



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:38 PM BST

PDB ID : 2QB9  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin. This file contains the 30S subunit of the first 70S ribosome, with gentamicin bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-16  
Resolution : 3.54 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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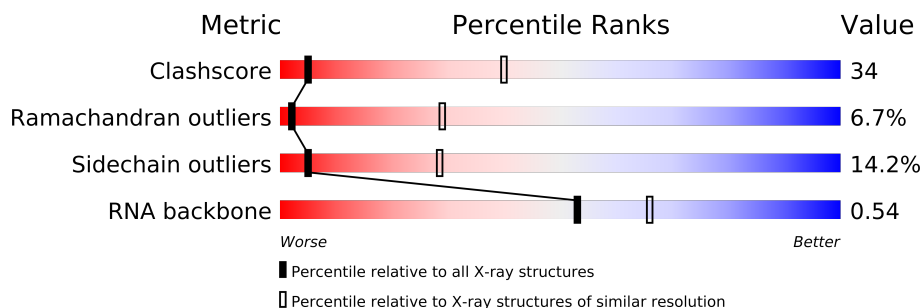
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.54 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	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RNA backbone	1838	1011 (4.30-2.76)

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  $\geq 3$ , 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	1542	
2	C	232	
3	D	205	
4	E	166	
5	F	135	
6	G	178	
7	H	129	
8	I	129	
9	J	103	
10	K	128	
11	L	123	
12	M	117	
13	N	100	
14	O	89	
15	P	82	

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Mol	Chain	Length	Quality of chain
16	Q	83	
17	R	74	
18	S	91	
19	T	86	
20	B	240	
21	U	70	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51820 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	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	B	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

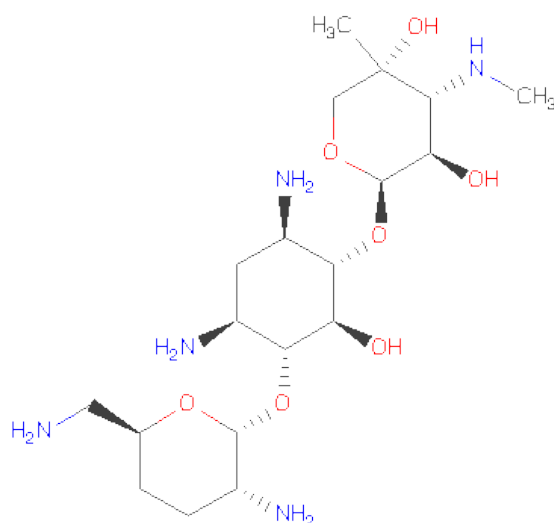
- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	60	Total	Mg	0	0
			60	60		

- Molecule 23 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-O-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C<sub>19</sub>H<sub>39</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			31	19	5	7		
23	A	1	Total	C	N	O	0	0
			31	19	5	7		
23	A	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	293	Total	O	0	0
			293	293		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	E	3	Total 3	O 3	0	0
24	L	2	Total 2	O 2	0	0
24	N	1	Total 1	O 1	0	0
24	T	1	Total 1	O 1	0	0

