



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 7A0S / pdb_00007a0s
Title : 50S Deinococcus radiodurans ribosome bounded with mycinamicin I
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Cimicata, G.; Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2020-08-10
Resolution : 3.22 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

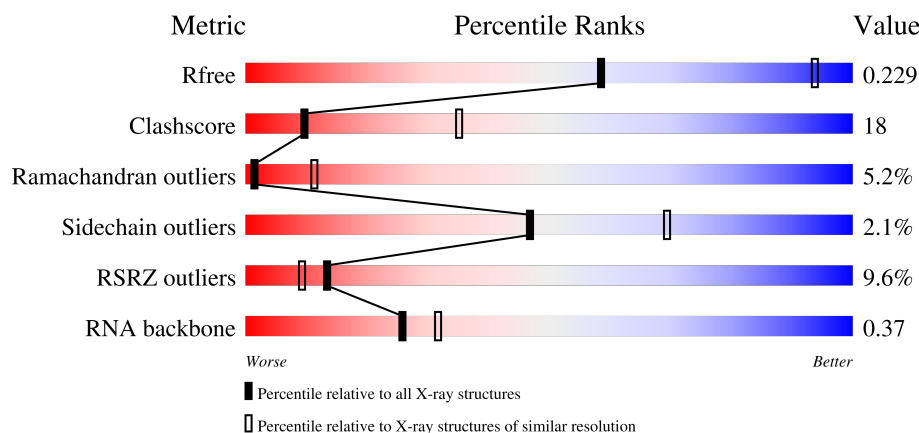
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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	2880	
2	Y	123	
3	A	274	
4	B	206	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	177	
7	E	171	
8	G	143	
9	H	134	
10	I	137	
11	J	136	
12	K	116	
13	L	104	
14	M	166	
15	N	117	
16	O	98	
17	P	134	
18	Q	93	
19	R	110	
20	S	175	
21	T	91	
22	U	74	
23	V	61	
24	W	55	
25	Z	58	
26	1	49	
27	2	47	
28	3	63	

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
30	MG	A	302	-	-	-	X
30	MG	A	303	-	-	-	X
30	MG	X	2906	-	-	-	X
30	MG	X	2915	-	-	-	X
30	MG	X	2917	-	-	-	X
30	MG	X	2919	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2927	-	-	-	X
30	MG	X	2940	-	-	-	X
30	MG	X	2942	-	-	-	X
30	MG	X	2944	-	-	-	X
30	MG	X	2948	-	-	-	X
30	MG	X	2950	-	-	-	X
30	MG	X	2951	-	-	-	X
30	MG	X	2953	-	-	-	X
30	MG	X	2960	-	-	-	X
30	MG	X	2974	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2985	-	-	-	X
30	MG	X	2989	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3004	-	-	-	X
30	MG	X	3005	-	-	-	X
30	MG	X	3015	-	-	-	X
30	MG	X	3022	-	-	-	X
30	MG	X	3024	-	-	-	X
30	MG	X	3043	-	-	-	X
30	MG	X	3056	-	-	-	X
30	MG	X	3073	-	-	-	X
30	MG	X	3097	-	-	-	X
30	MG	X	3101	-	-	-	X
30	MG	X	3116	-	-	-	X
30	MG	X	3117	-	-	-	X
30	MG	X	3120	-	-	-	X
30	MG	X	3130	-	-	-	X
30	MG	X	3159	-	-	-	X
30	MG	X	3161	-	-	-	X
30	MG	X	3164	-	-	-	X
30	MG	X	3166	-	-	-	X
30	MG	X	3190	-	-	-	X
30	MG	X	3208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3210	-	-	-	X
30	MG	X	3213	-	-	-	X
30	MG	X	3217	-	-	-	X
30	MG	X	3221	-	-	-	X
30	MG	X	3223	-	-	-	X
30	MG	X	3224	-	-	-	X
30	MG	X	3233	-	-	-	X
30	MG	Y	202	-	-	-	X
30	MG	Y	204	-	-	-	X
30	MG	Y	205	-	-	-	X
30	MG	Y	209	-	-	-	X
30	MG	Y	210	-	-	-	X
30	MG	Y	213	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 84486 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 RNA (2732-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2699	Total	C	N	O	P	5	0	0
			57935	25843	10696	18698	2698			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073
X	2779	A	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	272	Total	C	N	O	S	0	0	0
			2011	1248	396	364	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	206	Total	C	N	O	S	0	0	0
			1544	968	296	272	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	196	Total	C	N	O	S	0	0	0
			1479	918	284	274	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1375	874	243	251	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1110	701	208	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	137	Total	C	N	O	S	0	0	0
			982	603	194	184	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	135	Total	C	N	O	S	0	0	0
			1062	676	197	182	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			893	549	182	159	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			761	462	159	140			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O	0	0	0
			923	578	178	167			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			955	594	203	157	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	98	Total	C	N	O	S	0	0	0
			736	459	138	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	129	Total	C	N	O	S	0	0	0
			1014	640	198	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	92	Total	C	N	O	S	0	0	0
			705	445	131	127	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			771	473	147	150	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1288	809	224	250	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			537	334	105	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	74	Total	C	N	O		0	0	0
			519	319	106	94				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	54	Total	C	N	O	S	0	0	0
			438	270	89	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			448	275	92	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	49	Total	C	N	O		0	0	0
			314	199	53	62				

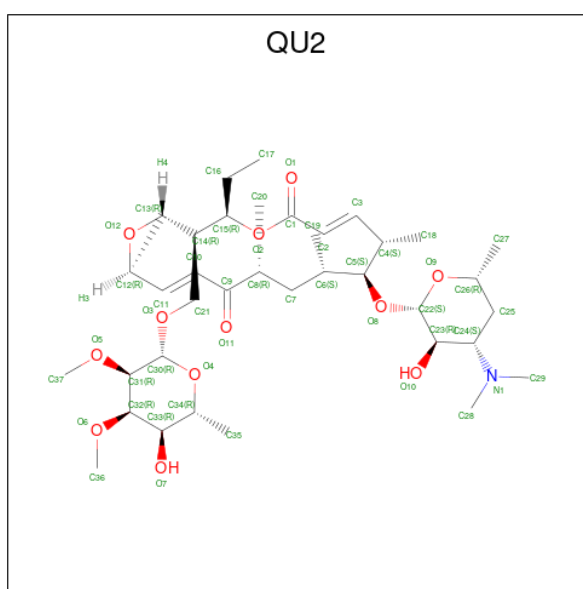
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	63	Total	C	N	O	S	0	0	0
			459	288	94	74	3			

- Molecule 29 is mycinamicin I (CCD ID: QU2) (formula: $C_{37}H_{61}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	X	1	Total	C	N	O	0	0
			50	37	1	12		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

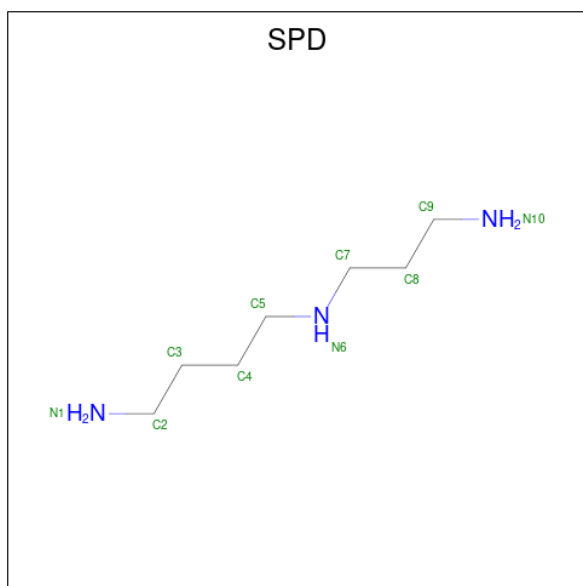
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	335	Total	Mg	0	0
			335	335		
30	Y	17	Total	Mg	0	0
			17	17		
30	A	3	Total	Mg	0	0
			3	3		
30	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	I	2	Total	Mg	0	0
			2	2		
30	J	1	Total	Mg	0	0
			1	1		
30	K	1	Total	Mg	0	0
			1	1		
30	M	1	Total	Mg	0	0
			1	1		
30	N	3	Total	Mg	0	0
			3	3		
30	2	2	Total	Mg	0	0
			2	2		
30	3	1	Total	Mg	0	0
			1	1		

- Molecule 31 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



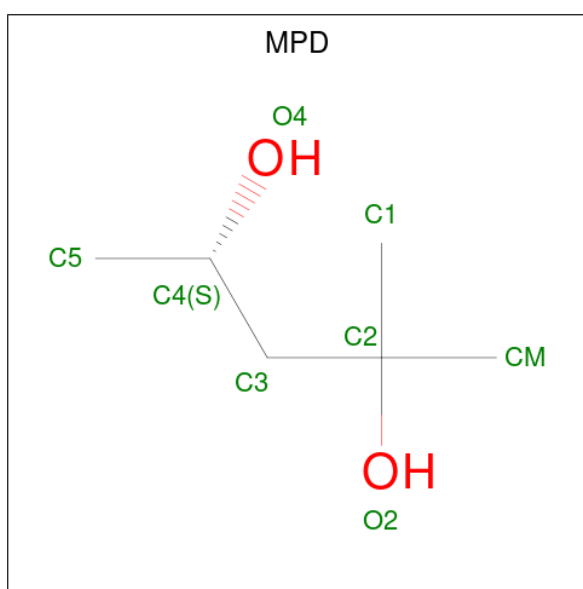
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

