



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:31 am GMT

PDB ID : 4WCE
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus*
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-04
Resolution : 3.53 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

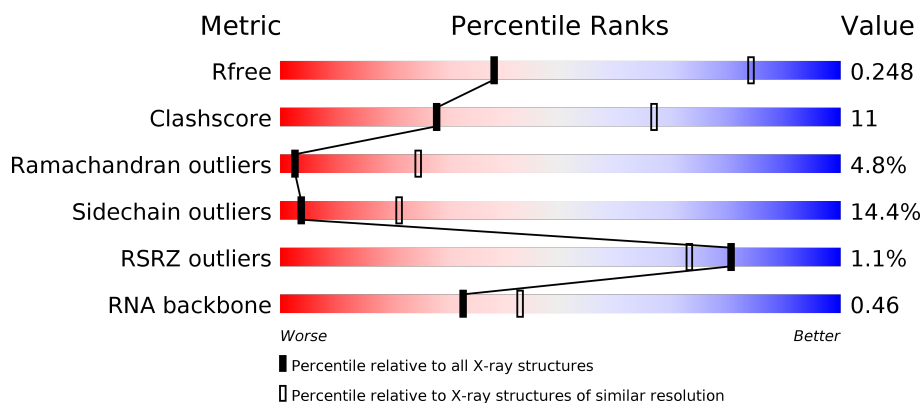
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.53 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.






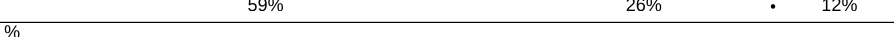


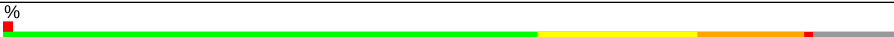
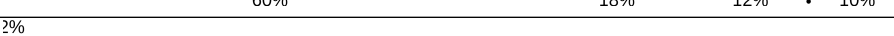



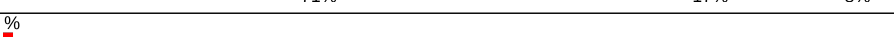



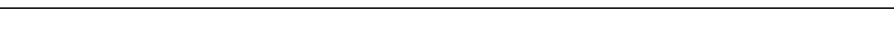








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)
RNA backbone	2435	1027 (4.18-2.86)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2923	
2	Y	114	
3	A	277	
4	B	220	

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3002	-	-	-	X
29	MPD	X	3006	-	-	-	X
29	MPD	X	3007	-	-	-	X
29	MPD	X	3008	-	-	-	X
29	MPD	X	3009	-	-	-	X
29	MPD	X	3010	-	-	-	X
29	MPD	Z	101	-	-	-	X
30	MN	X	3012	-	-	-	X
30	MN	X	3047	-	-	-	X
30	MN	X	3055	-	-	-	X
30	MN	X	3153	-	-	-	X
30	MN	X	3154	-	-	-	X
30	MN	X	3166	-	-	-	X
30	MN	X	3196	-	-	-	X
30	MN	X	3197	-	-	-	X
30	MN	X	3210	-	-	-	X
30	MN	X	3213	-	-	-	X
30	MN	X	3225	-	-	-	X
30	MN	X	3230	-	-	-	X
30	MN	X	3242	-	-	-	X
30	MN	X	3252	-	-	-	X
30	MN	X	3255	-	-	-	X
30	MN	X	3260	-	-	-	X
30	MN	X	3265	-	-	-	X
30	MN	X	3271	-	-	-	X
30	MN	X	3272	-	-	-	X
30	MN	X	3273	-	-	-	X
30	MN	X	3278	-	-	-	X
30	MN	X	3279	-	-	-	X
30	MN	X	3280	-	-	-	X
30	MN	X	3283	-	-	-	X
30	MN	X	3286	-	-	-	X
31	MG	X	3030	-	-	-	X
31	MG	X	3092	-	-	-	X
31	MG	X	3103	-	-	-	X
31	MG	X	3174	-	-	-	X
33	SPD	X	3312	-	-	-	X
33	SPD	X	3313	-	-	-	X
33	SPD	X	3314	-	-	-	X
33	SPD	X	3315	-	-	-	X
34	EOH	X	3316	-	-	-	X
34	EOH	X	3318	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	EOH	X	3322	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

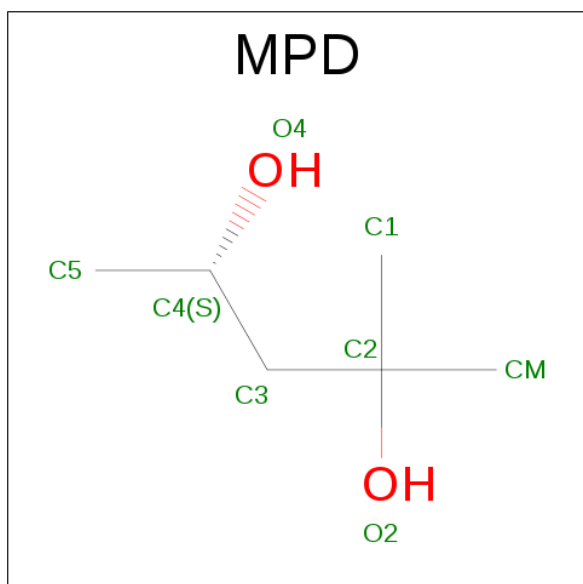
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	Z	1	Total	C	O	0	0
			8	6	2		

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	X	223	Total	Mn	0	0
			223	223		
30	R	2	Total	Mn	0	0
			2	2		
30	Y	2	Total	Mn	0	0
			2	2		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

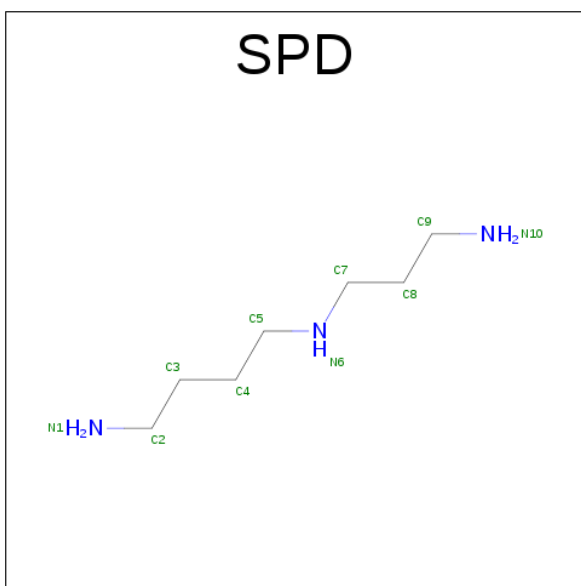
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



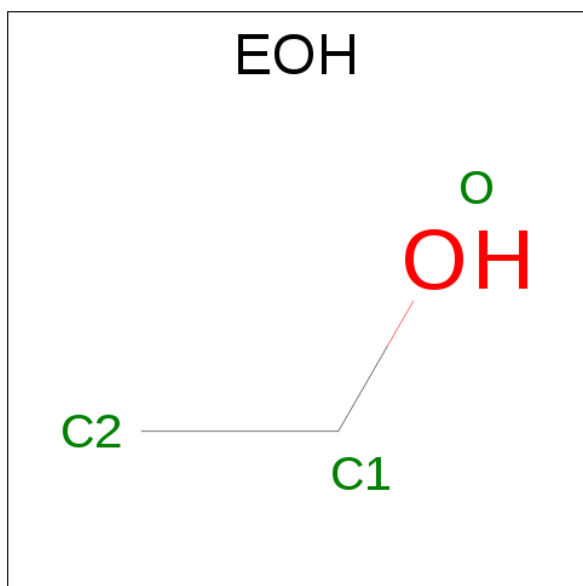
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

