



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:33 PM 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

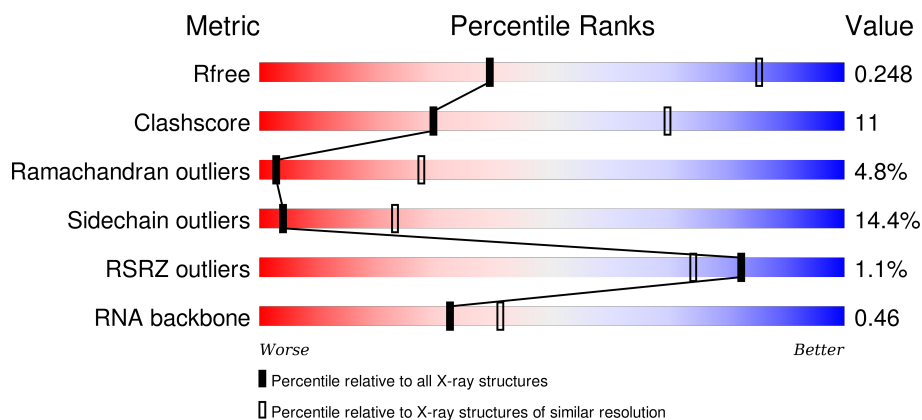
1 Overall quality at a glance

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.













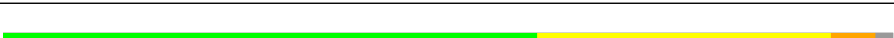

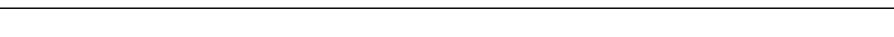
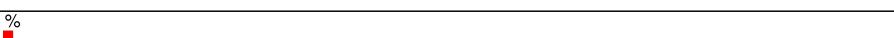
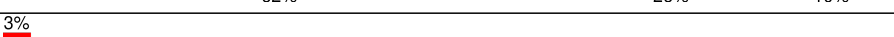
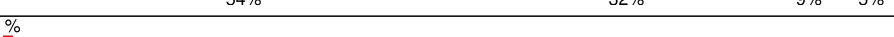

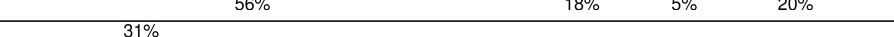

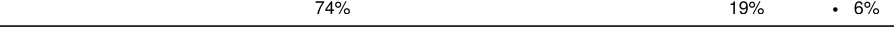
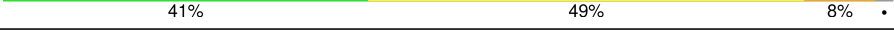



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)
RNA backbone	2183	1051 (4.22-2.80)

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. 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			

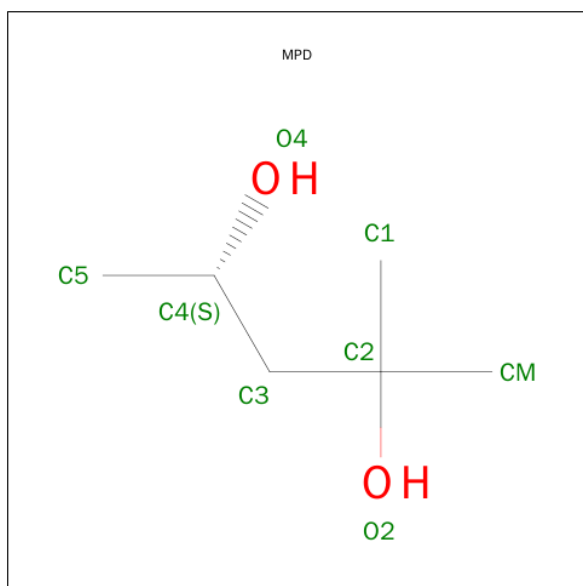
- Molecule 27 is a protein called 50S ribosomal protein L35.

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		

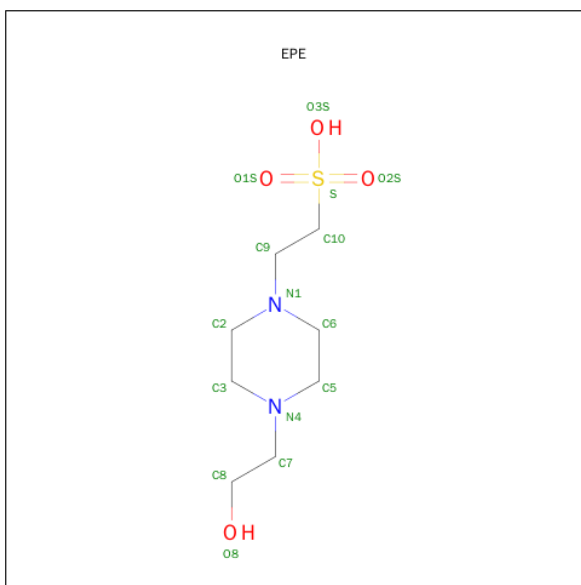
- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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).

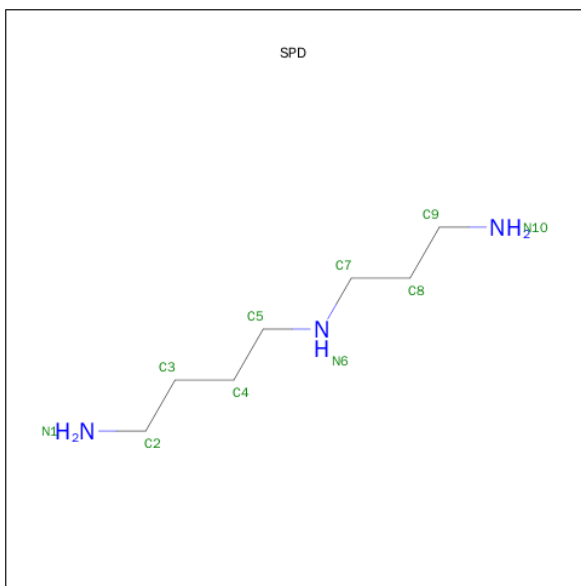
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

- 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: $C_7H_{19}N_3$).



