



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 11:31 PM EDT

PDB ID : 4WCE / pdb_00004wce
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

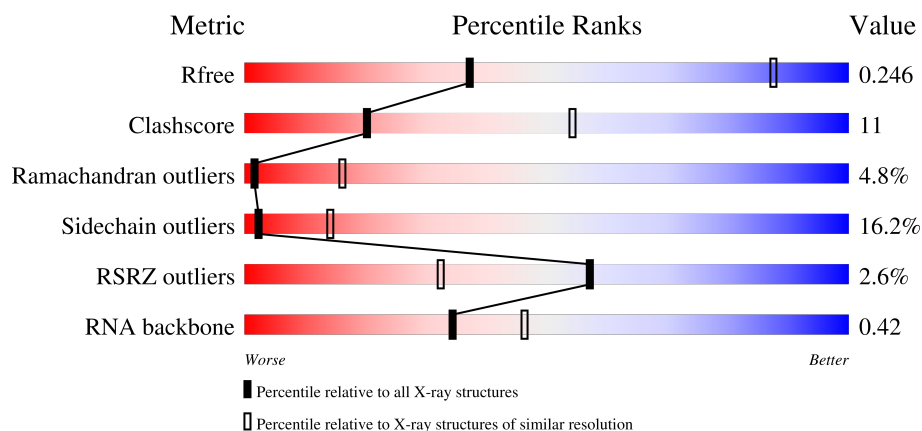
1 Overall quality at a glance

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.



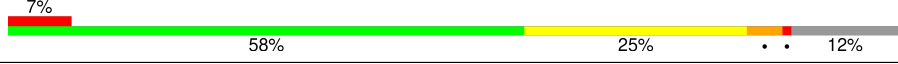
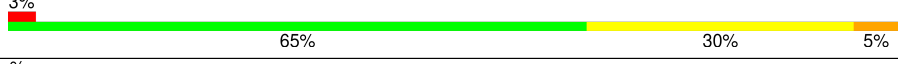
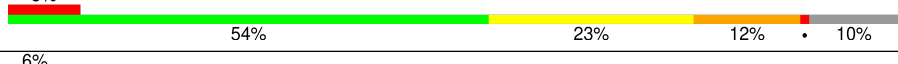
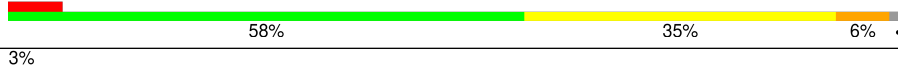
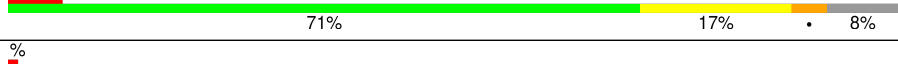
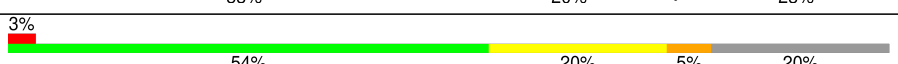
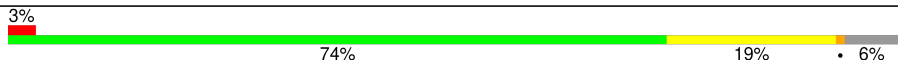
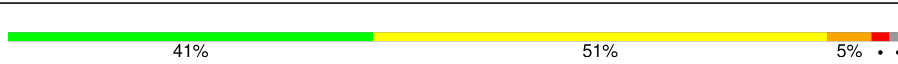
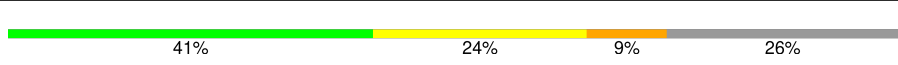
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	7% 46% 37% 10% 7%
2	Y	114	49% 47%
3	A	277	7% 65% 25% 7%
4	B	220	55% 36% 6%

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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	3008	-	-	-	X
29	MPD	Z	101	-	-	-	X
34	EOH	X	3317	-	-	-	X
34	EOH	X	3318	-	-	-	X
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			

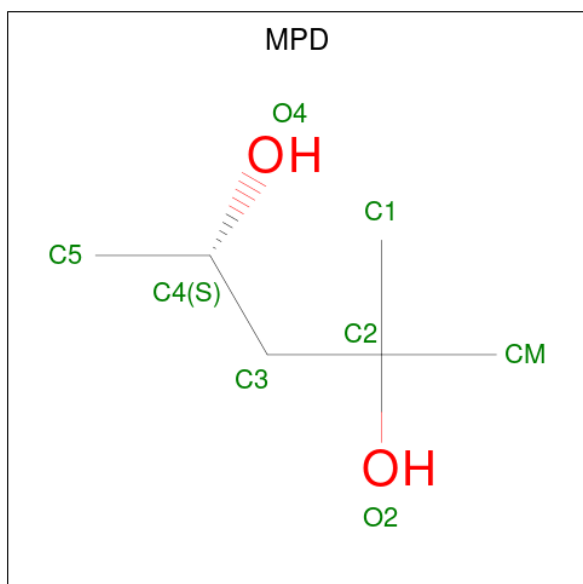
- Molecule 27 is a protein called 50S ribosomal protein L35.

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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	Z	1	Total	C	O	0	0
			8	6	2		

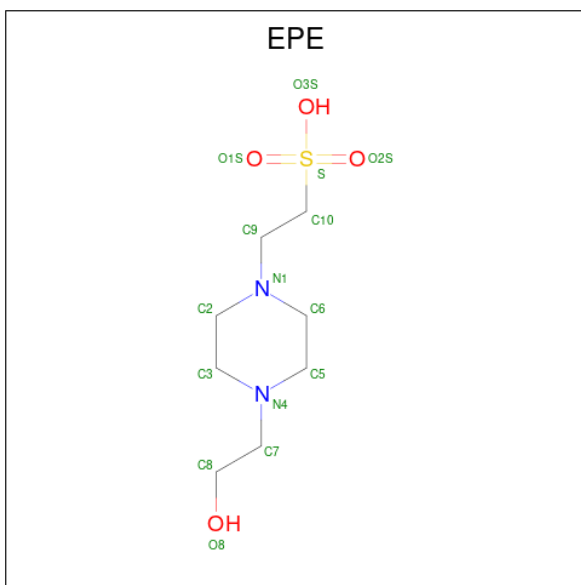
- Molecule 30 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

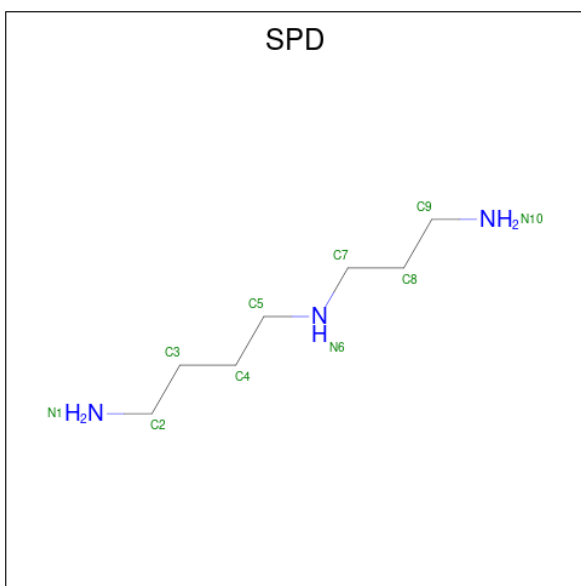
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	80	Total	Mg	0	0
			80	80		
31	Y	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	C	1	Total	Mg	0	0
			1	1		
31	G	3	Total	Mg	0	0
			3	3		
31	I	1	Total	Mg	0	0
			1	1		
31	O	1	Total	Mg	0	0
			1	1		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: 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 (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



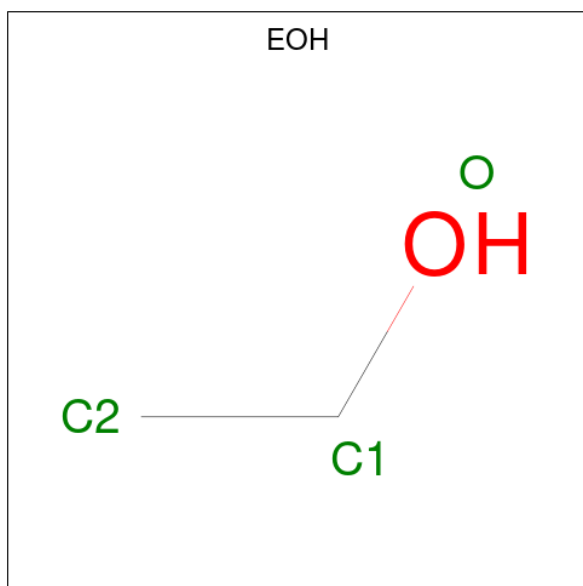
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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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 (CCD ID: EOH) (formula: C₂H₆O).