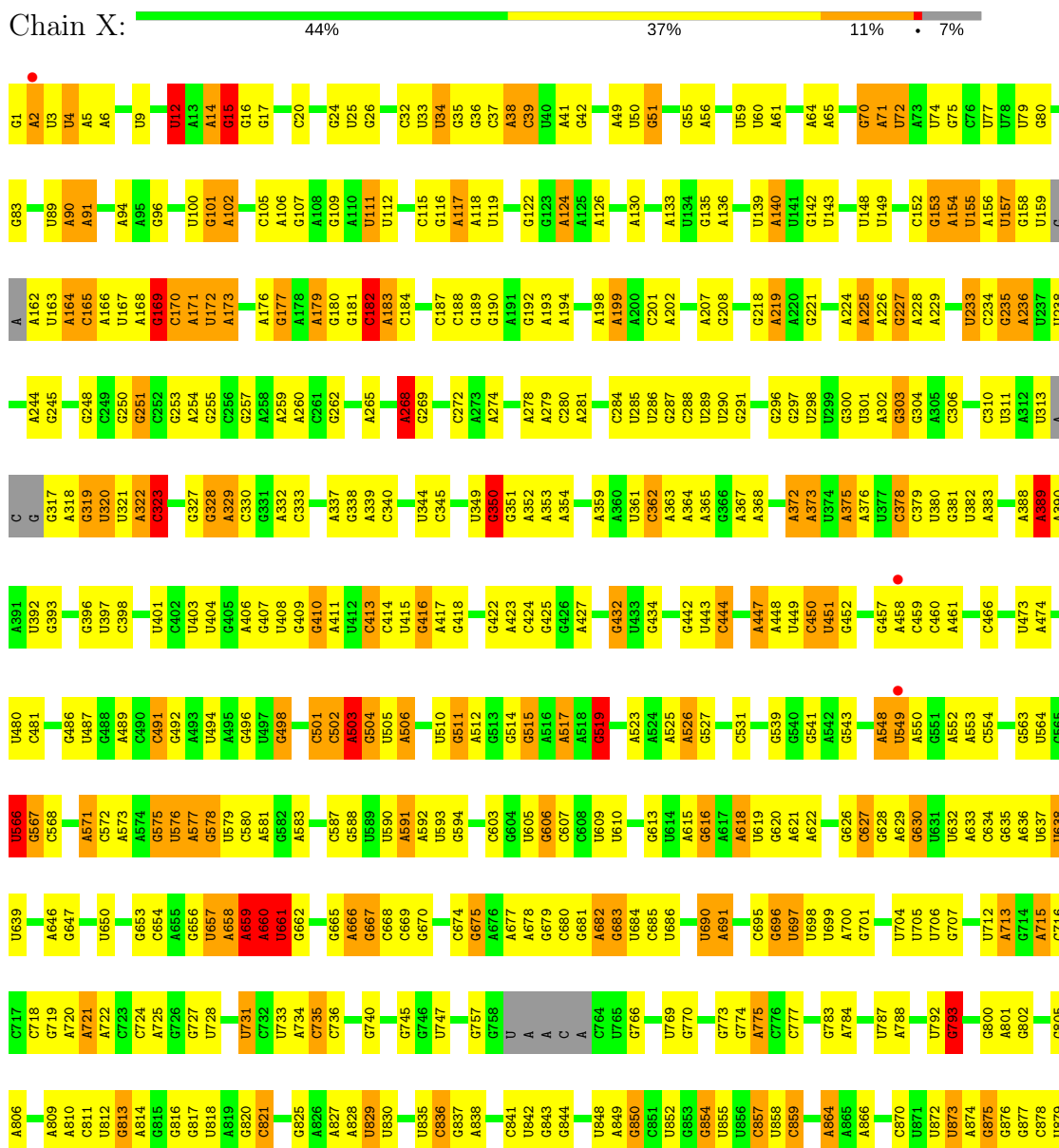


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots

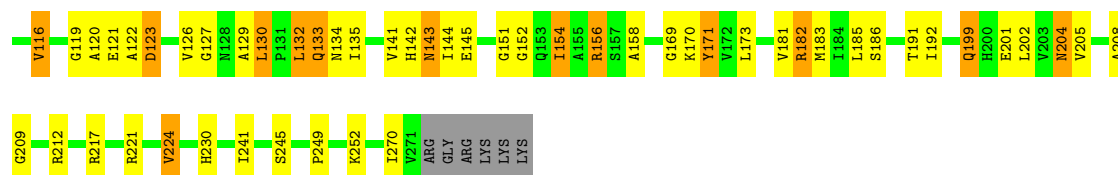
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 23S rRNA