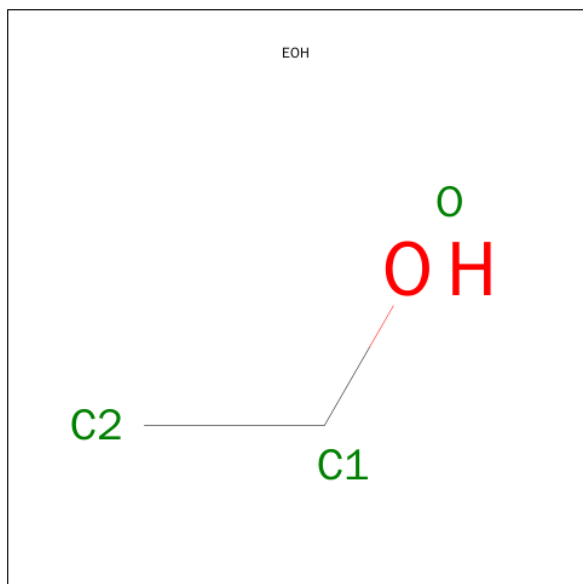
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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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: C₂H₆O).

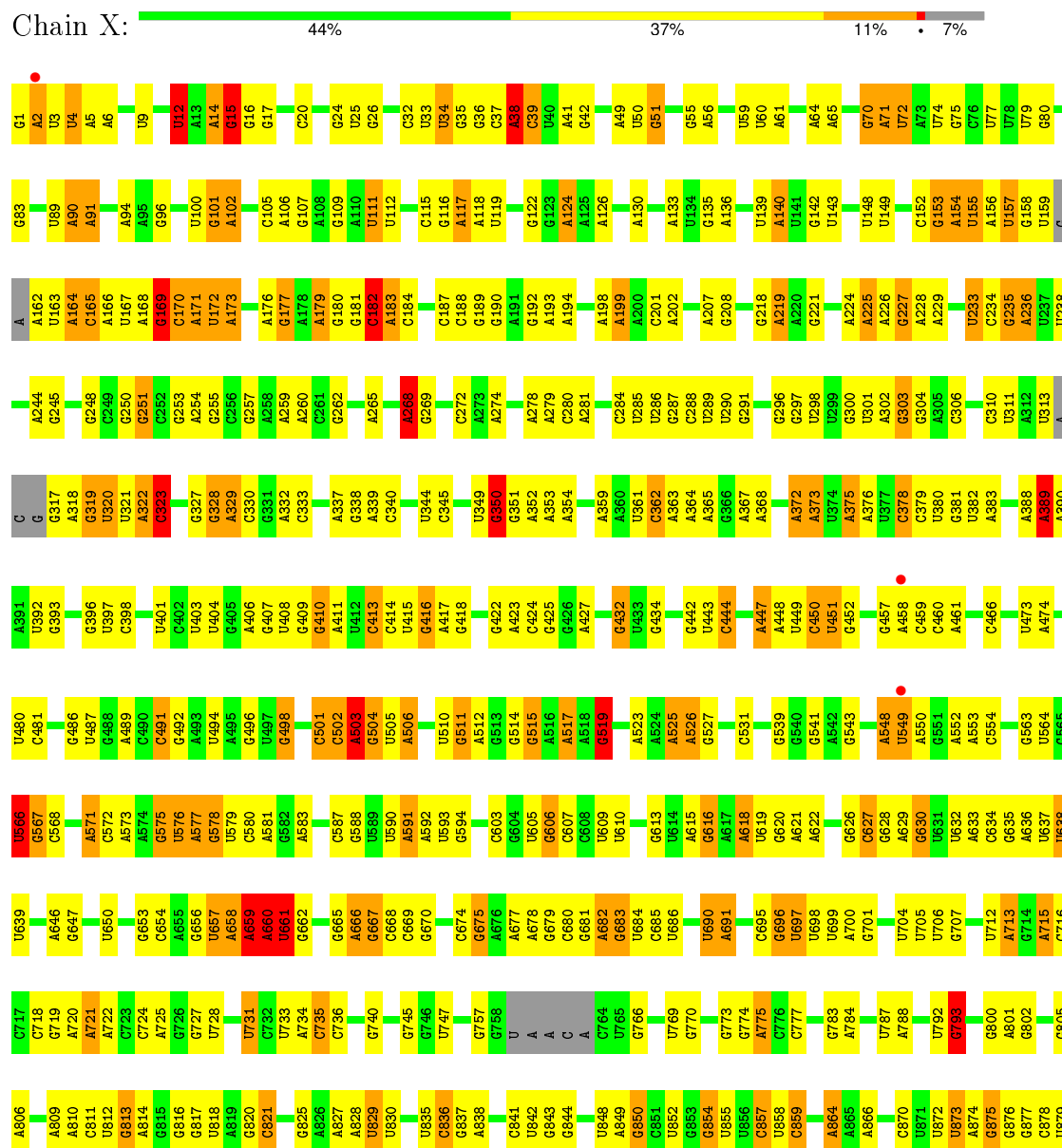


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

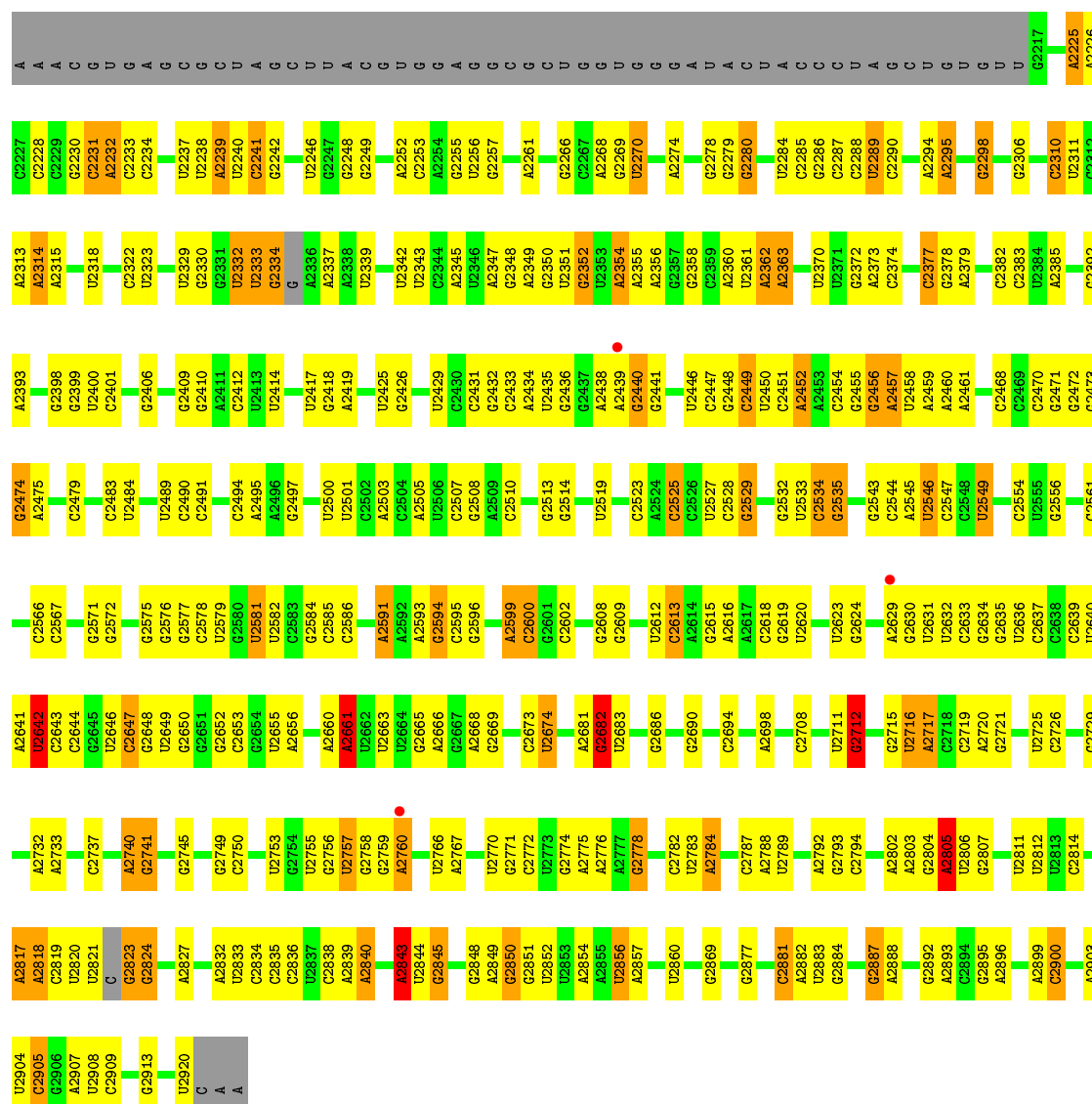
3 Residue-property plots

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

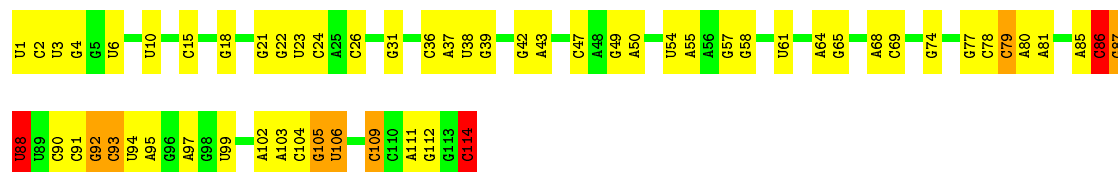
• Molecule 1: 23S rRNA



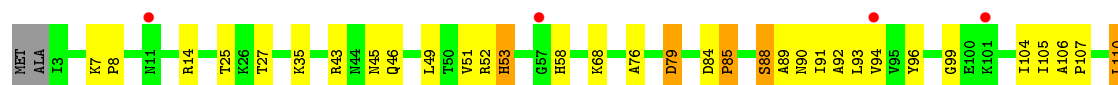
G2088	A1977	A1916	C1833	G1759	A1653	G1518	U1451		U1301	U1209	A	U1059	G966	A880
A2089	A1998	C1922	G1834	G1760	G1657	U1519	C1452	A1379	G1302	C1213	A	U1060	C967	A887
C2093	A1999	A1923	U1835	G1761	A1658	A	G1453	G1380	A1303	G1214	G	U1061	U970	U888
G2094	G1999	G1924	A1836	U1762		U1521	U1454	U1381	G1304	U1215	A	U1063	U971	U889
U2095	G2007	U1924	A1837	U1763	G1661	G1523	U	G1382	U1305	U	G	U1064	G990	G890
G2096	A2008	C1929	U1843	U1764	A1662	C1524	U	G1384	A1306	U1217	U	A1065	A977	A891
U2101	U2009	G1930	G1844	A1765	G1663	U	A1459	G1385	G1309	G1218	G	U1066	U892	U892
U2102	G2012	G1931	U1845	C1766	G1664	G1526	A		A1310	G1219	C	U1067	A985	U895
G2013	G2013	C1932	U1846	C1768	U1680	A1527	U1460	U1389	A1311	A	G	U1068	U896	U896
U2106	G2014	G1933	U1847	C1769	U1681	U1528	C1461	U1390	A1312	G1220	U	G1069	A989	A897
G2107	U2018	C1934	A1848	G1770	C1682	U1529	G1462	A1391	G1313	G1225	A	A1070	G990	U898
		C		A1771	U1683	A1530	A1463	G1392	A1314	G1226	U	A1071	U895	
		C		G1772	U1684	U	U1464		C1315	U1227	A	A1072	U896	A902
C2111	U2019	G	U1851		A1684	A	G1466	G1395	G1316	A1228	G	U1077	G997	G903
