



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:10 PM BST

PDB ID : 2VHM
Title : STRUCTURE OF PDF BINDING HELIX IN COMPLEX WITH THE RIBOSOME (PART 1 OF 4)
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Deposited on : 2007-11-22
Resolution : 3.74 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>

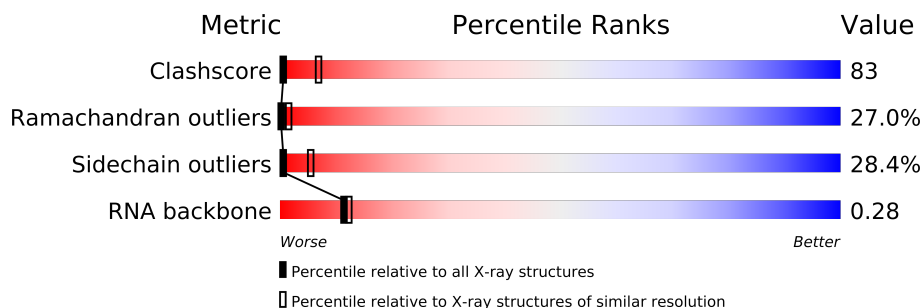
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.74 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	1072 (4.00-3.48)
Ramachandran outliers	78287	1023 (4.00-3.48)
Sidechain outliers	78261	1016 (4.00-3.48)
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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	54	
3	2	46	
4	3	64	
5	4	38	
6	5	16	
7	A	120	
8	B	2904	
9	C	273	
10	D	209	
11	E	201	
12	F	178	
13	G	176	
14	H	149	
15	I	141	

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Mol	Chain	Length	Quality of chain
16	J	142	
17	K	123	
18	L	144	
19	M	136	
20	N	127	
21	O	117	
22	P	114	
23	Q	117	
24	R	103	
25	S	110	
26	T	100	
27	U	103	
28	V	94	
29	W	84	
30	X	63	
31	Y	58	
32	Z	70	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90442 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 L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a protein called C-TERM HELIX PDF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	5	16	Total	C	N	O	0	0	0
			134	84	28	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	146	ALA	LEU	ENGINEERED MUTATION	UNP P0A6K3

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 8 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	J	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	K	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	L	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	N	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	O	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Q	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	T	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	U	103	Total	C	N	O			
			780	492	147	141	0	0	1

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	V	94	Total	C	N	O	S			
			753	479	137	134	3	0	0	0

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	W	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	X	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Y	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Z	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Z	110	Total	Mg		
			110	110	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	2	2	Total 2	O 2	0	0
34	B	488	Total 488	O 488	0	0
34	C	3	Total 3	O 3	0	0
34	D	1	Total 1	O 1	0	0
34	E	4	Total 4	O 4	0	0
34	J	2	Total 2	O 2	0	0
34	L	3	Total 3	O 3	0	0

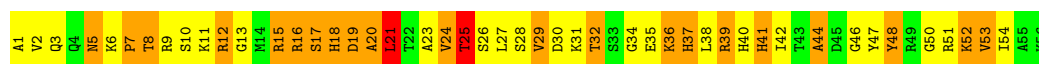
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

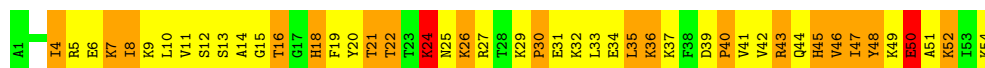
• Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0: 



• Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1: 



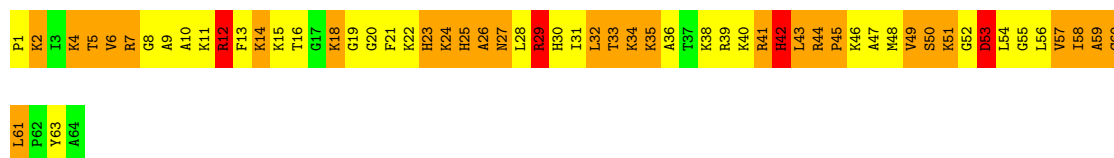
• Molecule 3: 50S RIBOSOMAL PROTEIN L34

Chain 2: 



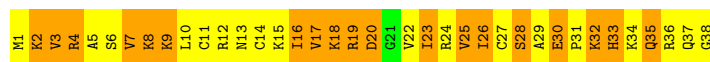
• Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3: 



• Molecule 5: 50S RIBOSOMAL PROTEIN L36

Chain 4: 



• Molecule 6: C-TERM HELIX PDF

Chain 5: 

A146
S147
P148
L149
K150
Q151
Q152
R153
I154
R155
Q156
K157
E158
K160
L161

• Molecule 7: 5S RIBOSOMAL RNA

Chain A:

U	G2	C3	C4	U5	G6	G7	C8	G9	G10	C11	G12	G13	G14	A15	G16	C17	G18	G19	G20	G21	U22	G23	G24	U25	G26	C27	C28	U29	C30	C31	U32	G33	A34	C35	G36	C37	C38	A39	U40	C41	C42	C43	C44	A45	A46	G107	U48	A109	C49	C110	G51	A52	C113	C54	A115	U55	G56	G117	A57	A58	A59	C60
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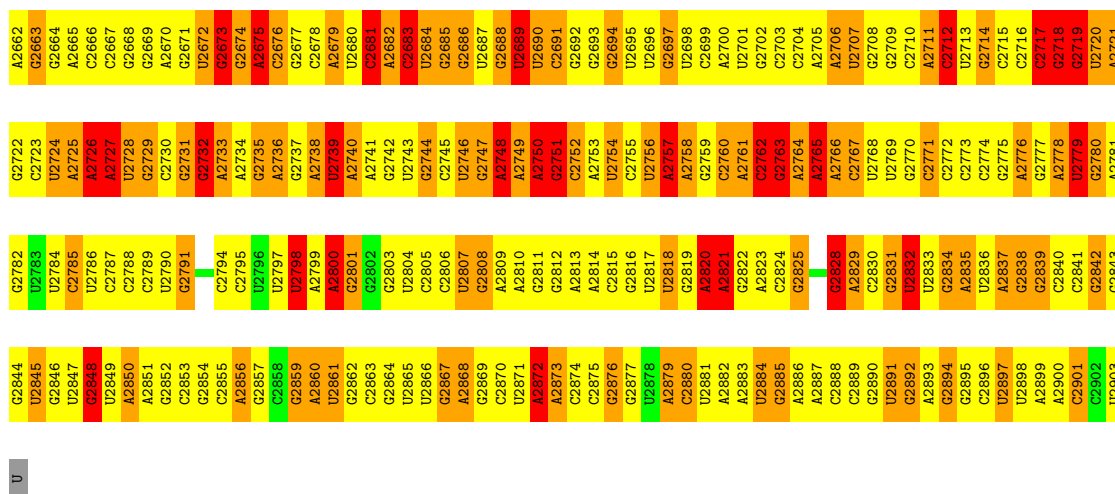
• Molecule 8: 23S RIBOSOMAL RNA