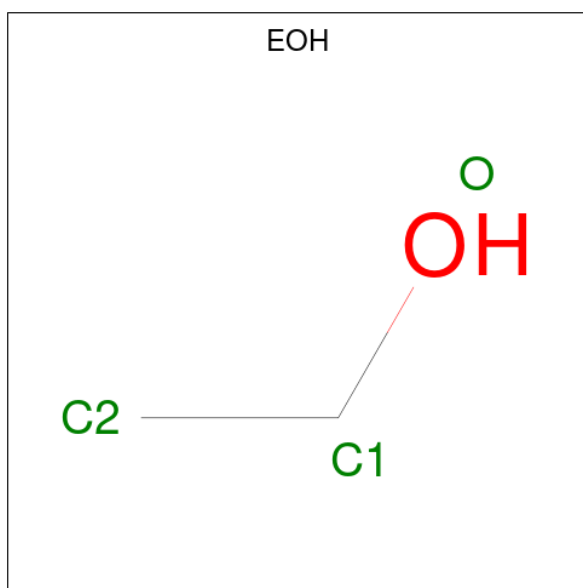


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Na	0	0
			1	1		

- Molecule 34 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



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

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Ca	0	0
			5	5		

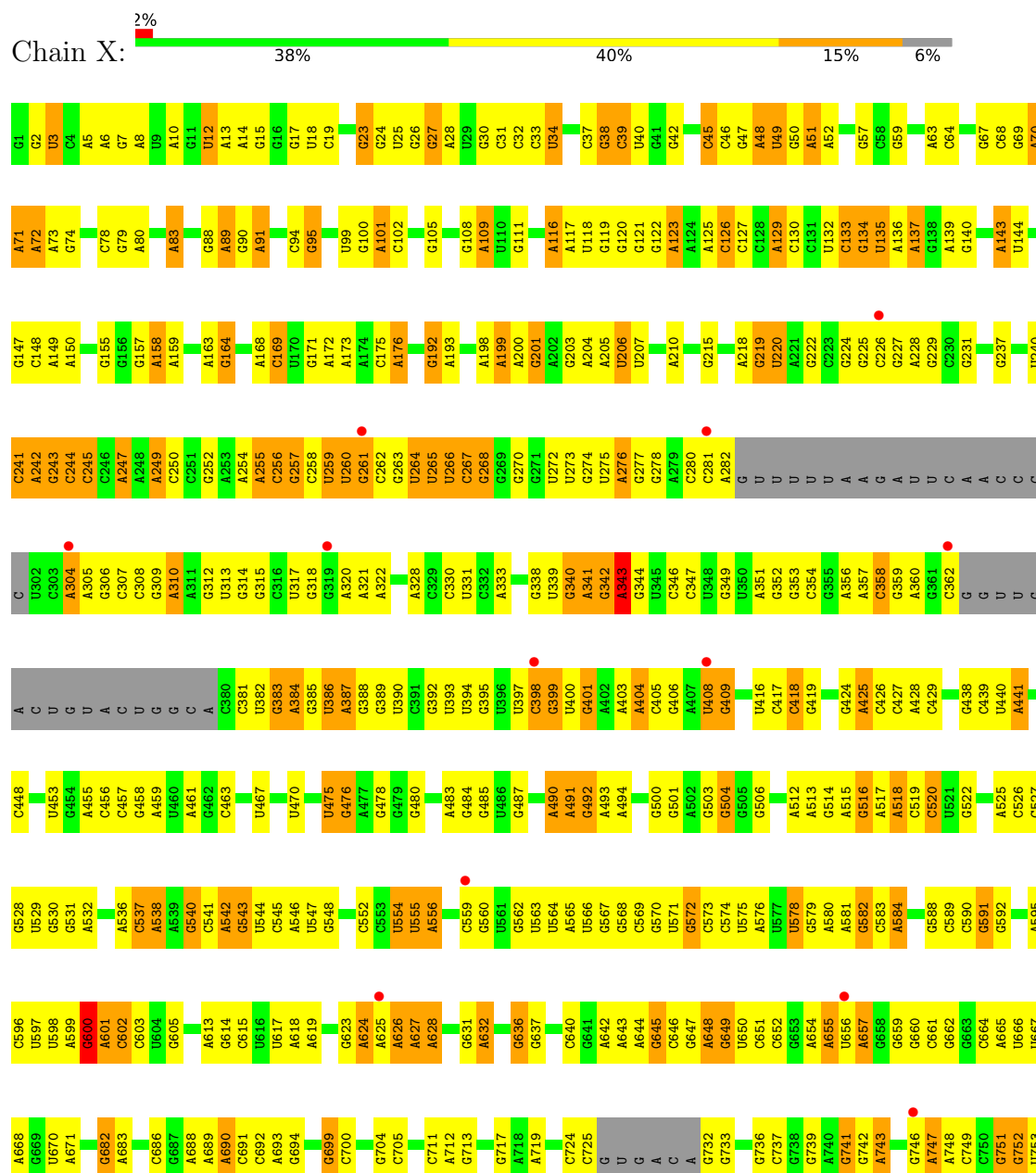
- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	X	1	Total	K	0	0
			1	1		

3 Residue-property plots

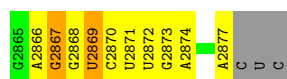
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA (2732-MER)

