



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:06 AM GMT

PDB ID : 2VHO
Title : STRUCTURE OF PDF BINDING HELIX IN COMPLEX WITH THE RIBOSOME (PART 3 OF 4)
Authors : Bingel-Erlenmeyer, R.; Kohler, R.; Kramer, G.; Sandikci, A.; Antolic, S.; Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.
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>

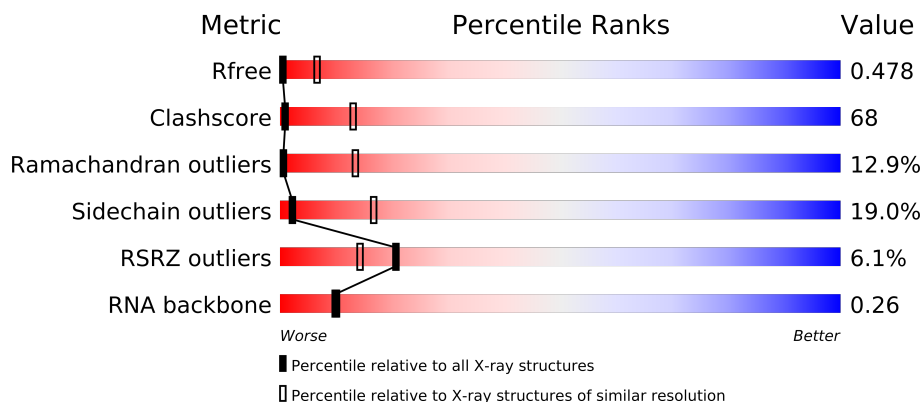
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : 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 3.74 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))
R_{free}	66092	1103 (4.04-3.40)
Clashscore	79885	1072 (4.00-3.48)
Ramachandran outliers	78287	1023 (4.00-3.48)
Sidechain outliers	78261	1016 (4.00-3.48)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	240	
3	C	232	
4	D	205	
5	E	166	
6	F	135	
7	G	178	
8	H	129	
9	I	129	
10	J	103	
11	K	128	
12	L	123	

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Mol	Chain	Length	Quality of chain
13	M	117	
14	N	100	
15	O	89	
16	P	82	
17	Q	83	
18	R	74	
19	S	91	
20	T	86	
21	U	71	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
22	MG	Z	4001	-	X
22	MG	Z	4004	-	X
22	MG	Z	4007	-	X
22	MG	Z	4012	-	X
22	MG	Z	4014	-	X
22	MG	Z	4016	-	X
22	MG	Z	4019	-	X
22	MG	Z	4020	-	X
22	MG	Z	4021	-	X
22	MG	Z	4022	-	X
22	MG	Z	4025	-	X
22	MG	Z	4031	-	X
22	MG	Z	4038	-	X
22	MG	Z	4043	-	X
22	MG	Z	4046	-	X
22	MG	Z	4049	-	X
22	MG	Z	4051	-	X
22	MG	Z	4055	-	X
22	MG	Z	4056	-	X
22	MG	Z	4060	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51738 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	151	Total	C	N	O	S	0	0	1
			1175	730	227	214	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	115	Total	C	N	O	S	0	0	1
			884	546	179	156	3			

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	81	Total	C	N	O	S	0	0	1
			649	411	122	113	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	56	Total	C	N	O	0	0	1
			456	288	87	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	1
			638	408	121	107	2			

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

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			

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

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

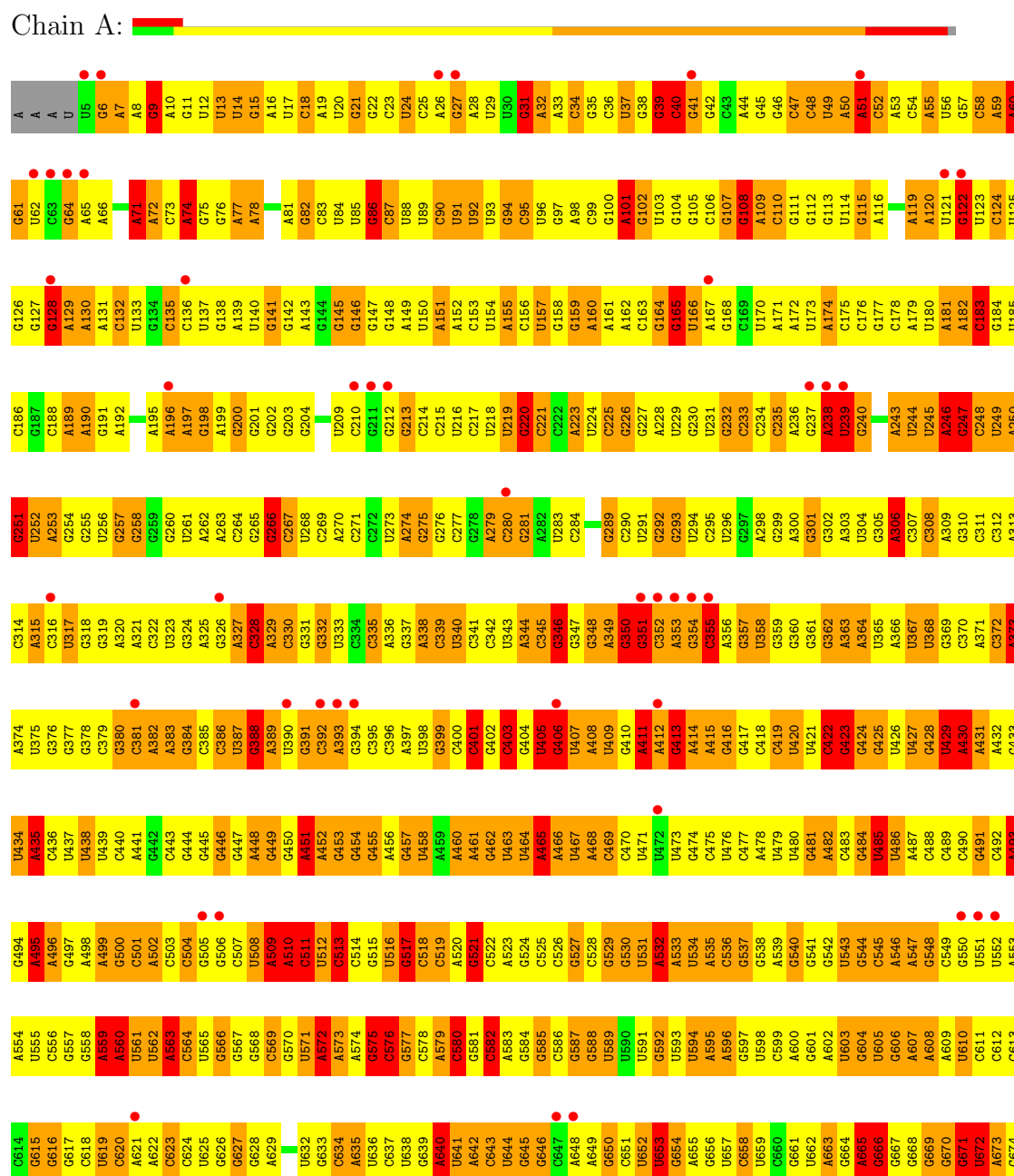
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	287	Total	O	0	0
			287	287		
23	E	2	Total	O	0	0
			2	2		
23	I	2	Total	O	0	0
			2	2		
23	L	2	Total	O	0	0
			2	2		
23	N	3	Total	O	0	0
			3	3		
23	P	1	Total	O	0	0
			1	1		
23	T	1	Total	O	0	0
			1	1		