Chain B:

G664	A603	G543	A483	A423	G363	G303	U243	A192	G122	G1
U665	G604	C544	C484	G424	U365	C304	A244	C183	G123	G2
A666	G605	U545	C485	G425	U365	C305	G245	C184	G124	U3
U667	U606	U546	C486	C426	C366	U306	C246	G185	A125	U65
A668	G607	A547	C487	U427	G367	G307	G247	G186	A126	C66
G669	A608	G548	G488	A428	A368	G308	C248	G187	A127	U67
A670	A609	G549	G489	A429	U369	A309	C249	G188	C128	G68
C671	C610	C550	C490	A430	G370	A310	G250	G189	C129	C69
C672	C611	G551	G491	U431	A371	A311	A251	A190	C130	G70
G673	G612	U552	A492	A432	C372	G312	G252	A191	A131	A71
A674	A613	G553	G493	C433	U373	G313	C253	C192	G132	U72
A675	A614	U554	G494	U434	A374	C314	G254	U193	U133	A73
A676	U615	G555	G495	A435	G375	G315	A255	G194	U133	A12
A677	A616	A556	G496	C436	C376	C316	A256	A195	U135	A74
C678	G617	U557	A497	U437	G377	G317	C257	A196	G136	A14
C679	G618	U558	G498	G438	C378	C318	G258	A197	U137	C76
G680	G619	G559	U499	A439	C379	G319	G259	C198	U137	G77
G681	G620	C560	G500	C440	G380	A320	G260	A199	U138	U78
G682	A621	U561	A501	U441	G381	U321	G261	U200	U139	C79
U683	G622	U562	A502	G442	A382	A322	A262	C201	C140	G80
G684	C623	A563	A503	A443	C383	C323	C263	U202	G141	G81
A685	A624	G564	A504	C444	A384	A324	C264	A203	A142	A82
U686	G625	C565	A505	C445	C385	G325	A265	U204	C143	G23
C687	A626	U566	G506	G446	G386	G326	G266	C205	C145	G24
U688	G627	U567	A507	A447	U387	G327	C267	U206	C146	G85
A689	G628	U568	A508	U448	G388	U328	C268	A207	A146	G86
G690	G629	U569	C509	U449	G389	G329	C269	C208	C147	U87
C691	G630	G570	C510	G450	U390	A330	A270	C209	U148	G88
A631	A631	U571	U511	U451	A391	C331	G271	C210	A149	A89
C632	A632	A572	G512	G452	U392	A332	A272	C211	U150	G30
G694	C633	U573	A513	A453	C393	G333	C273	G212	C151	A91
A695	A634	A574	A514	A454	C394	C334	C274	U153	A152	U92
G696	G635	A575	A515	C455	U395	C335	C275	G215	C153	C33
U697	G636	U576	C516	C456	G396	C336	C276	A216	U154	A94
A637	A637	G577	C517	A457	U397	G337	G277	A217	A155	A95
G698	G638	U578	G518	C458	C396	G338	A278	C218	C156	G36
A699	U639	G579	U519	U459	U399	U339	A279	A219	C157	C37
G700	G701	U580	G520	A460	A400	A340	U280	G220	U158	G98
C940	C940	C581	U521	C461	A401	C341	C281	A221	G159	U99
U702	U702	A582	A522	C462	A402	A342	A282	A222	A160	U100
U703	A643	G583	C523	C463	U403	C343	C283	A223	A161	C41
G704	A644	C584	G524	G464	A404	C344	U284	C223	U162	A101
A705	C645	C584	A524	U464	A404	A344	C284	U224	C163	A42
U706	U646	A586	G525	C465	U405	A345	G285	A225	C164	G43
G707	G647	G586	A526	A466	G406	A346	U286	C226	A165	A103
G708	G648	C587	C527	G467	G407	A347	G287	A227	C166	A104
U709	G649	U588	A528	G468	G408	A348	U288	C228	U166	C105
U710	C650	U589	A529	C469	G409	U349	G289	C229	A167	C106
G711	G651	A590	G530	A470	G410	C350	U290	C229	G168	G107
G712	U652	U591	C531	A471	G411	C351	G291	A231	G169	G48
G713	A653	A592	A532	A472	C412	A352	U292	G232	U170	A49
U714	A654	U593	G533	C473	C413	C353	U293	A233	A171	G51
A715	A655	U594	U534	G474	C414	A354	A294	U234	A172	A52
A716	G656	C595	G535	C475	A415	U355	C295	U235	A173	A53
C717	U657	U596	G536	C476	U416	C356	U296	C236	U174	G64
A718	U658	G597	G537	A477	C417	C357	G297	C237	A176	G54
C719	G659	U598	A538	A478	C418	U358	C298	C238	G175	C115
U720	C660	A599	G539	A479	U419	G359	A299	C239	A177	C116
A721	A661	G600	C540	A480	C420	U360	A300	C240	G178	G57
A722	G662	C601	A541	C481	C421	C361	A301	A241	C179	A118
									G180	U59
										G60

