



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:17 PM BST

PDB ID : 4V4R
Title : Crystal structure of the whole ribosomal complex.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.;
Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-09-30
Resolution : 5.90 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>

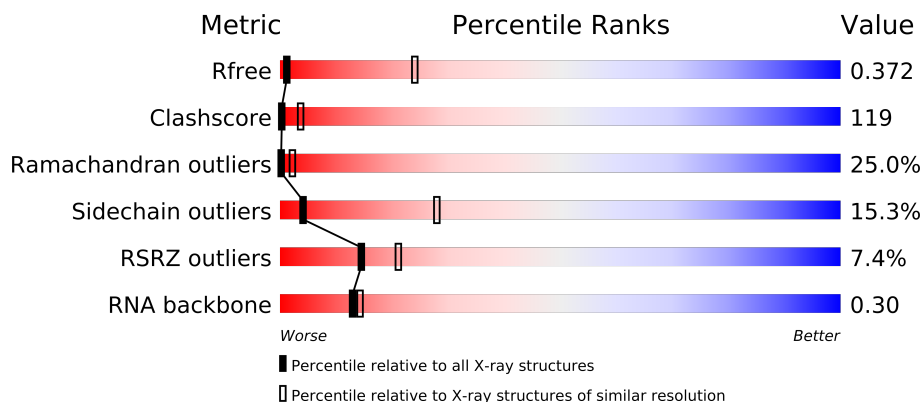
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
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) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 5.90 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	1089 (8.20-3.50)
Clashscore	79885	1024 (8.20-3.52)
Ramachandran outliers	78287	1282 (8.20-3.50)
Sidechain outliers	78261	1258 (8.20-3.50)
RSRZ outliers	66119	1088 (8.20-3.50)
RNA backbone	1838	1042 (8.70-2.80)

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	AA	1522	
2	AV	76	
3	AW	76	
4	AX	18	
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	

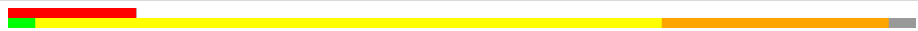

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Mol	Chain	Length	Quality of chain
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	AY	354	
26	BB	123	
27	BA	2916	
28	BD	173	
29	BE	338	
30	BF	246	
31	BG	176	
32	BH	177	
33	BI	149	
34	BN	145	
35	BO	122	
36	BP	164	
37	BQ	138	
38	BS	186	
39	BT	66	
40	BW	113	
41	BX	84	
42	BY	119	
43	BZ	253	
44	BR	118	
45	BU	118	
46	BV	100	
47	B2	70	
48	B3	60	
49	B0	91	
50	B4	73	
51	B5	60	
52	B6	82	
53	B7	47	
54	B8	64	

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Mol	Chain	Length	Quality of chain
55	B9	36	
56	BK	141	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142780 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	AA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-R(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*C
P*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AX	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AR	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 25 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	AY	333	Total	C	0	0	333
			333	333			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2814	Total	C	N	O	P	0	0	0
			60600	26974	11331	19482	2813			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	GB 48268

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BP	84	Total	C	N	O	0	0	0
			639	391	109	139			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BW	108	Total	C	N	O	0	0	0
			860	542	169	149			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 42 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BY	110	Total	C	N	O	0	0	0
			879	531	166	182			

- Molecule 43 is a protein called 50S ribosomal protein CTC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BR	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BU	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

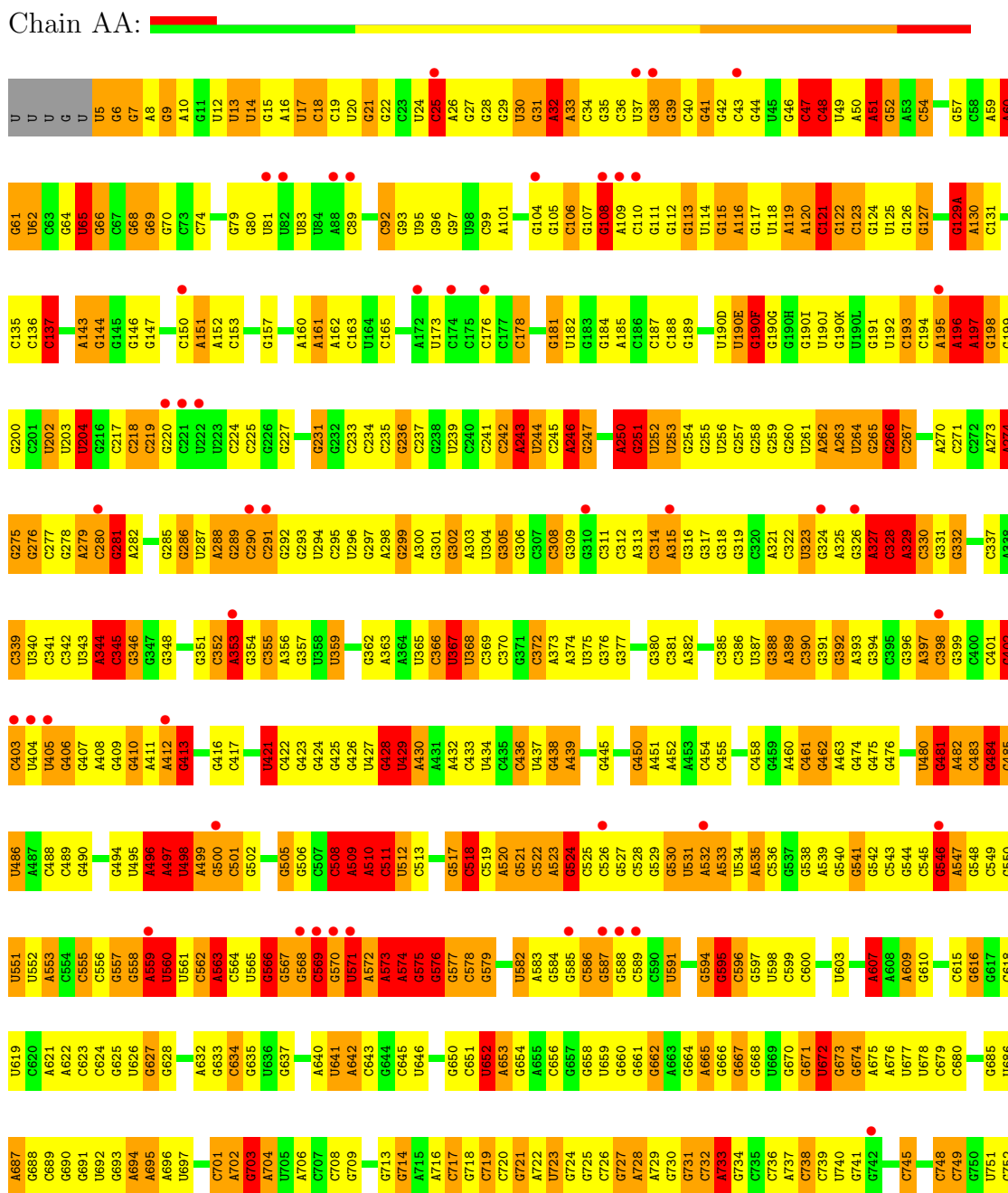
- Molecule 56 is a protein called 50S ribosomal protein L11.