U2112	U2020	U	U1854	G1775	G1687	A	G1467	C1400	A1323	U1229	C1144	U1078	G998	G902
G2113	A2024	G	G1855	A1776	U1688	G	U1468	G1401	G1328	G1230	U1145	U1079	U999	G904
U2114		A	A1856	U1788	G1689	G1596	G1469	A1402	G1329	U1240	C1146	U1080	U905	U905
		C	C1857	C1781	U1690	U1597	A1471	G1405	U1326	U1241	A1147	U1081	A906	A906
U2119	G2027	U	U1857	A1782	G1691	A	G1470		C1327	A1242	U1148	U1082	G1001	G907
G2120		A	C1864	U1787	G1692	U1598	C1472		G1328	U1243	U1149	U1083	U1002	
A2121	U2031	U	G1865	A1788	G1693	A1533	A	G1408	C1329	U1244	U1150	U1084	U1003	A911
G2122	A2032	G	U1866	U1789	G1694	U1540	G1467	U1409	G1330	U1245	G1151	U1085	G1005	U916
A2123		A	U1867	G1790	G1695	C1542	U1477	U1410	U1330	U1246	U1152	U1086	G1006	
	G2036	G	G1868	G1791	G1696	G1543	A1478	G1411	C1331	U1247	C1153	U1087	U1007	G822
G2126	G2037	U	C1870	U1792	U1697	U1544		G1412	G1335	U1248	U1154	U1088	G1008	A923
G	A2040	U	U1879	C1793	A1698	U1545	U1481	G1413	G1336	U1249	U1155	U1089	G1009	G924
G		C	A1875	U1794	A1699	U1546	G1487	G1414	A1337	U1250	U1156	U1090	U1013	G925
A	A2047	C	G1876	A1795	U1701	C1547	U1488	U1415	U1338	U1251	U1157	U1091	U1014	G
C	G2048	U	U1877	U1796	C1702	U1548	A1489	U1416	U1339	U1252	U1158	U1092	G1015	G
A	U2049	A	U1880	A1800	U1703	G1550	U1490	G1417	G1340	U1253	U1159	U1093	G1016	C
G	A2050	U	G1885	U1806	U1704	U1551	C1481	U1421	G1346	U1254	C1167	U1094	G1017	C
C	C2051	G	A1886	G1803	A1705	U	U1482	A1422	G1347	U1255	U1160	U1095	A1018	C
U	U2053	U	G1887	U1807	G1710	A	U1493	C1423	U1348	U1256	U1161	U1096	A1019	C
U	G2056	U	U1888	U1808	G1711	G1555	G1494	A1424	U1349	U1257	U1162	U1097	A1020	U
C	A2057	C	G1889	U1809	G1712	C1556	C1495	U1425	U1350	U1258	U1163	U1098	A1021	C