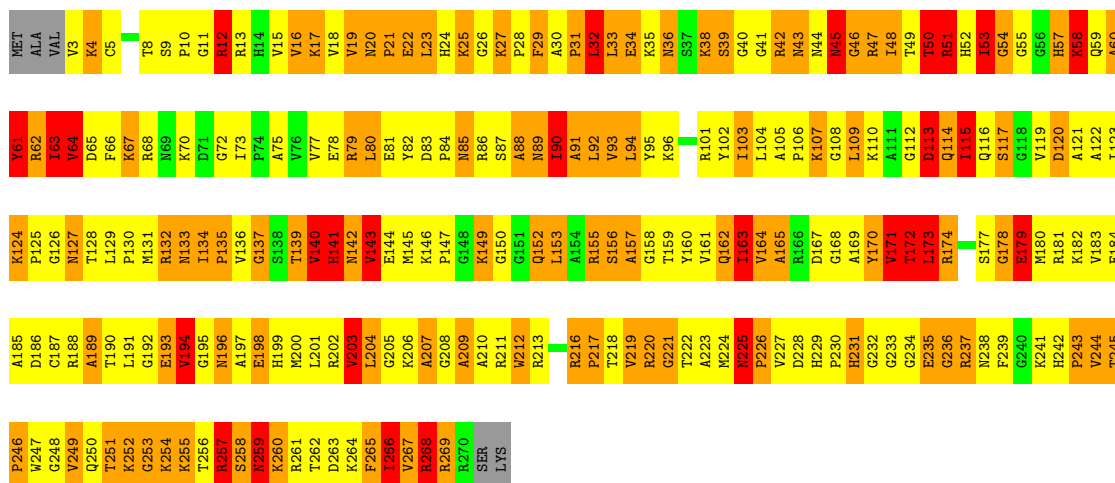
C1639	U1578	G1517	C1450	U1390	C1330	C1270	G1210	A1147	A1086	G1024	C964	G904	A844	G784	U724
A1640	U1579	C1518	C1451	U1391	G1331	G1271	C1211	U1148	G1087	G1025	C965	A905	A845	G785	G725
A1641	A1580	G1519	G1452	A1392	G1332	U1272	G1212	U1149	A1088	G1026	G966	U906	U846	G786	G726
G1642	G1581	U1520	A1453	G1393	G1333	U1273	A1213	C1150	A1089	A1027	U967	G907	U847	C787	A727
G1643	G1582	G1521	C1454	U1394	G1334	A1274	G1214	A1151	C968	A1028	C968	C908	C848	A788	G728
C1644	A1583	A1522	G1455	A1395	C1335	A1275	G1215	G1091	G969	A1029	G969	A909	A849	A789	G729
G1645	U1584	U1523	G1456	U1396	A1336	A1276	G1216	C1092	U870	C1030	U870	A910	U850	U790	A730
C1646	G1585	G1524	U1457	U1397	G1337	G1277	U1217	G1154	G971	G1031	G971	A911	C851	C791	C731
U1647	C1586	A1525	U1458	C1398	G1338	C1278	G1218	U1094	U1093	G1032	A972	C912	U852	A792	C732
U1648	A1586	C1526	G1459	G1399	G1339	G1279	U1219	A1095	A973	U1033	C973	G913	C853	A793	G733
G1649	G1587	G1527	U1460	U1400	U1340	G1280	G1220	A1096	A1096	G1034	G974	G914	C854	A794	A734
U1650	G1588	A1528	C1461	G1401	G1341	G1281	C1221	C1158	U1097	U1035	A975	C915	G855	C795	A735
A1650	U1589	U1529	C1462	U1402	A1342	U1282	G1222	U1159	A1098	G1036	G976	G916	G856	C796	C736
G1651	A1590	G1530	U1465	A1403	G1343	G1283	G1223	G1160	G1099	G1037	G977	A917	G857	C797	C737
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G1653	C1592	U1532	U1466	U1405	C1345	A1285	G1225	G1162	U1101	G1039	A979	U919	G859	G799	A739
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G1674	G1613	A1553	C1488	G1426	A1366	C1306	A1246	U1184	G1122	U1061	A1000	G940	G	A820	G760
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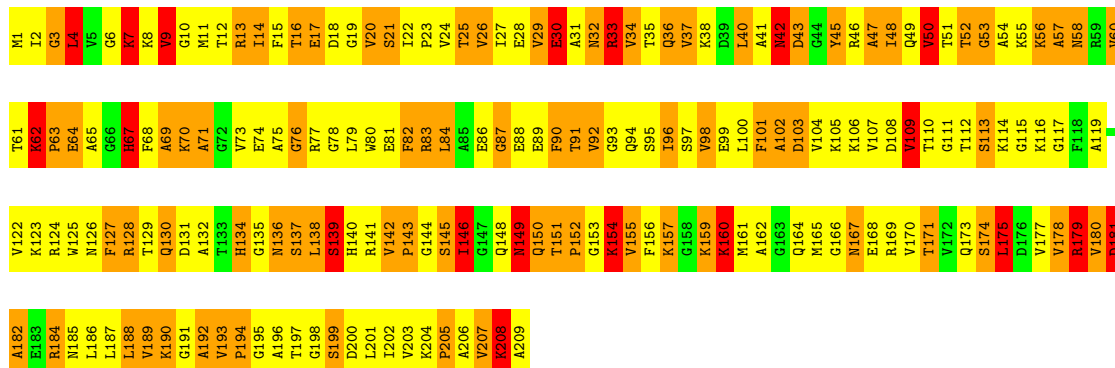
• Molecule 9: 50S RIBOSOMAL PROTEIN L2

Chain C:



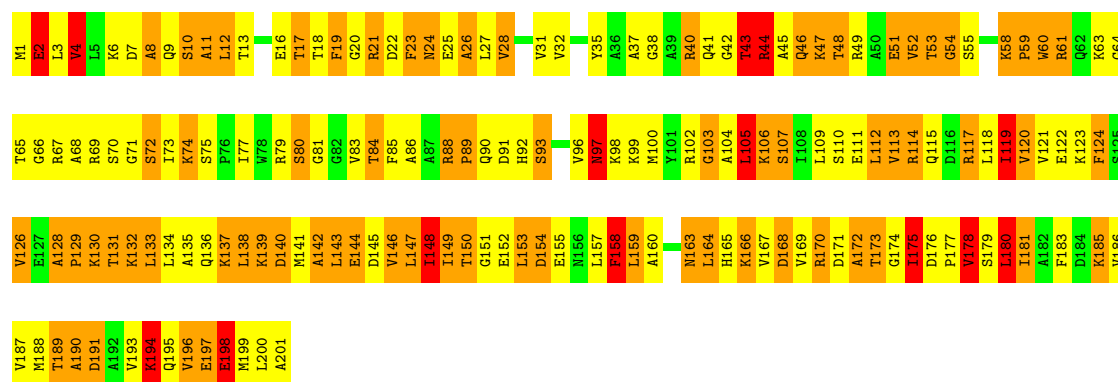
• Molecule 10: 50S RIBOSOMAL PROTEIN L3

Chain D:



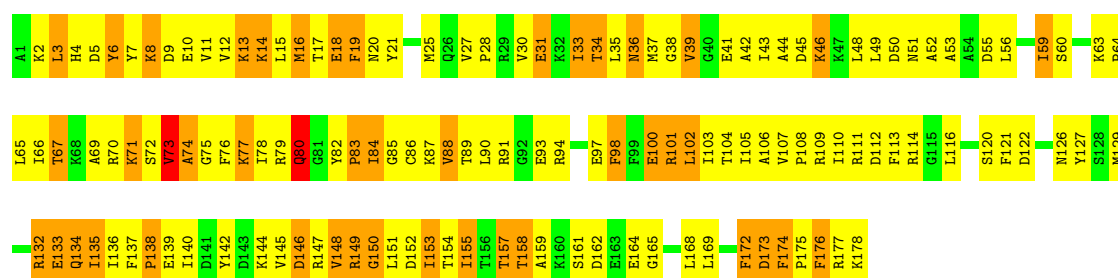
• Molecule 11: 50S RIBOSOMAL PROTEIN L4

Chain E:



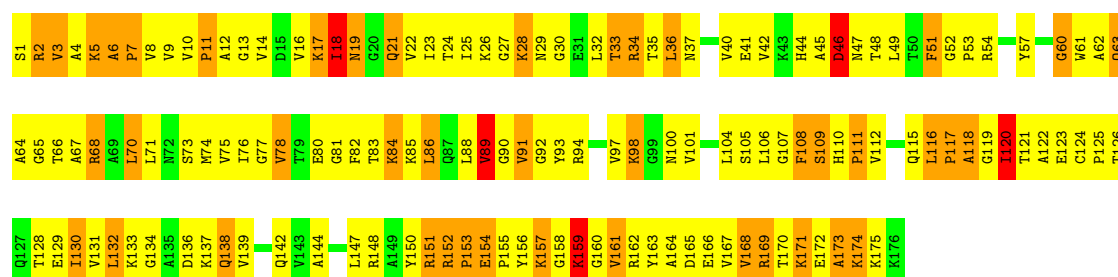
• Molecule 12: 50S RIBOSOMAL PROTEIN L5

Chain F:



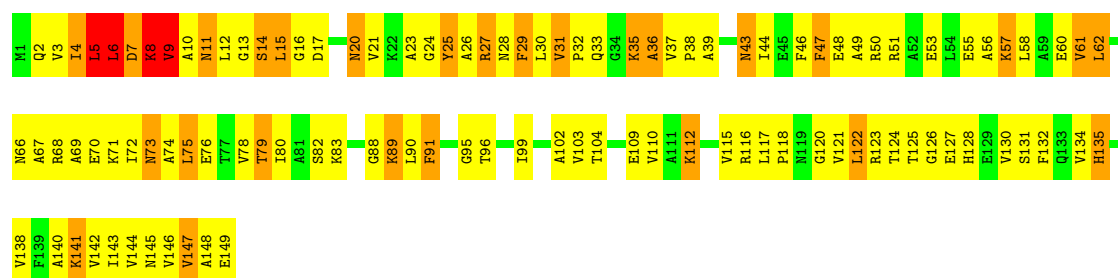
• Molecule 13: 50S RIBOSOMAL PROTEIN L6

Chain G:



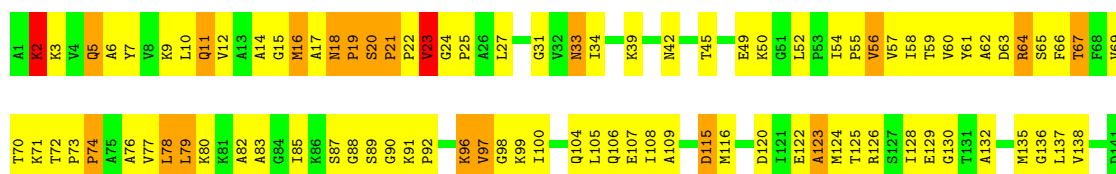
• Molecule 14: 50S RIBOSOMAL PROTEIN L9

Chain H:



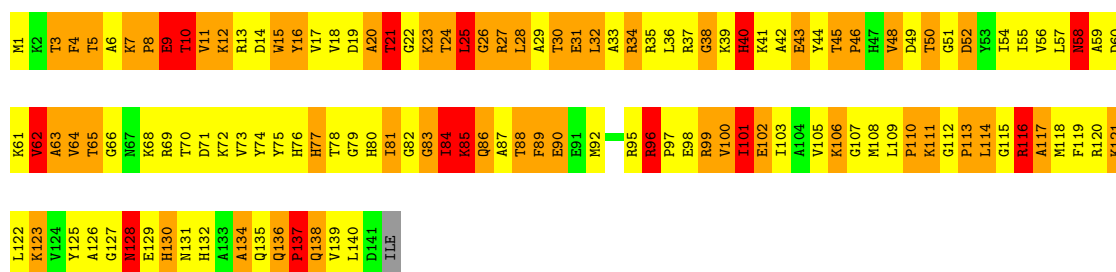
• Molecule 15: 50S RIBOSOMAL PROTEIN L11