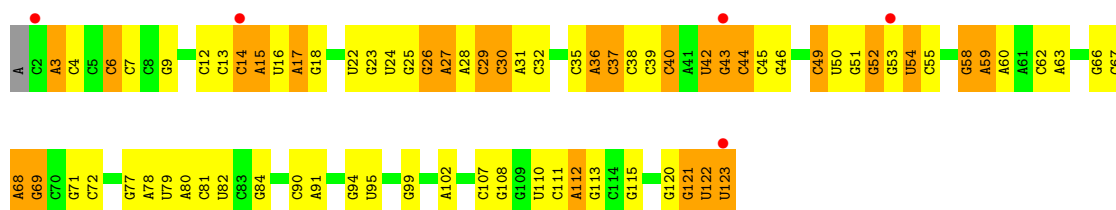


G1760	G1761	C1687	A1588	C1514	G1443	A1367	U1194	C1127	G1062	A986	C	G754
G1762	U1688	U1688	C1593	A1516	C1444	G1368	U1197	G1128	C1063	U	C	C755
G1763	U1689	C1517	U1594	C1517	A1445	G1369	U1197	A1129	C1064	A991	C	C756
U1764	U1690	C1518	U1595	C1518	U1446	G1370	G1201	U1130	A1065	A992	A	U757
G1765	G1691	C1519	U1595	G1519	U1447	A1372	U1202	U1130	A1066	C993	C	C758
U1766	C1692	G1520	U1601	G1520	A1448	G1373	U1207	G1133	C1067	A994	C	C759
U1699	A1693	U1521	G1602	U1521	C1451	U1287	G1207	G1134	A1068	A995	A	U760
U1770	A1603	C1522	A1603	C1522	U1452	A1288	G1210	G1135	G1069	C996	G	G761
A1771	U1695	A	A	C	U1453	A1289	G1210	G1136	U1071	A1001	C	A762
C1772	C1698	A	A	U1526	U1454	G1298	U1211	G1137	U1072	U1005	U	A763
C1773	A1698	U1530	A1607	U1530	U1455	G1381	U1212	A1138	G1073	U1006	C	A766
A1774	G1700	C1531	U1608	U1530	G1460	C1385	U1213	A1139	G1074	C1006	A	G772
A1775	A1610	G1536	A1624	C1531	A1463	A1386	G1217	U1141	U1076	A1007	C	G773
U1776	U1705	U1537	C1623	G1536	A1464	A1391	G1220	G1142	U1077	C1009	A911	A774
U1777	A1706	A1538	A1624	G1536	G1465	U1392	G1221	A1143	G1078	U1009	A912	U775
U1778	C1708	U1537	A1626	U1537	C1466	U1392	G1223	U1144	U1079	C1016	G776	
C1779	U1709	A1538	A1626	A1538	U1467	G1397	G1223	G1145	A1080	C1017	A777	
A1780	U1710	U1539	A1626	U1539	U1468	A1397	A1224	G1146	C1082	C1018	G778	
C1781	G1711	C1540	A1634	C1540	U1469	G1398	G1225	G1148	C1083	A1020	A846	
A1782	G1635	G1541	G1635	G1541	G1470	C1399	A1226	G1149	A1084	A1021	A846	
G1785	G1636	G1542	G1636	G1542	G1470	A1400	G1227	A1149	A923	A923	A923	U780
C1786	A1714	G1543	G1642	G1543	U1473	A1400	A1227	C1152	C1085	A1022	C924	G781
U1787	A1715	A1544	G1642	G1544	U1474	G1402	G1229	C1152	C1086	U1023	C924	U782
C1788	G1716	G1545	U1645	G1545	U1475	G1403	C1229	A1153	C1087	G1024	A930	G783
U1789	A1717	U1546	U1646	C1546	G1476	C1404	C1234	A1154	A1088	C850	A930	C850
G1790	U1718	C	U1647	U	C1477	C1404	C1234	G1155	C1089	U1026	A936	A877
C1791	G1719	C	U1647	U	U1478	A1408	A1242	U1156	C1090	G1027	C937	G788
C1792	C1648	C	C1648	C	G1479	U1409	A1242	C1160	C1091	G1028	C937	G789
A1793	U1723	C	A1649	C	U1482	U1410	G1246	U1161	U1092	G1029	C939	U790
U1794	C1724	U	A1650	C	C1411	C1411	G1247	A1162	U1093	U1030	C940	G791
C1795	G1725	C	G1483	U	G1483	C1412	G1248	C1163	C1094	U1031	U859	U792
A1796	C1726	C	G1484	C	U1484	U1413	G1249	C1164	A1095	A1032	U941	G793
C1727	C1652	G	U1485	G	G1485	U1413	G1249	C1164	A1096	G1033	U942	A794
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U1798	C1654	C	A1654	C	C1486	C1418	A1250	G1185	A1097	U1034	A944	A796
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C1801	U1732	C	U1656	C	C1487	G1419	A1255	A1171	A1099	G1036	U946	C869
U1800	U1656	C	U1656	C	G1488	C1488	C1256	U1172	G1100	U1037	C947	C798
A1802	A1657	G1558	A1657	G1558	C1489	C1489	U1257	G1173	U1101	C948	C948	U800
G1803	G1659	A1560	G1659	A1560	U1490	C1422	G1258	G1174	G1102	G102	G949	A801
U1804	C1662	A1561	C1662	A1561	G1495	G1422	G1258	U1175	C1103	A1043	A952	A802
G1805	G1736	U1562	G1662	U1562	U1426	U1426	G1261	U1176	G1104	U1044	A952	C803
C1806	C1663	U1563	G1663	U1563	C1497	G1427	G1261	U1176	U1105	G1045	U105	C804
A1807	U1739	U1564	G1664	U1564	G1498	G1427	C1264	A1179	A1106	C877	A956	C805
C1808	G1740	C1665	C1665	C1665	A1499	A1429	G1265	A1180	G957	U1047	G957	A806
G1809	C1745	G1571	C1665	G1571	U1500	G1430	G1266	C1181	U1048	A883	C959	A807
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A1811	U1670	A1573	A1669	G1573	U1501	G1431	A1267	U1182	U1112	C1049	U1050	U810
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A1813	A1671	C1575	A1671	C1575	G1503	A1433	G1269	G1184	A1114	C1052	A966	A886
C1816	U1749	C1575	A1671	C1575	U1504	U1434	C1270	C	C1115	G1053	A966	A886
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U1820	A1753	G1584	U1679	G1584	A1509	C1358	G1276	G	A1057	U1056	A971	A817
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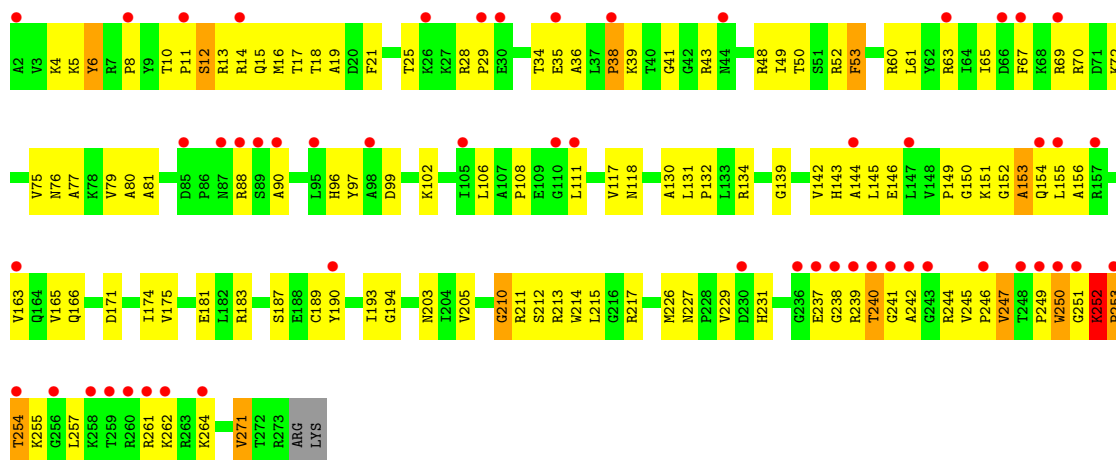
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C2790	U2706	U2542	U2471	C2402	C2329	A2266	U2180	C	U2057	C1988	C	G1827
C2791	G2707	A2543	U2471	C2403	C2330	A2267	A2181	U	U2058	U1989	U	C1908
C2792	U2708	A2544	U2471	A2404	A2331	G2268		G		C1990	U	C1830
G2793	U2709	A2545	G2474	A2405	G2332	G2269	G2186	G	A2063	U1991	U	G1831
G2794	G2710	G2546	C2475	C2406	A2333	U2270	A2187	C	U2064	C1992	A	G1834
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C2800	C2722	G2553	A2481	A2412	U2344	A2276	C2193	G	G2070	A1998	U	A1920
A2801	U2723	A2556	A2482	G2415	A2348	A2277	C2194	G	U1999	U1999	U	U1843
U2807	G2724	C2557	U2483	A2418	G2351	A2278	C2196	G	A2002	A2002	U	C1844
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A2811	G2727	U2560	G2486	C2421	G2354	C2281	U2199	C	U2005	U2005	G	C1925
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G2839	A2744	G2583	C2500	A2433	A2367	A2288	G2217	G	U2088	C2019	U	U1870
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G2841	G2746	C2585	U2502	C2435	G2369	C2295	U2219	U	U1946	G2021	U	A1872
G2842	U2750	U2586	G2503	C2436	U2370	U2296	A2220	A	C1948	U2024	U	G1873
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G2855	U2763	C2605	U2526	C2454	U2388	G2313		U	G2039	A1964	U	G
G2856	U2764	C2606	G2527	U2455	G2389	A2314	U2241	G	A2040	U1965	U	U
G2857	U2765	C2607	G2528	U2456	G2390	A2315		G	A2041	G1972	U	A
G2858	U2766	A2608	G2529	U2457	A2391	G2316	A2245	A	A2042	C1975	U	A
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G2860	U2768	U2616	G2531	C2459	G2393	U2318	A2247	U	A2045	C1977	U	A
G2861	U2769	U2617	U2532	G2460	C2394			U	C2046	U1978	U	U
G2862	U2770	U2618	U2533	G2461	G2395	U2322	A2253	G	C2047	C1979	U	A
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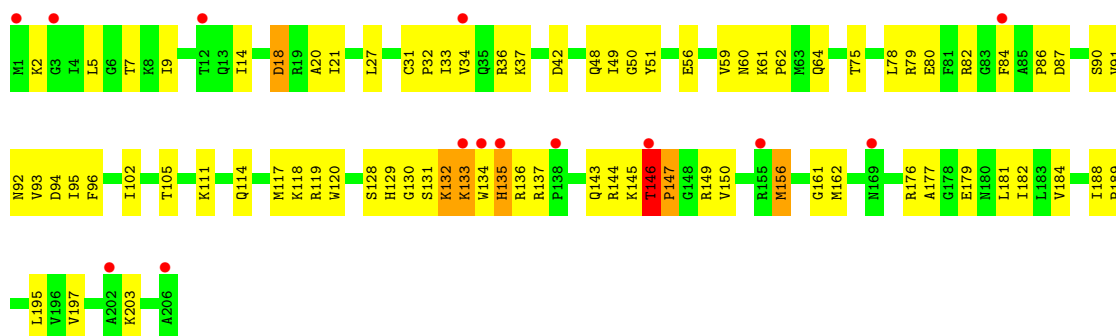
• Molecule 2: RNA (122-MER)