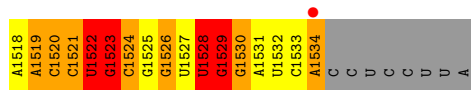
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S RIBOSOMAL RNA

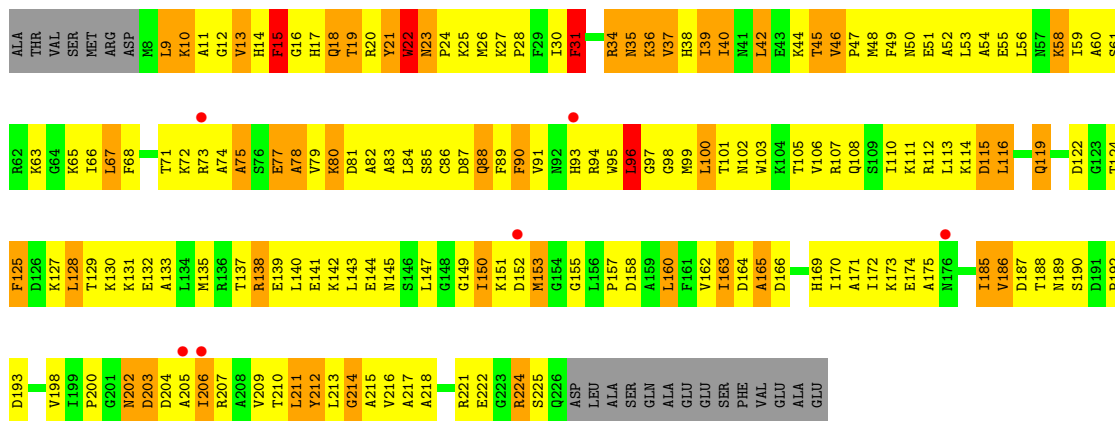


G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	A1500	A1501	A1502	A1503	G1504	G1505	G1506	A1507	A1508	G1509	G1510	G1511	G1512	A1513	G1514	G1515	G1516	G1517				
A1398	C1399	C1400	G1401	C1402	C1403	C1404	G1405	A1346	C1407	A1408	C1409	A1410	C1411	C1412	A1413	A1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	A1430	A1431	G1432	G1433	A1434	G1435	G1436	G1437	G1438	G1439	G1440	A1441	G1442	C1443	U1444	U1445	A1446	A1447	C1448	G1449	U1450	U1451	C1452	G1453	G1454	G1455	G1456	G1457				
G1276	C1277	G1278	G1279	A1280	C1281	C1282	U1283	C1284	A1285	U1286	A1287	A1288	A1289	C1290	U1291	G1353	G1354	G1355	G1356	A1357	U1358	C1359	A1360	G1361	A1362	A1363	G1364	G1365	G1366	C1367	A1368	C1369	U1370	G1371	U1372	G1373	A1374	G1375	G1376	A1377	C1378	G1379	U1380	A1381	C1382	C1383	C1384	G1385	G1386	G1387	C1388	C1389	U1390	U1391	G1392	U1393	A1394	G1395	A1396	C1397			
A1216	C1217	C1218	A1219	G1220	G1221	G1222	C1223	U1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	G1233	G1234	U1235	A1236	G1237	A1238	A1239	U1240	G1241	G1242	C1243	G1244	C1245	A1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1258	C1259	G1260	A1261	C1262	C1263	U1264	C1265	G1266	C1267	U1268	A1269	G1270	A1271	G1272	C1273	A1274	A1275				
G1156	A1157	C1158	U1159	G1160	A1161	C1162	A1163	G1164	U1165	G1166	A1167	U1168	A1169	A1170	A1171	C1172	U1173	G1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	U1183	G1184	G1185	G1186	G1187	A1188	U1189	G1190	A1191	C1192	G1193	U1194	C1195	A1196	A1197	G1198	U1199	C1200	A1201	U1202	C1203	A1204	U1205	G1206	G1207	C1208	G1209	C1210	A1211	U1212	A1213	C1214	G1215				
C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	G1053	C1113	G1114	U1115	A1116	A1117	U1118	C1119	C1120	U1121	U1122	U1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	C1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	A1145	A1146	C1147	U1148	C1149	A1150	A1151	U1152	G1153	G1154	A1155			
A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1044	C1045	A1046	U1047	G1048	U1049	G1050	A1051	U1052	G1053	C1054	A1055	U1056	A1057	G1058	G1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074	U1075	U1076	G1077	U1078	G1079	A1080	A1081	A1082	U1083	G1084	U1085	U1086	G1087	U1088	G1089	U1090	U1091	A1092	A1093	U1095					