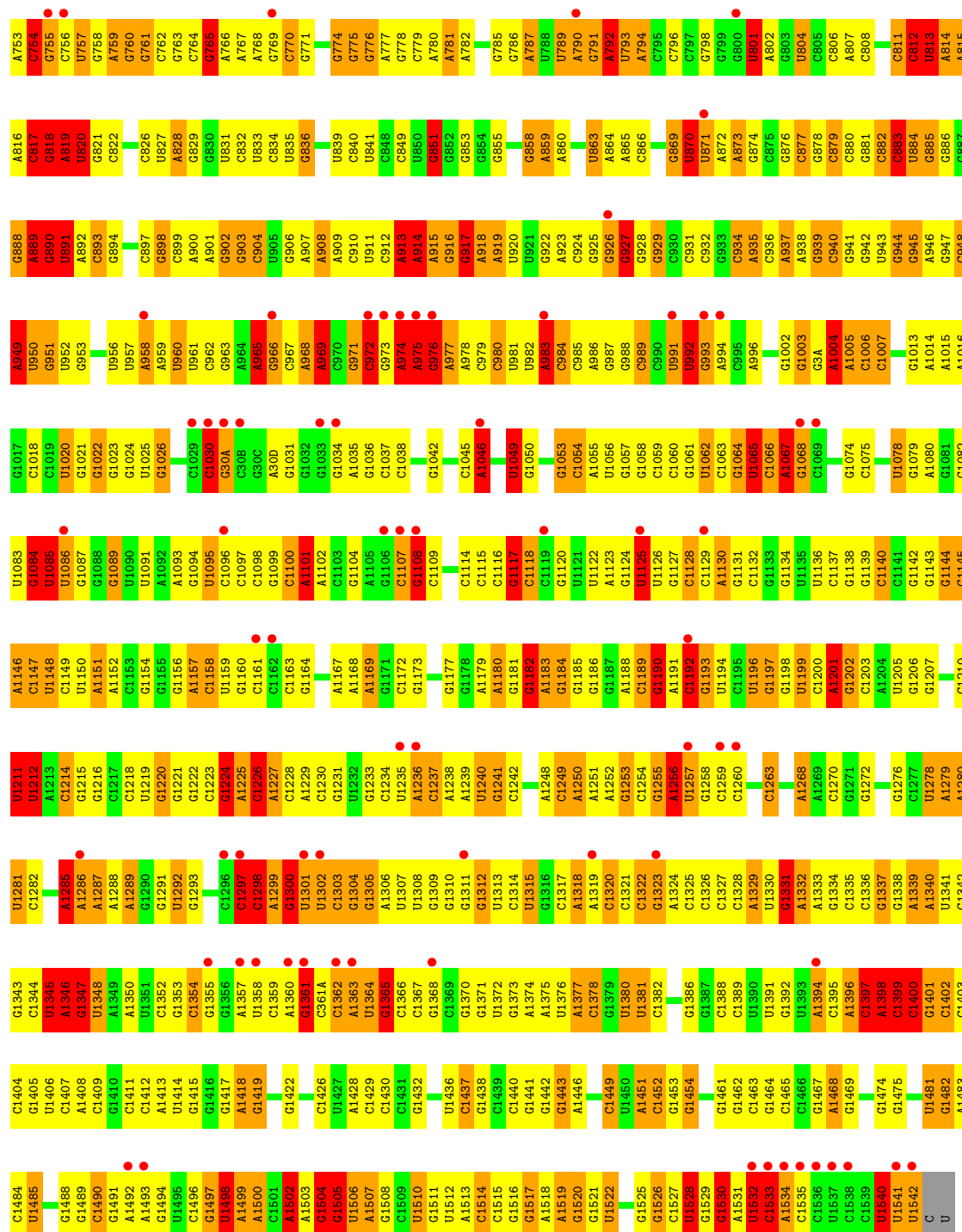
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

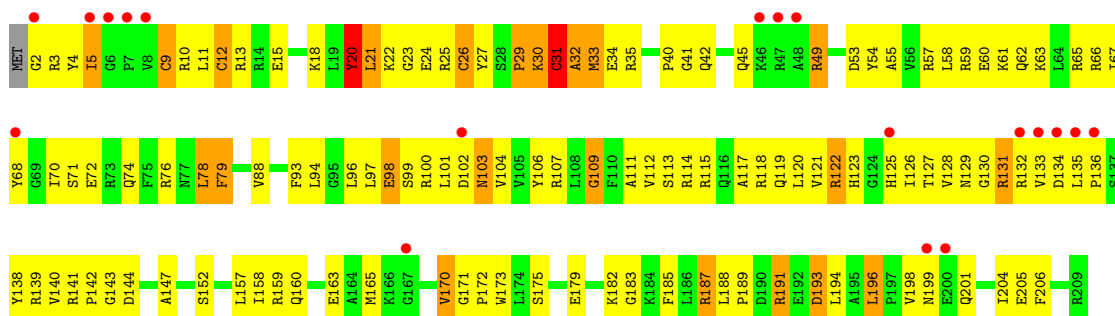
3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

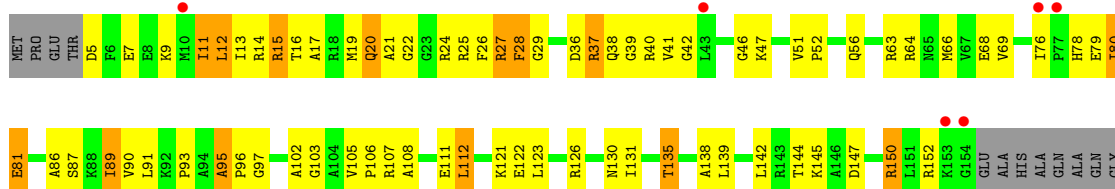






• Molecule 8: 30S ribosomal protein S5

Chain AE:



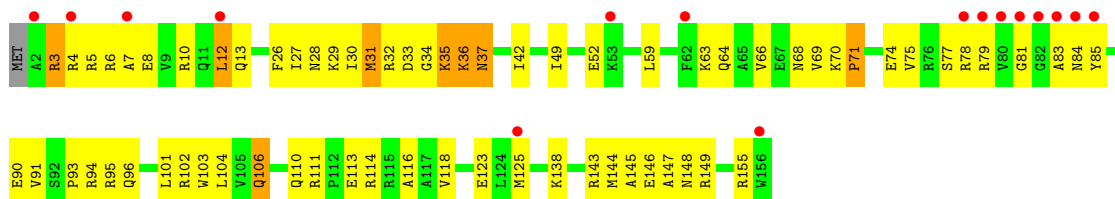
• Molecule 9: 30S ribosomal protein S6

Chain AF:



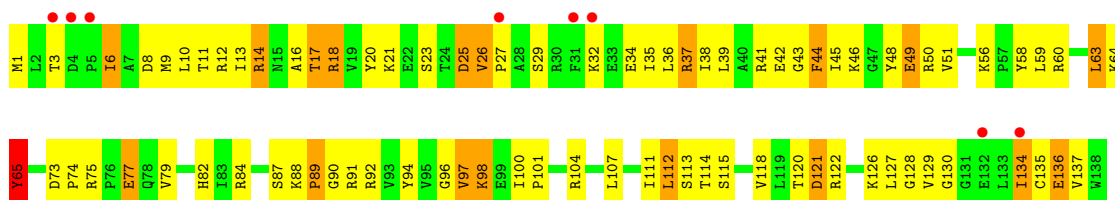
• Molecule 10: 30S ribosomal protein S7

Chain AG:



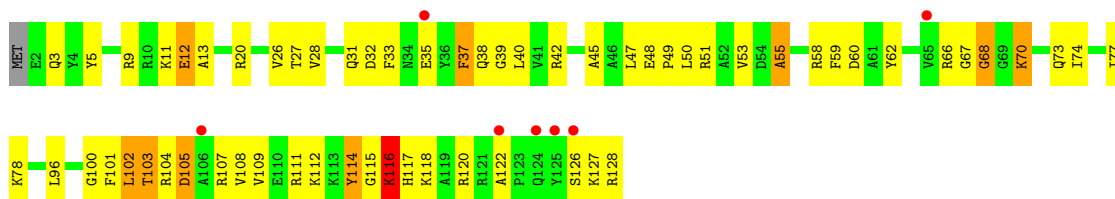
• Molecule 11: 30S ribosomal protein S8

Chain AH:



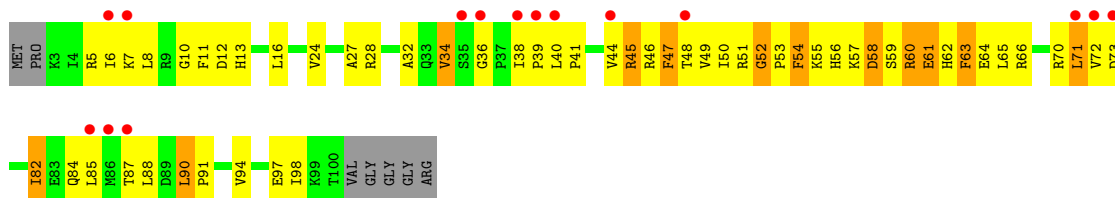
• Molecule 12: 30S ribosomal protein S9

Chain AI:



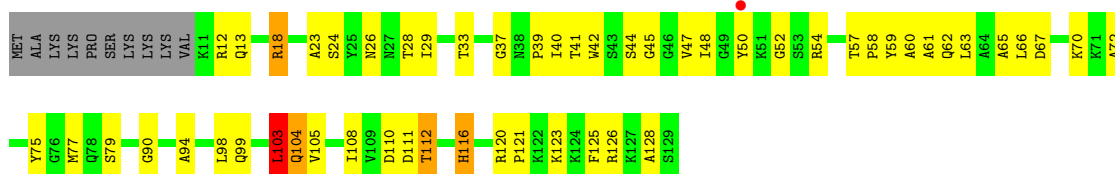
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



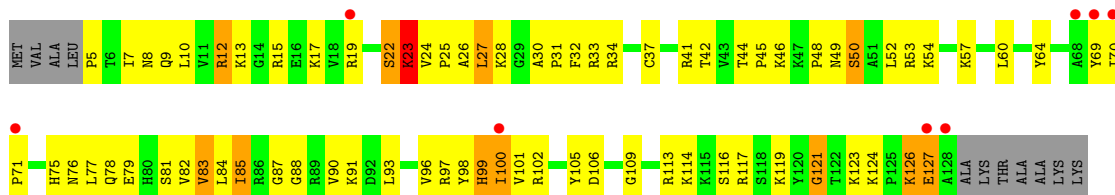
• Molecule 14: 30S ribosomal protein S11