• Molecule 3: 50S ribosomal protein L2

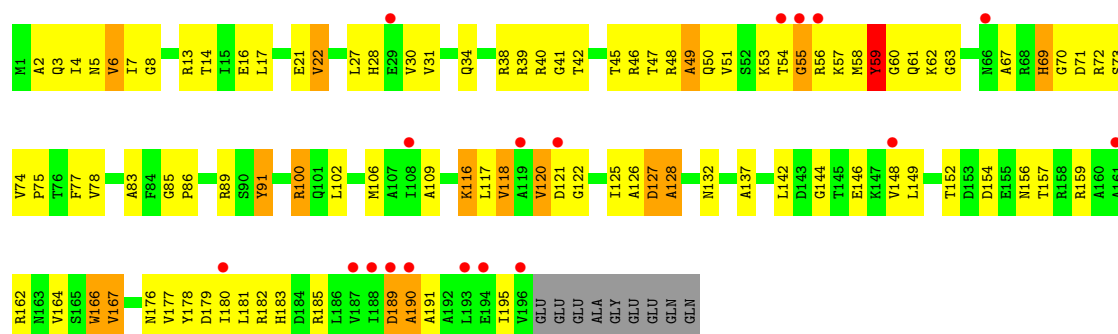


• Molecule 4: 50S ribosomal protein L3

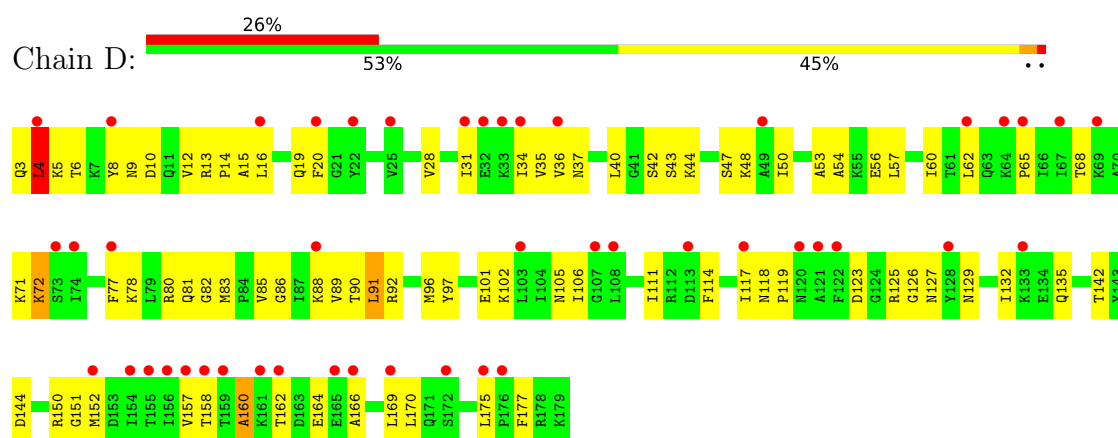


• Molecule 5: 50S ribosomal protein L4

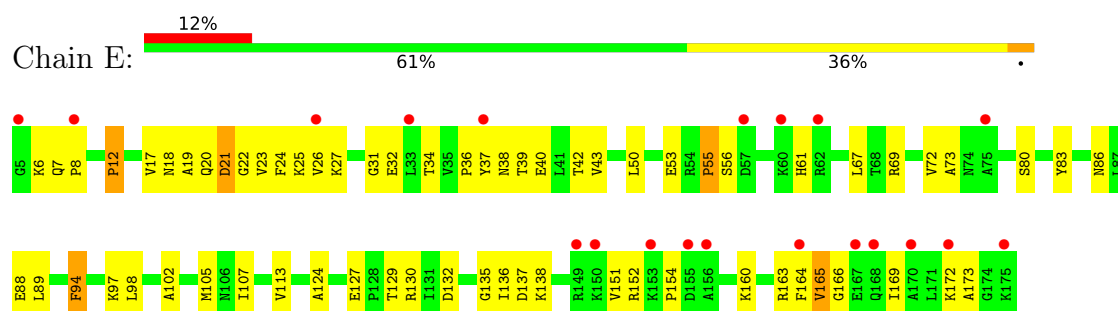




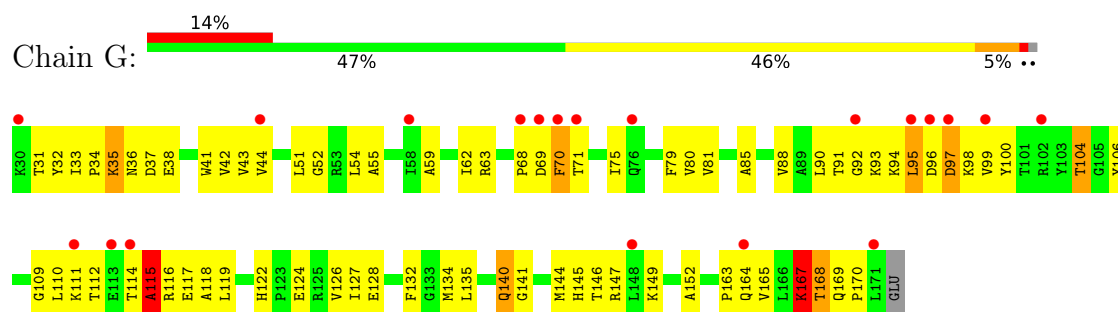
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

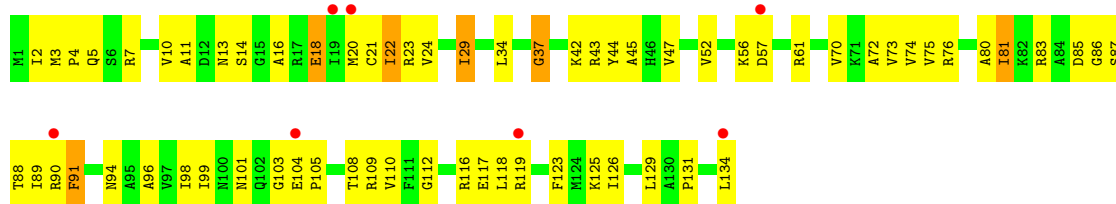


• Molecule 8: 50S ribosomal protein L13

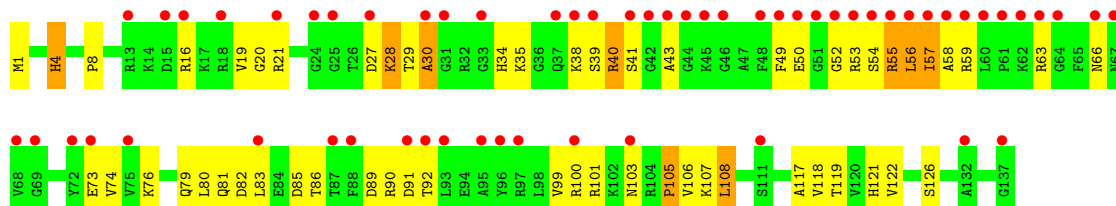
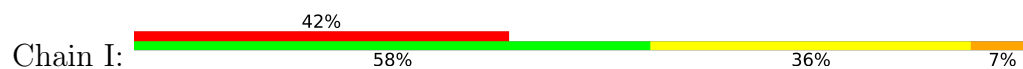


• Molecule 9: 50S ribosomal protein L14

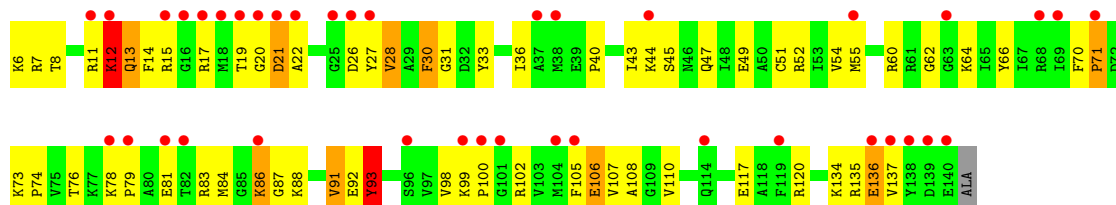




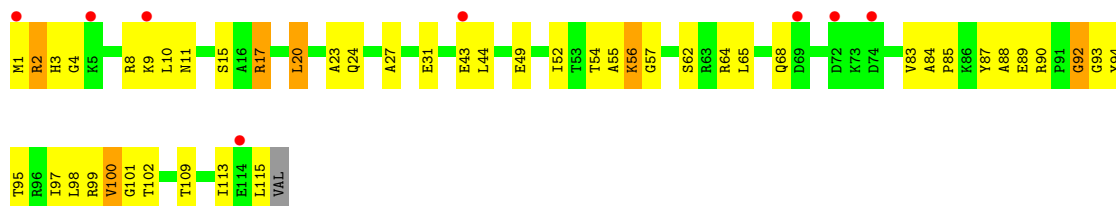
• Molecule 10: 50S ribosomal protein L15



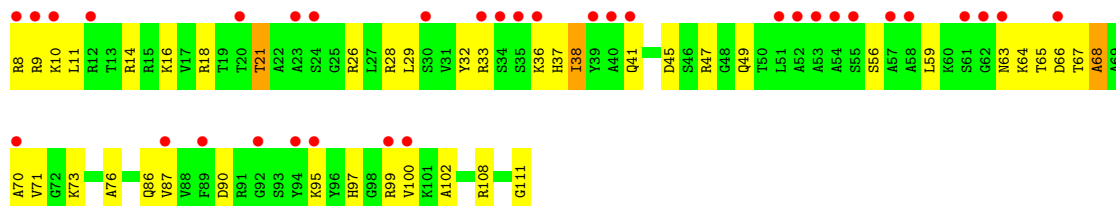
• Molecule 11: 50S ribosomal protein L16



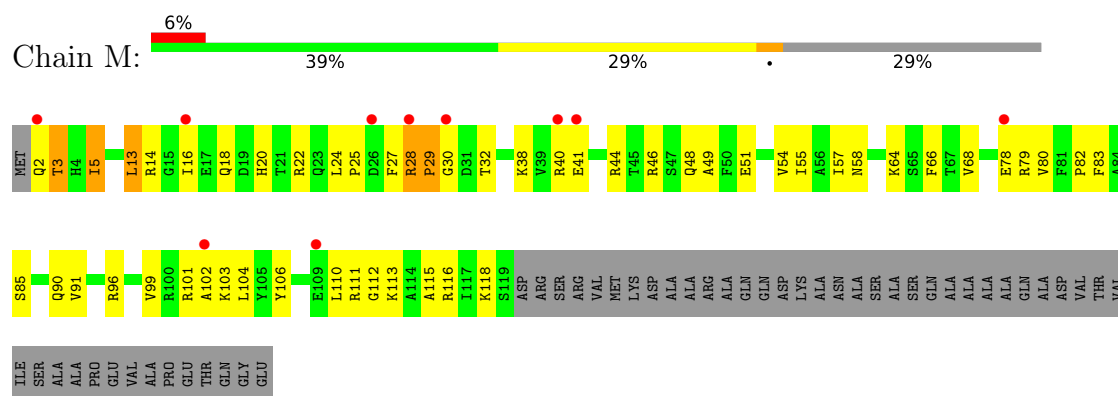
• Molecule 12: 50S ribosomal protein L17