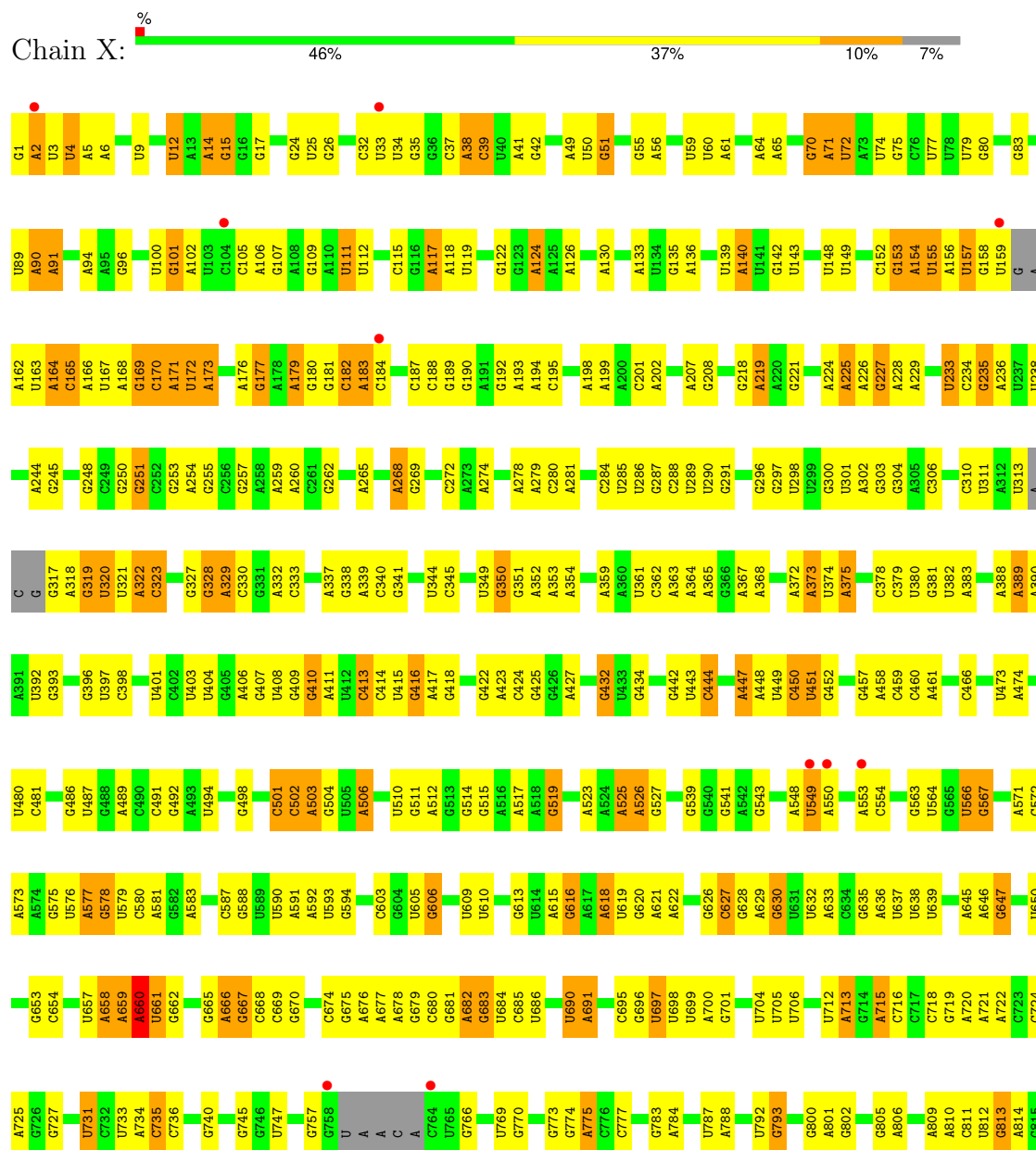


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

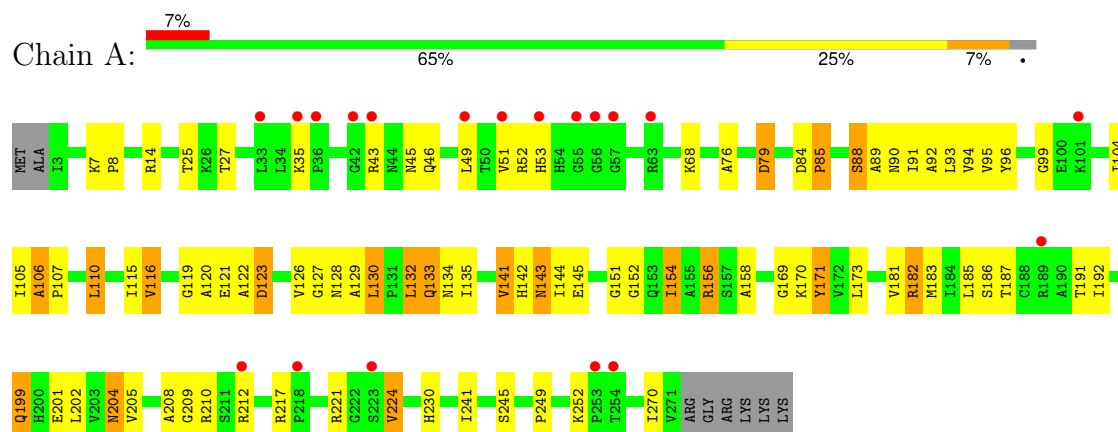


C1865	G	U1788	G1889	C1595	G	G1467	C1400	C1315	A1222	G	U1067	A985	U895	G816
C1867	U1789	G1596	A1690	G1596	G	G1468	G1401	G1316	G1225	U	G1068	A989	U896	G817
U1868	G1790	U1597	C1691	U1597	C	G1469	A1402	A1323	G1226	A	G1069	G990	U897	U818
C1869	G1791	U1598	C1692	U1598	A	G1470	G1405	A1324	U1227	U	A1070	U995	U898	A819
G1870	C1792	G1599	G1693	G1599	A	C1471	G1406	A1325	A1228	A	A1071	U996	C821	G820
C1870	C1793	G1600	G1694	U1600	U1540	C1472	G1408	C1326	G1229	G	U1072	U997	A902	G821
A1874	C1794	U1603	U1695	U1603	C1541	G1476	G1409	C1327	A1230	U1077	U998	G903	G825	G825
A1875	A1796	C1604	A1605	C1604	C1542	U1477	A1410	C1328	U1240	G1078	U999	G904	A826	A826
G1876	A1800	U1605	U1606	U1605	G1543	A1478	G1411	C1329	A1241	G1086	U999	U905	A827	A827
A1880	G1803	U1609	G1610	U1609	G1544	U1481	G1412	U1330	A1242	U1087	U1000	U906	A828	A828
G1885	U1806	G1611	C1612	G1611	G1545	G1487	G1414	C1331	U1248	C1088	A1001	U907	U829	U829
A1886	U1807	G1613	C1613	G1613	U1546	G1488	A1415	A1337	U1249	G1089	U1002	A911	U830	U830
G1887	U1808	A1614	G1614	U1808	C1547	A1489	A1416	U1338	U1250	A1090	A1003	U916	U835	U835
U1888	G1809	G1615	A1615	G1809	C1548	A1490	G1417	U1339	G1251	U1091	A1004	U917	C836	C836
G1889	U1810	A1616	G1616	U1810	G1550	G1491	G1421	G1340	G1252	U1092	G1005	G922	G837	G837
G1890	G1718	A1617	A1617	U	U	G1492	A1422	G1345	U1272	A1093	C1008	A923	U841	U841
U1891	U1730	U1623	U1623	A	A	U1493	G1423	G1347	G1273	U1097	U1013	G924	U842	U842
U1892	G1731	U1624	U1624	G1555	G1555	U1494	G1425	U1348	G1274	A1098	U1014	G925	G843	G843
A1893	U1732	U1625	U1625	G1556	G1556	G1495	G1426	U1349	A1275	G1099	C1015	G	G844	G844
G1894	U1737	A1628	A1628	U1557	U1557	G1496	G1429	C1352	G1276	G	C	C	A847	A847
C1895	C1738	U1629	U1629	C1558	C1558	U1497	G1430	A1353	G1277	A	C	C	U848	U848
U1896	G1739	U1630	U1630	G1559	G1559	U1498	U1431	G1354	G1278	U	C	C	U849	U849
C	G1740	G1631	G1631	U1560	U1560	U1499	A1432	A1355	G1279	U	U	C	G850	G850
U	U1741	A1632	A1632	G1561	G1561	U1500	U1433	G1356	G1280	U	U	C	C851	C851
C	A1744	A	A	U1562	U1562	U1501	U1434	G1357	G1281	U	U	C	U852	U852
G1900	G1745	A	A	U1563	U1563	U1502	G1435	A1358	G1282	U	U	C	G853	G853
C1901	G1746	A	A	U1564	U1564	U1503	C1436	A1359	U1281	U	U	C	G854	G854
G1902	G1747	A	A	U1565	U1565	U1504	U1437	U1366	U1282	U	U	C	U855	U855
U1906	G1748	A1635	A1635	G1566	G1566	U1505	G1438	U1367	G1283	U	U	C	U856	U856
U1907	G1749	U1636	U1636	U1567	U1567	U1506	U1439	C1370	U1284	U	U	C	C857	C857
A1908	U1755	A1637	A1637	U1568	U1568	U1507	G1440	U1371	G1285	A	U	C	U858	U858
C1909	U1756	G1638	G1638	G1569	G1569	U1508	C1441	C1372	G1286	G	A	C	C859	C859
G1910	U1757	G1639	G1639	G	G	U1510	G1442	U1373	A1289	U	U	C	A864	A864
A1911	U1760	U1640	U1640	U1572	U1572	U1512	C1445	G1374	G1290	U	U	C	A865	A865
A1912	G1761	C1643	C1643	G1573	G1573	U1513	U1446	G1375	G1291	U	U	C	A866	A866
C	G1762	C1644	C1644	G1574	G1574	U1514	U1447	G1376	A1292	U	U	C	C870	C870
A1916	U1763	U1650	U1650	A1575	A1575	U1515	A1448	U1380	G1294	U	U	C	U871	U871
C1922	U1764	G1651	G1651	A1576	A1576	U1516	U1450	G1381	C1295	U	U	C	U872	U872
A1923	A1765	C1652	C1652	A1577	A1577	U1517	U1451	U1382	C1296	U	U	C	U873	U873
G1924	C1766	A1653	A1653	U1578	U1578	U1518	G1452	G1383	U1297	U	U	C	A874	A874
C	C1767	U1654	U1654	C	C	A	G1453	G1384	G1300	U	U	C	G875	G875
C1929	C1768	G1657	G1657	U	U	U1519	U1454	G1385	G1301	U	U	C	G876	G876
G1930	C1769	A1658	A1658	U	U	G1521	U	U	G1302	U	U	C	G877	G877
G1931	G1770	U1659	U1659	G	G	G1522	U	U	A1303	U	U	C	C878	C878
C1932	A1771	U1660	U1660	U	U	C1523	U	U	A1306	U	U	C	A880	A880
G1933	G1772	U1680	U1680	C	C	C1524	U	U	G1309	U	U	C	G887	G887
U1934	G1775	C1682	C1682	U	U	U	A	U	U1215	U	U	C	U889	U889
C	U1776	U1681	U1681	U	U	G1526	A1459	U1388	C1213	U	U	C	U890	U890
C	G1777	U1682	U1682	U	U	A1527	U1460	A1390	G1214	U	U	C	A891	A891
U1854	G1781	C1683	C1683	U	U	G1528	G1461	G1391	U1216	U	U	C	U892	U892
G1855	A1782	A1684	A1684	C	C	U1530	A1463	G1392	A1311	U	U	C		
A1856	U1787	U1687	U1687	G1591	G1591	U	U	G1395	A1312	U	U	C		
C1857		U1688	U1688	A1592	A1592	U	U	G1398	G1313	U	U	C		
C1864				U1594	U1594	A	U	C1399	A1314	U	U	C		