G	C2058	U	U1890	U1809	G1713	C1557	U1496	G1429	C1351	U1259	U1164	U1099	A1022	U
A	A2059	U	U1891	U1810	G1714	C1558	U1497	U1430	C1352	U1260	U1165	U1100	A1023	C
G	G2059	U	U1892	U1811	A1721	U1559	U1498	U1431	G1353	U1261	U1166	U1101	A1024	C
A	A2060	U	U1893	U1812	C1730	G1560	U1499	U1432	A1354	U1262	U1167	U1102	A1025	U
G	U2061	U	G1894	A1813	U1731	A1561	G1500	U1433	G1355	U1263	U1168	U1103	G1026	C
U	G2062	C	U1895	U1814	U1732	C1562	G1501	U1434	G1356	U1264	U1169	U1104	G1027	C
U	C2063	U	U1896	C1815	U1733	U1563	A1502	U1435	G1357	U1265	U1170	U1105	G1028	G
A	A2064	U	U	U1816	U1734	G1564	U1503	C1436	A1358	U1266	U1171	U1106	G1029	G
G	C2070	C	C	C1817	U1735	U1565	U1504	U1437	A1359	U1267	U1172	U1107	G1030	C
U	C2071	U	U1900	A1818	G1739	U1566	G1505	U1438	G1360	U1268	U1173	U1108	G1031	C
A		U	G1901	G1819	G1740	U1567	U1506	U1439	U1366	U1269	U1174	U1109	G1032	C
G	G2077	U	G1902	U1823		U1568	C1508	A1440	C1367	U1270	U1175	U1110	G1033	C
G	A2078	G	G1983	C1824	A1744	G1569	G1509	U1441	C1368	U1271	U1176	U1111	A1034	C
A	G2079	A	U1906	U1825	A1745	U1510	U1510	C1442	G1369	U1272	U1177	U1112	G1035	C
G	G2080	G	G1907	U1826	G1746	G1572	C1511	U1445	C1370	U1273	U1178	U1113	G1036	C
C	A2081	C	U1908	C1827	G1747	U1573	U1512	U1446	C1371	U1274	U1179	U1114	G1037	C
C	G2082	C	U1909	U1828	U1755	G1574	A1513	U1447	C1372	U1275	U1180	U1115	G1038	C
U	G2083	U	G1910	A1829	U1756	U1575	A1514	U1448	U1373	U1276	U1181	U1116	G1039	C
U	G2084	U	U1911	A1830	U1757	G1576	G1515	U1449	C1374	U1277	U1182	U1117	G1040	C
U		U	A1912	A1831	U1758	A1577	C1516	U1450	G1375	U1278	U1183	U1118	G1041	C
G	A2087	U				A1578	A1517		G1376	U1279	U1184	U1119	G1042	C