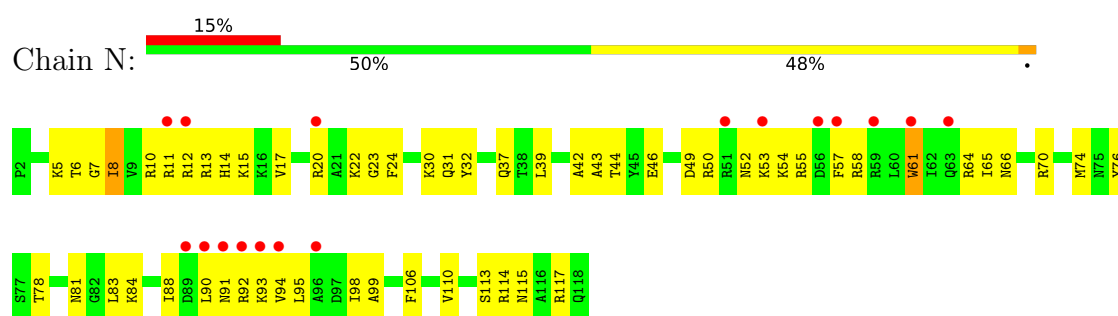
• Molecule 13: 50S ribosomal protein L18



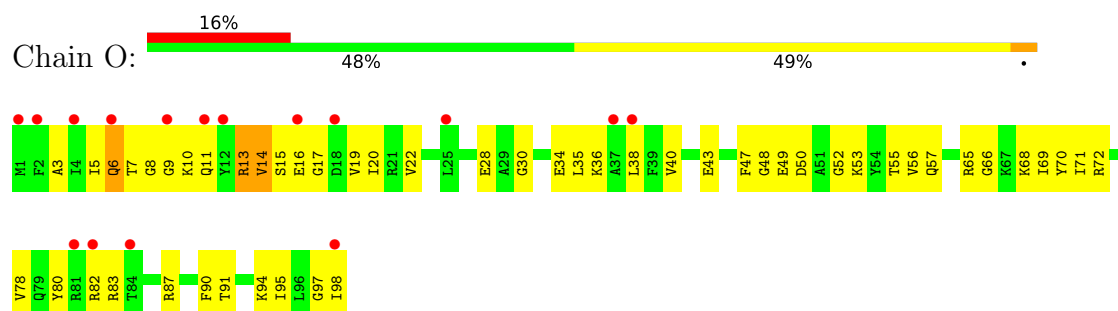
- Molecule 14: 50S ribosomal protein L19



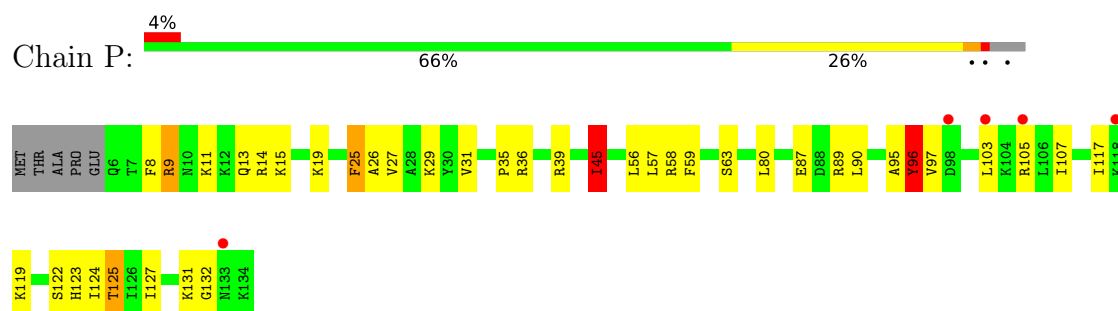
- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21

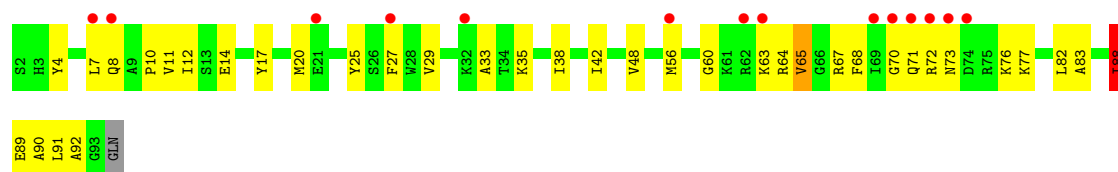


- Molecule 17: 50S ribosomal protein L22

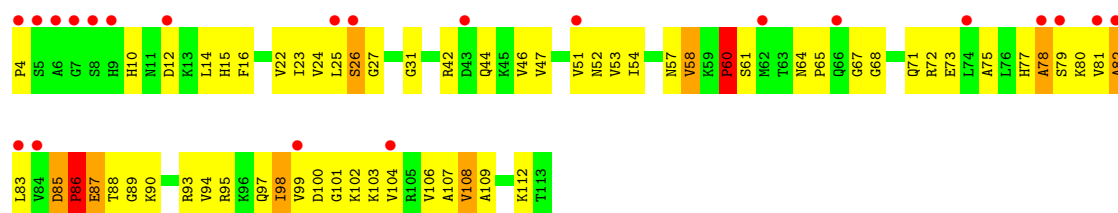
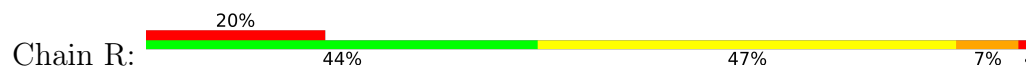


- Molecule 18: 50S ribosomal protein L23

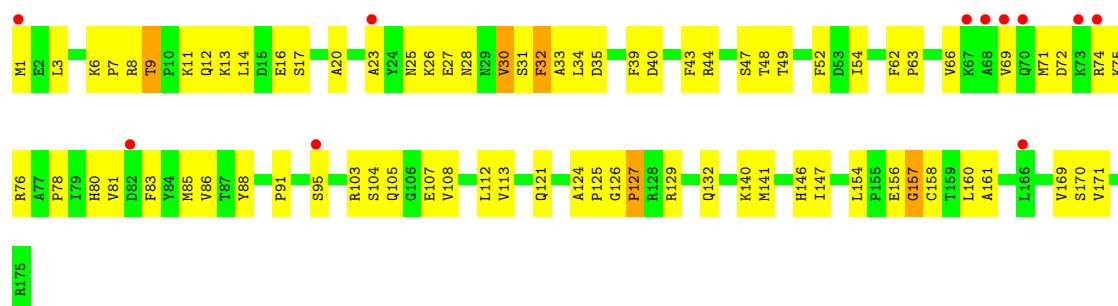




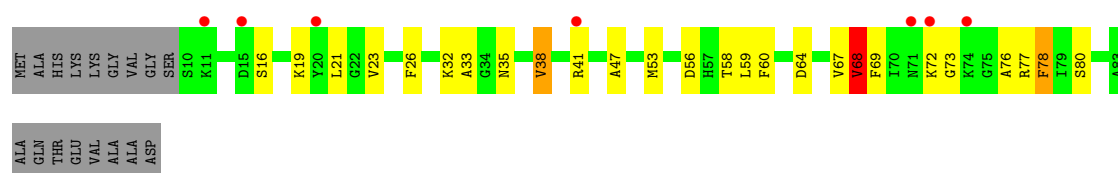
• Molecule 19: 50S ribosomal protein L24



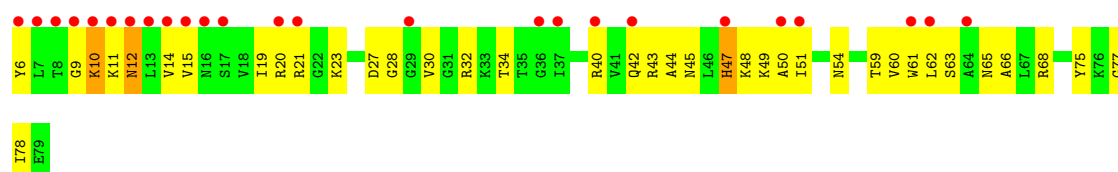
• Molecule 20: 50S ribosomal protein L25



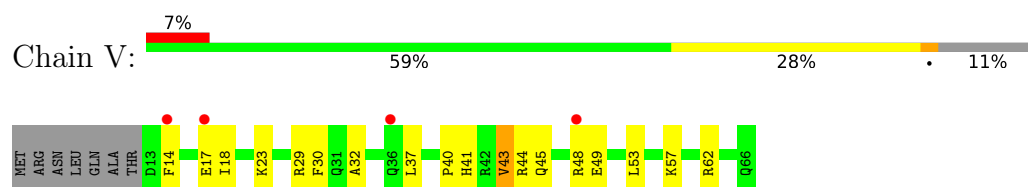
• Molecule 21: 50S ribosomal protein L27



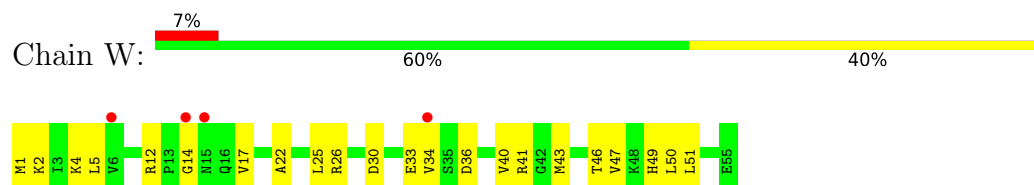
• Molecule 22: 50S ribosomal protein L28



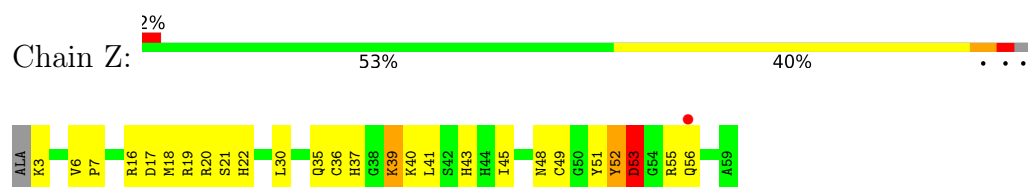
• Molecule 23: 50S ribosomal protein L29