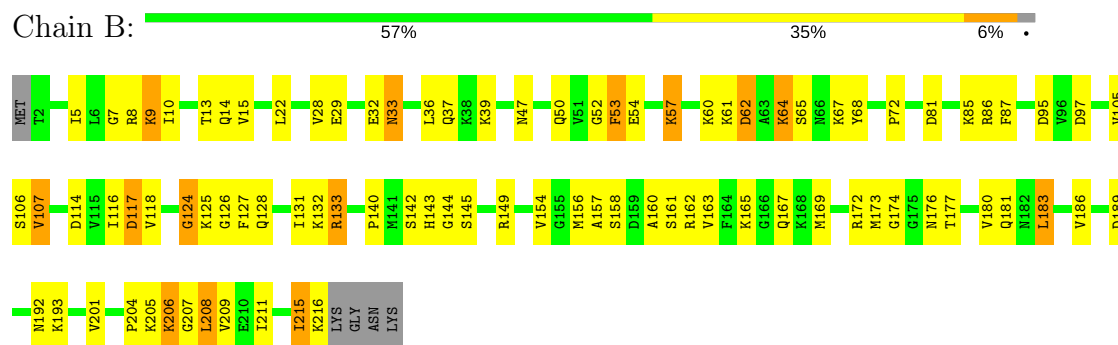


G2088	A1967	C1833	G1759	A1653	C	G1518	U1451	G1301	U1209	A	A1059	C966	A880
A2089	A1998	G1834	G1760	G1657	A	U1519	C1452	G1302	C1213	A	U1060	C967	A887
C2093	A1999	U1835	G1761	G1658	U	A	G1453	G1303	C1214	G	U1061	U970	G888
G2094	G1999	A1836	U1762	A1658	U	A1521	U1454	G1304	U1215	G	U1062	U971	U889
U2095	G2007	G1837	U1763	C1661	A	G1522	U	U1305	U	A	U1064	G990	G890
G2096	A2008	U1843	A1765	G1662	G	G1524	U	U1306	U1217	U	A1065	A977	A891
U2101	U2009	G1844	C1766	G1663	U	U1526	A	G1309	G1218	G	U1066	U892	U892
U2102	G2012	U1845	G1767	G1664	C	U	A1459	A1310	G1219	C	U1067	A985	U895
G2013	G2012	C1846	C1768	U1680	U	A1527	U1460	A1311	A1222	G	G1068	A989	U896
U1847	G2013	U1847	C1769	U1681	U	G1528	C1461	A1312	A1223	U	G1069	G990	A897
A1848	G2014	A1848	C1770	C1682	C	U1529	G1462	G1313	G1225	A	A1070	U995	U898
G2107	G2014	G1851	A1771	U1683	G1591	A1530	U1464	A1314	G1226	A	A1071	U995	U898
U2018	U2018	G	G1772	A1684	A1592	U	G1465	C1315	U1227	U	A1072	U995	A902
G2019	G2019	U1854	G1775	A1684	U	U	G1466	G1316	A1228	G	U1077	G996	G903
U2020	U2019	G1855	A1776	G1687	A1594	A	G1467	A1323	U1228	A	U1078	G997	G904
G2112	G2020	U1856	G1777	U1688	G1595	G	U1468	A1324	G1229	U	U1079	G998	U905
U2113	A2024	C1857	C1781	G1689	U1597	C	G1469	U1325	U1230	U	U1080	U999	U906
G2119	G2027	U1881	A1782	A1690	U1598	A	G1470	C1326	U1240	U	G1086	G1000	A906
G2121	G2031	C1864	G1787	G1691	U1599	A	A1471	C1327	A1241	U	U1087	A1001	G907
A2122	A2032	G1865	U1788	G1692	U1603	A1539	C1472	C1328	U1242	U	U1088	U1002	A911
A2123	A2032	G1867	A1789	U1693	U1604	A1540	U1476	U1329	U1243	U	U1089	G1003	U916
G2126	G2036	U1888	G1790	G1694	G1542	C1541	U1477	U1330	U1248	U	U1090	G1005	U916
G	G2037	G1889	G1791	G1695	G1543	C1544	A1478	U1331	U1249	U	U1091	G1006	U916
G	A2040	C1870	C1792	A1698	G1544	U	U1481	C1335	G1257	U	U1092	U1007	G922
G	A2047	G1885	C1793	A1699	U1545	U	G1482	G1336	G1257	U	U1093	G1008	A923
C	G2048	A1875	G1794	C1700	A1546	A	U1483	U1337	A1264	U	U1094	G1009	G924
A	G2049	U1886	U1701	G1701	C1547	U	G1487	U1338	U1265	U	U1097	U1014	G
C	U2050	G1887	A1796	C1702	U1548	U	A1488	U1339	U1266	U	U1098	G1015	G
G	A2050	A1889	U1796	U1703	C1549	U	A1489	U1340	C1288	U	U1099	G1016	C
C	C2051	U1890	A1800	U1708	G1550	U	G1490	G1346	A1269	U	G	C	C
U	C2052	G1885	G1800	A1708	U	U	C1491	U1347	U1272	U	U1099	A1018	C
U	U2053	G1887	G1803	G1710	A	A	U1492	U1348	U1273	U	U	A1023	C
U	G2056	U1890	U1806	G1711	G1555	G1556	G1493	U1349	G1274	U	U	A1024	C
C	A2057	G1891	U1807	G1718	C1557	C1557	G1494	U1350	A1275	U	U	A1025	U
C	G2058	U1892	U1808	G1718	U1558	U	G1495	C1351	G1276	U	U	A1026	C
G	A2059	A1811	A1812	A1721	U1559	A	U1497	C1352	C1277	U	U	A1027	G
A	A2060	U1893	A1813	G1730	G1560	U	U1498	A1353	C1278	U	U	G1028	G
G	U2061	G1894	A1814	G1731	A1561	U	U1499	G1354	C1279	U	U	C1029	G
U	G2062	C1895	U1815	U1732	G1562	U	G1500	A1355	U1280	U	U	C1030	G
U	C2063	U1896	C1815	U1732	C1563	U	A1502	G1356	U1281	U	U	U	C
A	A2064	U	A1816	U1737	U1563	U	U1503	A1358	A1282	U	U	G	C942
G	C2070	C	A1817	C1738	G1564	U	U1504	A1359	G1283	A	U	G1033	C943
U	C2071	U	A1818	G1739	U1565	U	C1436	G1360	U1284	A	U	A1034	A945
A	U1982	G1900	G1819	G1740	G1566	U	G1505	G1360	A1285	C	U	A1037	A946
G	U1983	C1901	U1823	G1740	U1567	U	G1506	U1366	G1286	A	U	C1038	U947
G	A2077	G1902	U1824	G1744	U1568	U	C1508	U1367	A1288	A	U	C1039	U948
G	G2078	U1906	U1825	A1745	G1569	U	G1509	C1368	G1290	C	U	A1040	A955
G	G2079	U1907	U1826	G1746	U1510	U	U1510	G1369	G1291	C	U	G1041	A956
C	G2080	A1908	G1827	G1747	G1511	U	C1442	C1370	A1292	A	U	C1042	A956
C	C2081	C1987	U1828	G1747	U1512	U	U1446	C1371	A1293	U	U	U1043	C959
U	G2083	G1910	A1829	U1755	A1513	U	A1447	C1372	G1294	C	U	A1053	C960
U	G2084	U1911	A1830	U1756	A1514	U	U1448	U1373	C1295	A	U	G961	G961
U	A2087	U1912	A1831	U1757	G1515	U	C1516	G1374	C1296	U	U	U1056	U964
G				A1758	A1517	U	A1517	G1376	G1300	U	U	U1058	G965