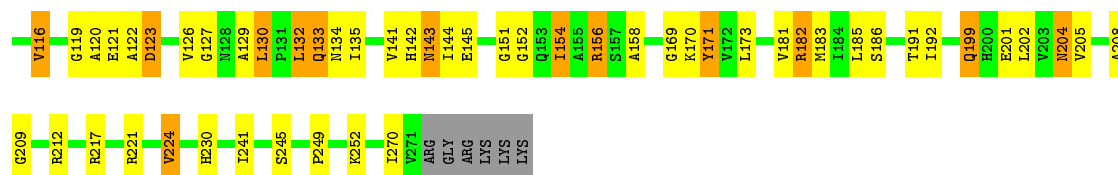


• Molecule 2: 5S rRNA

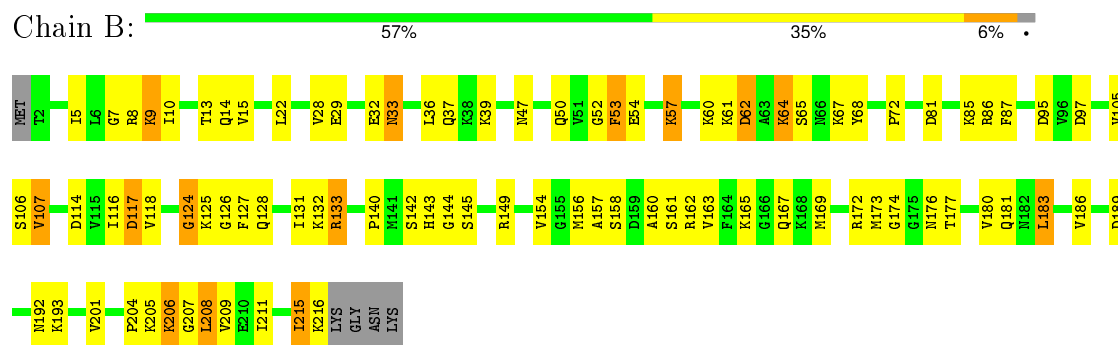


• Molecule 3: 50S ribosomal protein L2

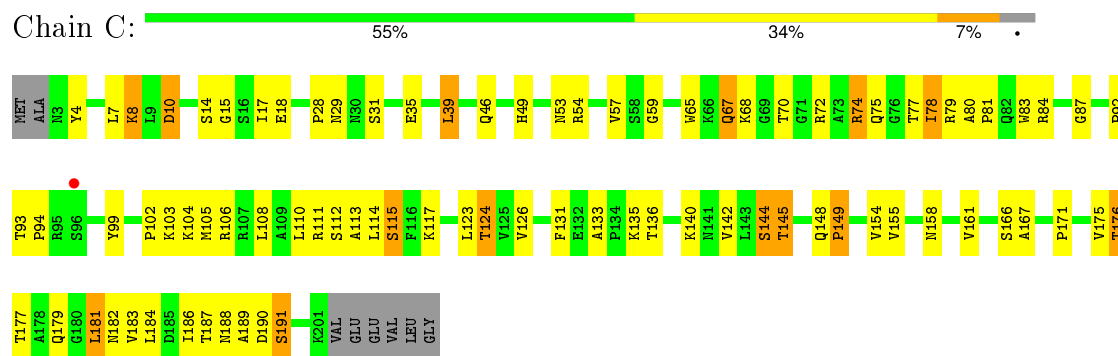




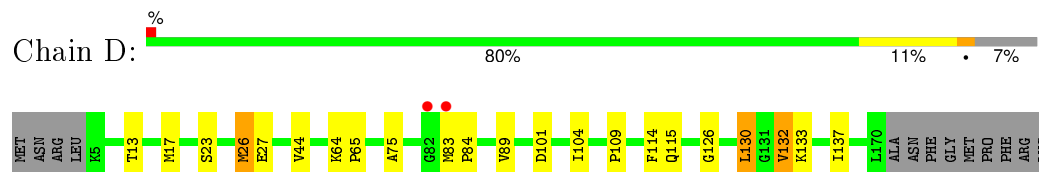
• Molecule 4: 50S ribosomal protein L3



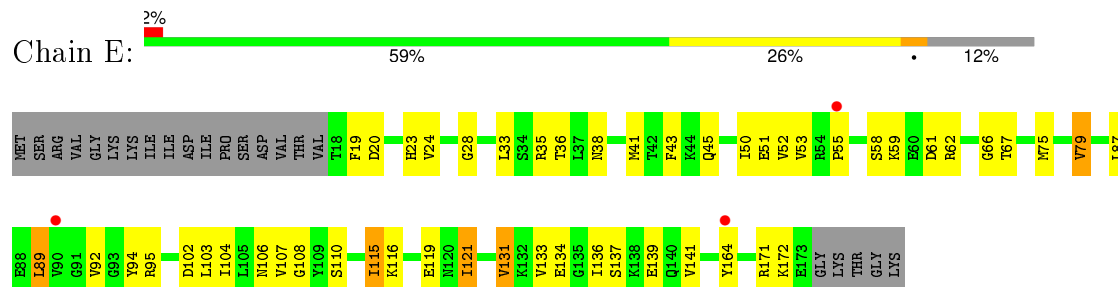
• Molecule 5: 50S ribosomal protein L4



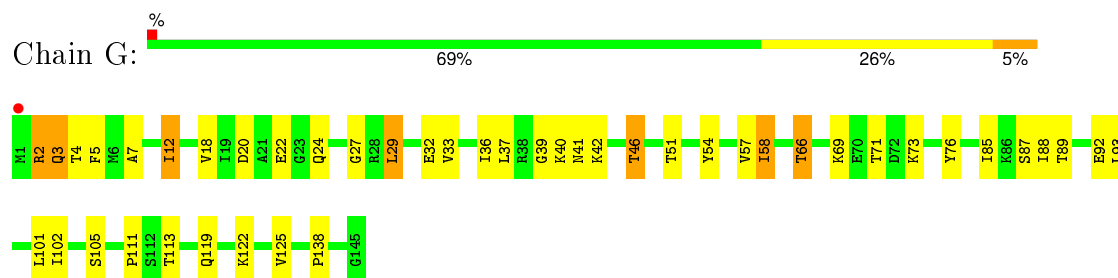
• Molecule 6: 50S ribosomal protein L5



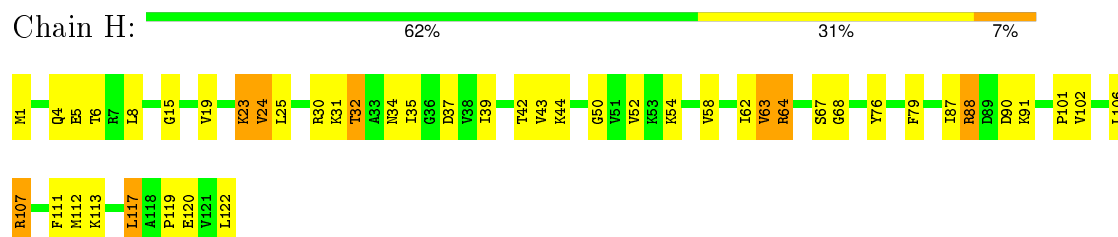
• Molecule 7: 50S ribosomal protein L6