A975	G976	A977	A978	C979	C980	U981	U982	A983	C984	C985	U986	G987	G988	U989	U990	U991	U992	G993	A994	C995	C996	C997	C998	C999	A1000	C1001	G1002	U1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	G1015	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	U965	G966	A967	A968	A969	C970	C971	C972	G1033	G1034	A1035		
U855	C856	C857	C858	C859	A860	C861	C862	U863	U864	C865	C866	G867	C868	C869	U870	A871	U872	G873	A874	U875	C876	C877	C878	C879	C880	C881	C882	C883	U884	G885	A886	G887	U888	U889	A890	A891	U892	C893	C894	C895	C896	C897	C898	C899	A900	A901	C902	G903	U904	U905	A906	A907	A908	A909	C910	U911	C912	C913	A914				
A915	U916	A917	A918	A919	U920	U921	G922	A923	C924	A925	G926	G927	C928	C929	C930	C931	C932	G933	C934	C935	C936	A937	A938	C939	C940	G941	U942	U943	U944	C945	A946	G947	C948	A949	U950	U951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	U965	G966	A967	A968	A969	C970	C971	C972	G1033	G1034	A1035			
C795	C796	C797	U798	C799	G800	U801	A802	U803	U804	C805	C806	A807	C808	C809	C810	C811	G812	U813	A814	A815	A816	U757	C758	A818	C819	U820	G821	U822	C823	G824	A825	C826	C827	U828	G829	U830	C831	G832	C833	U834	U835	C836	U837	C838	C839	C840	A781	A782	C783	U843	G844	A845	G846	G847	U787	A788	U789	A790	C910	C851	C852	U793	A794
C735	C736	C737	U677	C738	C739	U740	G741	G742	A743	G744	G745	U686	A747	A748	G749	C750	U691	U751	G752	A753	C754	G755	C756	U757	C758	A759	G760	G761	U762	G763	A764	G765	A766	U767	U768	C769	C770	G771	C772	G773	G774	G775	G776	A777	C778	C779	A780	A781	A782	C783	U784	A785	G786	U787	A788	U789	A790	C910	C851	C852	U793	A794	
A875	A876	U677	U678	C679	C680	U740	G741	G742	A743	G744	G745	U686	A747	A748	G749	C750	U691	U751	G752	A753	C754	G755	C756	U757	C758	A759	G760	G761	U762	G763	A764	G765	A766	U767	U768	C769	C770	G771	C772	G773	G774	G775	G776	A777	C778	C779	A780	A781	A782	C783	U784	A785	G786	U787	A788	U789	A790	C910	C851	C852	U793	A794	



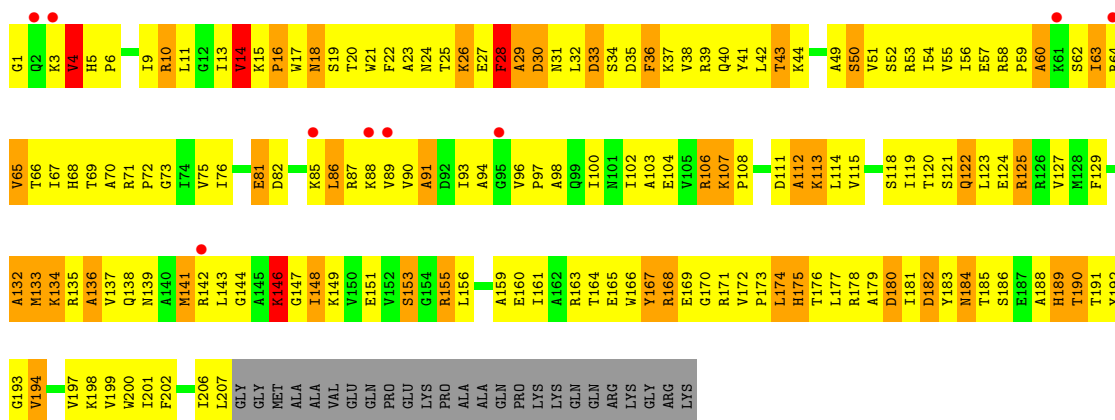
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



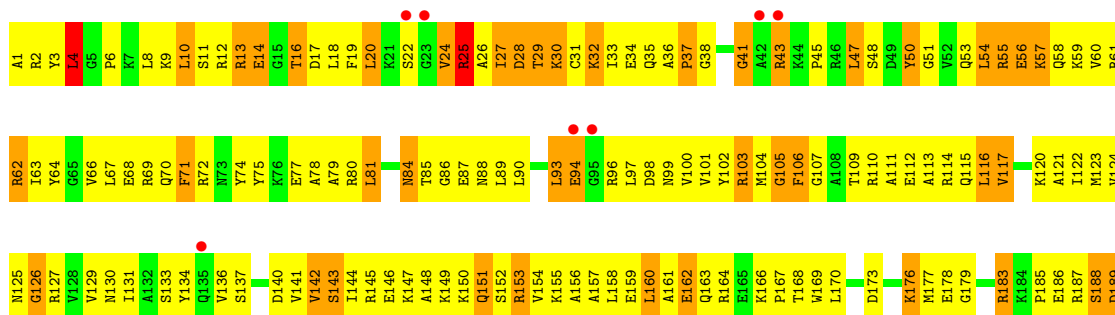
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