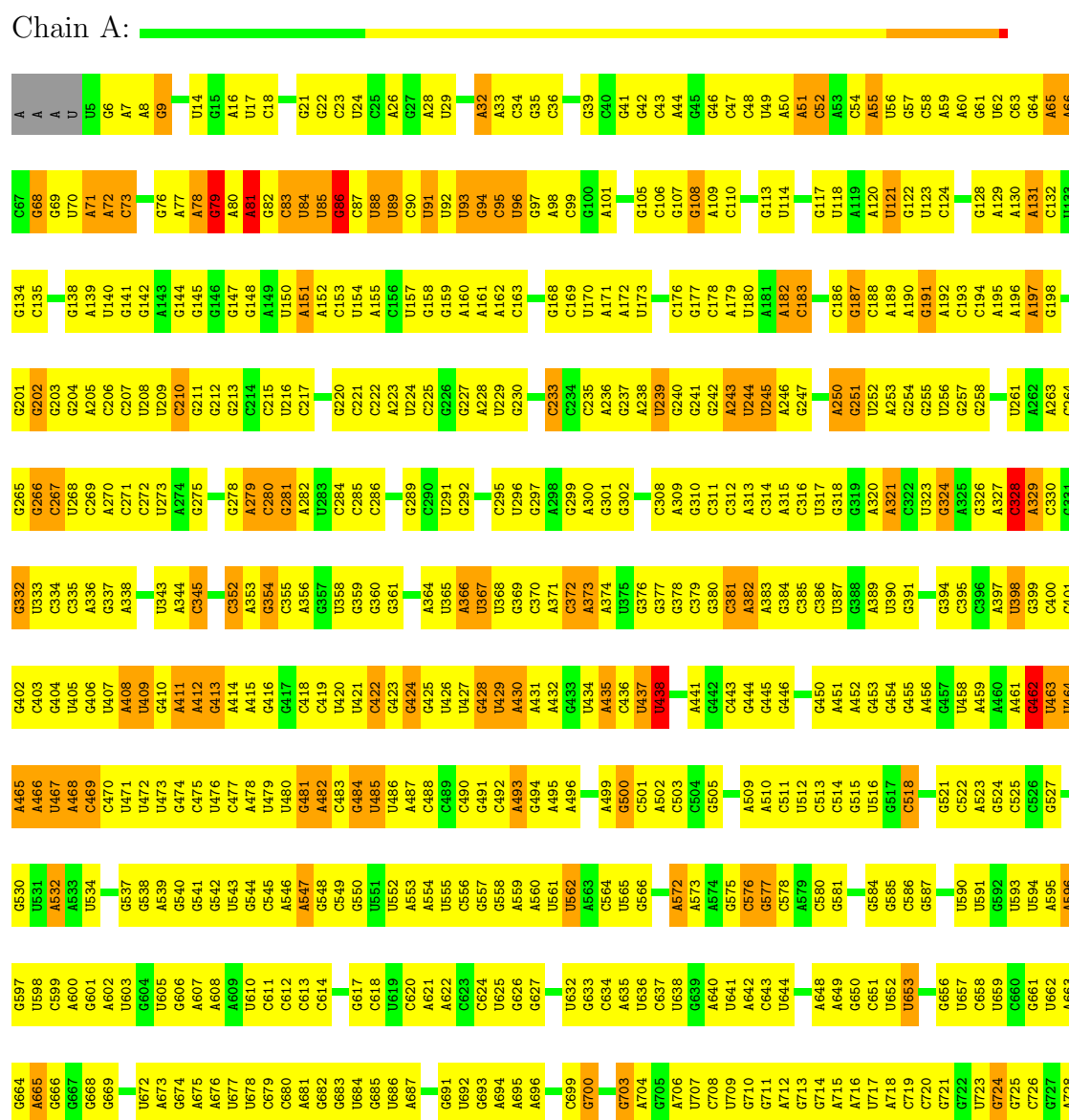


### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: 16S rRNA

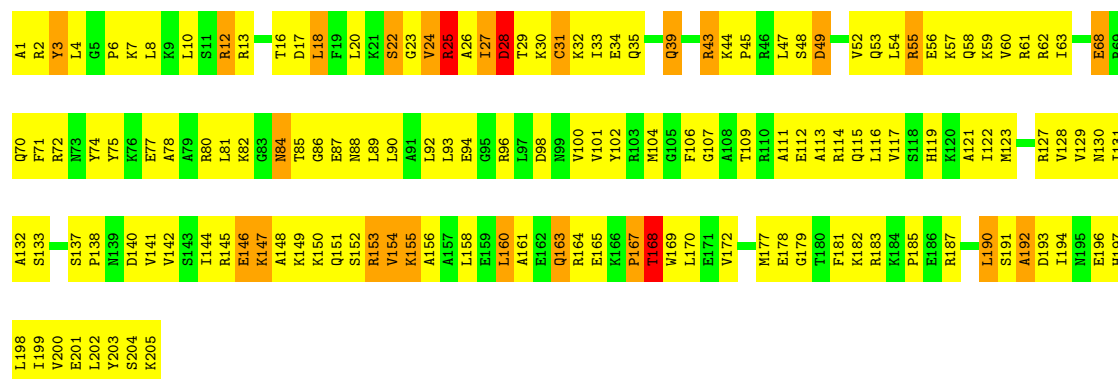


A729	G809	G885	U960	A1021	G1084	A1152	A1219	C1284	G1347	U1425	C1501	G1
G730	C810	G886	U961	A1022	U1085	G1153	G1220	A1285	U1348	G1426	A1502	Q2
G731	C811	G889	G962	U1023	U1086	C1158	G1221	U1286	A1349	G1432	A1503	K3
G732	G812	G890	G963	U1024	U1090	U1159	G1222	U1287	A1350	U1433	G1504	V4
G733	U813	G895	A964	U1025	U1091	G1160	C1223	A1288	C1351	U1434	U1506	H5
G734	A814	G896	U965	U1026	U1092	U1161	U1224	A1289	C1352	U1435	U1507	G8
G735	A815	G898	G966	C1027	A1093	C1162	A1225	G1290	U1353	U1436	A1508	I9
G736	A816	C896	G967	U1028	A1094	C1163	C1226	U1291	G1356	U1437	C1509	R10
G737	C817	C897	A969	U1029	G1095	G1164	A1227	U1292	A1357	G1439	C1510	L11
G738	G818	C899	G970	U1030	U1096	U1165	C1228	C1293	U1358	U1440	G1511	G12
G739	A819	A900	G971	U1031	C1097	U1166	A1229	C1296	C1359	A1441	U1512	I13
U740	U820	G903	G972	G1032	C1098	A1167	C1230	G1297	C1362	A1446	U1513	Y14
U741	G821	U904	G973	G1033	G1099	U1168	C1231	U1298	A1363	U1447	G1514	K15
A747	U822	U905	A974	G1034	A1100	U1169	C1234	U1299	A1364	U1448	G1515	P16
G748	C823	U906	A975	A1035	A1101	A1170	U1235	G1300	U1365	U1450	G1516	W17
U751	A825	A907	A977	C1037	A1102	A1171	A1236	C1301	G1366	U1451	G1517	R18
U755	C826	A908	A978	C1038	A1103	C1172	C1237	C1302	G1367	U1452	U1518	S19
G755	G827	A909	C979	U1039	A1105	U1173	A1238	C1303	C1368	U1453	A1519	T20
G756	U828	C910	G980	U1040	G1106	G1174	A1239	G1304	U1369	U1454	C1520	W21
G763	G829	A914	U981	G1041	C1107	G1175	U1240	G1305	C1369	G1455	C1521	N24
G764	G833	G917	U982	A1042	G1108	A1176	G1241	U1306	G1370	U1456	U1522	T25
G765	U834	C984	A983	U1043	G1109	G1177	C1242	U1307	G1371	G1457	G1523	K26
A766	U835	A918	C985	A1044	A1110	U1178	G1243	U1308	U1372	G1458	C1524	E27
A767	G836	A919	U986	C1046	A1111	A1179	G1244	G1309	G1373	G1459	G1525	F28
A769	C839	U920	G987	G1047	A1112	A1180	C1245	G1310	A1374	C1460	G1526	Q99
G770	C840	U921	U988	U1049	U1118	G1182	A1246	A1311	U1381	G1461	U1527	I100
G771	C841	A923	U989	C990	C1119	G1183	U1247	U1312	C1382	U1462	U1528	N01
A777	U842	C924	U991	G1050	C1120	G1184	C1249	U1313	C1383	U1463	G1529	E04
G778	U843	G925	U992	G1053	U1121	G1185	A1250	U1315	G1386	U1464	U1530	V05
G779	G844	G926	G993	C1054	U1122	G1186	A1251	U1316	G1387	A1468	A1531	D35
A780	A845	G927	A994	A1055	U1123	G1190	A1252	C1317	C1388	C1469	U1532	R106
A781	G846	G928	C995	U1056	G1124	U1191	G1253	U1318	C1389	U1470	C1533	K107
A782	G847	U996	A996	G1057	U1125	C1192	A1254	A1319	U1390	U1471	A1534	P108
C783	C848	G933	U997	C1058	U1126	U1196	G1255	C1320	U1391	U1472	C	D180
A784	G849	C934	C998	C1059	G1127	A1196	A1256	U1321	G1392	G1473	C	L110
G785	C857	C936	C999	U1060	A1130	U1197	G1257	C1322	U1393	U1474	C	D111
G786	G858	G939	A1000	C1061	G1131	G1198	C1258	G1323	A1394	U1477	U	A112
G787	G859	G940	C1001	U1062	C1132	U1199	C1259	U1324	C1397	U1478	U	K113
A787	U860	C941	G1002	C1063	G1133	C1200	A1261	C1325	C1398	C1479	U	L114
G791	G861	G945	G1003	U1064	U1134	U1201	C1262	U1326	C1400	A1480	U	V115
A792	C861	G946	A1004	C1065	U1135	U1202	C1263	G1331	G1401	G1481	A	A47
U793	A864	A946	A1005	C1066	C1136	C1203	A1269	A1332	C1404	G1482		K48
G795	A865	A947	U1007	G1067	C1137	A1204	G1270	A1333	C1405	A1483		S50
C796	G868	C948	U1008	C1068	G1138	U1205	A1271	U1334	U1406	C1484		A49
C797	C869	A949	U1009	U1070	C1140	G1207	G1272	U1335	U1407	U1485		V55
U798	U870	U950	C1010	G1071	G1141	C1208	C1273	C1336	C1409	G1486		I66
G802	G874	U951	C1011	U1072	G1142	C1209	A1274	G1337	A1410	G1487		E57
G803	U875	G953	G1012	G1073	G1143	U1210	A1275	G1338	C1411	G1488		R58
U804	A878	U955	A1014	U1074	A1144	U1211	G1276	A1339	C1412	U1489		P59