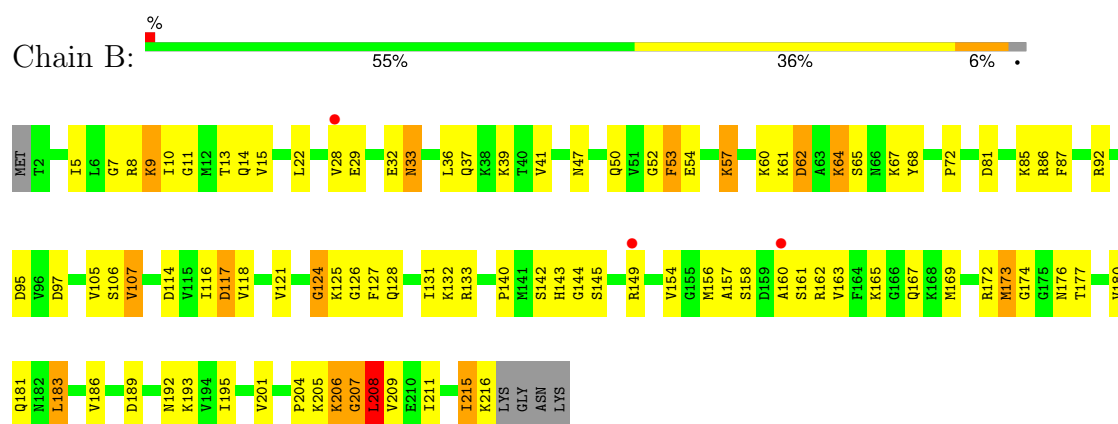




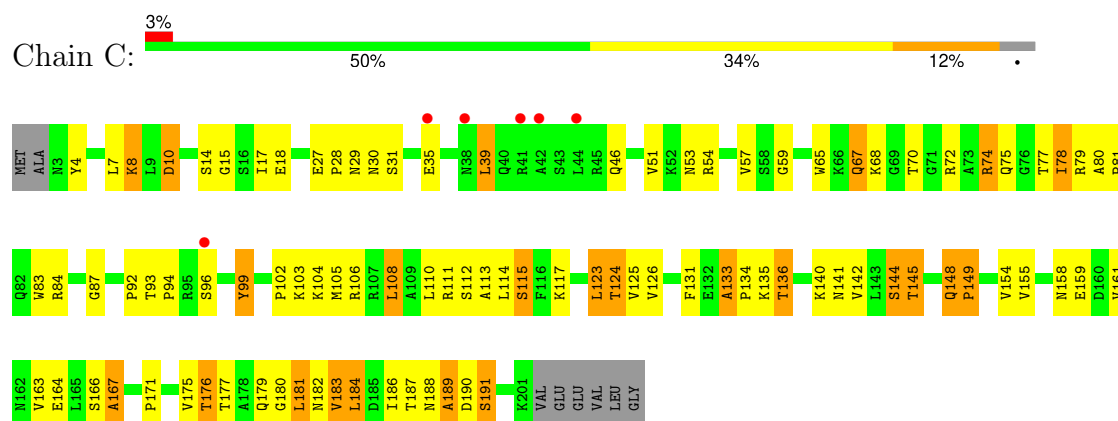
• Molecule 3: 50S ribosomal protein L2



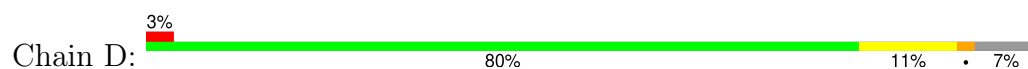
• Molecule 4: 50S ribosomal protein L3

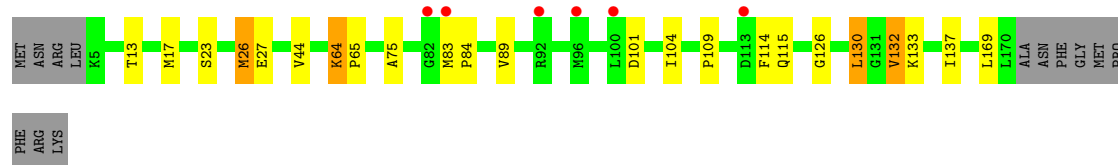


• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

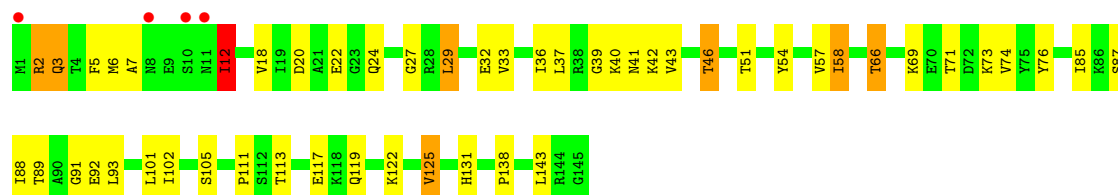




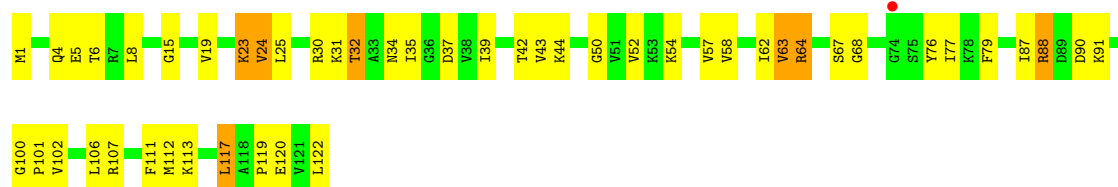
- Molecule 7: 50S ribosomal protein L6



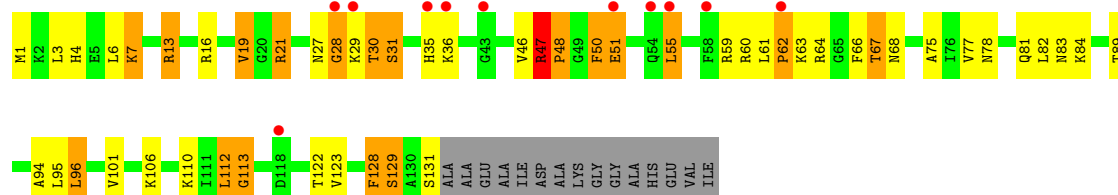
- Molecule 8: 50S ribosomal protein L13



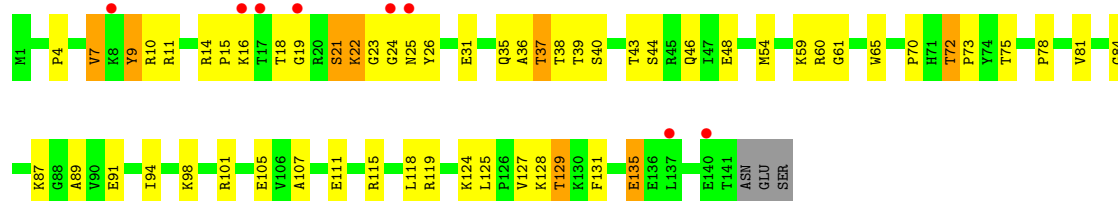
- Molecule 9: 50S ribosomal protein L14



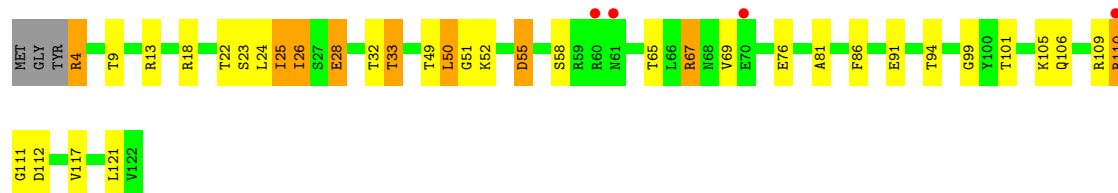
- Molecule 10: 50S ribosomal protein L15