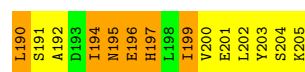
Chain C:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

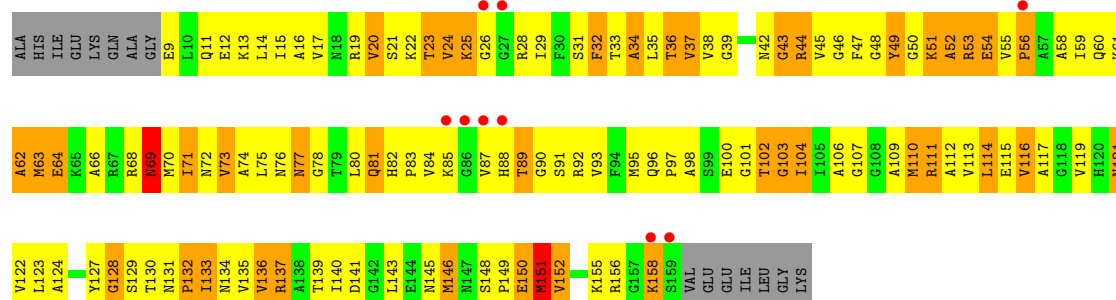
Chain D:





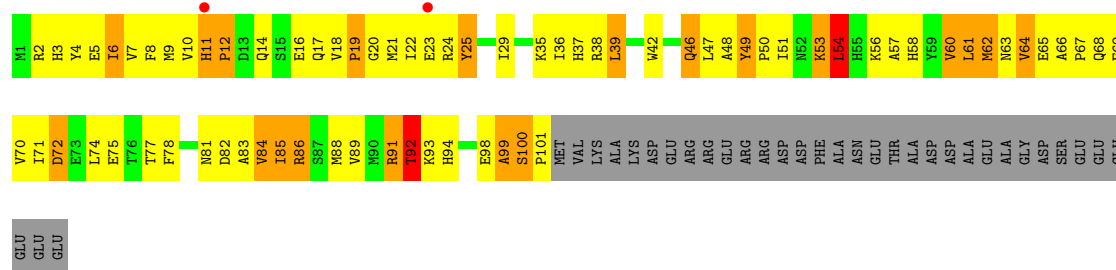
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



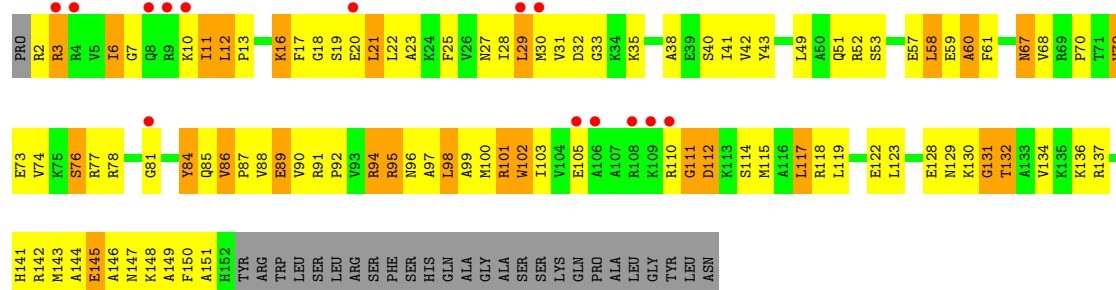
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



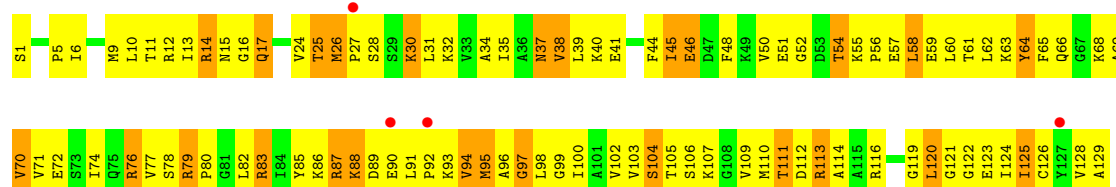
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



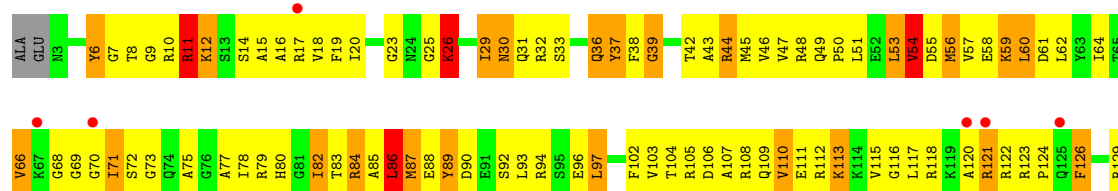
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



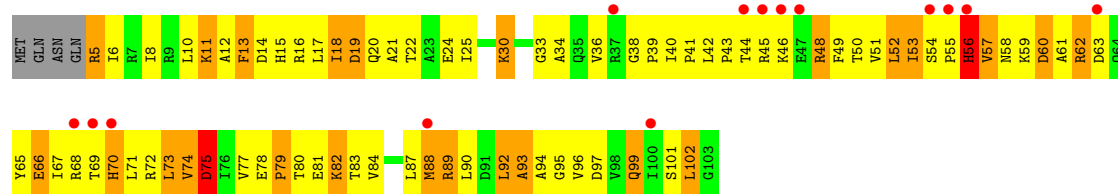
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