G805	C882	U956	G1015	G1077	A1145	U1212	G1277	A1340	C1413	U1490		A60
C806	U884	U957	G1016	U1078	A1146	A1213	G1278	U1341	U1418	G1491		K61
A807	C883	U958	A1017	G1079	C1147	C1214	G1279	C1342	A1495	U1492		S62
C808	C882	U959	G1018	U1081	U1148	G1215	A1280	G1343	C1496	U1493		I63
G809	U884	A959	A1019	A1081	A1150	C1217	C1281	U1344	G1423	U1494		R64
			G1020		A1151	C1218	U1283	A1346	U1424			V65
												T66
												I67
H68	R141	R142	R143	R144	R145	R146	R147	R148	R149	R150	R151	R152
T69	R153	R154	R155	R156	R157	R158	R159	R160	R161	R162	R163	R164
A70	R165	R166	R167	R168	R169	R170	R171	R172	R173	R174	R175	R176
R71	R177	R178	R179	R180	R181	R182	R183	R184	R185	R186	R187	R188
P72	R189	R190	R191	R192	R193	R194	R195	R196	R197	R198	R199	R200
V75	R201	R202	R203	R204	R205	R206	R207	R208	R209	R210	R211	R212
I76	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224
E81	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236
D82	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246	R247	R248
V83	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260
L86	R261	R262	R263	R264	R265	R266	R267	R268	R269	R270	R271	R272
R87	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284
K88	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296
V89	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308
A91	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320
R163	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332
R164	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344
E165	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356
G166	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368
W167	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380
R168	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392
Q99	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404
I100	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416
N01	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428
E04	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440
V05	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452
R106	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464
K107	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476
P108	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488
D109	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500
E109	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512
L110	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524
D181	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536
D182	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548
Y183	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560
R184	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572
T185	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584
A188	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596
H189	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608
T190	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620
T191	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632
Y192	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644
G193	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656
R126	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668
I54	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680
V55	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692
I66	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704
F129	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716
E57	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728
R58	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740
P59	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752
A60	R753											