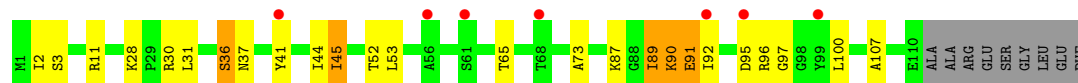
- Molecule 11: 50S ribosomal protein L16



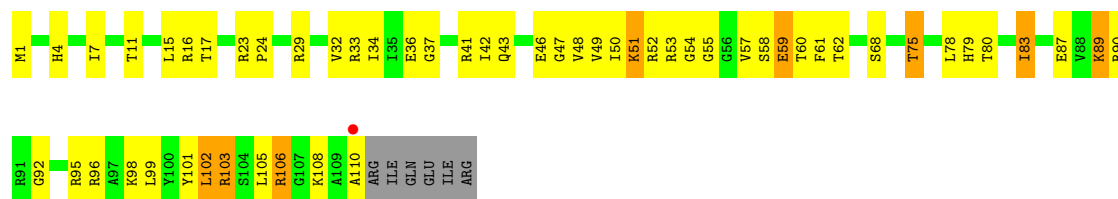
- Molecule 12: 50S ribosomal protein L17



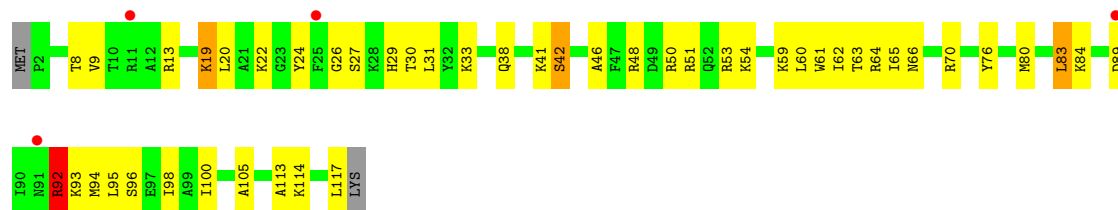
- Molecule 13: 50S ribosomal protein L18



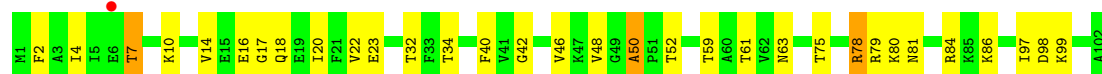
- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



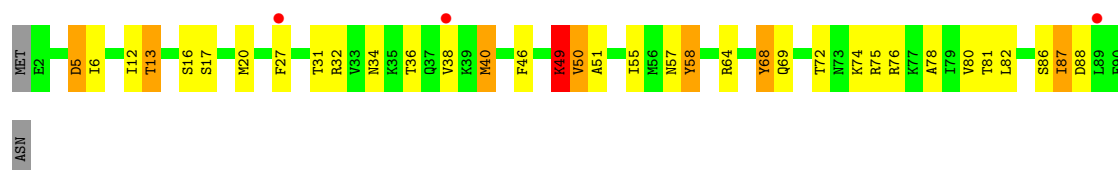
- Molecule 16: 50S ribosomal protein L21



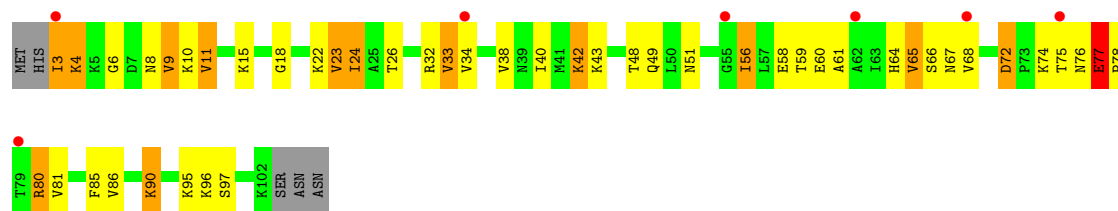
• Molecule 17: 50S ribosomal protein L22



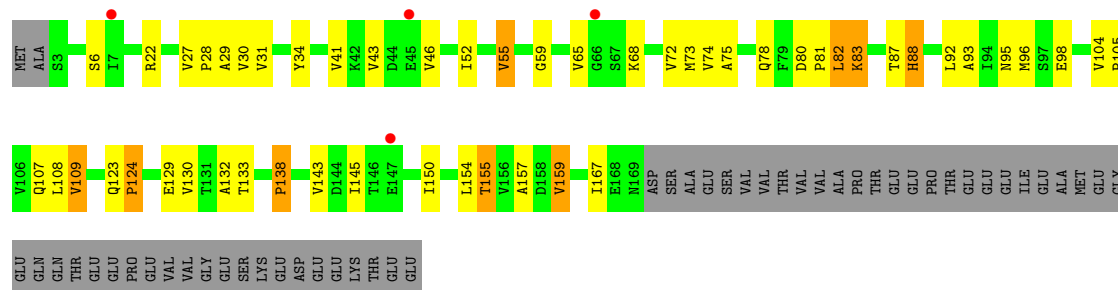
• Molecule 18: 50S ribosomal protein L23



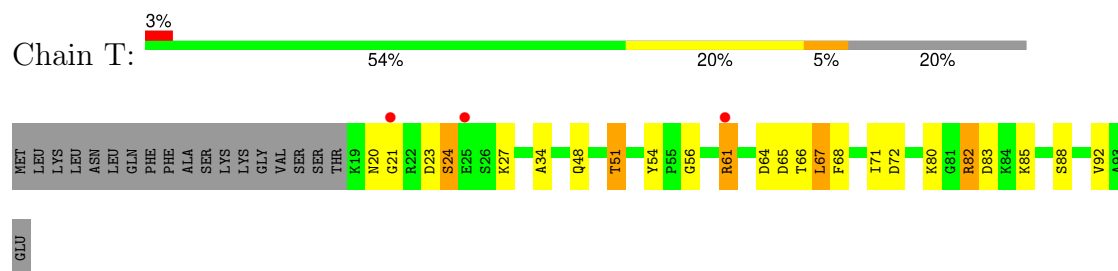
• Molecule 19: 50S ribosomal protein L24



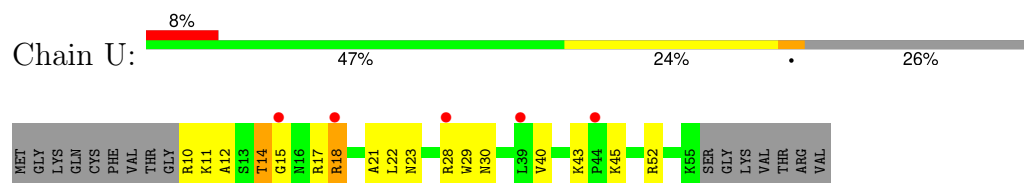
• Molecule 20: 50S ribosomal protein L25



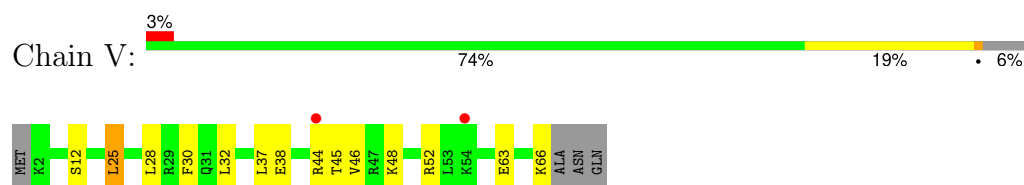
- Molecule 21: 50S ribosomal protein L27



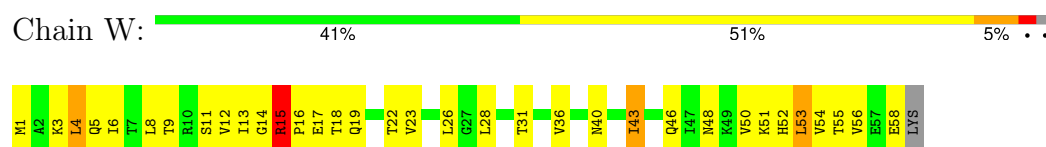
- Molecule 22: 50S ribosomal protein L28



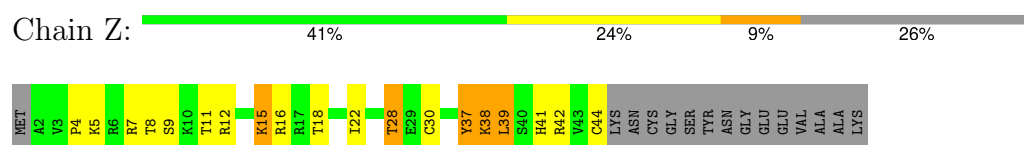
- Molecule 23: 50S ribosomal protein L29



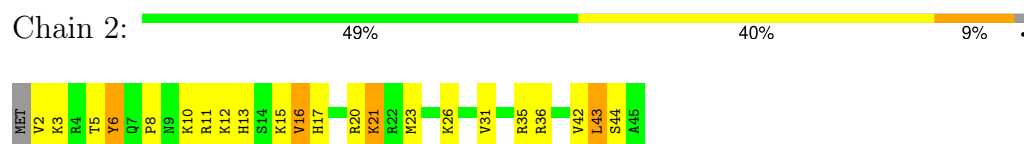
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32