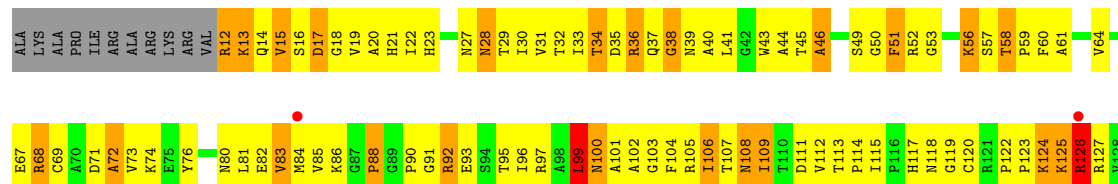
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



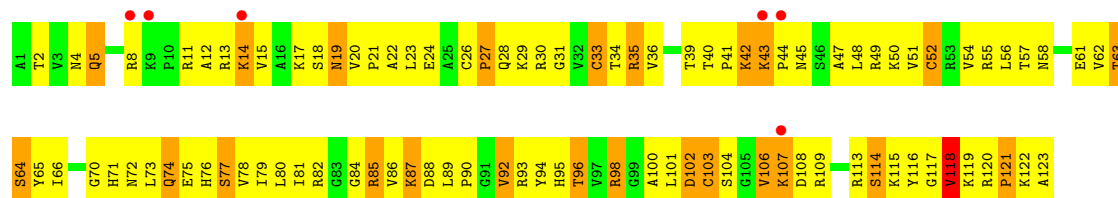
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



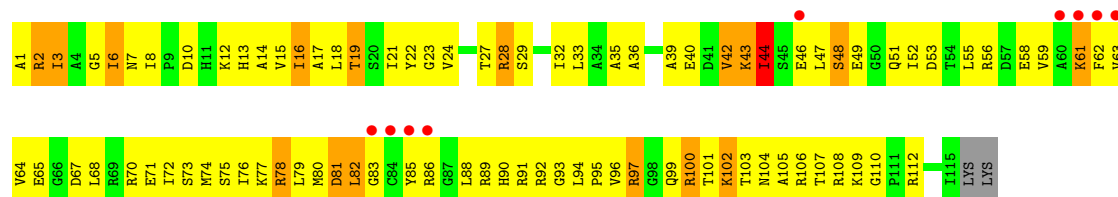
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



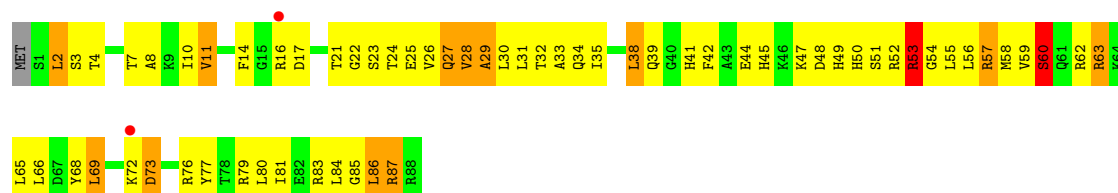
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:



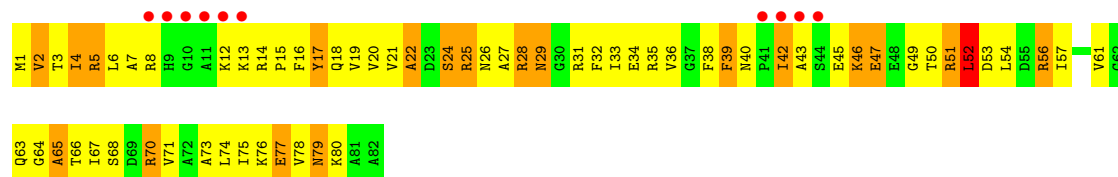
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



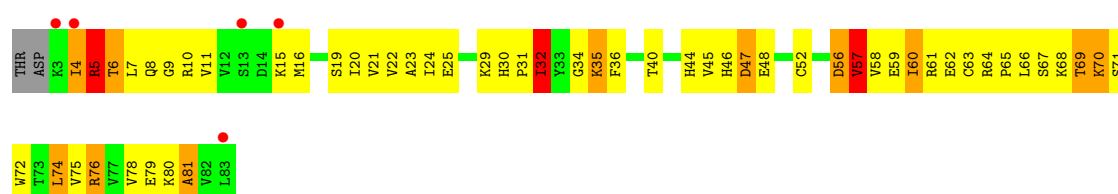
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



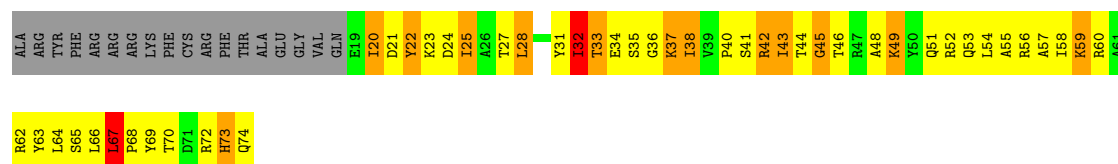
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



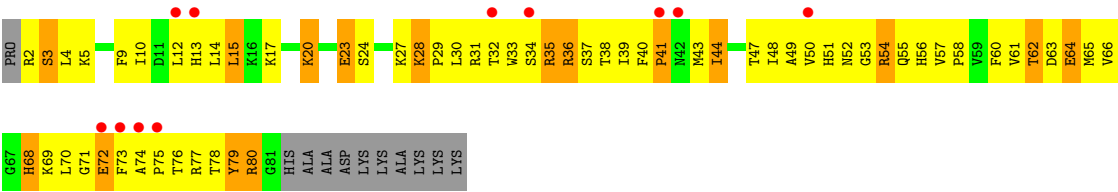
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