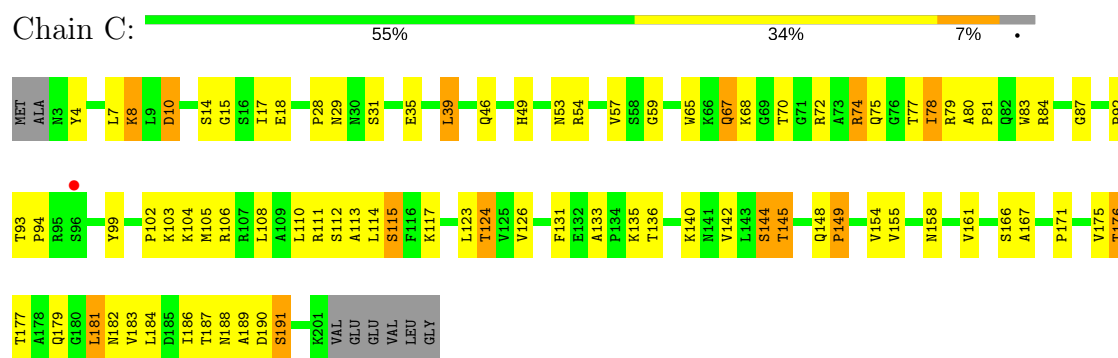




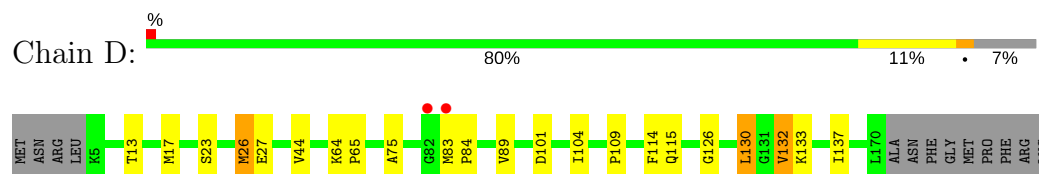
• Molecule 4: 50S ribosomal protein L3



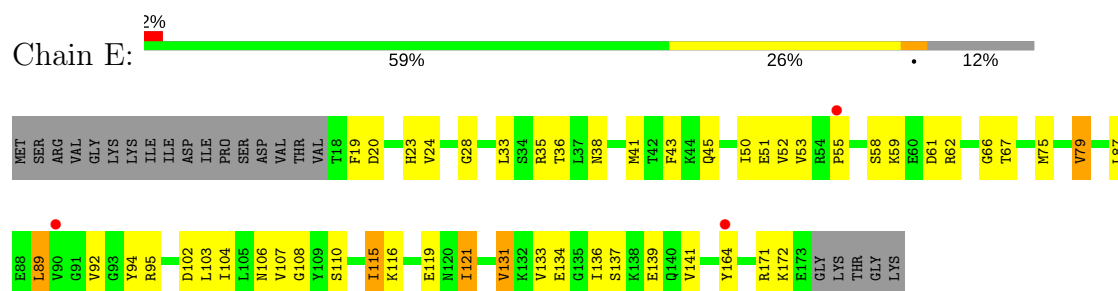
• Molecule 5: 50S ribosomal protein L4



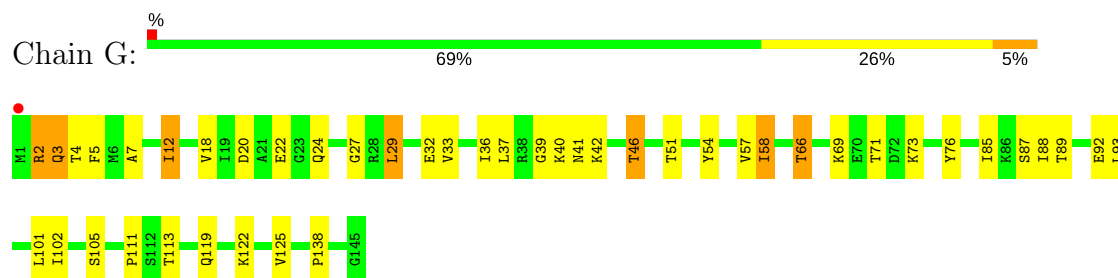
• Molecule 6: 50S ribosomal protein L5



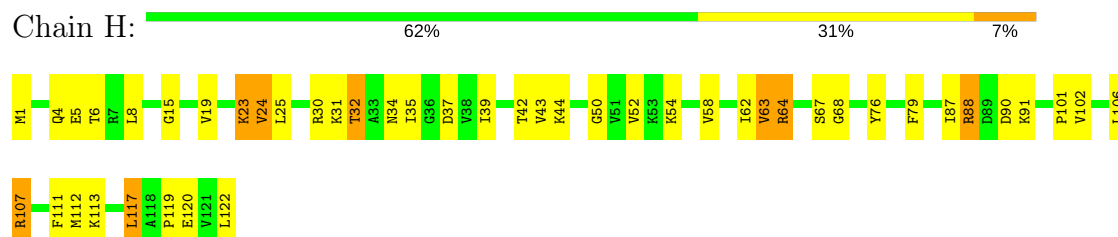
• Molecule 7: 50S ribosomal protein L6



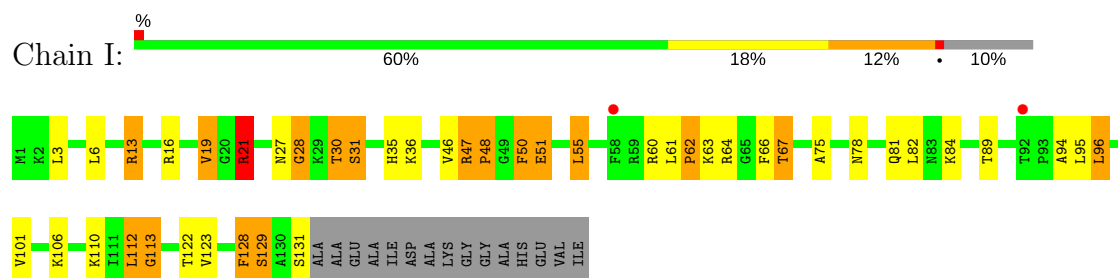
• Molecule 8: 50S ribosomal protein L13



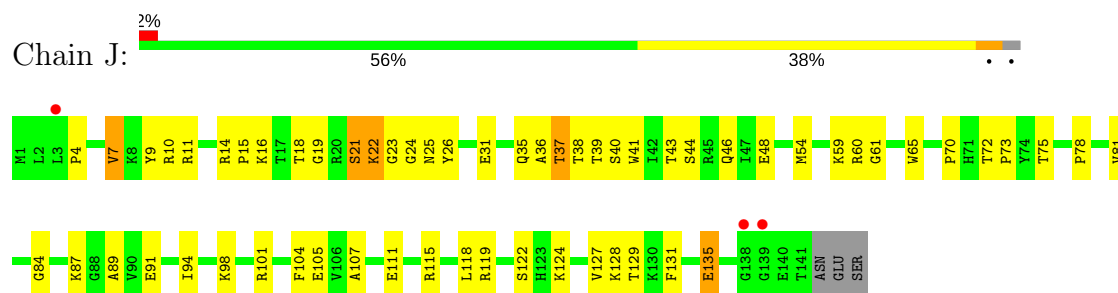
• Molecule 9: 50S ribosomal protein L14



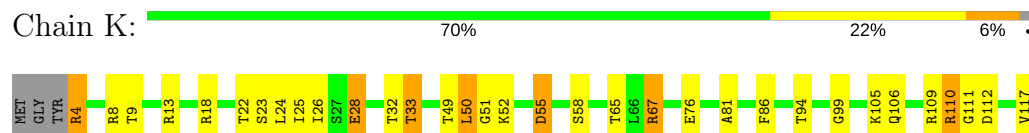
• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L17

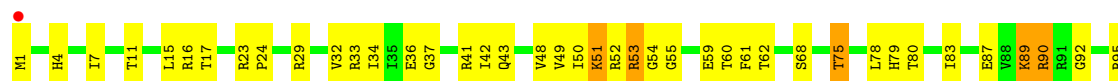


• Molecule 13: 50S ribosomal protein L18

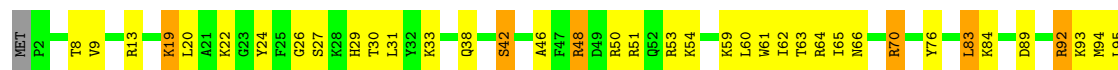




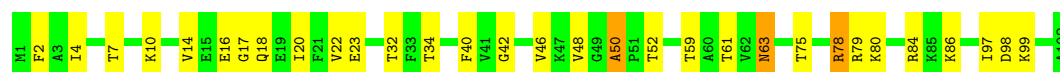
- Molecule 14: 50S ribosomal protein L19



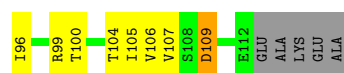
- Molecule 15: 50S ribosomal protein L20



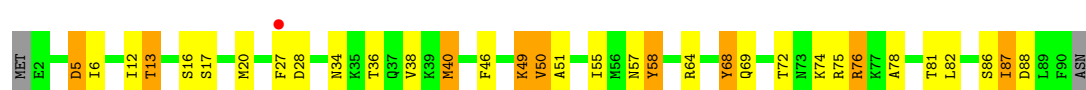
- Molecule 16: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L22

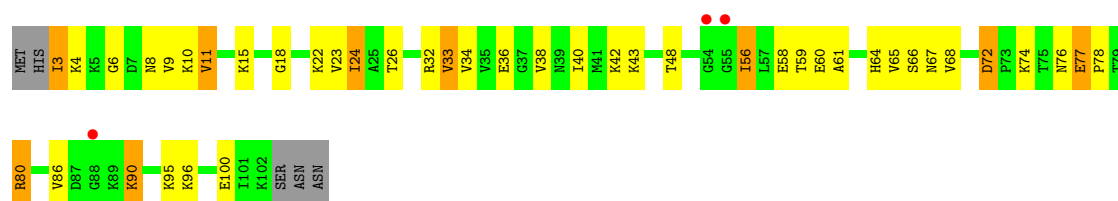


- Molecule 18: 50S ribosomal protein L23

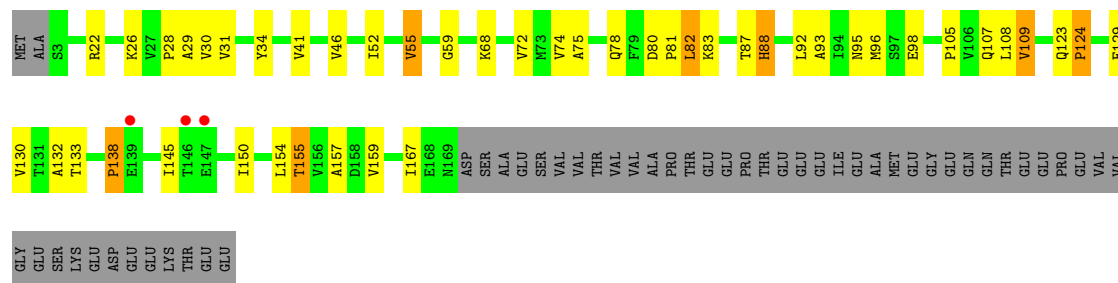


- Molecule 19: 50S ribosomal protein L24

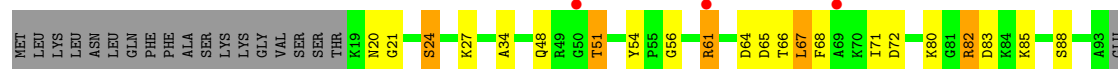




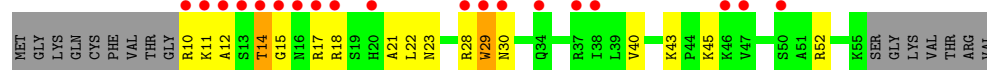
• Molecule 20: 50S ribosomal protein L25



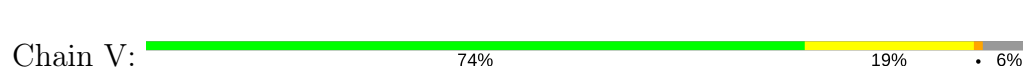
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



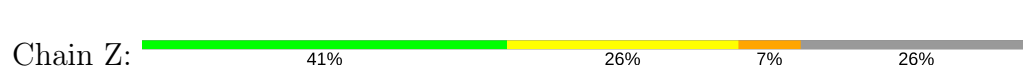
• Molecule 23: 50S ribosomal protein L29

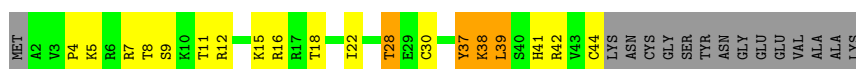


• Molecule 24: 50S ribosomal protein L30



• Molecule 25: 50S ribosomal protein L32





- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.206 , 0.248	Depositor DCC
R_{free} test set	11858 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, EOH, MPD, EPE, SPD

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	X	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

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	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	17
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	2	19
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	29
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	17
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	1	9
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	13	53
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	1	8
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	3	27
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	20	63
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	3	26
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	4	32
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	29
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	7	43
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	29
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	1	9
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	13	53
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	9
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	11	50
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	24
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	5	37
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	24