Chain AK:



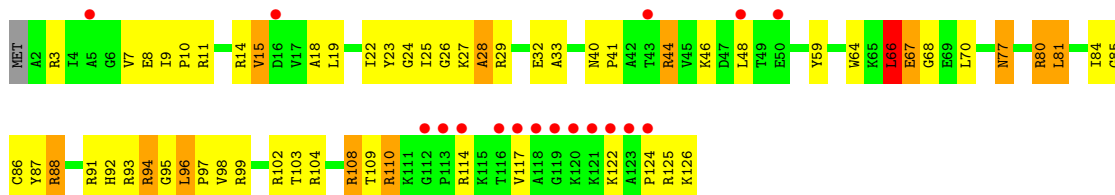
• Molecule 15: 30S ribosomal protein S12

Chain AL:



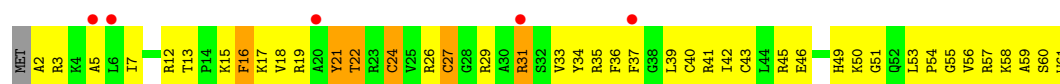
• Molecule 16: 30S ribosomal protein S13

Chain AM:



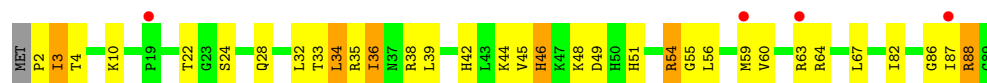
• Molecule 17: 30S ribosomal protein S14

Chain AN:



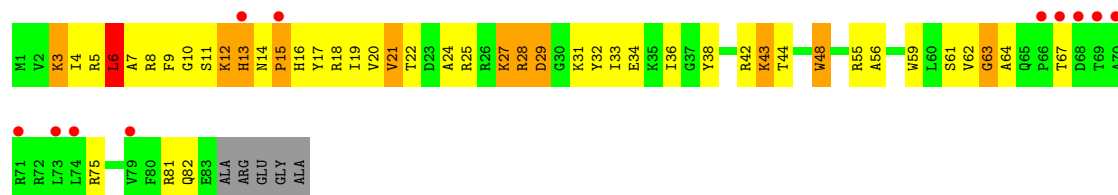
- Molecule 18: 30S ribosomal protein S15

Chain AO:



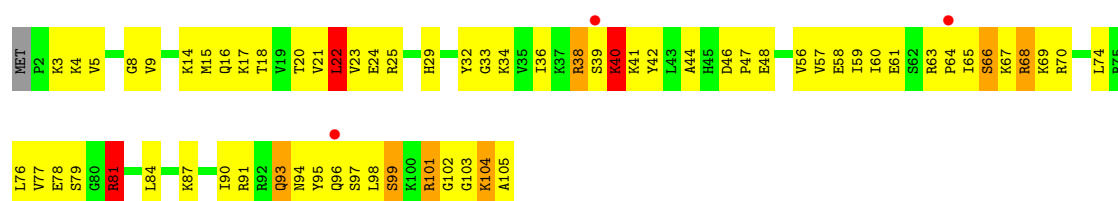
- Molecule 19: 30S ribosomal protein S16

Chain AP:



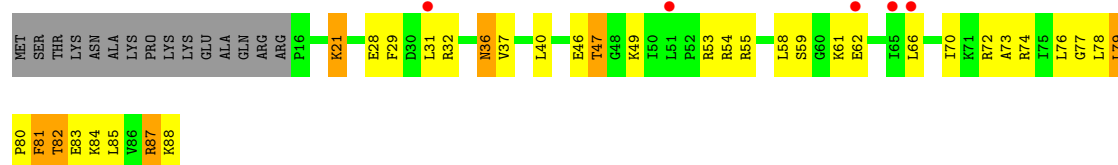
- Molecule 20: 30S ribosomal protein S17

Chain AQ:



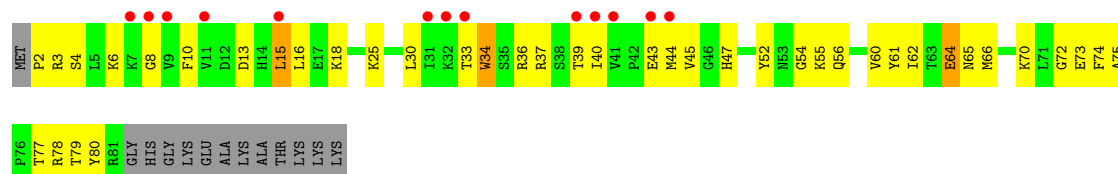
- Molecule 21: 30S ribosomal protein S18

Chain AR:



- Molecule 22: 30S ribosomal protein S19

Chain AS:



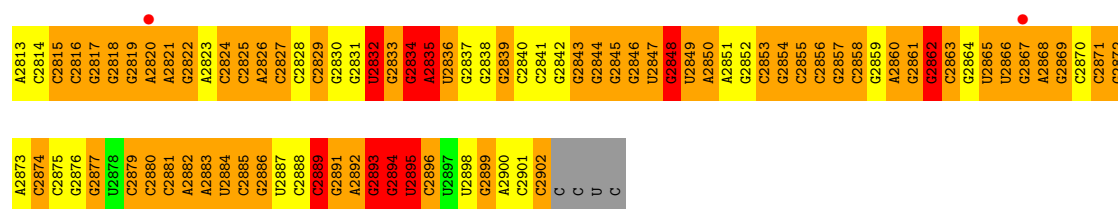
- Molecule 23: 30S ribosomal protein S20

Chain AT:



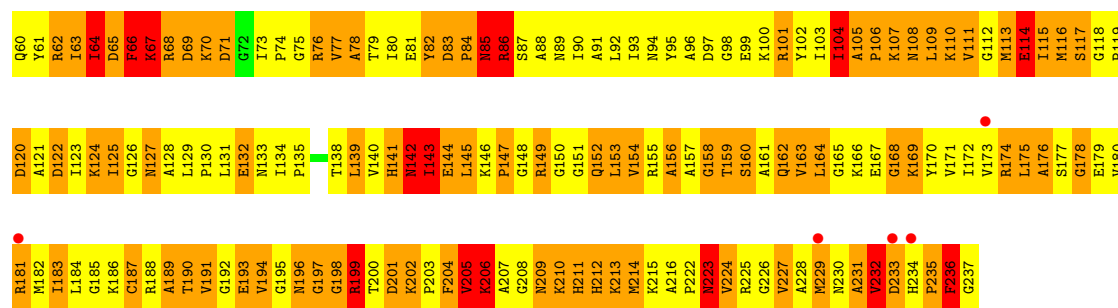
G1896	A1821	A1760	G1678	A545A	G1484	G1418	G1356	G1226	G1663	C1100	G1034
G1899	G1822	G1761	U1679	C1546	G1485	A1419	U1357	A1227	G1664	U1101	U1035
A1900	G1823	A1762	U1680	C1547	A1486	U1420	G1358	G1228	U1165	G1102	G1036
A1901	G1824	G1763	G1681	C1548	A1487	G1421	A1359	G1229	A1103	A1103	
G1902	G1825	G1764	G1682		G1488	G1422	A1360	C1230	U1105	C1104	C1040
G1903	G1826	G1765	G1683	G1552	U1489	G1423	G1361	U1234	G1669	G1106	C1041
G1904	C1827	U1766	G1684	A1553	A1490	G1424	C1362	U1235	G1170	G1107	G1044
G1905	G1828	G1767	G1685	A1554	G1491	G1425	G1363	G1236	A1171	U1108	A1045
G1906	A1829	G1768	G1686	G1555	G1492	G1426	G1364	G1237	A1046	C1109	A1046
G1907	G1830	G1769	G1687	G1556	A1493	A1427	A1365	G1238	G1173	G1109	
G1908	G1831	G1770	U1688	C1557	A1494	G1428	A1366	G1239	A1174	A1111	
G1909	C1832	C1771	A1689	C1558	A1495	G1429	A1367	U1240	U1175	G1112	G1049
C1908	G1833	G1772	G1690	G1559	A1496	G1430	G1368	U1241	G1176	G1113	A1050
G1910	U1834	A1773	G1693	G1560	U1497	U1431	G1369	A1241	A1177	G1114	G1051
G1911	G1835	C1774	C630A	G1561	C1498	G1432	C1370	A1242	C1178	G1115	A1054
A1912	G1836	U1775	G1694		C1499	U1433	G1371	G1243	G1179	G1116	G1055
A1913	G1837	G1776	A1632	G1562	G1500	A1434	G1372	G1244	G1180	G1117	G1056
G1914	C1838	U1777	G1633	G1563	G1501		A1373	G1245	C1181	G1118	G1057
U1915	G1839	U1778	G1697	G1564	C1502	G1437	G1374	A1246	G1182	C1119	G1058
A1916	G1840	U1779	G1698	A1569		U1438	C1375	A1247	G1183	G1120	G1059
U1917	U1841	A1780	G1699	A1570	C1506	U1439	C1376	G1248	G1184	G1121	U1060
A1918	G1842	C1781	A1637	A1571	A1507	G1440	G1377	U1249	C1185	G1122	U1061
A1919	C1843	A1701	C1638	A1572	A1508	G1441	A1378	G1250	G1186	G1123	G1062
G1920	C1844	G1783	U1639	G1573	C1509	G1442	A1379	G1251	G1187	C1124	G1063
G1921		A1784	G1640	C1574	A1510	G1443	G1380	G1252	U1188	G1125	G1064
G1922	A1847	A1785	G1641	C1575	A1511	G1444	G1381	A1253	A1189	U1126	U1065
U1923	A1848	U1786	G1705	U1576	G1512	A444A	G1382	A1254	G1190	A1127	U1066
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A1937	G1801	G1731	C1657	A1596	G1526	C1462	U1397	A1268	C1207	U1142	U1082
U1938	A1802	A1732	C1658	A1597	G1527	C1463	C1398	A1269	G1208	A1424	U1083
U1939	A1803	G1733		C1598	A1528	G1464	C1399	G1270	G1209	A1143	A1084
C1940	C1804	G1734	G1735	C1599	A1529	G1465	G1400	G1271	A1210	G1149	A1085
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U2755	U2696	U2636	G2576	G2516	G2457	C2396	A2336	G2276	G2211	C	C2085	C2025	C1962
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A2757	U2698	G2638	C2578	A2518	G2458	U2398	G2338	A2278	U2213	G	G2087	G2027	U1964
A2758	C2699	A2639	C2579	U2519	A2459	G2399	G2339	G2279	U2215	G	C2088	U2028	C1965
G2759	C2700	G2640	U2580	C2520	U2460	G2400	G2340	G2280	G2216	U	U2089	U2029	A1966
C2760	C2701	G2641	U2581	C2521	U2461	U2401	G2341	C2281	G2217	G	U2090	A2030	C1967
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G2762	C2703	G2643	G2583	G2523	U2463	C2403	C2343	G2283	G2219	G	U2092	G2032	G1969
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A2764	A2705	G2645	U2585	G2525	C2465	G2405	A2345	C2285	A2225	G	A2094	U2034	A1971
A2765	G2706	C2646	C2586	G2526	C2466	U2406	A2346	A2286	C2226	G	G2095	U2035	A1972
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A2778	C2719	G2659	C2599	G2539	G2479	U2419	C2359	G2299	G2239	A	U	G2048	C
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A2799	A2739	A2679	C2619	U2559	C2499	A2439	G2379	G2319	C2259	U	U	U2068	G2009
G2801	U2739	C2680	C2620	C2560	U2500	C2440	C2380	A2320	C2260	G	G	G2069	G2010
G2802	A2740	C2681	A2621	A2561	C2501	C2441	C2381	G2321	C2261	U	G	G2070	C2011
C2803	A2741	U2682	C2622	U2562	G2502	C2442	G2382	A2322	U2262	C	U	A2071	U2011
C2804	C2742	C2683	G2623	U2563	A2503	C2443	G2383	G2323	C2263	G	G	G2072	G2012
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G2807	G2744	G2685	G2625	A2565	G2505	G2445	C2385	G2325	U2265	A	A	U2074	A2014
U2808	C2745	G2686	A2566	A2566	U2506	G2446	C2386	C2326	A2266	C	C	U2075	A2015
A2809	U2746	U2687	G2627	C2567	C2507	G2447	U2387	A2327	A2267	C	C	U2076	U2016
C2810	G2747	U2688	C2628	C2568	G2508	A2448	A2388	A2328	A2268	C	C	A2077	U2017
G2811	A2748	G2689	A2629	U2569	G2509	G2449	G2389	G2329	A2269	C	C	G2078	G2018
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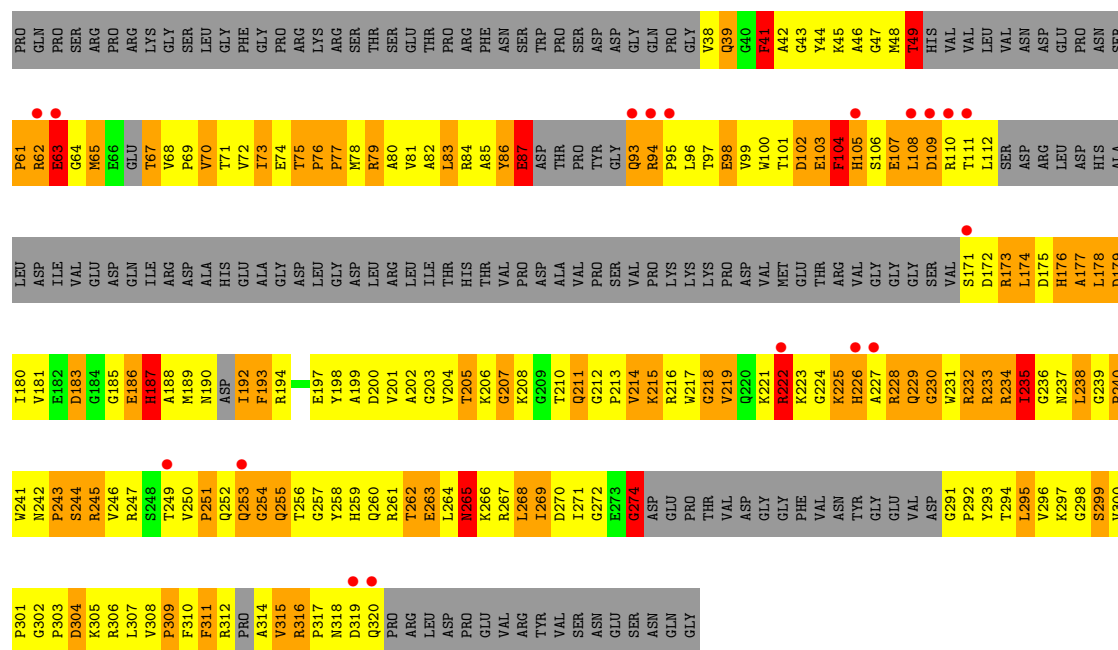
• Molecule 28: 50S ribosomal protein L2

Chain BD:



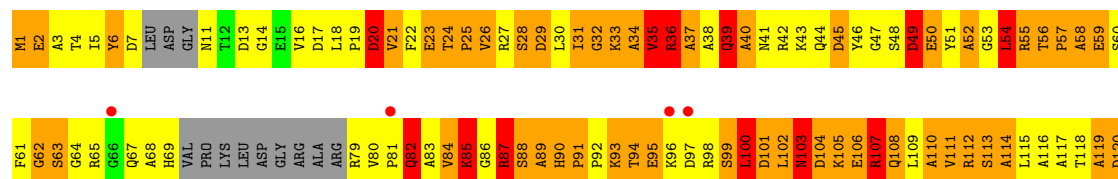
• Molecule 29: 50S ribosomal protein L3

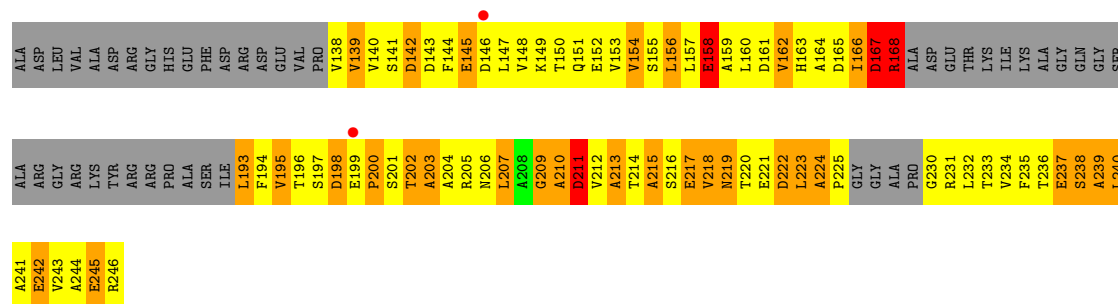
Chain BE:



• Molecule 30: 50S ribosomal protein L4

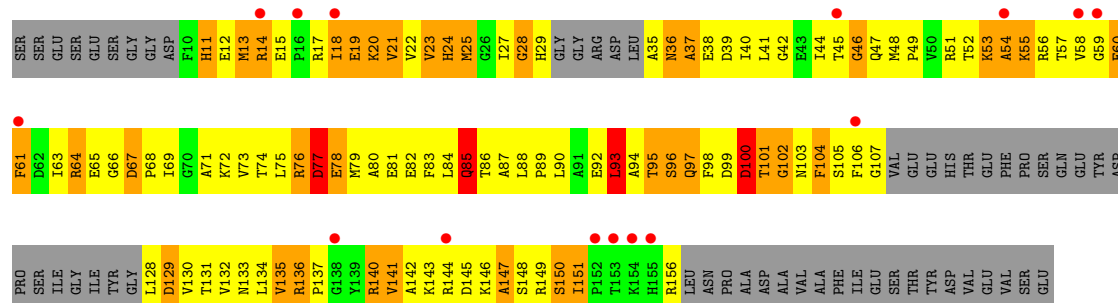
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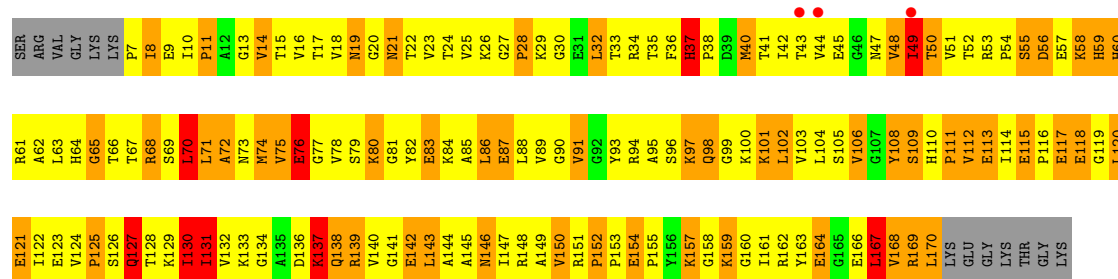
• Molecule 31: 50S ribosomal protein L5

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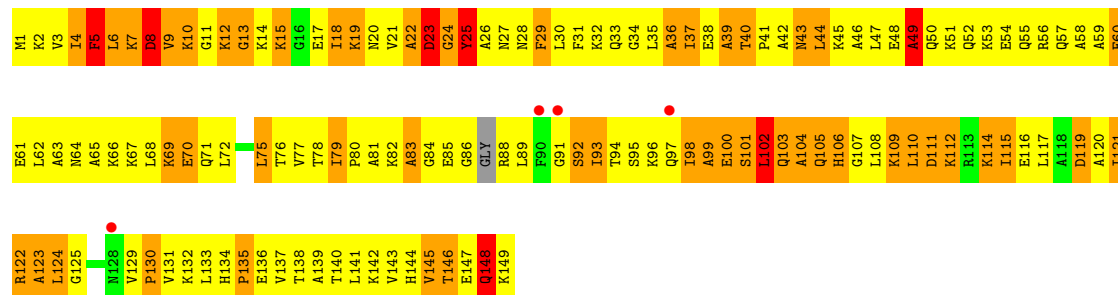
• Molecule 32: 50S ribosomal protein L6

Chain BH:



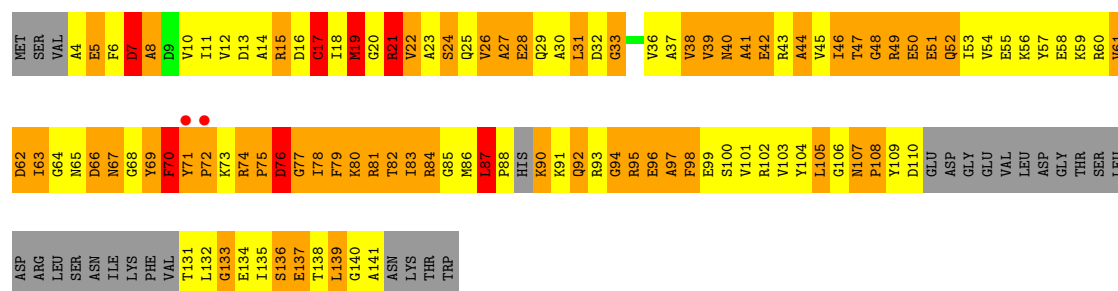
• Molecule 33: 50S ribosomal protein L9

Chain BI:



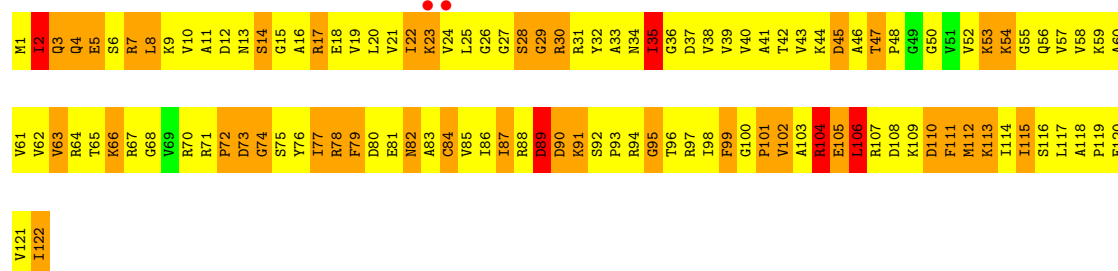
• Molecule 34: 50S ribosomal protein L13

Chain BN:



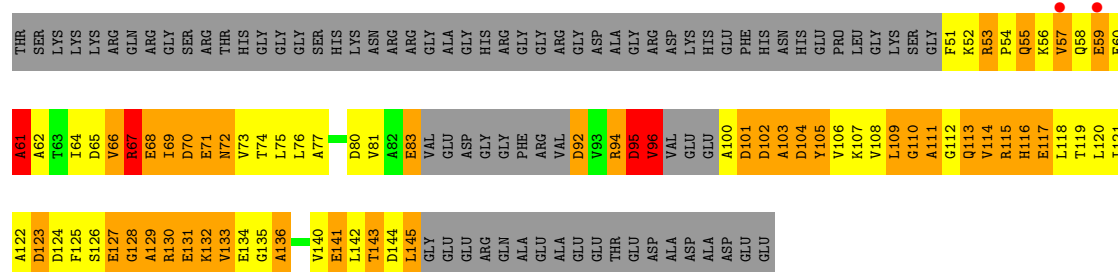
- Molecule 35: 50S ribosomal protein L14

Chain BO:



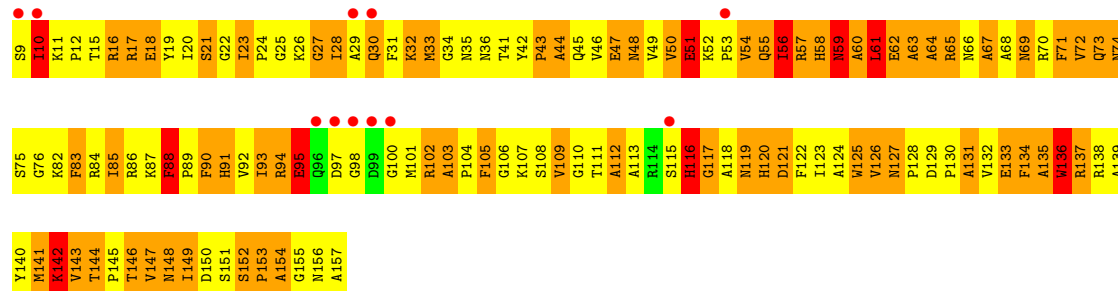
- Molecule 36: 50S ribosomal protein L15

Chain BP:



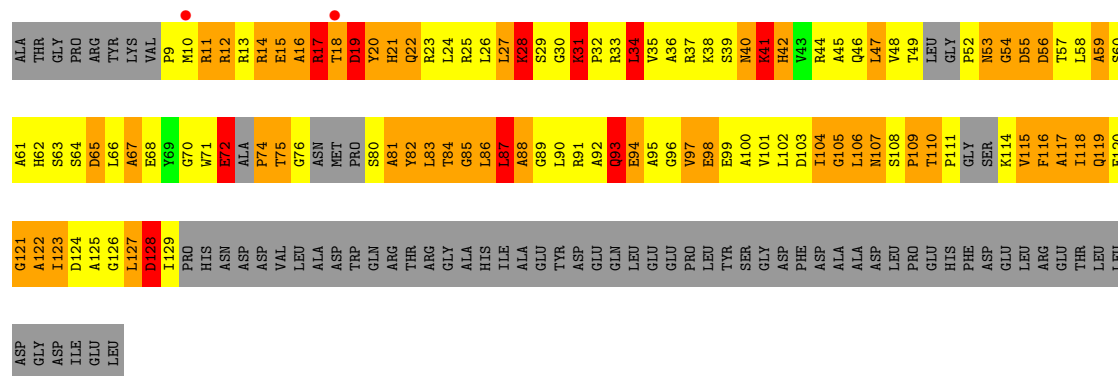
- Molecule 37: 50S ribosomal protein L16

Chain BQ:



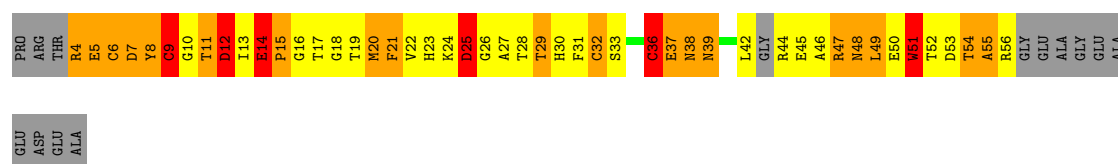
- Molecule 38: 50S ribosomal protein L18

Chain BS:



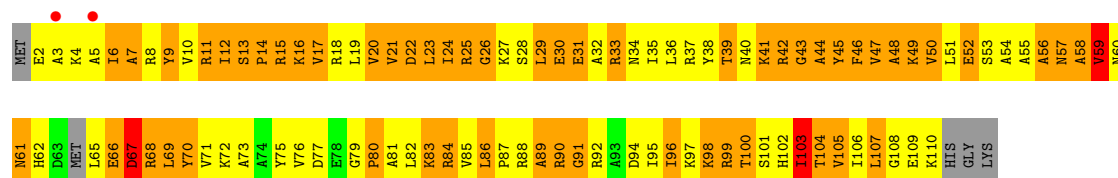
• Molecule 39: 50S ribosomal protein L19

Chain BT:



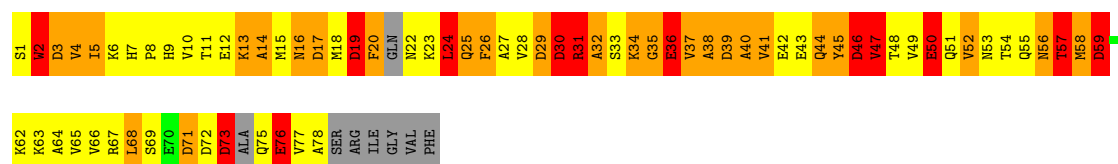
• Molecule 40: 50S ribosomal protein L22

Chain BW:



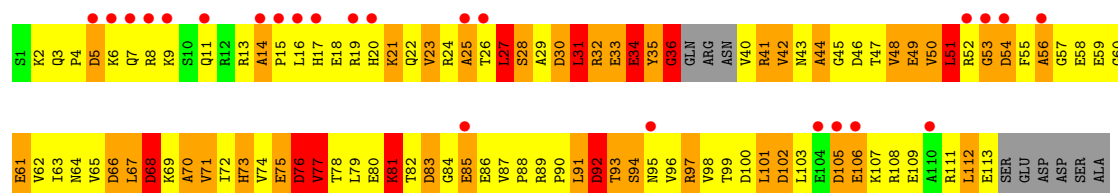
• Molecule 41: 50S ribosomal protein L23

Chain BX:



• Molecule 42: 50S ribosomal protein 24

Chain BY:



• Molecule 43: 50S ribosomal protein CTC

Chain BZ:





- Molecule 48: 50S ribosomal protein L30

Chain B3:



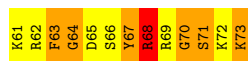
- Molecule 49: 50S ribosomal protein L27

Chain B0:



- Molecule 50: 50S ribosomal protein L31

Chain B4:



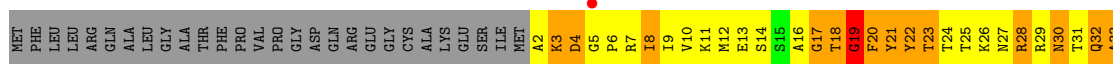
- Molecule 51: 50S ribosomal protein L32

Chain B5:



- Molecule 52: 50S ribosomal protein L33

Chain B6:



- Molecule 53: 50S ribosomal protein L34

Chain B7:



- Molecule 54: 50S ribosomal protein L35

R94	R95	I96	K99	V100	T101	E106	E107	F114	D115	N116	N117	A118	L121	A124	M125	K126	I127	G130	T131	S134	M135	G136	I137	E138	V139	V140	ASP	MET	ALA	LYS	VAL	ALA	Q8	I9	K10	L11	Q12	L13	P14	A15	G16	K17	A18	T19	P20	A21	P22	P23	V24	G25	L28	I35	F42	K43	A44	K49	A50	G51	M52	I53	L54	P55	V56	I70	K71	T72	P73	P74	K80	I85	K86	G88	S89	S90	E91	P92	V93
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	518.99Å 518.99Å 365.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 5.90 49.92 – 5.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-5.90) 94.5 (49.92-5.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 5.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.351 , 0.371 0.350 , 0.372	Depositor DCC
R_{free} test set	7425 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	223.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 148368 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	142780	wwPDB-VP
Average B, all atoms (Å ²)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: YYG, PSU

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	AA	1.25	68/36411 (0.2%)	1.47	415/56769 (0.7%)
2	AV	2.34	3/1813 (0.2%)	1.16	11/2823 (0.4%)
3	AW	1.82	17/1739 (1.0%)	1.97	36/2698 (1.3%)
4	AX	0.18	0/139	0.66	0/213
5	AB	0.63	1/1935 (0.1%)	0.66	4/2609 (0.2%)
6	AC	0.60	2/1636 (0.1%)	1.10	6/2205 (0.3%)
7	AD	0.65	4/1733 (0.2%)	0.97	9/2318 (0.4%)
8	AE	0.46	0/1161	0.61	1/1561 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.60	1/1276 (0.1%)	0.59	2/1709 (0.1%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.87	1/900 (0.1%)	0.56	0/1213
15	AL	0.49	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	AM	1.15	2/1008 (0.2%)	1.16	3/1347 (0.2%)
17	AN	0.49	1/501 (0.2%)	0.64	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.15	2/870 (0.2%)	1.38	5/1159 (0.4%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.48	0/277
26	BB	1.11	5/2950 (0.2%)	1.43	23/4602 (0.5%)
27	BA	1.21	152/67844 (0.2%)	1.45	897/105838 (0.8%)
28	BD	0.37	0/1328	0.61	0/1783
29	BE	0.64	3/1540 (0.2%)	1.07	7/2078 (0.3%)
30	BF	0.69	3/1444 (0.2%)	0.82	1/1954 (0.1%)
31	BG	0.25	0/971	0.46	0/1304
32	BH	0.58	1/1272 (0.1%)	0.48	0/1721
33	BI	0.39	1/1156 (0.1%)	0.64	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BN	0.35	0/927	0.55	0/1245
35	BO	0.32	0/946	0.57	0/1269
36	BP	1.55	3/643 (0.5%)	1.32	5/870 (0.6%)
37	BQ	0.32	0/1106	0.53	0/1490
38	BS	0.79	2/877 (0.2%)	0.87	5/1179 (0.4%)
39	BT	0.39	0/412	0.70	0/554
40	BW	0.37	0/869	0.59	0/1166
41	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
42	BY	0.25	0/887	0.83	3/1195 (0.3%)
43	BZ	0.32	1/1385 (0.1%)	0.55	3/1883 (0.2%)
44	BR	0.31	0/867	0.49	0/1162
45	BU	0.70	1/994 (0.1%)	0.65	3/1323 (0.2%)
46	BV	0.75	1/796 (0.1%)	0.89	3/1058 (0.3%)
47	B2	0.37	0/497	1.00	2/668 (0.3%)
48	B3	0.31	0/482	0.50	0/646
49	B0	0.29	0/649	1.15	3/860 (0.3%)
50	B4	0.77	2/620 (0.3%)	0.57	0/831
51	B5	0.36	0/469	0.79	3/629 (0.5%)
52	B6	0.32	0/438	0.55	1/583 (0.2%)
53	B7	0.38	0/387	0.64	0/509
54	B8	0.73	2/503 (0.4%)	1.23	5/657 (0.8%)
55	B9	0.33	0/286	0.59	0/375
56	BK	0.30	0/1010	0.60	3/1349 (0.2%)
All	All	1.11	281/154800 (0.2%)	1.32	1469/231824 (0.6%)

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
3	AW	1	5
5	AB	0	1
6	AC	0	2
7	AD	0	1
15	AL	0	1
16	AM	0	1
20	AQ	0	2
28	BD	0	1
29	BE	0	3
30	BF	0	3
32	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	BI	0	1
36	BP	0	1
38	BS	0	1
41	BX	0	1
42	BY	0	1
47	B2	0	1
54	B8	0	1
56	BK	0	1
All	All	1	29

The worst 5 of 281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2199	A	O3'-P	-71.12	0.75	1.61
2	AV	45	G	O3'-P	-70.03	0.77	1.61
2	AV	65	G	O3'-P	-62.91	0.85	1.61
27	BA	2196	C	O3'-P	-59.20	0.90	1.61
1	AA	1211	U	O3'-P	-53.33	0.97	1.61