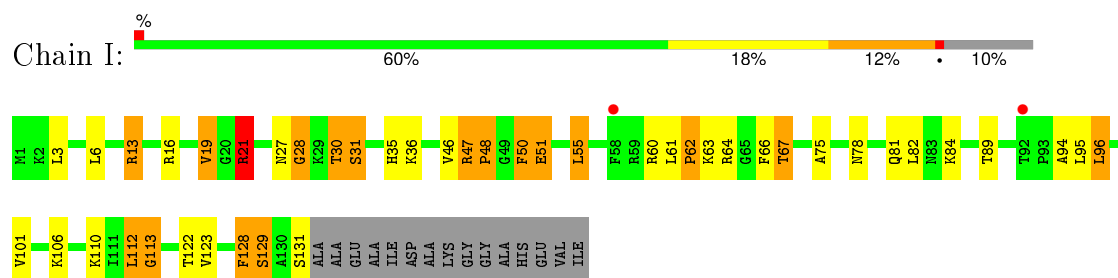
• Molecule 8: 50S ribosomal protein L13



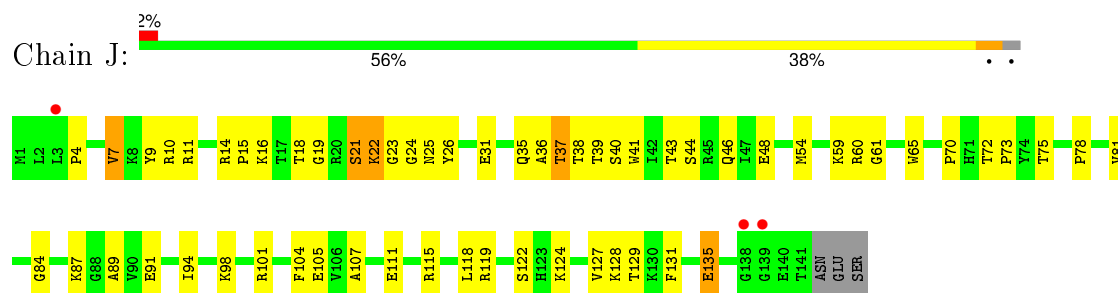
- Molecule 9: 50S ribosomal protein L14



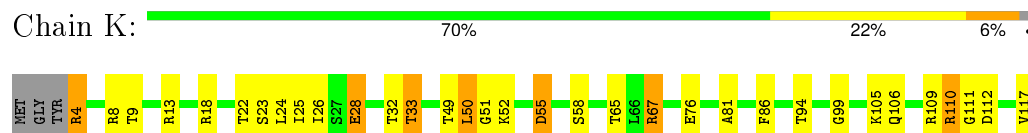
- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17

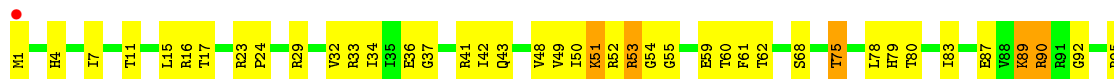


- Molecule 13: 50S ribosomal protein L18

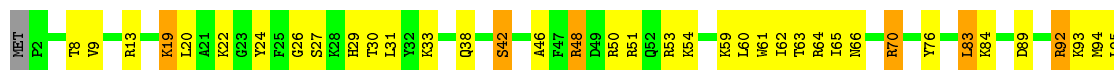




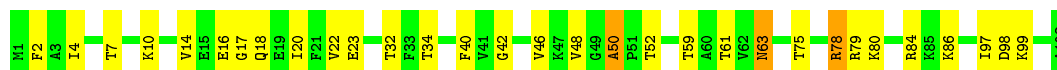
- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L23