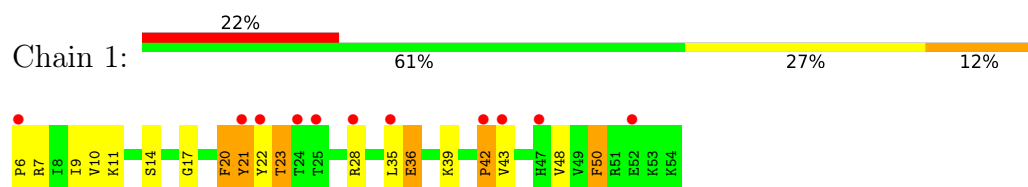
• Molecule 24: 50S ribosomal protein L30



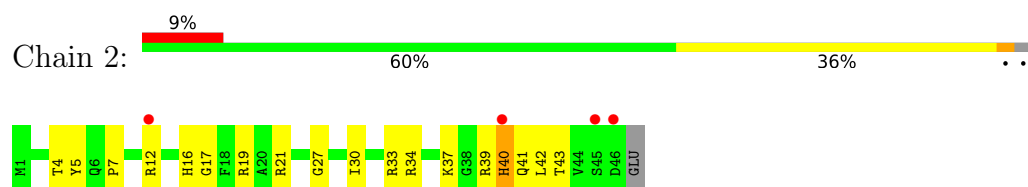
• Molecule 25: 50S ribosomal protein L32



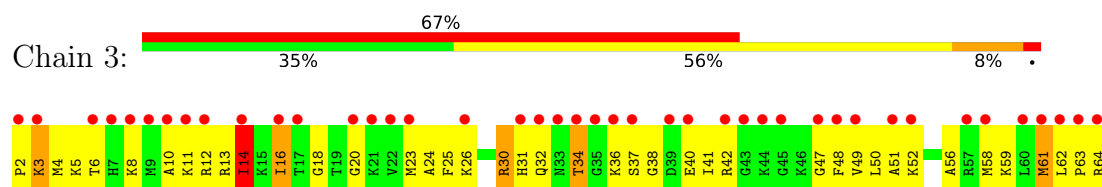
• Molecule 26: 50S ribosomal protein L33



• Molecule 27: 50S ribosomal protein L34



• Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.00Å 410.74Å 697.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.22 49.67 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.67-3.22) 99.3 (49.67-3.22)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.224 , 0.253 0.223 , 0.229	Depositor DCC
R_{free} test set	19448 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 28.4	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	0.95	EDS
Total number of atoms	84486	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: CA, EOH, MPD, K, NA, SPD, QU2, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.45	0/64872	0.68	15/101178 (0.0%)
2	Y	0.34	0/2904	0.58	0/4525
3	A	0.40	0/2050	0.76	2/2772 (0.1%)
4	B	0.62	0/1572	0.93	2/2112 (0.1%)
5	C	0.54	0/1502	0.88	1/2035 (0.0%)
6	D	0.28	0/1393	0.64	0/1873
7	E	0.29	0/1308	0.57	0/1771
8	G	0.55	1/1134 (0.1%)	0.83	0/1535
9	H	0.71	0/1007	1.04	1/1352 (0.1%)
10	I	0.56	0/994	0.99	2/1338 (0.1%)
11	J	0.52	0/1085	0.93	1/1451 (0.1%)
12	K	0.72	0/901	1.19	5/1208 (0.4%)
13	L	0.36	0/767	0.72	0/1027
14	M	0.70	0/936	0.98	0/1257
15	N	0.63	0/971	1.04	3/1296 (0.2%)
16	O	0.49	0/743	0.92	0/995
17	P	0.67	0/1027	0.92	1/1375 (0.1%)
18	Q	0.48	0/716	0.82	0/963
19	R	0.47	0/781	0.85	0/1062
20	S	0.30	0/1313	0.60	0/1796
21	T	0.48	0/543	0.85	0/722
22	U	0.46	0/524	0.82	0/707
23	V	0.33	0/441	0.58	0/586
24	W	0.43	0/426	0.75	0/568
25	Z	0.77	1/460 (0.2%)	1.34	2/618 (0.3%)
26	1	0.43	0/317	0.77	0/434
27	2	0.46	0/387	0.88	0/509
28	3	0.52	0/464	0.94	0/611
All	All	0.47	2/91538 (0.0%)	0.72	35/137676 (0.0%)

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	2
4	B	0	2
5	C	0	2
8	G	0	3
10	I	0	4
11	J	0	6
12	K	0	1
14	M	0	1
16	O	0	1
17	P	0	2
19	R	0	3
20	S	0	1
21	T	0	1
22	U	0	1
25	Z	0	2
28	3	0	4
All	All	0	36

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	56	GLN	CD-OE1	5.83	1.34	1.23
8	G	140	GLN	CG-CD	-5.24	1.39	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	50	ARG	CB-CG-CD	-9.90	88.53	111.30
9	H	37	GLY	N-CA-C	7.93	121.20	111.45
1	X	1288	A	N9-C1'-C2'	7.51	123.26	112.00
25	Z	56	GLN	CG-CD-NE2	-7.30	105.45	116.40
1	X	1391	A	C4'-C3'-O3'	6.85	119.67	109.40

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	210	GLY	Peptide
3	A	271	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	B	132	LYS	Peptide
4	B	146	THR	Peptide
5	C	49	ALA	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	57935	0	29196	1270	0
2	Y	2598	0	1328	75	0
3	A	2011	0	2012	132	0
4	B	1544	0	1605	87	0
5	C	1479	0	1488	116	0
6	D	1375	0	1433	68	0
7	E	1286	0	1336	59	0
8	G	1110	0	1133	83	0
9	H	997	0	1046	70	0
10	I	982	0	973	62	0
11	J	1062	0	1067	64	0
12	K	893	0	944	40	0
13	L	761	0	776	47	0
14	M	923	0	942	55	0
15	N	955	0	974	60	0
16	O	736	0	735	45	0
17	P	1014	0	1085	48	0
18	Q	705	0	717	37	0
19	R	771	0	740	53	0
20	S	1288	0	1237	68	0
21	T	537	0	537	21	0
22	U	519	0	501	37	0
23	V	438	0	456	13	0
24	W	424	0	470	17	0
25	Z	448	0	448	35	0
26	1	314	0	249	16	0
27	2	383	0	414	19	0
28	3	459	0	486	57	0
29	X	50	0	0	0	0
30	2	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	1	0	0	0	0
30	A	3	0	0	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	K	1	0	0	0	0
30	M	1	0	0	0	0
30	N	3	0	0	0	0
30	X	335	0	0	0	0
30	Y	17	0	0	0	0
31	X	80	0	124	18	0
32	X	32	0	55	2	0
33	X	1	0	0	0	0
34	X	3	0	6	0	0
35	X	5	0	0	0	0
36	X	1	0	0	0	0
All	All	84486	0	54513	2434	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 18.

The worst 5 of 2434 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)
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.30	1.10
1:X:243:G:H2'	1:X:244:C:H5'	1.32	1.07
18:Q:89:GLU:HB2	18:Q:91:LEU:HD22	1.38	1.06
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.38	1.05
1:X:566:U:O3'	8:G:140:GLN:NE2	1.88	1.04

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	270/274 (98%)	221 (82%)	30 (11%)	19 (7%)	1	6
4	B	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	3	23
5	C	194/205 (95%)	152 (78%)	29 (15%)	13 (7%)	1	7
6	D	175/177 (99%)	140 (80%)	29 (17%)	6 (3%)	3	19
7	E	169/171 (99%)	144 (85%)	18 (11%)	7 (4%)	2	16
8	G	140/143 (98%)	111 (79%)	18 (13%)	11 (8%)	1	4
9	H	132/134 (98%)	120 (91%)	9 (7%)	3 (2%)	5	27
10	I	135/137 (98%)	109 (81%)	18 (13%)	8 (6%)	1	9
11	J	133/136 (98%)	102 (77%)	22 (16%)	9 (7%)	1	6
12	K	113/116 (97%)	101 (89%)	8 (7%)	4 (4%)	3	19
13	L	102/104 (98%)	80 (78%)	17 (17%)	5 (5%)	1	12
14	M	116/166 (70%)	100 (86%)	9 (8%)	7 (6%)	1	9
15	N	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	4	25
16	O	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	1	11
17	P	127/134 (95%)	119 (94%)	8 (6%)	0	100	100
18	Q	90/93 (97%)	80 (89%)	8 (9%)	2 (2%)	5	28
19	R	108/110 (98%)	73 (68%)	19 (18%)	16 (15%)	0	1
20	S	173/175 (99%)	136 (79%)	28 (16%)	9 (5%)	1	11
21	T	72/91 (79%)	61 (85%)	8 (11%)	3 (4%)	2	15
22	U	72/74 (97%)	51 (71%)	17 (24%)	4 (6%)	1	10
23	V	52/61 (85%)	48 (92%)	3 (6%)	1 (2%)	6	31
24	W	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
25	Z	55/58 (95%)	44 (80%)	7 (13%)	4 (7%)	1	5
26	1	47/49 (96%)	33 (70%)	8 (17%)	6 (13%)	0	1
27	2	44/47 (94%)	38 (86%)	4 (9%)	2 (4%)	2	14
28	3	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	0	4
All	All	3048/3194 (95%)	2511 (82%)	379 (12%)	158 (5%)	1	11