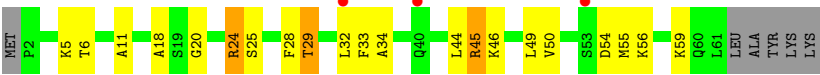


- Molecule 26: 50S ribosomal protein L34

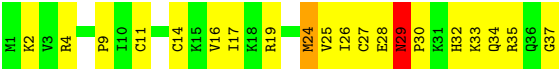


- Molecule 27: 50S ribosomal protein L35





• 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) 95.9 (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 0.201 , 0.246	Depositor DCC
R_{free} test set	11858 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 35.2	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, EPE, MPD, SPD, EOH, MN

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	0.35	0/65032	0.53	1/101388 (0.0%)
2	Y	0.29	0/2717	0.45	0/4232
3	A	0.40	0/1717	0.99	7/2361 (0.3%)
4	B	0.42	0/1581	1.00	5/2129 (0.2%)
5	C	0.68	0/1338	1.21	15/1831 (0.8%)
6	D	0.38	0/869	0.92	2/1205 (0.2%)
7	E	0.42	0/982	0.98	4/1354 (0.3%)
8	G	0.49	0/1128	1.00	4/1525 (0.3%)
9	H	0.38	0/891	0.90	2/1203 (0.2%)
10	I	0.86	0/868	1.29	6/1172 (0.5%)
11	J	0.38	0/1092	0.93	4/1473 (0.3%)
12	K	0.43	0/911	0.87	1/1219 (0.1%)
13	L	0.38	0/711	0.91	2/970 (0.2%)
14	M	0.67	0/838	1.17	2/1132 (0.2%)
15	N	0.48	0/944	0.87	1/1252 (0.1%)
16	O	0.36	0/761	1.18	4/1022 (0.4%)
17	P	0.77	0/870	1.21	3/1171 (0.3%)
18	Q	0.58	0/633	1.02	1/859 (0.1%)
19	R	0.43	0/688	1.01	5/930 (0.5%)
20	S	0.41	0/1109	1.02	7/1522 (0.5%)
21	T	0.33	0/574	0.83	1/763 (0.1%)
22	U	0.45	0/305	0.96	1/419 (0.2%)
23	V	0.34	0/487	0.78	0/654
24	W	0.68	0/451	1.03	2/607 (0.3%)
25	Z	0.59	0/345	1.00	0/460
26	2	0.59	0/366	0.97	0/480
27	3	0.43	0/424	0.99	2/566 (0.4%)
28	4	0.54	0/280	1.08	2/371 (0.5%)
All	All	0.39	0/88912	0.66	84/134270 (0.1%)

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

There are no bond length outliers.

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-16.98	102.27	119.76
16	O	50	ALA	C-N-CA	-16.98	102.27	119.76
10	I	47	ARG	N-CA-C	9.51	116.53	108.07
5	C	148	GLN	N-CA-C	8.94	116.17	108.13
4	B	11	GLY	N-CA-C	8.79	123.20	110.80

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	856	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	62	0
5	C	1320	0	1171	56	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1106	0	1072	30	0
9	H	884	0	902	26	0
10	I	859	0	772	41	0
11	J	1068	0	1078	41	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	42	0
15	N	932	0	995	38	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	22	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	10	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	20	0
26	2	362	0	398	14	0
27	3	420	0	405	6	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
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	1421	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 1421 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)
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
2:Y:15:C:H42	2:Y:105:G:H21	1.19	0.88

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	11
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1	12
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	2	19
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	11
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	0	6
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	9	38
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	4	28
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0	6
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	2	18
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	14	48
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2	17
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	2	21
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	5	29
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	2	19
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	0	6
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	9	38
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	0	6
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	7	36
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	16
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	3
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	25
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	16

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%)	102 (85%)	18 (15%)	3	17
4	B	153/177 (86%)	134 (88%)	19 (12%)	4	23
5	C	106/169 (63%)	83 (78%)	23 (22%)	1	6
6	D	18/158 (11%)	16 (89%)	2 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	67/155 (43%)	55 (82%)	12 (18%)	2	10
8	G	111/123 (90%)	95 (86%)	16 (14%)	3	18
9	H	91/100 (91%)	77 (85%)	14 (15%)	2	16
10	I	67/112 (60%)	51 (76%)	16 (24%)	1	4
11	J	103/119 (87%)	91 (88%)	12 (12%)	5	25
12	K	91/102 (89%)	78 (86%)	13 (14%)	3	18
13	L	47/95 (50%)	40 (85%)	7 (15%)	3	17
14	M	80/102 (78%)	65 (81%)	15 (19%)	1	9
15	N	93/98 (95%)	80 (86%)	13 (14%)	3	19
16	O	71/86 (83%)	61 (86%)	10 (14%)	3	19
17	P	91/94 (97%)	85 (93%)	6 (7%)	15	42
18	Q	53/82 (65%)	38 (72%)	15 (28%)	0	3
19	R	63/90 (70%)	42 (67%)	21 (33%)	0	2
20	S	91/190 (48%)	79 (87%)	12 (13%)	4	21
21	T	56/75 (75%)	47 (84%)	9 (16%)	2	14
22	U	18/52 (35%)	18 (100%)	0	100	100
23	V	47/62 (76%)	42 (89%)	5 (11%)	6	28
24	W	52/53 (98%)	41 (79%)	11 (21%)	1	6
25	Z	38/51 (74%)	29 (76%)	9 (24%)	1	4
26	2	37/40 (92%)	29 (78%)	8 (22%)	1	6
27	3	37/57 (65%)	31 (84%)	6 (16%)	2	14
28	4	30/35 (86%)	26 (87%)	4 (13%)	4	21
All	All	1831/2701 (68%)	1535 (84%)	296 (16%)	2	14

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	97	SER
27	3	6	THR
20	S	55	VAL
24	W	4	LEU
9	H	57	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	72	HIS
24	W	46	GLN
18	Q	54	ASN
25	Z	19	HIS
23	V	27	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	628 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0
All	All	2804/3037 (92%)	641 (22%)	18 (0%)

5 of 641 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	1576	A
1	X	2823	G
1	X	2457	A
1	X	1503	U
1	X	1575	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.64	0
33	SPD	X	3315	-	9,9,9	0.22	0	8,8,8	0.25	0
34	EOH	X	3316	-	2,2,2	0.68	0	1,1,1	0.41	0
29	MPD	X	3003	-	7,7,7	0.29	0	9,10,10	0.39	0
29	MPD	X	3006	-	7,7,7	0.40	0	9,10,10	0.10	0
29	MPD	X	3004	-	7,7,7	0.52	0	9,10,10	0.23	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.78	0
29	MPD	Z	101	-	7,7,7	0.28	0	9,10,10	0.41	0
29	MPD	X	3010	-	7,7,7	0.55	0	9,10,10	0.41	0
34	EOH	X	3321	-	2,2,2	0.59	0	1,1,1	0.63	0
29	MPD	X	3002	-	7,7,7	0.86	0	9,10,10	0.57	0
29	MPD	X	3009	-	7,7,7	0.58	0	9,10,10	0.30	0
29	MPD	X	3005	-	7,7,7	0.60	0	9,10,10	0.26	0
32	EPE	X	3311	-	15,15,15	1.29	1 (6%)	19,20,20	0.37	0
34	EOH	X	3322	-	2,2,2	0.55	0	1,1,1	0.67	0
29	MPD	X	3007	-	7,7,7	0.80	1 (14%)	9,10,10	0.43	0
29	MPD	X	3011	-	7,7,7	0.80	0	9,10,10	0.47	0
29	MPD	X	3008	-	7,7,7	0.61	0	9,10,10	0.37	0
34	EOH	X	3317	-	2,2,2	0.54	0	1,1,1	0.67	0
33	SPD	X	3313	-	9,9,9	0.18	0	8,8,8	0.28	0
33	SPD	X	3312	-	9,9,9	0.27	0	8,8,8	0.36	0
29	MPD	X	3001	-	7,7,7	0.30	0	9,10,10	0.49	0
34	EOH	X	3318	-	2,2,2	0.57	0	1,1,1	0.66	0
33	SPD	X	3314	-	9,9,9	0.13	0	8,8,8	0.21	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	3005	-	-	3/5/5/5	-
29	MPD	X	3004	-	-	2/5/5/5	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
29	MPD	X	3008	-	-	2/5/5/5	-
29	MPD	X	3010	-	-	4/5/5/5	-
29	MPD	Z	101	-	-	2/5/5/5	-
29	MPD	X	3007	-	-	5/5/5/5	-
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3011	-	-	2/5/5/5	-
29	MPD	X	3002	-	-	3/5/5/5	-
29	MPD	X	3001	-	-	2/5/5/5	-
33	SPD	X	3312	-	-	2/7/7/7	-
33	SPD	X	3314	-	-	2/7/7/7	-
33	SPD	X	3315	-	-	2/7/7/7	-
29	MPD	X	3003	-	-	4/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-
29	MPD	X	3009	-	-	1/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.79	1.70	1.77
29	X	3007	MPD	C3-C2	-2.01	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3002	MPD	C2-C3-C4-O4
29	X	3002	MPD	C2-C3-C4-C5
29	X	3003	MPD	C2-C3-C4-C5
29	X	3006	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4