The worst 5 of 1469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	712(A)	A	P-O3'-C3'	-48.47	61.54	119.70
1	AA	196	A	P-O3'-C3'	44.40	172.99	119.70
3	AW	25	C	O3'-P-O5'	-43.47	21.42	104.00
27	BA	2199	A	O3'-P-O5'	-43.09	22.13	104.00
26	BB	24	G	P-O3'-C3'	29.89	155.56	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	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	AA	32551	0	16464	1922	4
2	AV	1622	0	823	187	0
3	AW	1638	0	835	231	0
4	AX	136	0	63	35	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	104	0
7	AD	1703	0	1762	190	0
8	AE	1146	0	1206	57	0
9	AF	843	0	857	27	0
10	AG	1257	0	1294	138	0
11	AH	1116	0	1177	79	0
12	AI	1011	0	1041	80	0
13	AJ	794	0	840	118	0
14	AK	885	0	904	50	0
15	AL	970	0	1056	79	0
16	AM	997	0	1071	129	0
17	AN	492	0	529	111	0
18	AO	734	0	771	31	0
19	AP	700	0	720	68	0
20	AQ	857	0	929	96	0
21	AR	597	0	668	31	0
22	AS	647	0	672	146	0
23	AT	762	0	859	43	0
24	AU	208	0	221	22	0
25	AY	333	0	0	47	0
26	BB	2637	0	1338	198	0
27	BA	60600	0	30513	10823	139
28	BD	1308	0	1345	1087	0
29	BE	1507	0	1474	1127	3
30	BF	1430	0	1359	1069	0
31	BG	957	0	950	685	0
32	BH	1251	0	1289	743	0
33	BI	1145	0	1225	635	4
34	BN	917	0	896	775	1
35	BO	937	0	993	614	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BP	639	0	605	490	0
37	BQ	1081	0	1048	916	0
38	BS	866	0	867	686	0
39	BT	406	0	360	166	0
40	BW	860	0	911	559	0
41	BX	602	0	558	457	0
42	BY	879	0	860	748	0
43	BZ	1360	0	1377	887	0
44	BR	855	0	904	580	0
45	BU	978	0	995	924	0
46	BV	787	0	783	652	0
47	B2	494	0	504	385	0
48	B3	477	0	528	446	0
49	B0	641	0	657	501	0
50	B4	604	0	587	493	0
51	B5	457	0	457	293	0
52	B6	431	0	454	288	0
53	B7	383	0	409	396	0
54	B8	496	0	541	358	0
55	B9	285	0	312	203	0
56	BK	999	0	1068	144	0
All	All	142780	0	94554	28108	146

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 119.

The worst 5 of 28108 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:B5:33:CYS:SG	51:B5:36:CYS:HB2	1.24	1.69
27:BA:2470:G:C2	27:BA:2471:C:C5	1.81	1.68
27:BA:994:C:C2	45:BU:53:LYS:HD3	1.16	1.68
53:B7:30:ILE:HA	53:B7:33:ARG:CD	1.21	1.67
27:BA:2580:U:C6	27:BA:2581:G:C8	1.82	1.66

The worst 5 of 146 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:BA:6:A:C4'	27:BA:2902:C:O2'[8_554]	0.49	1.71
1:AA:359:U:OP1	33:BI:82:LYS:NZ[3_454]	0.68	1.52
27:BA:6:A:N9	27:BA:2902:C:C6[8_554]	0.88	1.32
27:BA:1:G:O6	27:BA:2898:U:C2[8_554]	0.92	1.28

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:BA:6:A:O4'	27:BA:2902:C:C2'[8.554]	0.97	1.23

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	
5	AB	232/256 (91%)	183 (79%)	34 (15%)	15 (6%)	2	35
6	AC	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1	28
7	AD	206/209 (99%)	156 (76%)	34 (16%)	16 (8%)	1	28
8	AE	146/162 (90%)	114 (78%)	29 (20%)	3 (2%)	11	65
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	5	49
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	8	60
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	2	30
12	AI	125/128 (98%)	87 (70%)	30 (24%)	8 (6%)	2	35
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	23
14	AK	117/129 (91%)	89 (76%)	23 (20%)	5 (4%)	4	47
15	AL	122/135 (90%)	91 (75%)	14 (12%)	17 (14%)	0	11
16	AM	123/126 (98%)	96 (78%)	21 (17%)	6 (5%)	3	43
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	2	32
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	19	77
19	AP	81/88 (92%)	64 (79%)	10 (12%)	7 (9%)	1	25
20	AQ	102/105 (97%)	78 (76%)	17 (17%)	7 (7%)	2	32
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	26
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	5	50
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	36
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	24
28	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BE	183/338 (54%)	89 (49%)	35 (19%)	59 (32%)	0	1
30	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
31	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
32	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	1
33	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	1
34	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
35	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	2
36	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
37	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
38	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
39	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
40	BW	104/113 (92%)	42 (40%)	15 (14%)	47 (45%)	0	0
41	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
42	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
43	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
44	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
45	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
46	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
47	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
48	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
49	B0	84/91 (92%)	33 (39%)	16 (19%)	35 (42%)	0	0
50	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
51	B5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0	0
52	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
53	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
54	B8	61/64 (95%)	23 (38%)	9 (15%)	29 (48%)	0	0
55	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	1
56	BK	124/141 (88%)	93 (75%)	26 (21%)	5 (4%)	5	49
All	All	5320/6250 (85%)	2968 (56%)	1021 (19%)	1331 (25%)	0	2

5 of 1331 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	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	
5	AB	202/220 (92%)	173 (86%)	29 (14%)	5	31
6	AC	160/188 (85%)	146 (91%)	14 (9%)	14	57
7	AD	180/181 (99%)	162 (90%)	18 (10%)	11	50
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2	17
9	AF	90/90 (100%)	83 (92%)	7 (8%)	18	63
10	AG	126/127 (99%)	116 (92%)	10 (8%)	18	62
11	AH	119/119 (100%)	91 (76%)	28 (24%)	1	9
12	AI	98/99 (99%)	90 (92%)	8 (8%)	17	60
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	7	38
14	AK	90/99 (91%)	85 (94%)	5 (6%)	30	75
15	AL	104/111 (94%)	93 (89%)	11 (11%)	10	47
16	AM	100/101 (99%)	87 (87%)	13 (13%)	6	36
17	AN	49/50 (98%)	43 (88%)	6 (12%)	7	39
18	AO	79/80 (99%)	70 (89%)	9 (11%)	8	42
19	AP	72/74 (97%)	62 (86%)	10 (14%)	5	33
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	13	53
21	AR	64/77 (83%)	57 (89%)	7 (11%)	9	46
22	AS	71/80 (89%)	64 (90%)	7 (10%)	11	50
23	AT	76/82 (93%)	68 (90%)	8 (10%)	10	47
24	AU	19/22 (86%)	19 (100%)	0	100	100
28	BD	135/135 (100%)	99 (73%)	36 (27%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	156/284 (55%)	128 (82%)	28 (18%)	2	19
30	BF	152/193 (79%)	124 (82%)	28 (18%)	2	17
31	BG	102/147 (69%)	93 (91%)	9 (9%)	14	57
32	BH	137/147 (93%)	111 (81%)	26 (19%)	2	16
33	BI	119/119 (100%)	98 (82%)	21 (18%)	3	20
34	BN	95/121 (78%)	80 (84%)	15 (16%)	4	27
35	BO	101/101 (100%)	81 (80%)	20 (20%)	2	14
36	BP	67/126 (53%)	56 (84%)	11 (16%)	3	24
37	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	8
38	BS	89/149 (60%)	73 (82%)	16 (18%)	2	18
39	BT	44/52 (85%)	30 (68%)	14 (32%)	0	4
40	BW	88/92 (96%)	74 (84%)	14 (16%)	4	26
41	BX	67/73 (92%)	44 (66%)	23 (34%)	0	3
42	BY	97/105 (92%)	80 (82%)	17 (18%)	3	20
43	BZ	151/203 (74%)	129 (85%)	22 (15%)	5	30
44	BR	89/101 (88%)	71 (80%)	18 (20%)	2	14
45	BU	96/97 (99%)	68 (71%)	28 (29%)	0	5
46	BV	79/79 (100%)	69 (87%)	10 (13%)	6	37
47	B2	51/56 (91%)	37 (72%)	14 (28%)	0	6
48	B3	52/52 (100%)	47 (90%)	5 (10%)	12	52
49	B0	64/67 (96%)	57 (89%)	7 (11%)	9	46
50	B4	66/66 (100%)	54 (82%)	12 (18%)	2	18
51	B5	51/53 (96%)	43 (84%)	8 (16%)	4	27
52	B6	46/69 (67%)	39 (85%)	7 (15%)	4	28
53	B7	39/40 (98%)	31 (80%)	8 (20%)	2	13
54	B8	50/51 (98%)	39 (78%)	11 (22%)	1	11
55	B9	34/35 (97%)	30 (88%)	4 (12%)	8	41
56	BK	108/113 (96%)	105 (97%)	3 (3%)	56	88
All	All	4533/5148 (88%)	3840 (85%)	693 (15%)	4	28