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	90	ALA
3	A	153	ALA
3	A	242	ALA
3	A	247	VAL
3	A	252	LYS

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	197/215 (92%)	195 (99%)	2 (1%)	68	78
4	B	155/155 (100%)	152 (98%)	3 (2%)	50	71
5	C	151/163 (93%)	145 (96%)	6 (4%)	28	59
6	D	147/153 (96%)	145 (99%)	2 (1%)	59	75
7	E	136/136 (100%)	136 (100%)	0	100	100
8	G	117/119 (98%)	115 (98%)	2 (2%)	53	72
9	H	103/103 (100%)	100 (97%)	3 (3%)	37	64
10	I	93/105 (89%)	90 (97%)	3 (3%)	34	63
11	J	104/110 (94%)	101 (97%)	3 (3%)	37	64
12	K	91/93 (98%)	85 (93%)	6 (7%)	15	45
13	L	69/74 (93%)	68 (99%)	1 (1%)	59	75
14	M	97/134 (72%)	95 (98%)	2 (2%)	47	69
15	N	91/96 (95%)	90 (99%)	1 (1%)	65	77
16	O	71/78 (91%)	71 (100%)	0	100	100
17	P	107/115 (93%)	102 (95%)	5 (5%)	23	55
18	Q	71/75 (95%)	69 (97%)	2 (3%)	38	65
19	R	77/91 (85%)	77 (100%)	0	100	100
20	S	134/149 (90%)	132 (98%)	2 (2%)	57	74
21	T	51/67 (76%)	49 (96%)	2 (4%)	28	60
22	U	45/59 (76%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	43/49 (88%)	43 (100%)	0	100	100
24	W	48/48 (100%)	47 (98%)	1 (2%)	47	69
25	Z	50/51 (98%)	50 (100%)	0	100	100
26	1	22/44 (50%)	21 (96%)	1 (4%)	24	56
27	2	39/40 (98%)	38 (97%)	1 (3%)	40	66
28	3	42/50 (84%)	41 (98%)	1 (2%)	43	68
All	All	2351/2572 (91%)	2302 (98%)	49 (2%)	47	69

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	102	THR
17	P	25	PHE
12	K	109	THR
14	M	13	LEU
17	P	96	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	115	ASN
19	R	15	HIS
25	Z	56	GLN
5	C	183	HIS
5	C	176	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2686/2880 (93%)	753 (28%)	76 (2%)
2	Y	121/123 (98%)	33 (27%)	4 (3%)
All	All	2807/3003 (93%)	786 (28%)	80 (2%)

5 of 786 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U
1	X	10	A

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Mol	Chain	Res	Type
1	X	12	U
1	X	13	A
1	X	14	A

5 of 80 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1920	A
1	X	2705	A
1	X	2180	U
1	X	2325	A
1	X	2848	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 [i](#)

Of 388 ligands modelled in this entry, 374 are monoatomic - leaving 14 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	$\# Z > 2$
31	SPD	X	3244	1	9,9,9	0.27	0	8,8,8	0.83	0
32	MPD	X	3247	-	7,7,7	0.40	0	9,10,10	0.72	0
31	SPD	X	3241	1	9,9,9	0.31	0	8,8,8	0.80	0
31	SPD	X	3242	1	9,9,9	0.61	0	8,8,8	0.95	0
31	SPD	X	3243	1	9,9,9	0.64	0	8,8,8	1.15	1 (12%)
34	EOH	X	3250	-	2,2,2	0.51	0	1,1,1	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SPD	X	3237	1	9,9,9	0.69	0	8,8,8	1.19	1 (12%)
31	SPD	X	3238	1	9,9,9	0.86	0	8,8,8	2.09	3 (37%)
32	MPD	X	3246	-	7,7,7	0.56	0	9,10,10	1.14	1 (11%)
31	SPD	X	3240	1	9,9,9	0.67	0	8,8,8	1.37	1 (12%)
32	MPD	X	3248	-	7,7,7	0.63	0	9,10,10	0.42	0
29	QU2	X	2901	-	53,53,53	1.04	4 (7%)	69,76,76	1.88	14 (20%)
31	SPD	X	3239	1	9,9,9	0.69	0	8,8,8	1.88	2 (25%)
32	MPD	X	3245	-	7,7,7	0.57	0	9,10,10	0.39	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
31	SPD	X	3244	1	-	2/7/7/7	-
32	MPD	X	3247	-	-	3/5/5/5	-
31	SPD	X	3241	1	-	1/7/7/7	-
31	SPD	X	3242	1	-	1/7/7/7	-
31	SPD	X	3243	1	-	3/7/7/7	-
31	SPD	X	3237	1	-	4/7/7/7	-
31	SPD	X	3238	1	-	1/7/7/7	-
32	MPD	X	3246	-	-	3/5/5/5	-
31	SPD	X	3240	1	-	1/7/7/7	-
32	MPD	X	3248	-	-	4/5/5/5	-
29	QU2	X	2901	-	-	21/57/98/98	0/3/4/4
31	SPD	X	3239	1	-	2/7/7/7	-
32	MPD	X	3245	-	-	1/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	QU2	C32-C31	3.98	1.60	1.52
29	X	2901	QU2	C7-C8	3.28	1.62	1.54
29	X	2901	QU2	C7-C6	2.35	1.57	1.54
29	X	2901	QU2	O6-C32	2.12	1.47	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	QU2	C8-C7-C6	5.52	124.99	115.09
29	X	2901	QU2	C5-C4-C3	5.31	126.35	109.46
31	X	3238	SPD	C7-N6-C5	4.51	134.73	113.40
29	X	2901	QU2	O8-C22-C23	4.30	118.67	108.09
29	X	2901	QU2	C36-O6-C32	4.09	124.97	114.47

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

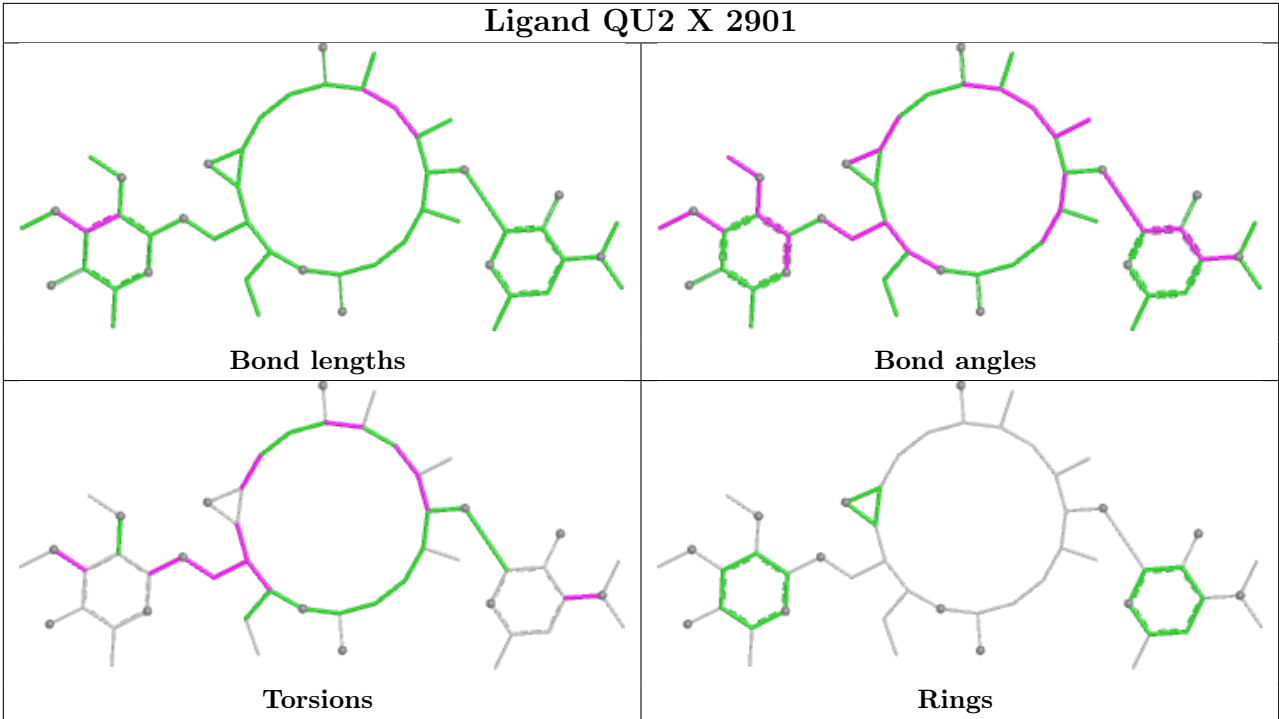
Mol	Chain	Res	Type	Atoms
29	X	2901	QU2	C10-C11-C12-C13
29	X	2901	QU2	C10-C11-C12-O12
29	X	2901	QU2	C12-C13-C14-C15
29	X	2901	QU2	O12-C13-C14-C15
29	X	2901	QU2	O12-C13-C14-C21

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	3244	SPD	1	0
31	X	3242	SPD	1	0
31	X	3243	SPD	5	0
31	X	3238	SPD	5	0
32	X	3246	MPD	1	0
31	X	3240	SPD	3	0
32	X	3248	MPD	1	0
31	X	3239	SPD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	724:C	O3'	725:C	P	4.40