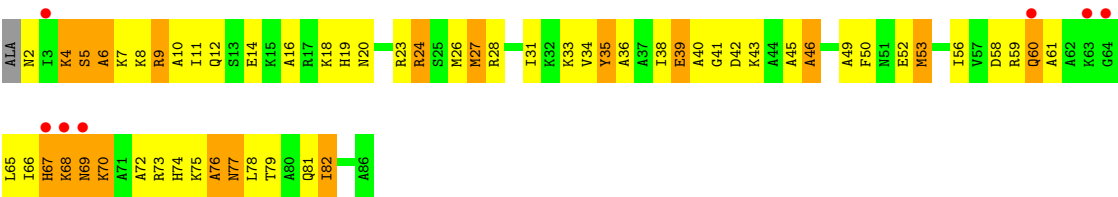
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



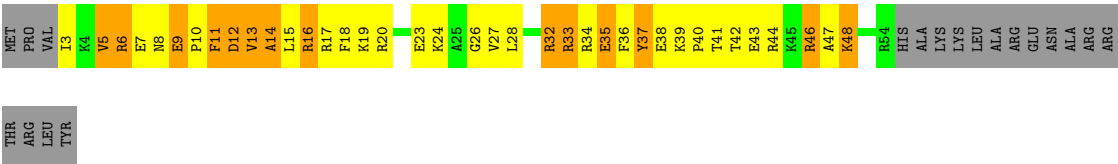
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: 30S RIBOSOMAL PROTEIN S21

Chain U:



4 Data and refinement statistics

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 49.74 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (49.74-3.74)	Depositor EDS
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 0.471 , 0.478	Depositor DCC
R_{free} test set	5522 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , -10.0	EDS
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
F_o, F_c correlation	0.57	EDS
Total number of atoms	51738	wwPDB-VP
Average B, all atoms (Å ²)	164.0	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	A	0.70	4/36761 (0.0%)	1.42	407/57346 (0.7%)
2	B	0.32	0/1736	0.54	0/2340
3	C	0.33	0/1652	0.53	0/2227
4	D	0.36	0/1665	0.62	0/2227
5	E	0.37	0/1119	0.56	0/1506
6	F	0.40	1/836 (0.1%)	0.57	0/1130
7	G	0.33	0/1188	0.52	0/1593
8	H	0.32	0/989	0.55	0/1326
9	I	0.29	0/1034	0.51	0/1375
10	J	0.33	1/797 (0.1%)	0.53	0/1079
11	K	0.35	0/893	0.61	0/1205
12	L	0.33	0/969	0.58	0/1300
13	M	0.29	0/893	0.50	0/1195
14	N	0.29	0/785	0.51	0/1043
15	O	0.33	0/724	0.55	0/966
16	P	0.30	0/659	0.51	0/884
17	Q	0.37	0/658	0.59	0/883
18	R	0.40	0/463	0.62	0/623
19	S	0.32	1/653 (0.2%)	0.50	0/879
20	T	0.32	0/671	0.49	0/888
21	U	0.42	0/431	0.56	0/572
All	All	0.61	7/55576 (0.0%)	1.22	407/82587 (0.5%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	765	G	N9-C4	6.00	1.42	1.38
1	A	603	U	C1'-N1	5.69	1.57	1.48
6	F	100	SER	C-N	-5.50	1.23	1.34
19	S	80	ARG	C-N	-5.27	1.23	1.33
1	A	717	U	C1'-N1	5.26	1.56	1.48

The worst 5 of 407 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1529	G	C1'-O4'-C4'	-12.81	99.66	109.90
1	A	563	A	C1'-O4'-C4'	-12.33	100.04	109.90
1	A	779	C	P-O3'-C3'	-12.32	104.92	119.70
1	A	765	G	O4'-C1'-N9	11.87	117.70	108.20
1	A	306	A	O4'-C1'-N9	11.54	117.44	108.20

There are no chirality outliers.

There are no planarity outliers.

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	16522	3622	0
2	B	1705	0	1732	245	0
3	C	1625	0	1699	214	0
4	D	1643	0	1710	284	0
5	E	1106	0	1148	176	0
6	F	818	0	808	113	0
7	G	1175	0	1230	116	0
8	H	979	0	1034	141	0
9	I	1022	0	1070	141	0
10	J	787	0	828	99	0
11	K	877	0	887	127	0
12	L	955	0	1019	145	0
13	M	884	0	944	120	0
14	N	774	0	827	138	0
15	O	716	0	742	94	0
16	P	649	0	666	109	0
17	Q	649	0	691	70	0
18	R	456	0	478	75	0
19	S	638	0	665	112	0
20	T	665	0	714	85	0
21	U	426	0	449	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Z	60	0	0	0	0
23	A	287	0	0	26	0
23	E	2	0	0	0	0
23	I	2	0	0	0	0
23	L	2	0	0	0	0
23	N	3	0	0	0	0
23	P	1	0	0	0	0
23	T	1	0	0	0	0
All	All	51738	0	35863	5867	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 68.