LEU  
GLY  
GLY  
MET  
ALA  
ALA  
VAL  
GLU  
GLN  
PRO  
GLU  
LYS  
PRO  
ALA  
ALA  
GLN  
PRO  
LYS  
LYS  
LYS  
GLN  
GLN  
ARG  
LYS  
GLY  
ARG  
LYS

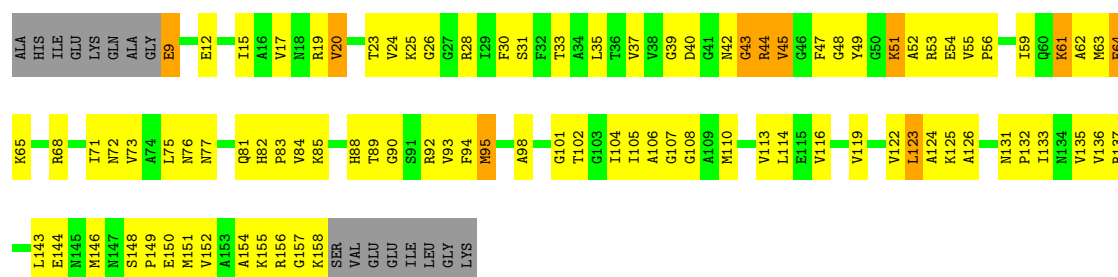
• Molecule 3: 30S ribosomal protein S4

Chain D:



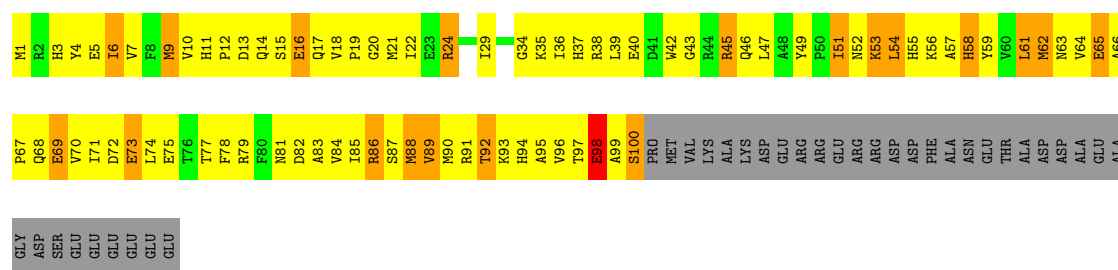
• Molecule 4: 30S ribosomal protein S5

Chain E:



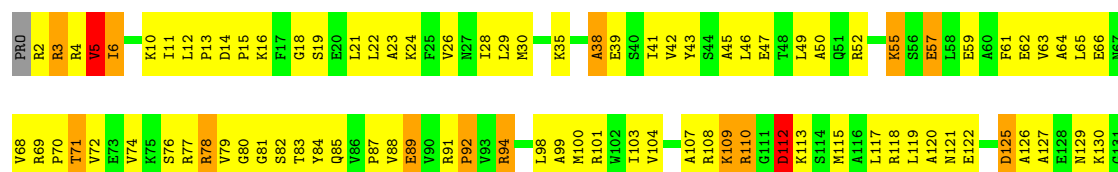
• Molecule 5: 30S ribosomal protein S6

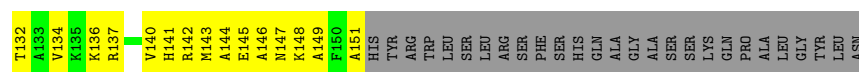
Chain F:



• Molecule 6: 30S ribosomal protein S7

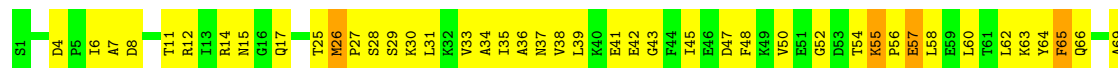
Chain G:





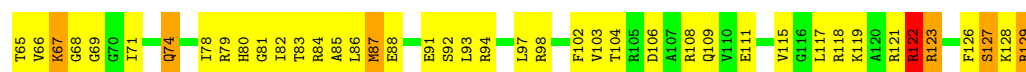
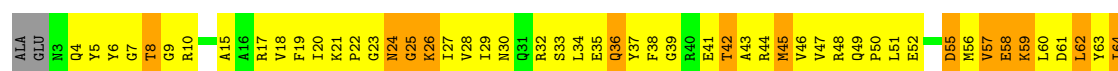
• Molecule 7: 30S ribosomal protein S8

Chain H:



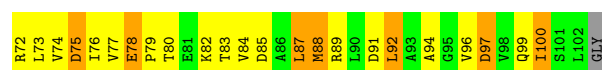
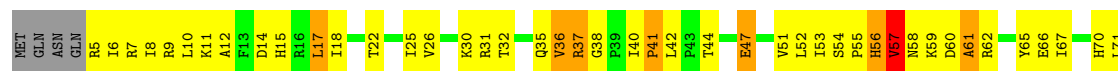
• Molecule 8: 30S ribosomal protein S9

Chain I:



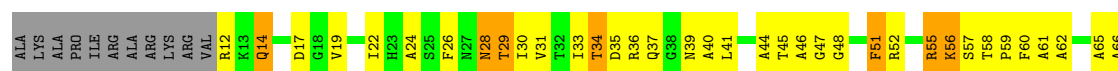
• Molecule 9: 30S ribosomal protein S10

Chain J:



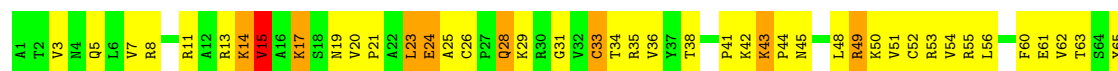
• Molecule 10: 30S ribosomal protein S11

Chain K:



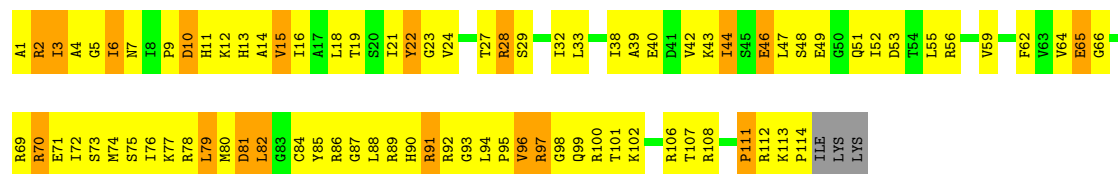
• Molecule 11: 30S ribosomal protein S12

Chain L:



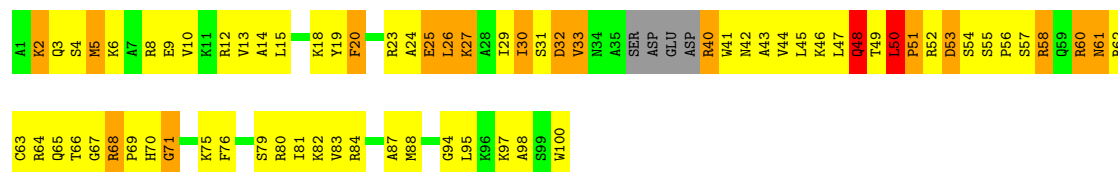
• Molecule 12: 30S ribosomal protein S13

Chain M: 



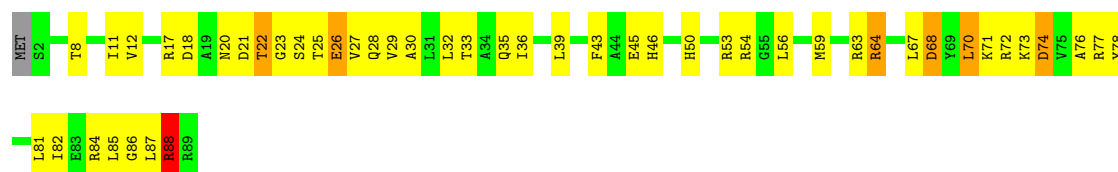
- Molecule 13: 30S ribosomal protein S14

Chain N: 



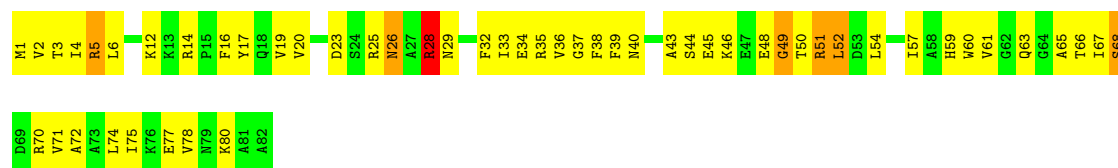
- Molecule 14: 30S ribosomal protein S15

Chain O: 



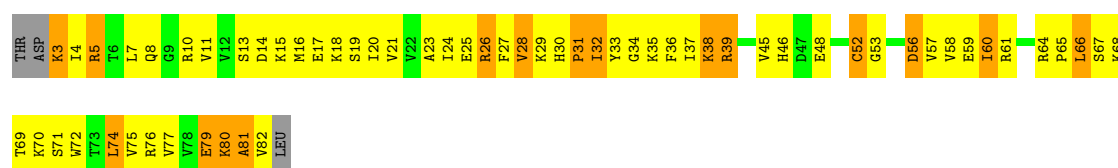
- Molecule 15: 30S ribosomal protein S16

Chain P: 



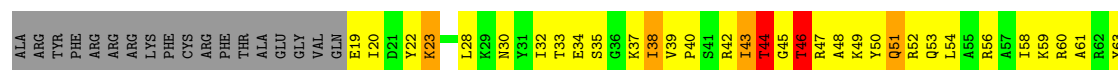
- Molecule 16: 30S ribosomal protein S17

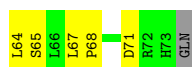
Chain Q: 



- Molecule 17: 30S ribosomal protein S18

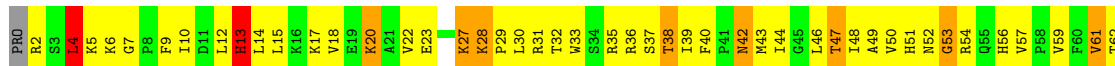
Chain R: 





- Molecule 18: 30S ribosomal protein S19

Chain S:



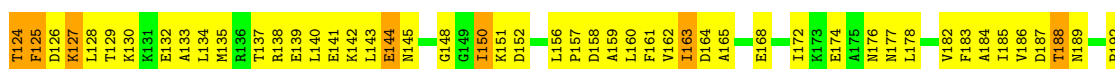
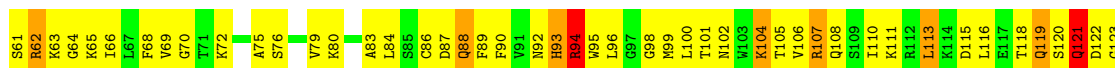
- Molecule 19: 30S ribosomal protein S20

Chain T:



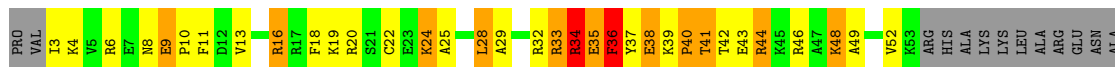
- Molecule 20: 30S ribosomal protein S2

Chain B:



- Molecule 21: 30S ribosomal protein S21

Chain U:



## 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, $\alpha$ , $\beta$ , $\gamma$	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.54	Depositor
% Data completeness (in resolution range)	88.8 (70.00-3.54)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.281 , 0.320	Depositor
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.234	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 627888 reflections (0.000%)	Xtriage
Total number of atoms	51820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, LLL

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	0.26	2/36762 (0.0%)	0.76	22/57350 (0.0%)
2	C	0.23	0/1651	0.44	0/2225
3	D	0.23	0/1665	0.44	0/2227
4	E	0.23	0/1118	0.45	0/1504
5	F	0.24	0/835	0.44	0/1128
6	G	0.23	0/1187	0.45	0/1591
7	H	0.23	0/989	0.44	0/1326
8	I	0.24	0/1034	0.46	0/1375
9	J	0.22	0/796	0.48	0/1077
10	K	0.24	0/893	0.46	0/1205
11	L	0.22	0/969	0.48	0/1300
12	M	0.21	0/892	0.46	0/1193
13	N	0.24	0/785	0.45	0/1043
14	O	0.23	0/722	0.47	0/964
15	P	0.25	0/659	0.46	0/884
16	Q	0.24	0/657	0.46	0/881
17	R	0.23	0/462	0.46	0/621
18	S	0.25	0/652	0.46	0/877
19	T	0.24	0/671	0.39	0/888
20	B	0.25	0/1735	0.45	0/2338
21	U	0.26	0/430	0.47	0/570
All	All	0.25	2/55564 (0.0%)	0.68	22/82567 (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	0	15



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1213	A	P-OP2	-8.66	1.34	1.49
1	A	495	A	N3-C4	-5.07	1.31	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1213	A	O5'-P-OP2	-28.32	76.72	110.70
1	A	1212	U	OP2-P-O3'	-9.32	84.69	105.20
1	A	366	A	C2'-C3'-O3'	8.50	128.21	109.50
1	A	1213	A	O5'-P-OP1	8.30	120.66	110.70
1	A	1212	U	OP1-P-O3'	8.23	123.30	105.20

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	324	G	Sidechain
1	A	437	U	Sidechain
1	A	86	G	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	32831	0	16521	1235	0
2	C	1624	0	1699	150	0
3	D	1643	0	1710	174	0
4	E	1105	0	1148	94	0
5	F	817	0	808	97	0
6	G	1174	0	1230	105	0
7	H	979	0	1034	82	0
8	I	1022	0	1070	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	786	0	828	81	0
10	K	877	0	887	105	0
11	L	955	0	1019	95	0
12	M	883	0	944	105	0
13	N	774	0	827	108	0
14	O	714	0	734	41	0
15	P	649	0	666	65	0
16	Q	648	0	691	76	0
17	R	455	0	478	48	0
18	S	637	0	665	87	0
19	T	665	0	714	56	0
20	B	1704	0	1732	218	0
21	U	425	0	449	67	0
22	A	60	0	0	0	0
23	A	93	0	117	6	0
24	A	293	0	0	1	0
24	E	3	0	0	0	0
24	L	2	0	0	0	0
24	N	1	0	0	0	0
24	T	1	0	0	0	0
All	All	51820	0	35971	2933	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 34.

The worst 5 of 2933 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:N:63:CYS:HB3	13:N:67:GLY:H	1.16	1.06
5:F:3:HIS:HB2	5:F:92:THR:HA	1.31	1.05
20:B:33:ALA:HA	20:B:38:HIS:HA	1.38	1.05
8:I:51:LEU:HB3	8:I:56:MET:HG2	1.41	1.02
21:U:16:ARG:HE	21:U:16:ARG:HA	1.21	1.02