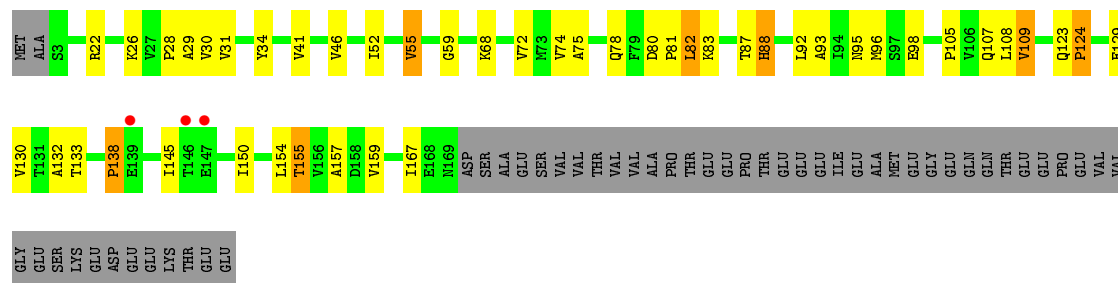


- Molecule 19: 50S ribosomal protein L24

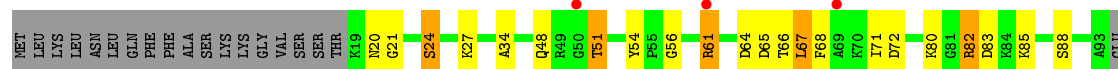




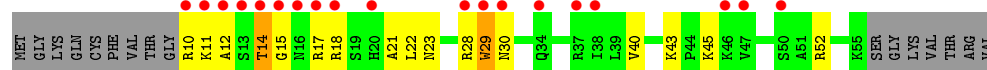
• Molecule 20: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29

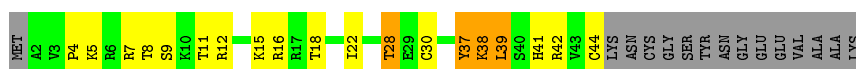


• Molecule 24: 50S ribosomal protein L30



• 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 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 236666 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	19
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	2	21
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	33
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	19
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	1	10
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	14	57
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	7	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	1	9
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	3	31
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	21	67
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	3	29
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	4	36
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	4	33
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	8	47
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	33
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	1	10
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	14	57
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	11
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	12	54
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%)	3	28
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	6	42
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	3	28

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	19
4	B	153/177 (86%)	136 (89%)	17 (11%)	8	35
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	15
6	D	18/158 (11%)	17 (94%)	1 (6%)	26	66
7	E	67/155 (43%)	58 (87%)	9 (13%)	5	26
8	G	111/123 (90%)	101 (91%)	10 (9%)	12	47
9	H	91/100 (91%)	78 (86%)	13 (14%)	4	24
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	6
11	J	103/119 (87%)	91 (88%)	12 (12%)	7	32
12	K	91/102 (89%)	81 (89%)	10 (11%)	8	36
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	15
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	14
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	21
16	O	71/86 (83%)	60 (84%)	11 (16%)	3	20
17	P	91/94 (97%)	84 (92%)	7 (8%)	16	54
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	4
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	4
20	S	91/190 (48%)	83 (91%)	8 (9%)	12	48
21	T	56/75 (75%)	48 (86%)	8 (14%)	4	24
22	U	18/52 (35%)	17 (94%)	1 (6%)	26	66
23	V	47/62 (76%)	42 (89%)	5 (11%)	8	38
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	6
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	8
26	2	37/40 (92%)	32 (86%)	5 (14%)	5	26
27	3	37/57 (65%)	33 (89%)	4 (11%)	8	37
28	4	30/35 (86%)	27 (90%)	3 (10%)	9	41
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	4	23

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	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0
All	All	2804/3037 (92%)	640 (22%)	18 (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

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1503	U
1	X	1510	U
1	X	1576	A
1	X	1091	G
1	X	1490	G

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	-	6,7,7	0.31	0	6,10,10	0.34	0
29	MPD	X	3002	-	6,7,7	0.48	0	6,10,10	0.24	0
29	MPD	X	3003	-	6,7,7	0.30	0	6,10,10	0.38	0
29	MPD	X	3004	-	6,7,7	0.42	0	6,10,10	0.11	0
29	MPD	X	3005	-	6,7,7	0.44	0	6,10,10	0.16	0
29	MPD	X	3006	-	6,7,7	0.34	0	6,10,10	0.10	0
29	MPD	X	3007	-	6,7,7	0.23	0	6,10,10	0.43	0
29	MPD	X	3008	-	6,7,7	0.44	0	6,10,10	0.15	0
29	MPD	X	3009	-	6,7,7	0.42	0	6,10,10	0.13	0
29	MPD	X	3010	-	6,7,7	0.36	0	6,10,10	0.16	0
29	MPD	X	3011	-	6,7,7	0.58	0	6,10,10	0.36	0
32	EPE	X	3311	-	15,15,15	1.20	1 (6%)	19,20,20	0.63	1 (5%)
33	SPD	X	3312	-	9,9,9	0.29	0	8,8,8	0.37	0
33	SPD	X	3313	-	9,9,9	0.21	0	8,8,8	0.30	0
33	SPD	X	3314	-	9,9,9	0.17	0	8,8,8	0.22	0
33	SPD	X	3315	-	9,9,9	0.25	0	8,8,8	0.26	0
34	EOH	X	3316	-	2,2,2	0.65	0	1,1,1	0.42	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.65	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	0
34	EOH	X	3319	-	2,2,2	0.49	0	1,1,1	0.75	0
34	EOH	X	3320	-	2,2,2	0.57	0	1,1,1	0.62	0
34	EOH	X	3321	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3322	-	2,2,2	0.53	0	1,1,1	0.65	0
29	MPD	Z	101	-	6,7,7	0.29	0	6,10,10	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
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 (1) 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