Chain I:



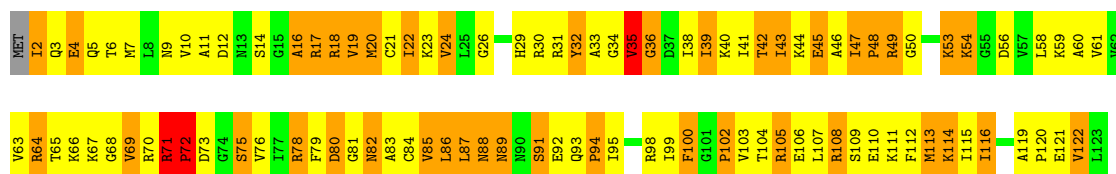
• Molecule 16: 50S RIBOSOMAL PROTEIN L13

Chain J:



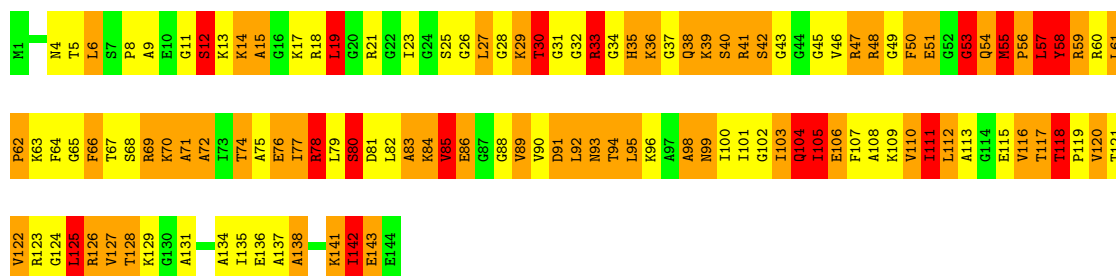
• Molecule 17: 50S RIBOSOMAL PROTEIN L14

Chain K:



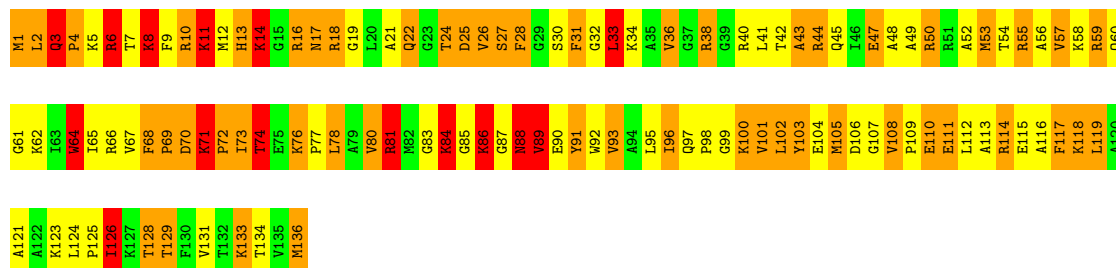
• Molecule 18: 50S RIBOSOMAL PROTEIN L15

Chain L:

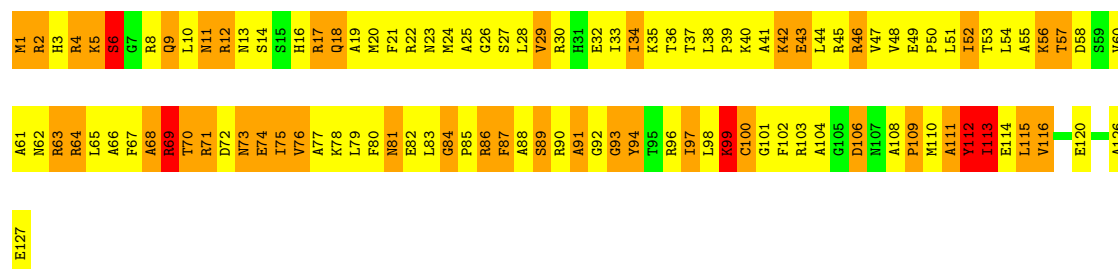


• Molecule 19: 50S RIBOSOMAL PROTEIN L16

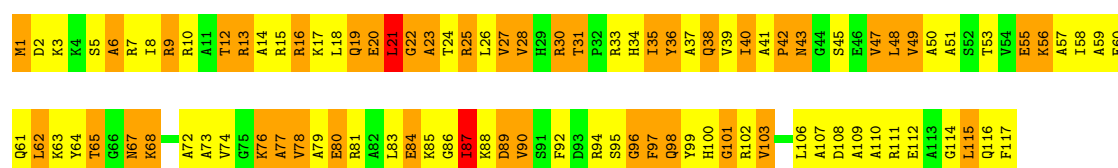
Chain M:



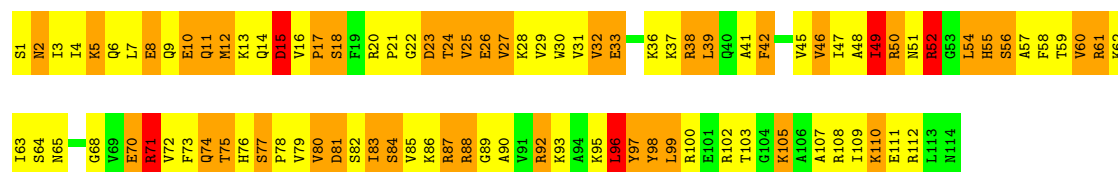
● Molecule 20: 50S RIBOSOMAL PROTEIN L17

Chain N: 