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA
3	A	126	VAL
3	A	141	VAL

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	
3	A	120/224 (54%)	101 (84%)	19 (16%)	3	17
4	B	153/177 (86%)	136 (89%)	17 (11%)	7	32
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	14
6	D	18/158 (11%)	17 (94%)	1 (6%)	25	62
7	E	67/155 (43%)	58 (87%)	9 (13%)	4	24
8	G	111/123 (90%)	101 (91%)	10 (9%)	11	42
9	H	91/100 (91%)	78 (86%)	13 (14%)	4	22
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	5
11	J	103/119 (87%)	91 (88%)	12 (12%)	6	30
12	K	91/102 (89%)	81 (89%)	10 (11%)	7	33
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	14
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	13
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	19
16	O	71/86 (83%)	60 (84%)	11 (16%)	3	18
17	P	91/94 (97%)	84 (92%)	7 (8%)	15	50
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	3
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	3
20	S	91/190 (48%)	83 (91%)	8 (9%)	12	44
21	T	56/75 (75%)	48 (86%)	8 (14%)	4	22
22	U	18/52 (35%)	17 (94%)	1 (6%)	25	62
23	V	47/62 (76%)	42 (89%)	5 (11%)	8	35
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	7
26	2	37/40 (92%)	32 (86%)	5 (14%)	4	24
27	3	37/57 (65%)	33 (89%)	4 (11%)	7	34
28	4	30/35 (86%)	27 (90%)	3 (10%)	9	37
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	4	21

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	33	THR
15	N	9	VAL
25	Z	5	LYS
12	K	76	GLU
14	M	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2688/2923 (91%)	627 (23%)	0
2	Y	113/114 (99%)	13 (11%)	0
All	All	2801/3037 (92%)	640 (22%)	0

5 of 640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A

There are no RNA pucker outliers to report.

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 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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	$\# Z > 2$
29	MPD	X	3001	-	7,7,7	0.31	0	9,10,10	0.43	0
29	MPD	X	3002	-	7,7,7	0.93	1 (14%)	9,10,10	0.48	0
29	MPD	X	3003	-	7,7,7	0.27	0	9,10,10	0.35	0
29	MPD	X	3004	-	7,7,7	0.55	0	9,10,10	0.18	0
29	MPD	X	3005	-	7,7,7	0.64	0	9,10,10	0.22	0
29	MPD	X	3006	-	7,7,7	0.44	0	9,10,10	0.09	0
29	MPD	X	3007	-	7,7,7	0.78	0	9,10,10	0.39	0
29	MPD	X	3008	-	7,7,7	0.66	0	9,10,10	0.30	0
29	MPD	X	3009	-	7,7,7	0.64	0	9,10,10	0.23	0
29	MPD	X	3010	-	7,7,7	0.61	0	9,10,10	0.32	0
29	MPD	X	3011	-	7,7,7	0.84	0	9,10,10	0.40	0
32	EPE	X	3311	-	15,15,15	1.20	1 (6%)	18,20,20	0.51	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.30	0
33	SPD	X	3314	-	9,9,9	0.15	0	8,8,8	0.21	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.26	0
34	EOH	X	3316	-	2,2,2	0.66	0	1,1,1	0.41	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.64	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.63	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.75	0
34	EOH	X	3320	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3321	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.64	0
29	MPD	Z	101	-	7,7,7	0.28	0	9,10,10	0.34	0