The worst 5 of 5867 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:C:H2'	1:A:236:A:C8	1.79	1.17
9:I:44:ARG:HG3	9:I:44:ARG:HH11	1.02	1.14
1:A:553:A:H2'	1:A:554:A:C8	1.81	1.13
1:A:843:U:H3'	1:A:844:G:H5'	1.30	1.12
21:U:36:PHE:HB3	21:U:40:PRO:HD3	1.26	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	217/240 (90%)	128 (59%)	65 (30%)	24 (11%)	1	17
3	C	205/232 (88%)	116 (57%)	59 (29%)	30 (15%)	0	10
4	D	203/205 (99%)	120 (59%)	57 (28%)	26 (13%)	0	14
5	E	149/166 (90%)	94 (63%)	33 (22%)	22 (15%)	0	9
6	F	99/135 (73%)	62 (63%)	25 (25%)	12 (12%)	1	15
7	G	149/178 (84%)	100 (67%)	34 (23%)	15 (10%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	127/129 (98%)	73 (58%)	42 (33%)	12 (9%)	1	24
9	I	125/129 (97%)	78 (62%)	35 (28%)	12 (10%)	1	22
10	J	97/103 (94%)	59 (61%)	23 (24%)	15 (16%)	0	8
11	K	115/128 (90%)	69 (60%)	31 (27%)	15 (13%)	0	13
12	L	121/123 (98%)	67 (55%)	37 (31%)	17 (14%)	0	11
13	M	113/117 (97%)	70 (62%)	32 (28%)	11 (10%)	1	22
14	N	92/100 (92%)	58 (63%)	18 (20%)	16 (17%)	0	6
15	O	86/89 (97%)	51 (59%)	26 (30%)	9 (10%)	1	18
16	P	80/82 (98%)	43 (54%)	22 (28%)	15 (19%)	0	5
17	Q	79/83 (95%)	53 (67%)	15 (19%)	11 (14%)	0	11
18	R	54/74 (73%)	25 (46%)	19 (35%)	10 (18%)	0	5
19	S	78/91 (86%)	52 (67%)	20 (26%)	6 (8%)	1	30
20	T	83/86 (96%)	51 (61%)	20 (24%)	12 (14%)	0	10
21	U	50/71 (70%)	26 (52%)	14 (28%)	10 (20%)	0	4
All	All	2322/2561 (91%)	1395 (60%)	627 (27%)	300 (13%)	0	13

5 of 300 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	19	THR
2	B	22	TRP
2	B	75	ALA
2	B	87	ASP
2	B	100	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/198 (91%)	143 (79%)	37 (21%)	2	13
3	C	170/189 (90%)	142 (84%)	28 (16%)	3	25
4	D	172/172 (100%)	137 (80%)	35 (20%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	113/125 (90%)	86 (76%)	27 (24%)	1	8
6	F	87/116 (75%)	71 (82%)	16 (18%)	2	18
7	G	123/146 (84%)	105 (85%)	18 (15%)	5	32
8	H	104/104 (100%)	78 (75%)	26 (25%)	1	8
9	I	105/106 (99%)	81 (77%)	24 (23%)	1	10
10	J	86/90 (96%)	68 (79%)	18 (21%)	1	13
11	K	90/98 (92%)	68 (76%)	22 (24%)	1	8
12	L	103/103 (100%)	82 (80%)	21 (20%)	2	14
13	M	92/95 (97%)	76 (83%)	16 (17%)	3	21
14	N	79/83 (95%)	66 (84%)	13 (16%)	3	25
15	O	76/77 (99%)	63 (83%)	13 (17%)	3	23
16	P	65/65 (100%)	54 (83%)	11 (17%)	3	24
17	Q	74/77 (96%)	65 (88%)	9 (12%)	7	42
18	R	48/64 (75%)	39 (81%)	9 (19%)	2	17
19	S	70/78 (90%)	59 (84%)	11 (16%)	4	28
20	T	65/65 (100%)	55 (85%)	10 (15%)	4	29
21	U	44/61 (72%)	39 (89%)	5 (11%)	8	45
All	All	1946/2112 (92%)	1577 (81%)	369 (19%)	2	17

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	37	ASN
9	I	108	ARG
18	R	54	LEU
8	H	58	LEU
9	I	6	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	67	ASN
9	I	31	GLN
19	S	56	HIS
7	G	85	GLN

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Mol	Chain	Res	Type
8	H	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1528/1542 (99%)	618 (40%)	204 (13%)

5 of 618 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	9	G
1	A	14	U
1	A	15	G

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	704	A
1	A	872	A
1	A	1380	U
1	A	712	A
1	A	804	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 ⓘ

Of 60 ligands modelled in this entry, 60 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1530/1542 (99%)	0.54	100 (6%) 18 13	70, 137, 279, 497	0
2	B	219/240 (91%)	0.03	6 (2%) 52 32	94, 175, 269, 316	0
3	C	207/232 (89%)	0.24	9 (4%) 34 22	87, 169, 255, 315	0
4	D	205/205 (100%)	0.19	7 (3%) 43 27	61, 139, 230, 325	0
5	E	151/166 (90%)	0.13	9 (5%) 21 15	75, 156, 254, 336	0
6	F	101/135 (74%)	0.19	2 (1%) 62 39	57, 140, 224, 279	0
7	G	151/178 (84%)	0.38	14 (9%) 9 8	94, 206, 288, 333	0
8	H	129/129 (100%)	0.26	4 (3%) 47 29	76, 157, 231, 297	0
9	I	127/129 (98%)	0.21	6 (4%) 30 20	90, 194, 271, 307	0
10	J	99/103 (96%)	0.89	14 (14%) 3 4	131, 254, 373, 423	0
11	K	117/128 (91%)	0.23	2 (1%) 67 44	54, 128, 245, 290	0
12	L	123/123 (100%)	0.27	6 (4%) 28 18	50, 138, 215, 332	0
13	M	115/117 (98%)	0.52	9 (7%) 13 10	144, 252, 315, 344	0
14	N	96/100 (96%)	1.07	18 (18%) 2 3	85, 188, 308, 367	0
15	O	88/89 (98%)	-0.02	2 (2%) 57 36	67, 133, 213, 255	0
16	P	82/82 (100%)	0.52	10 (12%) 5 5	90, 168, 269, 347	0
17	Q	81/83 (97%)	0.40	5 (6%) 20 14	101, 180, 266, 301	0
18	R	56/74 (75%)	0.01	0 100 100	66, 117, 216, 283	0
19	S	80/91 (87%)	0.88	11 (13%) 4 4	152, 267, 315, 366	0
20	T	85/86 (98%)	0.42	7 (8%) 12 10	76, 155, 224, 256	0
21	U	52/71 (73%)	0.08	0 100 100	91, 171, 256, 300	0
All	All	3894/4103 (94%)	0.41	241 (6%) 21 14	50, 156, 288, 497	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	84	CYS	13.0
19	S	73	PHE	8.5
13	M	83	GLY	8.5
17	Q	3	LYS	8.1
1	A	210	C	7.2