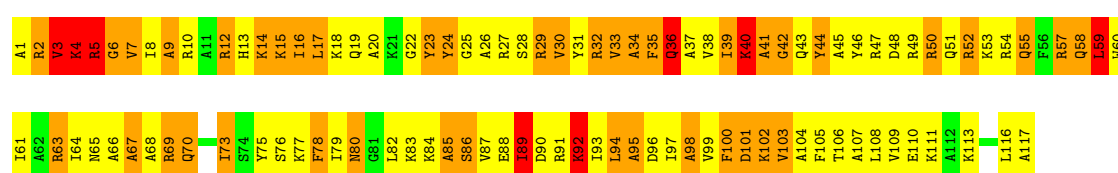
● Molecule 21: 50S RIBOSOMAL PROTEIN L18

Chain O: 

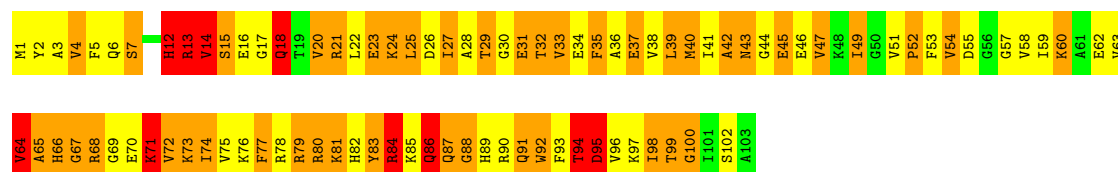
● Molecule 22: 50S RIBOSOMAL PROTEIN L19

Chain P: 

● Molecule 23: 50S RIBOSOMAL PROTEIN L20

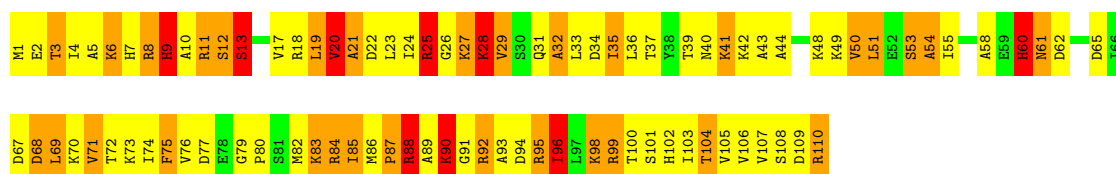
Chain Q: 

● Molecule 24: 50S RIBOSOMAL PROTEIN L21

Chain R: 

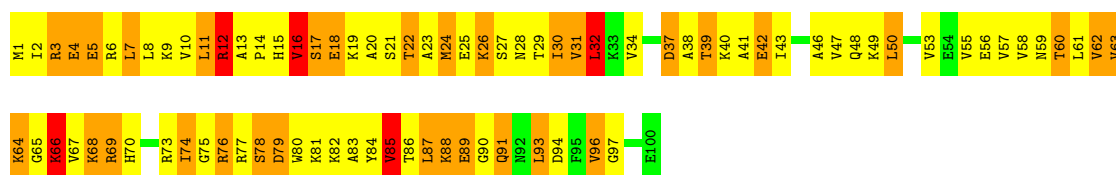
● Molecule 25: 50S RIBOSOMAL PROTEIN L22

Chain S: 



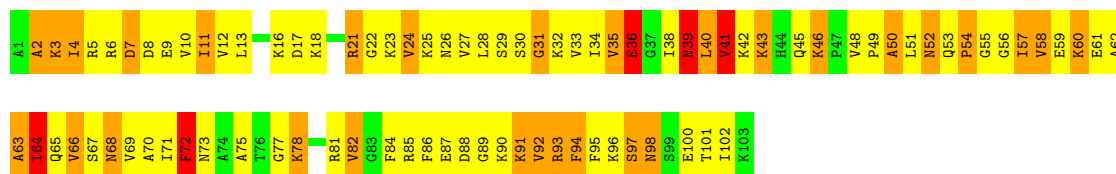
• Molecule 26: 50S RIBOSOMAL PROTEIN L23

Chain T:



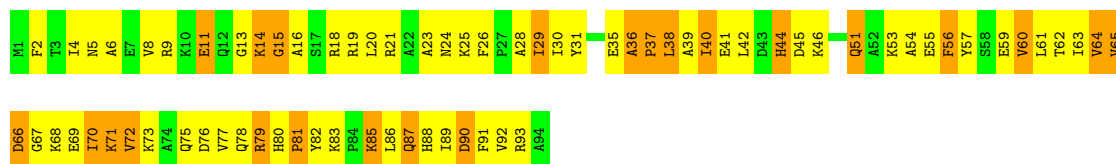
• Molecule 27: 50S RIBOSOMAL PROTEIN L24

Chain U:



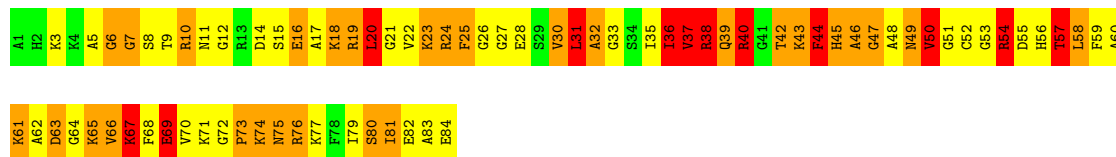
• Molecule 28: 50S RIBOSOMAL PROTEIN L25

Chain V:



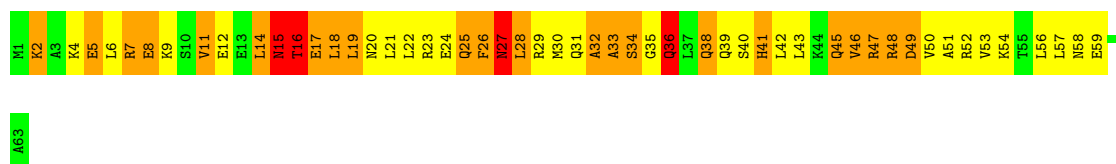
• Molecule 29: 50S RIBOSOMAL PROTEIN L27