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
29	MPD	X	3001	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3004	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3011	-	-	0/5/5/5	0/0/0/0
32	EPE	X	3311	-	-	0/9/19/19	0/1/1/1
33	SPD	X	3312	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3313	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3314	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3315	-	-	0/7/7/7	0/0/0/0
34	EOH	X	3316	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3317	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3318	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3319	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3320	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3321	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3322	-	-	0/0/0/0	0/0/0/0
29	MPD	Z	101	-	-	0/5/5/5	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.42	1.70	1.77
29	X	3002	MPD	C3-C2	2.27	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3003	MPD	4	0
29	X	3005	MPD	4	0
29	X	3007	MPD	4	0
29	X	3008	MPD	1	0
29	X	3011	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	2708/2923 (92%)	-0.47	9 (0%) 93 91	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 74 66	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 90 87	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 71	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.25	3 (1%) 67 59	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 82	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 74 66	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.05	3 (2%) 64 56	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 77	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.23	1 (1%) 80 73	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 51 42	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	3 (1%) 69 60	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 39 32	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 61 51	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.44	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 1 1	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	66 (1%) 80 73	6, 51, 123, 230	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	EOH	X	3322	3/3	0.91	0.47	20.93	34,34,34,34	0
30	MN	X	3255	1/1	0.92	0.56	17.35	35,35,35,35	0
30	MN	X	3252	1/1	0.96	0.30	13.45	17,17,17,17	0
30	MN	X	3260	1/1	0.96	0.30	11.96	40,40,40,40	0
30	MN	X	3225	1/1	0.96	0.41	11.47	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	EOH	X	3318	3/3	0.83	0.27	10.73	47,47,47,47	0
31	MG	X	3103	1/1	0.92	0.44	9.93	3,3,3,3	0
30	MN	X	3286	1/1	0.99	0.31	8.58	57,57,57,57	0
30	MN	X	3272	1/1	0.98	0.36	8.16	44,44,44,44	0
33	SPD	X	3312	10/10	0.77	0.30	8.12	47,47,47,47	0
30	MN	X	3283	1/1	0.98	0.34	6.93	14,14,14,14	0
29	MPD	X	3010	8/8	0.81	0.33	6.51	87,87,87,87	0
30	MN	X	3242	1/1	0.97	0.30	6.50	22,22,22,22	0
33	SPD	X	3314	10/10	0.87	0.48	6.38	26,26,26,26	0
29	MPD	X	3002	8/8	0.83	0.32	6.27	45,45,45,45	0
29	MPD	Z	101	8/8	0.90	0.35	6.27	48,48,48,48	0
29	MPD	X	3008	8/8	0.79	0.35	6.20	70,70,70,70	0
30	MN	X	3230	1/1	0.92	0.28	6.05	65,65,65,65	0
31	MG	X	3174	1/1	0.88	0.31	5.57	5,5,5,5	0
30	MN	X	3196	1/1	0.96	0.33	5.53	51,51,51,51	0
30	MN	X	3012	1/1	0.97	0.31	5.42	19,19,19,19	0
29	MPD	X	3009	8/8	0.92	0.14	5.36	76,76,76,76	0
30	MN	X	3280	1/1	0.98	0.27	5.27	39,39,39,39	0
30	MN	X	3166	1/1	0.97	0.23	5.19	62,62,62,62	0
30	MN	X	3197	1/1	0.98	0.24	5.19	34,34,34,34	0
34	EOH	X	3316	3/3	0.85	0.40	5.10	10,10,10,10	0
30	MN	X	3273	1/1	0.89	0.27	4.97	41,41,41,41	0
29	MPD	X	3007	8/8	0.96	0.28	4.80	9,9,9,9	0
31	MG	X	3092	1/1	0.96	0.14	4.76	20,20,20,20	0
30	MN	X	3055	1/1	0.61	0.21	4.49	94,94,94,94	0
30	MN	X	3278	1/1	0.97	0.30	4.35	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	4.14	95,95,95,95	0
31	MG	X	3030	1/1	0.97	0.21	3.66	15,15,15,15	0
30	MN	X	3271	1/1	0.99	0.25	3.52	17,17,17,17	0
29	MPD	X	3006	8/8	0.85	0.18	3.50	88,88,88,88	0
30	MN	X	3279	1/1	0.99	0.25	3.47	25,25,25,25	0
33	SPD	X	3313	10/10	0.86	0.29	2.89	30,30,30,30	0
30	MN	X	3047	1/1	0.97	0.20	2.79	69,69,69,69	0
30	MN	X	3210	1/1	0.98	0.20	2.65	57,57,57,57	0
33	SPD	X	3315	10/10	0.84	0.31	2.56	46,46,46,46	0
30	MN	X	3265	1/1	0.95	0.24	2.41	43,43,43,43	0
30	MN	X	3154	1/1	0.99	0.22	2.12	40,40,40,40	0
30	MN	X	3213	1/1	0.71	0.23	2.09	95,95,95,95	0
30	MN	X	3185	1/1	0.99	0.21	1.95	28,28,28,28	0
30	MN	X	3257	1/1	0.99	0.23	1.92	25,25,25,25	0
30	MN	X	3258	1/1	0.96	0.22	1.61	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MPD	X	3011	8/8	0.85	0.24	1.49	39,39,39,39	0
30	MN	X	3269	1/1	0.93	0.24	1.30	36,36,36,36	0
30	MN	X	3198	1/1	0.99	0.20	1.20	64,64,64,64	0
30	MN	X	3256	1/1	0.98	0.22	1.20	13,13,13,13	0
30	MN	X	3246	1/1	0.99	0.19	1.11	13,13,13,13	0
30	MN	X	3227	1/1	0.92	0.17	1.02	57,57,57,57	0
30	MN	X	3224	1/1	0.94	0.25	1.01	53,53,53,53	0
32	EPE	X	3311	15/15	0.95	0.18	0.87	57,57,57,57	0
31	MG	X	3080	1/1	0.97	0.19	0.73	33,33,33,33	0
30	MN	X	3244	1/1	0.90	0.18	0.68	57,57,57,57	0
30	MN	X	3231	1/1	0.93	0.24	0.65	74,74,74,74	0
30	MN	X	3078	1/1	0.97	0.20	0.63	78,78,78,78	0
30	MN	X	3251	1/1	0.98	0.19	0.62	8,8,8,8	0
29	MPD	X	3004	8/8	0.92	0.34	0.51	73,73,73,73	0
29	MPD	X	3005	8/8	0.94	0.17	0.46	65,65,65,65	0
30	MN	X	3167	1/1	0.99	0.20	0.45	57,57,57,57	0
30	MN	X	3164	1/1	0.98	0.23	0.42	48,48,48,48	0
30	MN	X	3324	1/1	0.96	0.18	0.36	12,12,12,12	0
30	MN	X	3140	1/1	0.82	0.16	0.31	71,71,71,71	0
29	MPD	X	3001	8/8	0.94	0.14	0.23	33,33,33,33	0
30	MN	X	3157	1/1	0.94	0.22	0.12	68,68,68,68	0
31	MG	X	3082	1/1	0.88	0.17	-0.05	31,31,31,31	0
30	MN	X	3163	1/1	0.98	0.16	-0.07	61,61,61,61	0
31	MG	X	3176	1/1	0.95	0.16	-0.19	14,14,14,14	0
30	MN	X	3058	1/1	0.91	0.15	-0.20	64,64,64,64	0
30	MN	X	3281	1/1	0.96	0.17	-0.25	40,40,40,40	0
29	MPD	X	3003	8/8	0.97	0.19	-0.27	21,21,21,21	0
30	MN	J	201	1/1	0.79	0.20	-0.45	78,78,78,78	0
30	MN	X	3326	1/1	0.99	0.18	-0.46	57,57,57,57	0
30	MN	X	3277	1/1	0.98	0.17	-0.59	35,35,35,35	0
30	MN	X	3171	1/1	0.95	0.15	-0.73	86,86,86,86	0
30	MN	X	3274	1/1	0.98	0.10	-0.85	36,36,36,36	0