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	C	204/232 (88%)	157 (77%)	34 (17%)	13 (6%)	2	30
3	D	203/205 (99%)	144 (71%)	45 (22%)	14 (7%)	2	28
4	E	148/166 (89%)	114 (77%)	30 (20%)	4 (3%)	8	57
5	F	98/135 (73%)	71 (72%)	17 (17%)	10 (10%)	1	15
6	G	148/178 (83%)	117 (79%)	22 (15%)	9 (6%)	2	31
7	H	127/129 (98%)	99 (78%)	24 (19%)	4 (3%)	7	54
8	I	125/129 (97%)	88 (70%)	28 (22%)	9 (7%)	2	26
9	J	96/103 (93%)	71 (74%)	15 (16%)	10 (10%)	1	15
10	K	115/128 (90%)	83 (72%)	26 (23%)	6 (5%)	3	36
11	L	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	2	29
12	M	112/117 (96%)	76 (68%)	28 (25%)	8 (7%)	2	27
13	N	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	1	13
14	O	86/89 (97%)	63 (73%)	19 (22%)	4 (5%)	4	40
15	P	80/82 (98%)	57 (71%)	19 (24%)	4 (5%)	3	38
16	Q	78/83 (94%)	56 (72%)	16 (20%)	6 (8%)	1	24
17	R	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	3	34
18	S	77/91 (85%)	60 (78%)	11 (14%)	6 (8%)	1	23
19	T	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	32
20	B	216/240 (90%)	149 (69%)	52 (24%)	15 (7%)	2	28
21	U	49/70 (70%)	28 (57%)	14 (29%)	7 (14%)	0	7
All	All	2311/2560 (90%)	1675 (72%)	481 (21%)	155 (7%)	2	29

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	14	VAL
2	C	54	ILE
2	C	205	GLU
3	D	24	VAL
3	D	192	ALA

### 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	C	170/189 (90%)	145 (85%)	25 (15%)	4	27
3	D	172/172 (100%)	148 (86%)	24 (14%)	5	29
4	E	113/125 (90%)	102 (90%)	11 (10%)	12	51
5	F	87/116 (75%)	70 (80%)	17 (20%)	2	12
6	G	123/146 (84%)	109 (89%)	14 (11%)	8	40
7	H	104/104 (100%)	97 (93%)	7 (7%)	23	71
8	I	105/106 (99%)	89 (85%)	16 (15%)	4	25
9	J	86/90 (96%)	74 (86%)	12 (14%)	5	29
10	K	90/98 (92%)	76 (84%)	14 (16%)	4	23
11	L	103/103 (100%)	92 (89%)	11 (11%)	10	45
12	M	92/95 (97%)	79 (86%)	13 (14%)	5	29
13	N	79/83 (95%)	64 (81%)	15 (19%)	2	13
14	O	76/77 (99%)	69 (91%)	7 (9%)	13	54
15	P	65/65 (100%)	59 (91%)	6 (9%)	13	54
16	Q	74/77 (96%)	59 (80%)	15 (20%)	2	10
17	R	48/64 (75%)	41 (85%)	7 (15%)	5	27
18	S	70/78 (90%)	56 (80%)	14 (20%)	2	11
19	T	65/65 (100%)	58 (89%)	7 (11%)	9	44
20	B	180/198 (91%)	149 (83%)	31 (17%)	3	18
21	U	44/60 (73%)	33 (75%)	11 (25%)	1	6
All	All	1946/2111 (92%)	1669 (86%)	277 (14%)	5	28

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	97	ASP
12	M	44	ILE
20	B	127	LYS
10	K	34	THR
11	L	14	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	21	HIS
11	L	19	ASN
20	B	35	ASN
10	K	80	ASN
11	L	45	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	246 (16%)	21 (1%)

5 of 246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	14	U
1	A	32	A
1	A	39	G
1	A	47	C

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	428	G
1	A	484	G
1	A	1201	A
1	A	372	C
1	A	1226	C

## 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 63 ligands modelled in this entry, 60 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	LLL	A	2356	-	33,33,33	3.19	14 (42%)	49,49,49	1.51	6 (12%)
23	LLL	A	2357	-	33,33,33	3.21	15 (45%)	49,49,49	1.55	5 (10%)
23	LLL	A	2358	-	33,33,33	3.17	14 (42%)	49,49,49	1.60	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LLL	A	2356	-	-	0/12/65/65	0/3/3/3
23	LLL	A	2357	-	-	0/12/65/65	0/3/3/3
23	LLL	A	2358	-	-	0/12/65/65	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2356	LLL	C22-C32	9.64	1.59	1.52
23	A	2358	LLL	C22-C32	9.41	1.59	1.52
23	A	2357	LLL	C22-C32	9.09	1.59	1.52
23	A	2357	LLL	C22-C12	7.59	1.58	1.52
23	A	2358	LLL	C22-C12	7.17	1.57	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2357	LLL	C93-N33-C33	6.07	117.30	113.85
23	A	2358	LLL	C93-N33-C33	5.76	117.13	113.85
23	A	2356	LLL	C93-N33-C33	5.27	116.85	113.85
23	A	2358	LLL	C53-O53-C13	5.12	118.52	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
23	A	2357	LLL	C53-O53-C13	4.69	117.90	111.22

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.