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	3011	MPD	1	0
29	X	3008	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2708/2923 (92%)	-0.32	37 (1%) 73 46	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.39	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	0.41	19 (7%) 22 14	43, 74, 106, 136	0
4	B	215/220 (97%)	0.07	3 (1%) 73 46	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.01	6 (3%) 52 29	12, 35, 71, 107	0
6	D	166/179 (92%)	0.40	6 (3%) 46 25	80, 102, 132, 150	0
7	E	156/178 (87%)	0.52	12 (7%) 19 13	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.18	4 (2%) 55 31	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.11	1 (0%) 82 58	17, 41, 74, 102	0
10	I	131/146 (89%)	0.53	11 (8%) 17 11	14, 47, 91, 108	0
11	J	141/144 (97%)	0.01	8 (5%) 29 17	25, 43, 97, 121	0
12	K	119/122 (97%)	0.17	4 (3%) 48 27	14, 37, 86, 97	0
13	L	110/119 (92%)	0.33	7 (6%) 25 15	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.24	1 (0%) 81 56	23, 43, 89, 115	0
15	N	116/118 (98%)	0.09	4 (3%) 48 27	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.27	1 (0%) 79 54	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.37	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	0.10	3 (3%) 48 27	39, 60, 93, 108	0
19	R	100/105 (95%)	0.46	7 (7%) 22 14	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.01	4 (2%) 59 34	42, 61, 120, 130	0
21	T	75/94 (79%)	0.08	3 (4%) 42 23	21, 39, 81, 102	0
22	U	46/62 (74%)	0.70	5 (10%) 10 7	60, 91, 122, 130	0
23	V	65/69 (94%)	0.13	2 (3%) 51 29	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.33	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%)	-0.02	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	-0.11	0 100 100	19, 41, 73, 93	0
27	3	60/66 (90%)	0.35	3 (5%) 34 19	10, 32, 69, 83	0
28	4	37/37 (100%)	0.17	0 100 100	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.09	151 (2%) 57 32	6, 51, 123, 230	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	96	SER	7.1
7	E	55	PRO	5.8
10	I	35	HIS	5.2
8	G	8	ASN	4.9
13	L	95	ASP	4.9