31	MG	X	3088	1/1	0.97	0.13	-0.85	36,36,36,36	0
31	MG	X	3310	1/1	0.94	0.13	-0.90	15,15,15,15	0
30	MN	X	3062	1/1	0.99	0.16	-0.95	42,42,42,42	0
30	MN	X	3150	1/1	0.99	0.13	-0.95	50,50,50,50	0
30	MN	R	201	1/1	0.96	0.10	-1.00	63,63,63,63	0
30	MN	X	3147	1/1	0.97	0.12	-1.02	82,82,82,82	0
30	MN	X	3061	1/1	0.93	0.12	-1.17	63,63,63,63	0
30	MN	X	3159	1/1	0.97	0.15	-1.20	42,42,42,42	0
30	MN	X	3112	1/1	0.96	0.06	-1.44	54,54,54,54	0
31	MG	B	302	1/1	0.98	0.11	-1.46	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3323	1/1	0.97	0.15	-1.53	42,42,42,42	0
30	MN	X	3229	1/1	0.93	0.13	-1.63	79,79,79,79	0
30	MN	X	3063	1/1	0.93	0.12	-1.68	60,60,60,60	0
31	MG	X	3037	1/1	0.96	0.12	-1.82	11,11,11,11	0
30	MN	X	3170	1/1	0.97	0.10	-1.93	54,54,54,54	0
30	MN	X	3288	1/1	0.91	0.11	-2.31	55,55,55,55	0
31	MG	X	3036	1/1	0.95	0.14	-	8,8,8,8	0
30	MN	X	3057	1/1	0.71	0.20	-	71,71,71,71	0
30	MN	X	3129	1/1	0.95	0.08	-	73,73,73,73	0
31	MG	X	3100	1/1	0.93	0.21	-	17,17,17,17	0
31	MG	X	3032	1/1	0.94	0.25	-	21,21,21,21	0
31	MG	X	3096	1/1	0.98	0.24	-	9,9,9,9	0
30	MN	X	3015	1/1	0.74	0.38	-	75,75,75,75	0
30	MN	X	3200	1/1	0.99	0.26	-	37,37,37,37	0
30	MN	X	3053	1/1	0.63	0.54	-	89,89,89,89	0
31	MG	X	3081	1/1	0.98	0.07	-	36,36,36,36	0
30	MN	X	3189	1/1	0.99	0.30	-	64,64,64,64	0
31	MG	X	3093	1/1	0.84	0.27	-	21,21,21,21	0
30	MN	X	3051	1/1	0.98	0.18	-	67,67,67,67	0
30	MN	X	3259	1/1	0.96	0.15	-	13,13,13,13	0
30	MN	X	3264	1/1	0.99	0.33	-	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	-	25,25,25,25	0
30	MN	X	3218	1/1	0.94	0.31	-	65,65,65,65	0
30	MN	X	3250	1/1	0.91	0.27	-	80,80,80,80	0
30	MN	X	3216	1/1	0.88	0.19	-	54,54,54,54	0
30	MN	X	3017	1/1	0.98	0.36	-	103,103,103,103	0
31	MG	X	3300	1/1	0.91	0.17	-	11,11,11,11	0
31	MG	X	3035	1/1	0.89	0.33	-	23,23,23,23	0
30	MN	X	3162	1/1	0.94	0.31	-	43,43,43,43	0
30	MN	X	3191	1/1	0.94	0.15	-	51,51,51,51	0
30	MN	X	3066	1/1	0.79	0.12	-	56,56,56,56	0
31	MG	X	3306	1/1	0.96	0.07	-	29,29,29,29	0
31	MG	C	301	1/1	0.90	0.26	-	2,2,2,2	0
31	MG	X	3020	1/1	0.97	0.25	-	20,20,20,20	0
30	MN	I	202	1/1	0.85	0.25	-	64,64,64,64	0
31	MG	X	3108	1/1	0.94	0.10	-	12,12,12,12	0
30	MN	X	3160	1/1	0.94	0.18	-	45,45,45,45	0
30	MN	X	3155	1/1	0.90	0.39	-	87,87,87,87	0
30	MN	X	3193	1/1	0.97	0.18	-	33,33,33,33	0
31	MG	X	3104	1/1	0.96	0.32	-	28,28,28,28	0
31	MG	X	3018	1/1	0.93	0.47	-	15,15,15,15	0
30	MN	X	3065	1/1	0.92	0.10	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3165	1/1	0.97	0.16	-	63,63,63,63	0
30	MN	X	3121	1/1	0.78	0.31	-	88,88,88,88	0
30	MN	X	3261	1/1	0.95	0.16	-	30,30,30,30	0
31	MG	X	3298	1/1	0.82	1.01	-	23,23,23,23	0
31	MG	Y	203	1/1	0.87	0.76	-	21,21,21,21	0
31	MG	X	3094	1/1	0.98	0.16	-	5,5,5,5	0
31	MG	X	3038	1/1	0.91	0.29	-	23,23,23,23	0
31	MG	X	3136	1/1	0.93	0.34	-	27,27,27,27	0
30	MN	X	3132	1/1	0.67	0.16	-	97,97,97,97	0
30	MN	X	3181	1/1	0.97	0.19	-	39,39,39,39	0
30	MN	X	3111	1/1	0.80	0.13	-	99,99,99,99	0
31	MG	X	3304	1/1	0.94	0.78	-	15,15,15,15	0
30	MN	X	3183	1/1	0.88	0.15	-	41,41,41,41	0
31	MG	X	3013	1/1	0.76	0.82	-	30,30,30,30	0
30	MN	X	3138	1/1	0.83	0.10	-	112,112,112,112	0
30	MN	X	3222	1/1	0.73	0.36	-	71,71,71,71	0
30	MN	X	3134	1/1	0.91	0.18	-	58,58,58,58	0
31	MG	X	3173	1/1	0.71	1.12	-	26,26,26,26	0
30	MN	X	3151	1/1	0.97	0.17	-	44,44,44,44	0
30	MN	X	3243	1/1	0.99	0.42	-	28,28,28,28	0
30	MN	X	3076	1/1	0.82	0.10	-	74,74,74,74	0
31	MG	X	3089	1/1	0.94	0.15	-	13,13,13,13	0
30	MN	X	3235	1/1	0.98	0.39	-	40,40,40,40	0
30	MN	X	3179	1/1	0.95	0.21	-	83,83,83,83	0
30	MN	X	3024	1/1	0.97	0.43	-	107,107,107,107	0
30	MN	X	3044	1/1	0.70	0.24	-	94,94,94,94	0
30	MN	X	3270	1/1	0.99	0.16	-	30,30,30,30	0
31	MG	X	3137	1/1	0.80	0.91	-	17,17,17,17	0
30	MN	Y	202	1/1	0.88	0.14	-	57,57,57,57	0
31	MG	O	201	1/1	0.92	0.28	-	7,7,7,7	0
30	MN	X	3177	1/1	0.95	0.21	-	82,82,82,82	0
30	MN	X	3180	1/1	0.96	0.54	-	76,76,76,76	0
31	MG	X	3023	1/1	0.78	0.29	-	37,37,37,37	0
31	MG	X	3307	1/1	0.96	0.04	-	21,21,21,21	0
30	MN	X	3234	1/1	0.99	0.18	-	17,17,17,17	0
30	MN	X	3049	1/1	0.96	0.39	-	82,82,82,82	0
30	MN	X	3043	1/1	0.98	0.11	-	61,61,61,61	0
31	MG	X	3101	1/1	0.98	0.35	-	9,9,9,9	0
30	MN	X	3118	1/1	0.87	0.31	-	101,101,101,101	0
31	MG	X	3102	1/1	0.96	0.34	-	6,6,6,6	0
31	MG	I	201	1/1	0.92	0.27	-	0,0,0,0	0
30	MN	X	3126	1/1	0.81	0.24	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3124	1/1	0.81	0.11	-	77,77,77,77	0
30	MN	X	3206	1/1	0.96	0.45	-	57,57,57,57	0
30	MN	R	202	1/1	0.96	0.23	-	58,58,58,58	0
30	MN	X	3071	1/1	0.96	0.08	-	69,69,69,69	0
30	MN	X	3130	1/1	0.81	0.13	-	102,102,102,102	0
30	MN	X	3073	1/1	0.88	0.14	-	86,86,86,86	0
30	MN	X	3050	1/1	0.74	0.47	-	99,99,99,99	0
31	MG	X	3295	1/1	0.94	0.68	-	18,18,18,18	0
30	MN	X	3046	1/1	0.93	0.30	-	94,94,94,94	0
31	MG	X	3116	1/1	0.99	0.14	-	20,20,20,20	0
31	MG	X	3099	1/1	0.94	0.14	-	26,26,26,26	0
31	MG	X	3114	1/1	0.82	0.57	-	36,36,36,36	0
30	MN	X	3161	1/1	0.97	0.23	-	46,46,46,46	0
31	MG	X	3029	1/1	0.97	0.39	-	19,19,19,19	0
31	MG	X	3095	1/1	0.84	0.34	-	26,26,26,26	0
30	MN	X	3169	1/1	0.89	0.67	-	78,78,78,78	0
30	MN	X	3214	1/1	0.98	0.11	-	81,81,81,81	0
30	MN	X	3133	1/1	0.73	0.32	-	98,98,98,98	0
30	MN	X	3068	1/1	0.87	0.22	-	70,70,70,70	0
30	MN	X	3119	1/1	0.93	0.15	-	63,63,63,63	0
31	MG	Y	205	1/1	0.88	0.14	-	12,12,12,12	0
30	MN	X	3239	1/1	0.97	0.36	-	15,15,15,15	0
30	MN	X	3048	1/1	0.95	0.10	-	59,59,59,59	0
31	MG	X	3172	1/1	0.87	0.80	-	27,27,27,27	0
31	MG	G	203	1/1	0.47	0.33	-	17,17,17,17	0
30	MN	X	3142	1/1	0.95	0.39	-	72,72,72,72	0
30	MN	X	3208	1/1	0.94	0.25	-	37,37,37,37	0
30	MN	X	3067	1/1	0.91	0.18	-	51,51,51,51	0
30	MN	X	3236	1/1	0.97	0.15	-	36,36,36,36	0
30	MN	X	3064	1/1	0.99	0.14	-	68,68,68,68	0
30	MN	X	3117	1/1	0.92	0.24	-	80,80,80,80	0
30	MN	X	3204	1/1	0.97	0.16	-	21,21,21,21	0
30	MN	X	3143	1/1	0.78	0.18	-	94,94,94,94	0
30	MN	X	3152	1/1	0.97	0.29	-	68,68,68,68	0
31	MG	X	3034	1/1	0.73	0.38	-	18,18,18,18	0
30	MN	X	3190	1/1	0.99	0.41	-	59,59,59,59	0
31	MG	X	3031	1/1	0.89	0.33	-	11,11,11,11	0
31	MG	X	3109	1/1	0.83	0.70	-	24,24,24,24	0
30	MN	X	3139	1/1	0.99	0.29	-	97,97,97,97	0
30	MN	X	3074	1/1	0.89	0.06	-	78,78,78,78	0