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	3311	EPE	O1S-S-C10	-2.19	105.32	106.87

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%) 94 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%) 76 68	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%) 91 88	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 81 73	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.25	3 (1%) 70 61	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 89 83	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%) 76 68	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 67 58	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%) 85 78	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%) 82 74	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 54 43	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	3 (1%) 71 63	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 42 33	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%) 64 54	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	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%) 82 74	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	20.99	34,34,34,34	0
30	MN	X	3255	1/1	0.92	0.56	17.42	35,35,35,35	0
30	MN	X	3252	1/1	0.96	0.30	14.07	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	11.40	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	10.92	47,47,47,47	0
31	MG	X	3103	1/1	0.92	0.44	10.10	3,3,3,3	0
30	MN	X	3286	1/1	0.99	0.31	8.64	57,57,57,57	0
30	MN	X	3272	1/1	0.98	0.36	8.18	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	6.85	14,14,14,14	0
29	MPD	X	3010	8/8	0.81	0.33	6.52	87,87,87,87	0
30	MN	X	3242	1/1	0.97	0.30	6.46	22,22,22,22	0
33	SPD	X	3314	10/10	0.87	0.48	6.36	26,26,26,26	0
29	MPD	X	3002	8/8	0.83	0.32	6.23	45,45,45,45	0
29	MPD	Z	101	8/8	0.90	0.35	6.23	48,48,48,48	0
29	MPD	X	3008	8/8	0.79	0.35	6.21	70,70,70,70	0
30	MN	X	3230	1/1	0.92	0.28	6.04	65,65,65,65	0
31	MG	X	3174	1/1	0.88	0.31	5.63	5,5,5,5	0
30	MN	X	3196	1/1	0.96	0.33	5.55	51,51,51,51	0
30	MN	X	3012	1/1	0.97	0.31	5.46	19,19,19,19	0
29	MPD	X	3009	8/8	0.92	0.14	5.29	76,76,76,76	0
30	MN	X	3197	1/1	0.98	0.24	5.25	34,34,34,34	0
30	MN	X	3166	1/1	0.97	0.23	5.19	62,62,62,62	0
30	MN	X	3280	1/1	0.98	0.27	5.13	39,39,39,39	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	4.94	41,41,41,41	0
29	MPD	X	3007	8/8	0.96	0.28	4.75	9,9,9,9	0
31	MG	X	3092	1/1	0.96	0.14	4.69	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	3.54	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	2.90	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	2.58	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	2.40	43,43,43,43	0
30	MN	X	3154	1/1	0.99	0.22	2.10	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	3257	1/1	0.99	0.23	1.94	25,25,25,25	0
30	MN	X	3185	1/1	0.99	0.21	1.93	28,28,28,28	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	1.48	39,39,39,39	0
30	MN	X	3269	1/1	0.93	0.24	1.33	36,36,36,36	0
30	MN	X	3198	1/1	0.99	0.20	1.18	64,64,64,64	0
30	MN	X	3256	1/1	0.98	0.22	1.18	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	3224	1/1	0.94	0.25	1.03	53,53,53,53	0
30	MN	X	3227	1/1	0.92	0.17	1.02	57,57,57,57	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	0.66	74,74,74,74	0
30	MN	X	3251	1/1	0.98	0.19	0.65	8,8,8,8	0
30	MN	X	3078	1/1	0.97	0.20	0.63	78,78,78,78	0
29	MPD	X	3004	8/8	0.92	0.34	0.50	73,73,73,73	0
30	MN	X	3167	1/1	0.99	0.20	0.46	57,57,57,57	0
29	MPD	X	3005	8/8	0.94	0.17	0.46	65,65,65,65	0
30	MN	X	3164	1/1	0.98	0.23	0.43	48,48,48,48	0
30	MN	X	3324	1/1	0.96	0.18	0.38	12,12,12,12	0
30	MN	X	3140	1/1	0.82	0.16	0.30	71,71,71,71	0
29	MPD	X	3001	8/8	0.94	0.14	0.22	33,33,33,33	0
30	MN	X	3157	1/1	0.94	0.22	0.12	68,68,68,68	0
30	MN	X	3163	1/1	0.98	0.16	-0.03	61,61,61,61	0
31	MG	X	3082	1/1	0.88	0.17	-0.06	31,31,31,31	0
31	MG	X	3176	1/1	0.95	0.16	-0.20	14,14,14,14	0
30	MN	X	3058	1/1	0.91	0.15	-0.20	64,64,64,64	0
29	MPD	X	3003	8/8	0.97	0.19	-0.23	21,21,21,21	0
30	MN	X	3281	1/1	0.96	0.17	-0.25	40,40,40,40	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	-0.84	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	-0.88	15,15,15,15	0
30	MN	X	3150	1/1	0.99	0.13	-0.95	50,50,50,50	0
30	MN	X	3062	1/1	0.99	0.16	-0.96	42,42,42,42	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	-1.19	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	-1.46	54,54,54,54	0
31	MG	B	302	1/1	0.98	0.11	-1.47	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	-1.78	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	-2.29	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	0.94	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	0.34	-	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	0.84	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	1.02	-	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	0.83	-	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	0.68	-	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	0.46	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	0.19	-	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	0.25	-	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	0.39	-	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	0.84	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	0.33	-	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	0.92	-	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	0.90	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	0.74	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	0.25	-	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	0.91	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	0.95	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.