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
34	EOH	X	3318	3/3	0.49	0.46	47,47,47,47	0
31	MG	X	3013	1/1	0.60	0.29	30,30,30,30	0
34	EOH	X	3316	3/3	0.61	0.27	10,10,10,10	0
34	EOH	X	3322	3/3	0.61	0.60	34,34,34,34	0
31	MG	X	3084	1/1	0.62	0.11	14,14,14,14	0
31	MG	X	3173	1/1	0.63	0.38	26,26,26,26	0
30	MN	X	3132	1/1	0.65	0.14	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MPD	X	3009	8/8	0.67	0.32	76,76,76,76	0
29	MPD	Z	101	8/8	0.69	0.57	48,48,48,48	0
34	EOH	X	3321	3/3	0.73	0.29	18,18,18,18	0
29	MPD	X	3008	8/8	0.74	0.46	70,70,70,70	0
29	MPD	X	3006	8/8	0.75	0.31	88,88,88,88	0
30	MN	X	3308	1/1	0.76	0.12	92,92,92,92	0
30	MN	X	3055	1/1	0.77	0.11	94,94,94,94	0
29	MPD	X	3001	8/8	0.77	0.24	33,33,33,33	0
31	MG	X	3023	1/1	0.78	0.11	37,37,37,37	0
31	MG	X	3175	1/1	0.78	0.13	0,0,0,0	0
30	MN	X	3042	1/1	0.78	0.08	104,104,104,104	0
34	EOH	X	3317	3/3	0.79	0.53	46,46,46,46	0
31	MG	X	3087	1/1	0.79	0.23	51,51,51,51	0
31	MG	G	203	1/1	0.80	0.08	17,17,17,17	0
31	MG	X	3038	1/1	0.80	0.19	23,23,23,23	0
34	EOH	X	3319	3/3	0.81	0.33	47,47,47,47	0
30	MN	X	3182	1/1	0.81	0.11	107,107,107,107	0
31	MG	X	3309	1/1	0.81	0.09	20,20,20,20	0
31	MG	X	3092	1/1	0.82	0.31	20,20,20,20	0
31	MG	X	3113	1/1	0.82	0.36	45,45,45,45	0
31	MG	X	3136	1/1	0.82	0.23	27,27,27,27	0
33	SPD	X	3313	10/10	0.82	0.29	30,30,30,30	0
30	MN	X	3290	1/1	0.82	0.08	89,89,89,89	0
30	MN	X	3121	1/1	0.83	0.08	88,88,88,88	0
29	MPD	X	3005	8/8	0.83	0.35	65,65,65,65	0
30	MN	X	3118	1/1	0.83	0.12	101,101,101,101	0
30	MN	X	3138	1/1	0.84	0.16	112,112,112,112	0
31	MG	X	3098	1/1	0.84	0.20	14,14,14,14	0
31	MG	X	3306	1/1	0.84	0.12	29,29,29,29	0
29	MPD	X	3002	8/8	0.85	0.36	45,45,45,45	0
31	MG	X	3109	1/1	0.85	0.20	24,24,24,24	0
30	MN	X	3292	1/1	0.85	0.16	99,99,99,99	0
31	MG	X	3081	1/1	0.85	0.11	36,36,36,36	0
31	MG	X	3096	1/1	0.85	0.21	9,9,9,9	0
33	SPD	X	3315	10/10	0.85	0.43	46,46,46,46	0
31	MG	X	3137	1/1	0.86	0.19	17,17,17,17	0
31	MG	X	3095	1/1	0.86	0.33	26,26,26,26	0
33	SPD	X	3312	10/10	0.86	0.35	47,47,47,47	0
30	MN	X	3184	1/1	0.86	0.19	88,88,88,88	0
33	SPD	X	3314	10/10	0.86	0.24	26,26,26,26	0
30	MN	X	3213	1/1	0.86	0.09	95,95,95,95	0
30	MN	X	3111	1/1	0.87	0.07	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3068	1/1	0.87	0.12	70,70,70,70	0
30	MN	X	3073	1/1	0.87	0.07	86,86,86,86	0
30	MN	X	3226	1/1	0.87	0.22	89,89,89,89	0
30	MN	X	3250	1/1	0.87	0.06	80,80,80,80	0
30	MN	X	3074	1/1	0.87	0.05	78,78,78,78	0
30	MN	X	3090	1/1	0.87	0.28	96,96,96,96	0
31	MG	X	3093	1/1	0.87	0.15	21,21,21,21	0
30	MN	X	3148	1/1	0.87	0.12	79,79,79,79	0
30	MN	B	303	1/1	0.87	0.14	102,102,102,102	0
31	MG	G	202	1/1	0.88	0.12	12,12,12,12	0
30	MN	X	3050	1/1	0.88	0.11	99,99,99,99	0
30	MN	X	3149	1/1	0.88	0.10	94,94,94,94	0
30	MN	X	3127	1/1	0.88	0.05	44,44,44,44	0
30	MN	X	3052	1/1	0.88	0.09	71,71,71,71	0
30	MN	X	3207	1/1	0.88	0.12	62,62,62,62	0
30	MN	X	3044	1/1	0.88	0.06	94,94,94,94	0
30	MN	R	202	1/1	0.88	0.08	58,58,58,58	0
31	MG	X	3302	1/1	0.88	0.15	20,20,20,20	0
30	MN	X	3219	1/1	0.88	0.12	53,53,53,53	0
31	MG	X	3018	1/1	0.88	0.25	15,15,15,15	0
31	MG	Y	203	1/1	0.88	0.26	21,21,21,21	0
30	MN	X	3143	1/1	0.89	0.13	94,94,94,94	0
29	MPD	X	3010	8/8	0.89	0.47	87,87,87,87	0
30	MN	X	3128	1/1	0.89	0.07	84,84,84,84	0
31	MG	X	3082	1/1	0.89	0.05	31,31,31,31	0
30	MN	X	3171	1/1	0.89	0.08	86,86,86,86	0
30	MN	X	3017	1/1	0.89	0.20	103,103,103,103	0
30	MN	X	3123	1/1	0.89	0.07	97,97,97,97	0
34	EOH	X	3320	3/3	0.89	0.48	28,28,28,28	0
31	MG	I	201	1/1	0.89	0.14	0,0,0,0	0
31	MG	X	3022	1/1	0.89	0.13	25,25,25,25	0
31	MG	X	3114	1/1	0.90	0.21	36,36,36,36	0
30	MN	X	3130	1/1	0.90	0.05	102,102,102,102	0
30	MN	X	3057	1/1	0.90	0.05	71,71,71,71	0
30	MN	X	3124	1/1	0.90	0.08	77,77,77,77	0
30	MN	X	3058	1/1	0.90	0.11	64,64,64,64	0
31	MG	X	3299	1/1	0.90	0.07	5,5,5,5	0
30	MN	X	3146	1/1	0.90	0.12	101,101,101,101	0
30	MN	X	3015	1/1	0.90	0.15	75,75,75,75	0
31	MG	X	3303	1/1	0.91	0.11	4,4,4,4	0
30	MN	X	3069	1/1	0.91	0.07	68,68,68,68	0
31	MG	X	3307	1/1	0.91	0.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3140	1/1	0.91	0.08	71,71,71,71	0
31	MG	X	3031	1/1	0.91	0.16	11,11,11,11	0
31	MG	G	201	1/1	0.91	0.04	19,19,19,19	0
31	MG	X	3099	1/1	0.91	0.09	26,26,26,26	0
31	MG	X	3101	1/1	0.91	0.20	9,9,9,9	0
31	MG	X	3107	1/1	0.91	0.18	18,18,18,18	0
31	MG	X	3035	1/1	0.91	0.05	23,23,23,23	0
30	MN	X	3155	1/1	0.91	0.09	87,87,87,87	0
31	MG	X	3079	1/1	0.91	0.32	27,27,27,27	0
30	MN	X	3157	1/1	0.91	0.07	68,68,68,68	0
30	MN	I	202	1/1	0.91	0.08	64,64,64,64	0
30	MN	X	3126	1/1	0.91	0.06	77,77,77,77	0
31	MG	X	3174	1/1	0.91	0.17	5,5,5,5	0
30	MN	X	3053	1/1	0.91	0.11	89,89,89,89	0
30	MN	X	3260	1/1	0.91	0.13	40,40,40,40	0
31	MG	X	3300	1/1	0.91	0.12	11,11,11,11	0
31	MG	X	3019	1/1	0.91	0.27	15,15,15,15	0
30	MN	X	3049	1/1	0.92	0.09	82,82,82,82	0
30	MN	X	3141	1/1	0.92	0.10	69,69,69,69	0
30	MN	X	3188	1/1	0.92	0.15	87,87,87,87	0
30	MN	X	3192	1/1	0.92	0.12	84,84,84,84	0
30	MN	X	3206	1/1	0.92	0.21	57,57,57,57	0
31	MG	X	3100	1/1	0.92	0.22	17,17,17,17	0
31	MG	X	3021	1/1	0.92	0.07	21,21,21,21	0
31	MG	X	3106	1/1	0.92	0.27	37,37,37,37	0
30	MN	X	3117	1/1	0.92	0.08	80,80,80,80	0
32	EPE	X	3311	15/15	0.92	0.18	57,57,57,57	0
29	MPD	X	3003	8/8	0.92	0.20	21,21,21,21	0
31	MG	X	3028	1/1	0.92	0.07	34,34,34,34	0
30	MN	X	3129	1/1	0.92	0.07	73,73,73,73	0
30	MN	X	3076	1/1	0.92	0.06	74,74,74,74	0
30	MN	X	3040	1/1	0.92	0.08	74,74,74,74	0
30	MN	X	3156	1/1	0.92	0.10	53,53,53,53	0
30	MN	X	3265	1/1	0.92	0.16	43,43,43,43	0
30	MN	X	3135	1/1	0.92	0.06	94,94,94,94	0
30	MN	X	3168	1/1	0.92	0.05	74,74,74,74	0
30	MN	X	3110	1/1	0.92	0.05	96,96,96,96	0
30	MN	X	3180	1/1	0.92	0.17	76,76,76,76	0
30	MN	X	3225	1/1	0.93	0.17	41,41,41,41	0
29	MPD	X	3004	8/8	0.93	0.42	73,73,73,73	0
30	MN	X	3233	1/1	0.93	0.09	63,63,63,63	0
30	MN	X	3054	1/1	0.93	0.21	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3254	1/1	0.93	0.05	48,48,48,48	0
31	MG	X	3026	1/1	0.93	0.32	18,18,18,18	0
30	MN	X	3142	1/1	0.93	0.13	72,72,72,72	0
30	MN	X	3186	1/1	0.93	0.09	51,51,51,51	0
31	MG	X	3032	1/1	0.93	0.07	21,21,21,21	0
30	MN	X	3287	1/1	0.93	0.12	78,78,78,78	0
30	MN	X	3133	1/1	0.93	0.08	98,98,98,98	0
30	MN	X	3166	1/1	0.93	0.11	62,62,62,62	0
30	MN	X	3024	1/1	0.93	0.19	107,107,107,107	0
30	MN	X	3169	1/1	0.93	0.15	78,78,78,78	0
30	MN	X	3125	1/1	0.93	0.14	79,79,79,79	0
31	MG	X	3295	1/1	0.93	0.32	18,18,18,18	0
30	MN	R	201	1/1	0.93	0.05	63,63,63,63	0
30	MN	X	3216	1/1	0.93	0.07	54,54,54,54	0
30	MN	X	3178	1/1	0.93	0.12	78,78,78,78	0
31	MG	X	3016	1/1	0.93	0.15	23,23,23,23	0
31	MG	X	3104	1/1	0.94	0.17	28,28,28,28	0
30	MN	X	3244	1/1	0.94	0.10	57,57,57,57	0
31	MG	X	3310	1/1	0.94	0.10	15,15,15,15	0
31	MG	Y	201	1/1	0.94	0.08	34,34,34,34	0
31	MG	X	3039	1/1	0.94	0.15	7,7,7,7	0
31	MG	X	3108	1/1	0.94	0.17	12,12,12,12	0
30	MN	X	3063	1/1	0.94	0.05	60,60,60,60	0
30	MN	X	3134	1/1	0.94	0.06	58,58,58,58	0
30	MN	X	3255	1/1	0.94	0.09	35,35,35,35	0
30	MN	X	3066	1/1	0.94	0.04	56,56,56,56	0
31	MG	X	3020	1/1	0.94	0.11	20,20,20,20	0
31	MG	X	3091	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3218	1/1	0.94	0.15	65,65,65,65	0
30	MN	X	3112	1/1	0.94	0.05	54,54,54,54	0
31	MG	X	3294	1/1	0.94	0.16	37,37,37,37	0
30	MN	X	3220	1/1	0.94	0.10	68,68,68,68	0
29	MPD	X	3011	8/8	0.94	0.25	39,39,39,39	0
30	MN	X	3152	1/1	0.94	0.08	68,68,68,68	0
30	MN	X	3228	1/1	0.94	0.05	85,85,85,85	0
30	MN	X	3229	1/1	0.94	0.07	79,79,79,79	0
29	MPD	X	3007	8/8	0.94	0.27	9,9,9,9	0
30	MN	X	3051	1/1	0.95	0.04	67,67,67,67	0
30	MN	X	3179	1/1	0.95	0.14	83,83,83,83	0