Chain W:

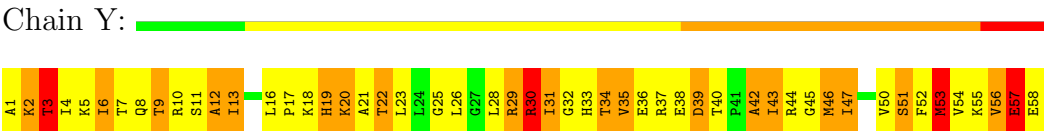


• Molecule 30: 50S RIBOSOMAL PROTEIN L29

Chain X:



● Molecule 31: 50S RIBOSOMAL PROTEIN L30



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	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74	Depositor
% Data completeness (in resolution range)	91.5 (50.00-3.74)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.323	Depositor
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 546832 reflections	Xtriage
Total number of atoms	90442	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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

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	0	0.41	0/450	0.71	0/599
2	1	0.42	0/448	0.69	0/594
3	2	0.46	0/380	0.76	0/498
4	3	0.52	0/513	0.79	0/676
5	4	0.43	0/303	0.69	0/397
6	5	0.64	0/134	0.72	0/176
7	A	0.76	3/2803 (0.1%)	1.48	39/4371 (0.9%)
8	B	0.82	7/68314 (0.0%)	1.58	975/106569 (0.9%)
9	C	0.51	0/2093	0.81	2/2815 (0.1%)
10	D	0.45	0/1586	0.72	0/2134
11	E	0.47	0/1571	0.77	0/2113
12	F	0.30	0/1444	0.53	0/1937
13	G	0.38	0/1343	0.62	0/1816
14	H	0.34	0/1122	0.60	0/1515
15	I	0.29	0/1046	0.52	0/1410
16	J	0.43	0/1136	0.71	0/1531
17	K	0.50	0/940	0.71	0/1260
18	L	0.46	0/1062	0.84	1/1413 (0.1%)
19	M	0.46	0/1093	0.73	0/1460
20	N	0.41	0/1021	0.66	0/1364
21	O	0.38	0/910	0.69	0/1219
22	P	0.44	0/929	0.77	1/1242 (0.1%)
23	Q	0.45	0/960	0.71	0/1278
24	R	0.41	0/829	0.72	0/1107
25	S	0.43	0/864	0.74	0/1156
26	T	0.45	0/785	0.68	0/1050
27	U	0.48	0/788	0.72	0/1053
28	V	0.34	0/766	0.52	0/1025
29	W	0.42	0/642	0.76	0/848
30	X	0.47	0/510	0.76	0/677
31	Y	0.36	0/453	0.66	0/605
32	Z	0.56	0/559	0.94	2/745 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.73	10/97797 (0.0%)	1.41	1020/146653 (0.7%)

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
13	G	0	1
16	J	0	1
18	L	0	1
19	M	0	1
22	P	0	3
32	Z	0	1
All	All	0	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	87	U	C1'-N1	6.70	1.58	1.48
8	B	2288	A	N1-C2	-6.29	1.28	1.34
8	B	1440	U	C1'-N1	6.07	1.57	1.48
8	B	2288	A	C2-N3	-5.73	1.28	1.33
8	B	2288	A	C5-C4	5.61	1.42	1.38

The worst 5 of 1020 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2288	A	C2-N3-C4	-70.19	75.50	110.60
8	B	2288	A	C6-N1-C2	-58.83	83.30	118.60
8	B	2288	A	N1-C2-N3	58.75	158.67	129.30
8	B	458	G	C1'-O4'-C4'	-14.23	98.51	109.90
8	B	1996	C	C1'-O4'-C4'	-13.99	98.71	109.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	109	SER	Peptide
16	J	9	GLU	Peptide
18	L	53	GLY	Peptide

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Mol	Chain	Res	Type	Group
19	M	88	ASN	Peptide
22	P	46	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	0	444	0	461	86	0
2	1	441	0	485	104	0
3	2	377	0	418	106	0
4	3	504	0	574	171	0
5	4	302	0	340	104	0
6	5	134	0	153	17	0
7	A	2507	0	1270	277	0
8	B	60995	0	30679	6963	0
9	C	2054	0	2122	603	0
10	D	1565	0	1616	443	0
11	E	1552	0	1619	432	0
12	F	1420	0	1460	172	0
13	G	1323	0	1374	196	0
14	H	1111	0	1148	159	0
15	I	1032	0	1088	100	0
16	J	1113	0	1147	293	0
17	K	931	0	1000	160	0
18	L	1053	0	1129	403	0
19	M	1074	0	1157	276	0
20	N	1008	0	1045	219	0
21	O	900	0	935	206	0
22	P	917	0	965	245	0
23	Q	947	0	1022	269	0
24	R	816	0	839	236	0
25	S	857	0	922	172	0
26	T	778	0	840	178	0
27	U	780	0	834	183	0
28	V	753	0	780	100	0
29	W	634	0	656	205	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	509	0	543	111	0
31	Y	449	0	491	66	0
32	Z	549	0	552	174	0
33	Z	110	0	0	0	0
34	2	2	0	0	2	0
34	B	488	0	0	65	0
34	C	3	0	0	1	0
34	D	1	0	0	0	0
34	E	4	0	0	2	0
34	J	2	0	0	2	0
34	L	3	0	0	1	0
All	All	90442	0	59664	12395	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 83.