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	BF	107	ARG
34	BN	79	PHE
50	B4	5	LEU
30	BF	245	GLU
32	BH	131	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	260	GLN
33	BI	64	ASN
49	B0	71	ASN
29	BE	318	ASN
30	BF	219	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1498/1522 (98%)	518 (34%)	166 (11%)
2	AV	74/76 (97%)	16 (21%)	4 (5%)
26	BB	122/123 (99%)	44 (36%)	3 (2%)
27	BA	2785/2916 (95%)	1488 (53%)	360 (12%)
3	AW	70/76 (92%)	14 (20%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4554/4731 (96%)	2080 (45%)	537 (11%)

5 of 2080 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 537 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	579	G
27	BA	1069	A
27	BA	2610	C

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Mol	Chain	Res	Type
27	BA	670	A
27	BA	801	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	YYG	AW	37	10,3	40,42,43	1.10	3 (7%)	50,62,65	11.20	12 (24%)
3	PSU	AW	39	3	19,21,22	0.96	0	23,30,33	0.82	0
3	PSU	AW	55	3	19,21,22	1.11	2 (10%)	23,30,33	1.02	2 (8%)

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
3	YYG	AW	37	10,3	1/1/8/9	0/25/42/43	0/4/4/4
3	PSU	AW	39	3	-	0/8/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/8/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C6-N1	2.72	1.43	1.37
3	AW	55	PSU	C4-N3	2.68	1.40	1.36
3	AW	37	YYG	P-OP1	2.46	1.49	1.46
3	AW	55	PSU	P-OP1	2.24	1.49	1.46
3	AW	37	YYG	C2-N1	-2.16	1.36	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	37	YYG	C6-C5-N7	-75.82	130.20	134.24
3	AW	37	YYG	C11-C12-N1	18.54	111.38	104.24
3	AW	37	YYG	C24-O23-C21	6.08	123.12	115.64
3	AW	37	YYG	C13-C12-C11	-5.35	123.50	131.05
3	AW	37	YYG	C3-N3-C4	4.55	125.54	118.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	BA	53
1	AA	40
3	AW	6
56	BK	5
2	AV	4
37	BQ	3
46	BV	2
45	BU	1

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Mol	Chain	Number of breaks
20	AQ	1
14	AK	1
8	AE	1
5	AB	1
6	AC	1
28	BD	1
36	BP	1
7	AD	1
26	BB	1
32	BH	1
16	AM	1

The worst 5 of 125 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	70:ILE	C	71:LYS	N	5.81
1	BK	73:PRO	C	74:PRO	N	5.30
1	BK	72:THR	C	73:PRO	N	5.11
1	AA	30(D):A	O3'	1031:G	P	4.82
1	BA	142(A):A	O3'	1143:A	P	4.82

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	AA	1515/1522 (99%)	0.45	118 (7%) 13 20	236, 236, 236, 236	0
2	AV	76/76 (100%)	0.47	6 (7%) 13 20	236, 236, 236, 236	0
3	AW	75/76 (98%)	0.89	12 (16%) 3 8	236, 236, 236, 236	0
4	AX	17/18 (94%)	3.86	12 (70%) 0 2	236, 236, 236, 236	0
5	AB	234/256 (91%)	0.24	7 (2%) 48 42	236, 236, 236, 236	0
6	AC	206/239 (86%)	0.22	7 (3%) 43 39	236, 236, 236, 236	0
7	AD	208/209 (99%)	0.55	19 (9%) 9 17	236, 236, 236, 236	0
8	AE	150/162 (92%)	0.32	6 (4%) 36 35	236, 236, 236, 236	0
9	AF	101/101 (100%)	0.24	6 (5%) 22 26	236, 236, 236, 236	0
10	AG	155/156 (99%)	0.40	16 (10%) 7 15	236, 236, 236, 236	0
11	AH	138/138 (100%)	0.18	8 (5%) 22 26	236, 236, 236, 236	0
12	AI	127/128 (99%)	0.39	7 (5%) 24 27	236, 236, 236, 236	0
13	AJ	98/105 (93%)	1.01	15 (15%) 3 8	236, 236, 236, 236	0
14	AK	119/129 (92%)	-0.11	1 (0%) 83 72	236, 236, 236, 236	0
15	AL	124/135 (91%)	0.34	8 (6%) 18 24	236, 236, 236, 236	0
16	AM	125/126 (99%)	0.76	17 (13%) 4 10	236, 236, 236, 236	0
17	AN	60/61 (98%)	0.60	5 (8%) 11 19	236, 236, 236, 236	0
18	AO	88/89 (98%)	0.43	4 (4%) 32 32	236, 236, 236, 236	0
19	AP	83/88 (94%)	0.74	11 (13%) 4 10	236, 236, 236, 236	0
20	AQ	104/105 (99%)	0.23	3 (2%) 49 43	236, 236, 236, 236	0
21	AR	73/88 (82%)	0.31	5 (6%) 17 23	236, 236, 236, 236	0
22	AS	80/93 (86%)	0.85	13 (16%) 2 7	236, 236, 236, 236	0
23	AT	99/106 (93%)	0.21	3 (3%) 48 42	236, 236, 236, 236	0
24	AU	24/27 (88%)	1.44	7 (29%) 1 4	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	AY	333/354 (94%)	1.95	122 (36%) 1 4	236, 236, 236, 236	0
26	BB	123/123 (100%)	0.15	2 (1%) 68 58	236, 236, 236, 236	0
27	BA	2814/2916 (96%)	0.26	163 (5%) 22 26	236, 236, 236, 236	0
28	BD	173/173 (100%)	0.02	5 (2%) 49 43	236, 236, 236, 236	0
29	BE	191/338 (56%)	0.44	18 (9%) 9 17	236, 236, 236, 236	0
30	BF	189/246 (76%)	0.25	6 (3%) 45 41	236, 236, 236, 236	0
31	BG	122/176 (69%)	0.74	15 (12%) 5 12	236, 236, 236, 236	0
32	BH	164/177 (92%)	-0.07	3 (1%) 65 55	236, 236, 236, 236	0
33	BI	148/149 (99%)	0.09	4 (2%) 52 45	236, 236, 236, 236	0
34	BN	117/145 (80%)	0.11	2 (1%) 67 56	236, 236, 236, 236	0
35	BO	122/122 (100%)	0.13	2 (1%) 68 58	236, 236, 236, 236	0
36	BP	84/164 (51%)	0.17	2 (2%) 56 47	236, 236, 236, 236	0
37	BQ	138/138 (100%)	0.49	11 (7%) 12 19	236, 236, 236, 236	0
38	BS	113/186 (60%)	0.09	2 (1%) 65 55	236, 236, 236, 236	0
39	BT	52/66 (78%)	0.56	0 100 100	236, 236, 236, 236	0
40	BW	108/113 (95%)	0.21	2 (1%) 64 53	236, 236, 236, 236	0
41	BX	76/84 (90%)	0.11	0 100 100	236, 236, 236, 236	0
42	BY	110/119 (92%)	0.97	24 (21%) 1 5	236, 236, 236, 236	0
43	BZ	177/253 (69%)	0.24	10 (5%) 24 27	236, 236, 236, 236	0
44	BR	105/118 (88%)	-0.11	1 (0%) 79 68	236, 236, 236, 236	0
45	BU	117/118 (99%)	0.04	5 (4%) 34 33	236, 236, 236, 236	0
46	BV	100/100 (100%)	0.18	5 (5%) 28 29	236, 236, 236, 236	0
47	B2	64/70 (91%)	-0.29	0 100 100	236, 236, 236, 236	0
48	B3	60/60 (100%)	-0.31	1 (1%) 67 56	236, 236, 236, 236	0
49	B0	86/91 (94%)	0.36	5 (5%) 22 26	236, 236, 236, 236	0
50	B4	73/73 (100%)	0.22	2 (2%) 52 45	236, 236, 236, 236	0
51	B5	58/60 (96%)	0.44	4 (6%) 17 23	236, 236, 236, 236	0
52	B6	53/82 (64%)	-0.02	1 (1%) 64 53	236, 236, 236, 236	0
53	B7	46/47 (97%)	0.20	4 (8%) 10 18	236, 236, 236, 236	0
54	B8	63/64 (98%)	0.09	0 100 100	236, 236, 236, 236	0
55	B9	35/36 (97%)	1.09	5 (14%) 3 9	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BK	133/141 (94%)	1.38	33 (24%) 1 5	236, 236, 236, 236	0
All	All	10426/11335 (91%)	0.39	775 (7%) 14 21	236, 236, 236, 236	0

The worst 5 of 775 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	AY	260	LYS	14.1
25	AY	284	ARG	13.6
25	AY	304	THR	11.9
25	AY	123	PHE	11.1
25	AY	287	LYS	10.6

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

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
3	YYG	AW	37	39/40	0.71	-	236,236,236,236	0
3	PSU	AW	55	20/21	0.15	-	236,236,236,236	0
3	PSU	AW	39	20/21	0.44	-	236,236,236,236	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.