30	MN	X	3287	1/1	0.97	0.31	-	78,78,78,78	0
30	MN	X	3070	1/1	0.95	0.10	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3106	1/1	0.85	0.22	-	37,37,37,37	0
30	MN	X	3215	1/1	0.99	0.28	-	26,26,26,26	0
30	MN	X	3202	1/1	0.93	0.23	-	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	-	20,20,20,20	0
30	MN	X	3263	1/1	0.94	0.33	-	52,52,52,52	0
30	MN	X	3188	1/1	0.94	0.45	-	87,87,87,87	0
30	MN	X	3146	1/1	0.90	0.23	-	101,101,101,101	0
31	MG	X	3115	1/1	0.91	0.72	-	1,1,1,1	1
30	MN	X	3158	1/1	0.85	0.22	-	62,62,62,62	0
31	MG	X	3107	1/1	0.91	0.58	-	18,18,18,18	0
30	MN	X	3293	1/1	0.81	0.19	-	70,70,70,70	0
30	MN	B	303	1/1	0.70	0.74	-	102,102,102,102	0
30	MN	X	3226	1/1	0.92	0.33	-	89,89,89,89	0
30	MN	X	3120	1/1	0.96	0.17	-	55,55,55,55	0
31	MG	X	3294	1/1	0.86	0.34	-	37,37,37,37	0
31	MG	X	3087	1/1	0.95	0.32	-	51,51,51,51	0
30	MN	X	3211	1/1	0.93	0.20	-	60,60,60,60	0
30	MN	X	3056	1/1	0.99	0.19	-	61,61,61,61	0
30	MN	X	3249	1/1	0.99	0.20	-	51,51,51,51	0
30	MN	X	3285	1/1	0.98	0.22	-	85,85,85,85	0
30	MN	X	3199	1/1	0.92	0.36	-	51,51,51,51	0
31	MG	X	3026	1/1	0.91	0.60	-	18,18,18,18	0
31	MG	X	3302	1/1	0.87	0.31	-	20,20,20,20	0
30	MN	X	3127	1/1	0.90	0.13	-	44,44,44,44	0
30	MN	X	3233	1/1	0.92	0.26	-	63,63,63,63	0
30	MN	X	3262	1/1	0.96	0.22	-	50,50,50,50	0
30	MN	X	3228	1/1	0.96	0.34	-	85,85,85,85	0
30	MN	X	3168	1/1	0.73	0.21	-	74,74,74,74	0
31	MG	X	3019	1/1	0.93	0.25	-	15,15,15,15	0
30	MN	X	3128	1/1	0.79	0.16	-	84,84,84,84	0
30	MN	X	3045	1/1	0.99	0.28	-	3,3,3,3	0
30	MN	X	3141	1/1	0.97	0.35	-	69,69,69,69	0
30	MN	X	3268	1/1	0.86	0.29	-	27,27,27,27	0
30	MN	X	3220	1/1	0.81	0.43	-	68,68,68,68	0
30	MN	X	3072	1/1	0.93	0.17	-	80,80,80,80	0
30	MN	X	3245	1/1	0.99	0.21	-	28,28,28,28	0
30	MN	Y	204	1/1	0.97	0.11	-	63,63,63,63	0
31	MG	X	3039	1/1	0.88	0.30	-	7,7,7,7	0
34	EOH	X	3317	3/3	0.71	0.52	-	46,46,46,46	0
30	MN	X	3125	1/1	0.85	0.32	-	79,79,79,79	0
30	MN	X	3241	1/1	0.97	0.28	-	20,20,20,20	0
30	MN	X	3131	1/1	0.85	0.49	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3221	1/1	0.94	0.12	-	46,46,46,46	0
31	MG	X	3033	1/1	0.98	0.20	-	19,19,19,19	0
30	MN	X	3240	1/1	0.96	0.19	-	28,28,28,28	0
30	MN	X	3182	1/1	0.77	0.38	-	107,107,107,107	0
31	MG	X	3305	1/1	0.90	0.91	-	15,15,15,15	0
30	MN	X	3025	1/1	0.96	0.21	-	52,52,52,52	0
30	MN	X	3014	1/1	0.97	0.20	-	12,12,12,12	0
30	MN	X	3276	1/1	0.88	0.17	-	42,42,42,42	0
30	MN	X	3187	1/1	0.94	0.28	-	74,74,74,74	0
30	MN	X	3282	1/1	0.97	0.21	-	49,49,49,49	0
31	MG	X	3175	1/1	0.80	0.30	-	0,0,0,0	0
30	MN	X	3041	1/1	0.91	0.22	-	84,84,84,84	0
30	MN	X	3135	1/1	0.83	0.15	-	94,94,94,94	0
30	MN	X	3060	1/1	0.98	0.15	-	51,51,51,51	0
31	MG	X	3016	1/1	0.75	0.38	-	23,23,23,23	0
30	MN	X	3205	1/1	0.98	0.27	-	61,61,61,61	0
31	MG	X	3105	1/1	0.95	0.24	-	35,35,35,35	0
30	MN	X	3195	1/1	0.98	0.21	-	30,30,30,30	0
30	MN	X	3149	1/1	0.93	0.28	-	94,94,94,94	0
30	MN	X	3156	1/1	0.95	0.22	-	53,53,53,53	0
30	MN	X	3291	1/1	0.93	0.52	-	94,94,94,94	0
30	MN	X	3219	1/1	0.97	0.31	-	53,53,53,53	0
30	MN	X	3059	1/1	0.84	0.10	-	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	-	89,89,89,89	0
31	MG	X	3144	1/1	0.96	0.19	-	8,8,8,8	0
31	MG	X	3297	1/1	0.92	0.31	-	5,5,5,5	0
30	MN	X	3209	1/1	0.94	0.20	-	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	-	4,4,4,4	0
30	MN	X	3186	1/1	0.92	0.29	-	51,51,51,51	0
30	MN	X	3290	1/1	0.90	0.18	-	89,89,89,89	0
31	MG	X	3022	1/1	0.91	0.60	-	25,25,25,25	0
30	MN	X	3238	1/1	0.98	0.22	-	34,34,34,34	0
31	MG	X	3021	1/1	0.95	0.18	-	21,21,21,21	0
30	MN	X	3148	1/1	0.75	0.25	-	79,79,79,79	0
30	MN	X	3275	1/1	0.99	0.18	-	30,30,30,30	0
30	MN	X	3292	1/1	0.97	0.28	-	99,99,99,99	0
30	MN	X	3267	1/1	0.94	0.31	-	48,48,48,48	0
31	MG	X	3097	1/1	0.91	0.22	-	14,14,14,14	0
30	MN	X	3178	1/1	0.92	0.46	-	78,78,78,78	0
31	MG	X	3028	1/1	0.90	0.29	-	34,34,34,34	0
30	MN	X	3232	1/1	0.98	0.30	-	55,55,55,55	0
30	MN	X	3042	1/1	0.84	0.11	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3253	1/1	0.97	0.34	-	26,26,26,26	0
30	MN	X	3052	1/1	0.83	0.21	-	71,71,71,71	0
30	MN	X	3207	1/1	0.92	0.44	-	62,62,62,62	0
30	MN	X	3075	1/1	0.97	0.11	-	76,76,76,76	0
30	MN	X	3145	1/1	0.99	0.16	-	51,51,51,51	0
34	EOH	X	3320	3/3	0.88	0.28	-	28,28,28,28	0
30	MN	X	3308	1/1	0.39	0.74	-	92,92,92,92	0
34	EOH	X	3321	3/3	0.88	0.31	-	18,18,18,18	0
30	MN	X	3217	1/1	0.98	0.27	-	38,38,38,38	0
30	MN	X	3223	1/1	0.89	0.24	-	60,60,60,60	0
31	MG	X	3085	1/1	0.91	0.21	-	9,9,9,9	0
30	MN	X	3212	1/1	0.97	0.26	-	56,56,56,56	0
30	MN	X	3069	1/1	0.94	0.14	-	68,68,68,68	0
30	MN	X	3110	1/1	0.95	0.13	-	96,96,96,96	0
30	MN	X	3325	1/1	0.96	0.22	-	59,59,59,59	0
31	MG	X	3299	1/1	0.93	0.26	-	5,5,5,5	0
34	EOH	X	3319	3/3	0.90	0.19	-	47,47,47,47	0
31	MG	G	201	1/1	0.86	0.20	-	19,19,19,19	0
30	MN	X	3040	1/1	0.95	0.19	-	74,74,74,74	0
31	MG	Y	201	1/1	0.88	0.11	-	34,34,34,34	0
31	MG	X	3113	1/1	0.65	1.07	-	45,45,45,45	0
30	MN	X	3289	1/1	0.97	0.28	-	57,57,57,57	0
30	MN	X	3237	1/1	0.99	0.23	-	47,47,47,47	0
30	MN	X	3123	1/1	0.83	0.42	-	97,97,97,97	0
31	MG	X	3296	1/1	0.96	0.48	-	9,9,9,9	0
31	MG	X	3091	1/1	0.96	0.44	-	30,30,30,30	0
30	MN	X	3090	1/1	0.84	0.35	-	96,96,96,96	0
30	MN	I	203	1/1	0.97	0.22	-	33,33,33,33	0
30	MN	X	3184	1/1	0.94	0.36	-	88,88,88,88	0
31	MG	X	3098	1/1	0.91	0.33	-	14,14,14,14	0
31	MG	X	3083	1/1	0.71	0.34	-	37,37,37,37	0
31	MG	X	3079	1/1	0.84	0.74	-	27,27,27,27	0
30	MN	X	3266	1/1	0.97	0.18	-	22,22,22,22	0
30	MN	X	3201	1/1	0.99	0.20	-	40,40,40,40	0
30	MN	X	3054	1/1	0.94	0.28	-	86,86,86,86	0
30	MN	X	3194	1/1	0.96	0.17	-	31,31,31,31	0
30	MN	X	3284	1/1	0.99	0.15	-	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	-	8,8,8,8	0
31	MG	G	202	1/1	0.94	0.37	-	12,12,12,12	0
31	MG	X	3086	1/1	0.96	0.10	-	26,26,26,26	0
31	MG	X	3084	1/1	0.76	0.14	-	14,14,14,14	0
30	MN	X	3254	1/1	0.83	0.23	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	B	301	1/1	0.89	0.14	-	0,0,0,0	0
30	MN	X	3203	1/1	0.98	0.37	-	27,27,27,27	0
31	MG	X	3027	1/1	0.94	0.19	-	29,29,29,29	0
30	MN	X	3077	1/1	0.98	0.20	-	78,78,78,78	0
30	MN	X	3248	1/1	0.99	0.28	-	37,37,37,37	0
30	MN	X	3192	1/1	0.90	0.32	-	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.