The worst 5 of 12395 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:B:1359:A:C2	8:B:1360:G:H1'	1.76	1.17
3:2:19:ARG:HG3	3:2:20:ALA:H	1.09	1.17
21:O:25:ARG:HG3	21:O:25:ARG:HH11	1.07	1.17
8:B:1813:G:H2'	8:B:1814:G:H5''	1.24	1.16
9:C:20:ASN:HB2	9:C:202:ARG:NH1	1.61	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	
1	0	54/56 (96%)	26 (48%)	13 (24%)	15 (28%)	0	1
2	1	52/54 (96%)	18 (35%)	15 (29%)	19 (36%)	0	0
3	2	44/46 (96%)	15 (34%)	16 (36%)	13 (30%)	0	1
4	3	62/64 (97%)	24 (39%)	17 (27%)	21 (34%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	36/38 (95%)	14 (39%)	13 (36%)	9 (25%)	0	2
6	5	14/16 (88%)	6 (43%)	5 (36%)	3 (21%)	0	3
9	C	266/273 (97%)	101 (38%)	67 (25%)	98 (37%)	0	0
10	D	207/209 (99%)	80 (39%)	56 (27%)	71 (34%)	0	0
11	E	199/201 (99%)	76 (38%)	58 (29%)	65 (33%)	0	0
12	F	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	5
13	G	174/176 (99%)	98 (56%)	42 (24%)	34 (20%)	0	4
14	H	147/149 (99%)	94 (64%)	34 (23%)	19 (13%)	0	13
15	I	139/141 (99%)	92 (66%)	33 (24%)	14 (10%)	1	20
16	J	139/142 (98%)	60 (43%)	34 (24%)	45 (32%)	0	0
17	K	120/123 (98%)	67 (56%)	30 (25%)	23 (19%)	0	4
18	L	142/144 (99%)	53 (37%)	37 (26%)	52 (37%)	0	0
19	M	134/136 (98%)	51 (38%)	46 (34%)	37 (28%)	0	1
20	N	125/127 (98%)	55 (44%)	43 (34%)	27 (22%)	0	3
21	O	115/117 (98%)	49 (43%)	40 (35%)	26 (23%)	0	3
22	P	112/114 (98%)	48 (43%)	30 (27%)	34 (30%)	0	1
23	Q	115/117 (98%)	62 (54%)	26 (23%)	27 (24%)	0	2
24	R	101/103 (98%)	31 (31%)	25 (25%)	45 (45%)	0	0
25	S	108/110 (98%)	58 (54%)	24 (22%)	26 (24%)	0	2
26	T	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	2
27	U	101/103 (98%)	40 (40%)	36 (36%)	25 (25%)	0	2
28	V	92/94 (98%)	58 (63%)	21 (23%)	13 (14%)	0	11
29	W	82/84 (98%)	20 (24%)	28 (34%)	34 (42%)	0	0
30	X	61/63 (97%)	17 (28%)	25 (41%)	19 (31%)	0	0
31	Y	56/58 (97%)	25 (45%)	17 (30%)	14 (25%)	0	2
32	Z	68/70 (97%)	30 (44%)	19 (28%)	19 (28%)	0	1
All	All	3339/3406 (98%)	1505 (45%)	931 (28%)	903 (27%)	0	1

5 of 903 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	19	ASP
1	0	21	LEU

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Mol	Chain	Res	Type
1	0	25	THR
1	0	29	VAL
1	0	36	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	
1	0	47/47 (100%)	34 (72%)	13 (28%)	0	6
2	1	48/48 (100%)	40 (83%)	8 (17%)	3	24
3	2	38/38 (100%)	18 (47%)	20 (53%)	0	0
4	3	51/51 (100%)	34 (67%)	17 (33%)	0	3
5	4	34/34 (100%)	21 (62%)	13 (38%)	0	1
6	5	15/15 (100%)	12 (80%)	3 (20%)	2	14
9	C	213/218 (98%)	150 (70%)	63 (30%)	0	5
10	D	164/164 (100%)	112 (68%)	52 (32%)	0	4
11	E	165/165 (100%)	120 (73%)	45 (27%)	0	6
12	F	149/149 (100%)	129 (87%)	20 (13%)	6	37
13	G	137/137 (100%)	103 (75%)	34 (25%)	1	8
14	H	114/114 (100%)	87 (76%)	27 (24%)	1	9
15	I	109/109 (100%)	93 (85%)	16 (15%)	4	31
16	J	114/116 (98%)	74 (65%)	40 (35%)	0	2
17	K	102/104 (98%)	68 (67%)	34 (33%)	0	3
18	L	103/103 (100%)	61 (59%)	42 (41%)	0	1
19	M	109/109 (100%)	59 (54%)	50 (46%)	0	0
20	N	103/103 (100%)	74 (72%)	29 (28%)	0	5
21	O	87/87 (100%)	64 (74%)	23 (26%)	1	7
22	P	99/99 (100%)	79 (80%)	20 (20%)	2	14
23	Q	89/89 (100%)	58 (65%)	31 (35%)	0	3
24	R	84/84 (100%)	59 (70%)	25 (30%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	S	93/93 (100%)	66 (71%)	27 (29%)	0	5
26	T	83/84 (99%)	60 (72%)	23 (28%)	0	6
27	U	83/84 (99%)	63 (76%)	20 (24%)	1	8
28	V	78/78 (100%)	63 (81%)	15 (19%)	2	16
29	W	62/62 (100%)	42 (68%)	20 (32%)	0	4
30	X	55/55 (100%)	40 (73%)	15 (27%)	0	6
31	Y	48/48 (100%)	33 (69%)	15 (31%)	0	5
32	Z	62/62 (100%)	44 (71%)	18 (29%)	0	5
All	All	2738/2749 (100%)	1960 (72%)	778 (28%)	0	5

5 of 778 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	J	58	ASN
18	L	112	LEU
29	W	37	VAL
16	J	102	GLU
17	K	80	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
15	I	11	GLN
18	L	99	ASN
28	V	80	HIS
15	I	33	ASN
16	J	132	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	116/120 (96%)	40 (34%)	12 (10%)
8	B	2839/2904 (97%)	1140 (40%)	396 (13%)
All	All	2955/3024 (97%)	1180 (39%)	408 (13%)

5 of 1180 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	6	G
7	A	7	G
7	A	9	G
7	A	12	C
7	A	13	G

5 of 408 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	1157	G
8	B	1490	A
8	B	2706	A
8	B	1211	C
8	B	1311	G

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 ⓘ

Of 110 ligands modelled in this entry, 110 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.