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	MG	Z	4025	1/1	0.86	39.65	32,32,32,32	1
22	MG	Z	4060	1/1	0.39	36.25	78,78,78,78	0
22	MG	Z	4043	1/1	1.19	16.85	54,54,54,54	0
22	MG	Z	4055	1/1	0.72	14.17	109,109,109,109	0
22	MG	Z	4049	1/1	0.36	12.93	29,29,29,29	0
22	MG	Z	4056	1/1	0.32	7.03	90,90,90,90	0
22	MG	Z	4019	1/1	0.26	6.00	64,64,64,64	0
22	MG	Z	4022	1/1	0.69	5.86	28,28,28,28	1
22	MG	Z	4046	1/1	0.86	5.20	86,86,86,86	0
22	MG	Z	4014	1/1	0.74	4.55	61,61,61,61	0
22	MG	Z	4031	1/1	0.42	4.23	34,34,34,34	0
22	MG	Z	4021	1/1	0.44	4.07	77,77,77,77	0
22	MG	Z	4007	1/1	0.38	3.97	81,81,81,81	0
22	MG	Z	4001	1/1	0.35	3.71	69,69,69,69	0
22	MG	Z	4016	1/1	0.37	2.85	59,59,59,59	0
22	MG	Z	4004	1/1	0.62	2.58	34,34,34,34	0
22	MG	Z	4051	1/1	0.36	2.55	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	Z	4020	1/1	0.28	2.48	11,11,11,11	0
22	MG	Z	4028	1/1	0.36	1.49	68,68,68,68	0
22	MG	Z	4009	1/1	0.29	1.40	34,34,34,34	0
22	MG	Z	4032	1/1	0.30	1.32	40,40,40,40	0
22	MG	Z	4054	1/1	0.27	1.31	33,33,33,33	0
22	MG	Z	4002	1/1	0.27	1.20	86,86,86,86	0
22	MG	Z	4038	1/1	0.61	1.16	27,27,27,27	0
22	MG	Z	4010	1/1	0.27	1.11	17,17,17,17	0
22	MG	Z	4036	1/1	0.45	0.94	30,30,30,30	0
22	MG	Z	4033	1/1	0.24	0.88	27,27,27,27	0
22	MG	Z	4023	1/1	0.24	0.73	14,14,14,14	0
22	MG	Z	4026	1/1	0.27	0.66	37,37,37,37	0
22	MG	Z	4044	1/1	0.42	0.63	69,69,69,69	0
22	MG	Z	4027	1/1	0.37	0.57	75,75,75,75	0
22	MG	Z	4012	1/1	0.52	0.56	54,54,54,54	0
22	MG	Z	4011	1/1	0.28	0.35	56,56,56,56	0
22	MG	Z	4045	1/1	0.27	0.29	25,25,25,25	0
22	MG	Z	4053	1/1	0.39	0.23	79,79,79,79	0
22	MG	Z	4042	1/1	0.27	0.22	49,49,49,49	0
22	MG	Z	4048	1/1	0.34	-0.32	62,62,62,62	0
22	MG	Z	4057	1/1	0.24	-0.64	27,27,27,27	0
22	MG	Z	4018	1/1	0.22	-0.79	42,42,42,42	0
22	MG	Z	4035	1/1	0.16	-1.52	48,48,48,48	0
22	MG	Z	4034	1/1	0.20	-1.64	90,90,90,90	0
22	MG	Z	4039	1/1	0.11	-1.83	58,58,58,58	0
22	MG	Z	4005	1/1	0.14	-1.91	59,59,59,59	0
22	MG	Z	4015	1/1	0.14	-2.07	44,44,44,44	0
22	MG	Z	4006	1/1	0.14	-2.26	42,42,42,42	0
22	MG	Z	4003	1/1	0.11	-2.55	29,29,29,29	0
22	MG	Z	4029	1/1	0.13	-2.68	61,61,61,61	0
22	MG	Z	4040	1/1	0.07	-2.76	50,50,50,50	0
22	MG	Z	4013	1/1	0.15	-3.27	73,73,73,73	0
22	MG	Z	4050	1/1	0.14	-3.81	73,73,73,73	0
22	MG	Z	4052	1/1	0.09	-3.92	51,51,51,51	0
22	MG	Z	4008	1/1	0.10	-4.05	21,21,21,21	0
22	MG	Z	4037	1/1	0.07	-4.06	5,5,5,5	0
22	MG	Z	4041	1/1	0.06	-4.36	31,31,31,31	0
22	MG	Z	4059	1/1	0.10	-4.50	29,29,29,29	0
22	MG	Z	4047	1/1	0.10	-4.66	59,59,59,59	0
22	MG	Z	4030	1/1	0.07	-5.24	44,44,44,44	0
22	MG	Z	4017	1/1	0.07	-6.67	47,47,47,47	0
22	MG	Z	4024	1/1	0.42	-	63,63,63,63	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	Z	4058	1/1	0.56	-	81,81,81,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.