31	MG	X	3296	1/1	0.95	0.13	9,9,9,9	0
31	MG	X	3298	1/1	0.95	0.24	23,23,23,23	0
30	MN	X	3293	1/1	0.95	0.05	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3048	1/1	0.95	0.06	59,59,59,59	0
31	MG	X	3301	1/1	0.95	0.13	8,8,8,8	0
31	MG	X	3085	1/1	0.95	0.10	9,9,9,9	0
30	MN	X	3323	1/1	0.95	0.07	42,42,42,42	0
31	MG	X	3305	1/1	0.95	0.27	15,15,15,15	0
30	MN	X	3041	1/1	0.95	0.04	84,84,84,84	0
30	MN	X	3070	1/1	0.95	0.05	78,78,78,78	0
30	MN	X	3059	1/1	0.95	0.04	61,61,61,61	0
30	MN	X	3187	1/1	0.95	0.04	74,74,74,74	0
30	MN	X	3061	1/1	0.95	0.05	63,63,63,63	0
30	MN	X	3231	1/1	0.95	0.10	74,74,74,74	0
30	MN	X	3190	1/1	0.95	0.11	59,59,59,59	0
30	MN	X	3131	1/1	0.95	0.16	89,89,89,89	0
30	MN	X	3196	1/1	0.95	0.13	51,51,51,51	0
30	MN	X	3252	1/1	0.95	0.07	17,17,17,17	0
30	MN	X	3046	1/1	0.95	0.13	94,94,94,94	0
30	MN	X	3064	1/1	0.95	0.04	68,68,68,68	0
30	MN	X	3257	1/1	0.95	0.12	25,25,25,25	0
30	MN	X	3210	1/1	0.95	0.07	57,57,57,57	0
30	MN	X	3177	1/1	0.95	0.09	82,82,82,82	0
30	MN	X	3272	1/1	0.95	0.14	44,44,44,44	0
31	MG	X	3115	1/1	0.95	0.23	1,1,1,1	1
31	MG	X	3034	1/1	0.95	0.11	18,18,18,18	0
30	MN	X	3274	1/1	0.95	0.07	36,36,36,36	0
31	MG	X	3037	1/1	0.95	0.09	11,11,11,11	0
30	MN	X	3282	1/1	0.95	0.06	49,49,49,49	0
30	MN	X	3214	1/1	0.95	0.06	81,81,81,81	0
31	MG	X	3030	1/1	0.96	0.07	15,15,15,15	0
30	MN	X	3276	1/1	0.96	0.08	42,42,42,42	0
30	MN	X	3277	1/1	0.96	0.05	35,35,35,35	0
30	MN	X	3205	1/1	0.96	0.06	61,61,61,61	0
30	MN	X	3283	1/1	0.96	0.12	14,14,14,14	0
31	MG	X	3036	1/1	0.96	0.11	8,8,8,8	0
30	MN	X	3285	1/1	0.96	0.09	85,85,85,85	0
30	MN	X	3183	1/1	0.96	0.04	41,41,41,41	0
30	MN	X	3288	1/1	0.96	0.05	55,55,55,55	0
30	MN	X	3289	1/1	0.96	0.06	57,57,57,57	0
30	MN	X	3077	1/1	0.96	0.03	78,78,78,78	0
30	MN	X	3291	1/1	0.96	0.16	94,94,94,94	0
31	MG	X	3083	1/1	0.96	0.32	37,37,37,37	0
30	MN	X	3230	1/1	0.96	0.12	65,65,65,65	0
30	MN	X	3153	1/1	0.96	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3086	1/1	0.96	0.12	26,26,26,26	0
30	MN	X	3211	1/1	0.96	0.08	60,60,60,60	0
30	MN	X	3236	1/1	0.96	0.05	36,36,36,36	0
30	MN	X	3325	1/1	0.96	0.10	59,59,59,59	0
30	MN	Y	204	1/1	0.96	0.05	63,63,63,63	0
31	MG	Y	205	1/1	0.96	0.08	12,12,12,12	0
31	MG	X	3094	1/1	0.96	0.15	5,5,5,5	0
30	MN	X	3012	1/1	0.96	0.14	19,19,19,19	0
30	MN	X	3147	1/1	0.96	0.04	82,82,82,82	0
30	MN	J	201	1/1	0.96	0.08	78,78,78,78	0
30	MN	X	3122	1/1	0.96	0.19	89,89,89,89	0
30	MN	X	3191	1/1	0.96	0.07	51,51,51,51	0
30	MN	X	3025	1/1	0.96	0.10	52,52,52,52	0
30	MN	X	3151	1/1	0.96	0.05	44,44,44,44	0
30	MN	X	3221	1/1	0.96	0.06	46,46,46,46	0
30	MN	X	3263	1/1	0.96	0.12	52,52,52,52	0
30	MN	X	3222	1/1	0.96	0.08	71,71,71,71	0
30	MN	X	3268	1/1	0.96	0.07	27,27,27,27	0
30	MN	X	3269	1/1	0.96	0.12	36,36,36,36	0
30	MN	X	3223	1/1	0.96	0.12	60,60,60,60	0
30	MN	X	3273	1/1	0.96	0.14	41,41,41,41	0
30	MN	X	3199	1/1	0.96	0.10	51,51,51,51	0
30	MN	X	3160	1/1	0.97	0.05	45,45,45,45	0
30	MN	X	3326	1/1	0.97	0.07	57,57,57,57	0
30	MN	Y	202	1/1	0.97	0.04	57,57,57,57	0
30	MN	X	3256	1/1	0.97	0.06	13,13,13,13	0
30	MN	X	3181	1/1	0.97	0.10	39,39,39,39	0
30	MN	X	3202	1/1	0.97	0.08	54,54,54,54	0
30	MN	X	3262	1/1	0.97	0.09	50,50,50,50	0
31	MG	X	3089	1/1	0.97	0.07	13,13,13,13	0
30	MN	X	3161	1/1	0.97	0.04	46,46,46,46	0
31	MG	X	3304	1/1	0.97	0.27	15,15,15,15	0
30	MN	X	3224	1/1	0.97	0.09	53,53,53,53	0
30	MN	X	3047	1/1	0.97	0.06	69,69,69,69	0
30	MN	X	3119	1/1	0.97	0.10	63,63,63,63	0
30	MN	X	3227	1/1	0.97	0.04	57,57,57,57	0
30	MN	X	3209	1/1	0.97	0.06	24,24,24,24	0
30	MN	X	3067	1/1	0.97	0.04	51,51,51,51	0
30	MN	X	3170	1/1	0.97	0.04	54,54,54,54	0
30	MN	X	3212	1/1	0.97	0.06	56,56,56,56	0
31	MG	B	301	1/1	0.97	0.07	0,0,0,0	0
30	MN	X	3232	1/1	0.97	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3139	1/1	0.97	0.08	97,97,97,97	0
30	MN	X	3284	1/1	0.97	0.07	21,21,21,21	0
30	MN	X	3235	1/1	0.97	0.15	40,40,40,40	0
31	MG	O	201	1/1	0.97	0.22	7,7,7,7	0
30	MN	X	3189	1/1	0.97	0.09	64,64,64,64	0
30	MN	X	3240	1/1	0.97	0.06	28,28,28,28	0
30	MN	X	3242	1/1	0.97	0.11	22,22,22,22	0
30	MN	X	3072	1/1	0.97	0.04	80,80,80,80	0
30	MN	X	3245	1/1	0.97	0.06	28,28,28,28	0
30	MN	X	3249	1/1	0.97	0.06	51,51,51,51	0
30	MN	X	3217	1/1	0.97	0.03	38,38,38,38	0
31	MG	X	3172	1/1	0.97	0.32	27,27,27,27	0
30	MN	X	3065	1/1	0.97	0.04	60,60,60,60	0
30	MN	X	3158	1/1	0.97	0.04	62,62,62,62	0
31	MG	X	3080	1/1	0.97	0.31	33,33,33,33	0
31	MG	X	3176	1/1	0.97	0.09	14,14,14,14	0
31	MG	X	3144	1/1	0.98	0.09	8,8,8,8	0
30	MN	X	3194	1/1	0.98	0.05	31,31,31,31	0
30	MN	X	3248	1/1	0.98	0.10	37,37,37,37	0
30	MN	X	3286	1/1	0.98	0.04	57,57,57,57	0
30	MN	X	3195	1/1	0.98	0.07	30,30,30,30	0
30	MN	X	3075	1/1	0.98	0.02	76,76,76,76	0
30	MN	X	3197	1/1	0.98	0.12	34,34,34,34	0
30	MN	X	3253	1/1	0.98	0.15	26,26,26,26	0
30	MN	X	3071	1/1	0.98	0.05	69,69,69,69	0
30	MN	X	3200	1/1	0.98	0.09	37,37,37,37	0
30	MN	X	3056	1/1	0.98	0.07	61,61,61,61	0
30	MN	X	3203	1/1	0.98	0.09	27,27,27,27	0
30	MN	X	3258	1/1	0.98	0.04	35,35,35,35	0
30	MN	X	3324	1/1	0.98	0.10	12,12,12,12	0
30	MN	X	3204	1/1	0.98	0.02	21,21,21,21	0
30	MN	X	3261	1/1	0.98	0.06	30,30,30,30	0
31	MG	X	3088	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3150	1/1	0.98	0.04	50,50,50,50	0
30	MN	X	3162	1/1	0.98	0.05	43,43,43,43	0
30	MN	X	3264	1/1	0.98	0.04	52,52,52,52	0
30	MN	X	3163	1/1	0.98	0.04	61,61,61,61	0
30	MN	X	3266	1/1	0.98	0.03	22,22,22,22	0
30	MN	X	3267	1/1	0.98	0.10	48,48,48,48	0
30	MN	X	3208	1/1	0.98	0.07	37,37,37,37	0
30	MN	X	3164	1/1	0.98	0.08	48,48,48,48	0
31	MG	B	302	1/1	0.98	0.05	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	C	301	1/1	0.98	0.04	2,2,2,2	0
30	MN	X	3271	1/1	0.98	0.09	17,17,17,17	0
30	MN	X	3165	1/1	0.98	0.04	63,63,63,63	0
30	MN	X	3078	1/1	0.98	0.07	78,78,78,78	0
31	MG	X	3102	1/1	0.98	0.13	6,6,6,6	0
31	MG	X	3103	1/1	0.98	0.10	3,3,3,3	0
30	MN	X	3043	1/1	0.98	0.04	61,61,61,61	0
31	MG	X	3105	1/1	0.98	0.20	35,35,35,35	0
30	MN	X	3120	1/1	0.98	0.03	55,55,55,55	0
30	MN	X	3154	1/1	0.98	0.03	40,40,40,40	0
30	MN	X	3278	1/1	0.98	0.04	35,35,35,35	0
30	MN	X	3279	1/1	0.98	0.03	25,25,25,25	0
30	MN	X	3280	1/1	0.98	0.07	39,39,39,39	0
31	MG	X	3029	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3281	1/1	0.98	0.03	40,40,40,40	0
31	MG	X	3116	1/1	0.98	0.05	20,20,20,20	0
30	MN	X	3145	1/1	0.98	0.04	51,51,51,51	0
30	MN	X	3060	1/1	0.98	0.02	51,51,51,51	0
30	MN	X	3247	1/1	0.99	0.08	25,25,25,25	0
30	MN	X	3201	1/1	0.99	0.02	40,40,40,40	0
30	MN	X	3193	1/1	0.99	0.04	33,33,33,33	0
30	MN	X	3045	1/1	0.99	0.11	3,3,3,3	0
30	MN	X	3270	1/1	0.99	0.03	30,30,30,30	0
30	MN	X	3251	1/1	0.99	0.13	8,8,8,8	0
30	MN	X	3167	1/1	0.99	0.03	57,57,57,57	0
31	MG	X	3027	1/1	0.99	0.04	29,29,29,29	0
30	MN	X	3234	1/1	0.99	0.04	17,17,17,17	0
30	MN	X	3159	1/1	0.99	0.04	42,42,42,42	0
30	MN	X	3275	1/1	0.99	0.06	30,30,30,30	0
30	MN	X	3215	1/1	0.99	0.07	26,26,26,26	0
30	MN	X	3237	1/1	0.99	0.05	47,47,47,47	0
31	MG	X	3097	1/1	0.99	0.03	14,14,14,14	0
31	MG	X	3033	1/1	0.99	0.07	19,19,19,19	0
30	MN	X	3238	1/1	0.99	0.06	34,34,34,34	0
31	MG	X	3297	1/1	0.99	0.05	5,5,5,5	0
30	MN	X	3239	1/1	0.99	0.07	15,15,15,15	0
30	MN	X	3259	1/1	0.99	0.05	13,13,13,13	0
30	MN	X	3062	1/1	0.99	0.03	42,42,42,42	0
30	MN	I	203	1/1	0.99	0.06	33,33,33,33	0
30	MN	X	3241	1/1	0.99	0.04	20,20,20,20	0
30	MN	X	3198	1/1	0.99	0.06	64,64,64,64	0
30	MN	X	3243	1/1	0.99	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3185	1/1	0.99	0.05	28,28,28,28	0
30	MN	X	3014	1/1	0.99	0.09	12,12,12,12	0
30	MN	X	3246	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.