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	2699/2880 (93%)	-0.22	54 (2%) 65 45	35, 122, 216, 317	2 (0%)
2	Y	122/123 (99%)	-0.00	5 (4%) 41 26	131, 174, 197, 204	0
3	A	272/274 (99%)	1.11	54 (19%) 3 2	102, 146, 172, 180	0
4	B	206/206 (100%)	0.44	14 (6%) 23 15	83, 99, 121, 130	0
5	C	196/205 (95%)	0.86	18 (9%) 14 10	94, 144, 175, 183	0
6	D	177/177 (100%)	1.38	46 (25%) 1 2	197, 222, 244, 253	0
7	E	171/171 (100%)	0.68	20 (11%) 9 7	130, 176, 217, 223	0
8	G	142/143 (99%)	0.89	20 (14%) 6 5	92, 121, 139, 144	0
9	H	134/134 (100%)	0.25	7 (5%) 33 21	86, 93, 104, 108	0
10	I	137/137 (100%)	2.06	58 (42%) 0 1	112, 159, 177, 179	0
11	J	135/136 (99%)	1.61	39 (28%) 1 1	133, 156, 174, 182	0
12	K	115/116 (99%)	0.23	8 (6%) 22 14	76, 81, 91, 93	0
13	L	104/104 (100%)	1.68	34 (32%) 1 1	158, 170, 176, 179	0
14	M	118/166 (71%)	0.52	10 (8%) 16 11	90, 98, 118, 124	0
15	N	117/117 (100%)	0.81	17 (14%) 6 5	87, 118, 147, 154	0
16	O	98/98 (100%)	0.82	16 (16%) 4 3	105, 139, 163, 169	0
17	P	129/134 (96%)	0.29	5 (3%) 43 27	83, 92, 118, 135	0
18	Q	92/93 (98%)	0.91	14 (15%) 5 4	114, 137, 155, 161	0
19	R	110/110 (100%)	1.06	22 (20%) 3 2	128, 135, 177, 198	0
20	S	175/175 (100%)	0.53	11 (6%) 26 16	161, 189, 202, 208	0
21	T	74/91 (81%)	0.71	7 (9%) 14 9	129, 139, 146, 151	0
22	U	74/74 (100%)	1.42	25 (33%) 1 1	129, 164, 191, 198	0
23	V	54/61 (88%)	0.35	4 (7%) 20 13	149, 159, 187, 199	0
24	W	55/55 (100%)	0.61	4 (7%) 21 13	130, 137, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/58 (98%)	0.22	1 (1%) 67 48	76, 91, 115, 122	0
26	1	49/49 (100%)	1.30	11 (22%) 2 2	158, 163, 167, 170	0
27	2	46/47 (97%)	0.83	4 (8%) 16 11	94, 110, 119, 123	0
28	3	63/63 (100%)	2.72	42 (66%) 0 0	136, 142, 153, 154	0
All	All	5921/6197 (95%)	0.38	570 (9%) 13 9	35, 133, 212, 317	2 (0%)

The worst 5 of 570 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	774	A	33.0
10	I	67	ASN	13.1
1	X	2045	A	11.7
11	J	21	ASP	8.5
10	I	68	VAL	7.6

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
30	MG	Y	208	1/1	0.20	0.30	180,180,180,180	0
30	MG	X	2968	1/1	0.25	0.35	114,114,114,114	0
30	MG	Y	210	1/1	0.25	0.54	149,149,149,149	0
30	MG	X	3223	1/1	0.28	0.68	137,137,137,137	0
30	MG	X	3224	1/1	0.34	0.63	133,133,133,133	0
30	MG	X	3164	1/1	0.36	0.40	149,149,149,149	0
30	MG	X	3199	1/1	0.36	0.39	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3024	1/1	0.36	0.82	122,122,122,122	0
30	MG	X	3166	1/1	0.48	0.41	139,139,139,139	0
30	MG	X	3120	1/1	0.49	0.59	110,110,110,110	0
30	MG	X	3190	1/1	0.50	1.11	183,183,183,183	0
30	MG	X	3097	1/1	0.50	0.56	132,132,132,132	0
30	MG	X	2951	1/1	0.51	0.62	115,115,115,115	0
30	MG	X	3043	1/1	0.53	0.64	120,120,120,120	0
30	MG	X	2978	1/1	0.54	0.77	95,95,95,95	0
30	MG	X	3073	1/1	0.55	0.41	137,137,137,137	0
30	MG	X	3210	1/1	0.55	0.54	99,99,99,99	0
30	MG	X	3058	1/1	0.55	0.37	156,156,156,156	0
30	MG	X	3204	1/1	0.56	0.25	161,161,161,161	0
30	MG	X	3208	1/1	0.57	0.48	104,104,104,104	0
30	MG	X	2950	1/1	0.57	0.53	122,122,122,122	0
30	MG	X	2971	1/1	0.58	0.29	149,149,149,149	0
30	MG	X	2953	1/1	0.58	0.75	125,125,125,125	0
30	MG	X	3188	1/1	0.58	0.36	131,131,131,131	0
30	MG	Y	205	1/1	0.59	0.53	123,123,123,123	0
30	MG	Y	206	1/1	0.59	0.29	148,148,148,148	0
30	MG	X	3101	1/1	0.60	0.46	128,128,128,128	0
30	MG	X	3059	1/1	0.60	0.23	149,149,149,149	0
30	MG	X	2928	1/1	0.62	0.32	127,127,127,127	0
30	MG	X	2948	1/1	0.62	0.65	103,103,103,103	0
30	MG	X	3168	1/1	0.62	0.26	135,135,135,135	0
30	MG	X	2985	1/1	0.62	0.69	101,101,101,101	0
30	MG	X	2989	1/1	0.62	0.63	111,111,111,111	0
30	MG	X	2983	1/1	0.63	0.74	121,121,121,121	0
30	MG	X	3103	1/1	0.63	0.35	145,145,145,145	0
30	MG	X	3009	1/1	0.63	0.33	123,123,123,123	0
30	MG	X	3117	1/1	0.64	0.64	130,130,130,130	0
30	MG	X	3191	1/1	0.64	0.17	146,146,146,146	0
30	MG	X	3083	1/1	0.64	0.28	104,104,104,104	0
30	MG	A	302	1/1	0.64	0.89	104,104,104,104	0
30	MG	X	3056	1/1	0.65	0.40	149,149,149,149	0
30	MG	X	3026	1/1	0.65	0.38	107,107,107,107	0
30	MG	X	3231	1/1	0.65	0.28	99,99,99,99	0
30	MG	Y	201	1/1	0.65	0.31	126,126,126,126	0
30	MG	Y	204	1/1	0.65	0.45	140,140,140,140	0
30	MG	X	3057	1/1	0.66	0.34	131,131,131,131	0
30	MG	X	3152	1/1	0.66	0.28	88,88,88,88	0
30	MG	X	3173	1/1	0.67	0.28	191,191,191,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3052	1/1	0.67	0.34	121,121,121,121	0
30	MG	Y	212	1/1	0.67	0.23	186,186,186,186	0
30	MG	X	2906	1/1	0.67	0.53	94,94,94,94	0
30	MG	X	3077	1/1	0.68	0.28	118,118,118,118	0
30	MG	X	2987	1/1	0.68	0.33	107,107,107,107	0
30	MG	Y	209	1/1	0.68	0.43	140,140,140,140	0
30	MG	X	2917	1/1	0.68	0.63	79,79,79,79	0
30	MG	X	3213	1/1	0.68	0.47	99,99,99,99	0
30	MG	X	2919	1/1	0.68	0.74	89,89,89,89	0
30	MG	Y	207	1/1	0.69	0.38	131,131,131,131	0
30	MG	Y	214	1/1	0.69	0.31	122,122,122,122	0
30	MG	X	3067	1/1	0.69	0.32	85,85,85,85	0
30	MG	X	3209	1/1	0.70	0.33	81,81,81,81	0
30	MG	X	3217	1/1	0.71	0.58	83,83,83,83	0
30	MG	X	3022	1/1	0.71	0.53	120,120,120,120	0
30	MG	X	3198	1/1	0.71	0.33	132,132,132,132	0
30	MG	X	3107	1/1	0.72	0.28	122,122,122,122	0
30	MG	Y	202	1/1	0.72	0.57	122,122,122,122	0
30	MG	X	2926	1/1	0.72	0.39	99,99,99,99	0
30	MG	X	2940	1/1	0.73	0.71	89,89,89,89	0
30	MG	X	2981	1/1	0.73	0.38	103,103,103,103	0
30	MG	X	3202	1/1	0.73	0.35	156,156,156,156	0
31	SPD	X	3238	10/10	0.73	0.35	79,79,79,79	0
30	MG	X	3159	1/1	0.74	0.46	143,143,143,143	0
30	MG	X	3161	1/1	0.74	0.48	107,107,107,107	0
30	MG	X	2927	1/1	0.74	0.61	77,77,77,77	0
30	MG	Y	211	1/1	0.74	0.25	173,173,173,173	0
30	MG	X	3130	1/1	0.75	1.09	143,143,143,143	0
30	MG	X	2942	1/1	0.76	0.44	73,73,73,73	0
30	MG	X	3165	1/1	0.76	0.35	144,144,144,144	0
30	MG	X	2974	1/1	0.76	0.58	86,86,86,86	0
30	MG	X	2939	1/1	0.76	0.26	93,93,93,93	0
30	MG	X	3230	1/1	0.76	0.29	119,119,119,119	0
30	MG	X	2938	1/1	0.76	0.36	104,104,104,104	0
30	MG	X	3234	1/1	0.76	0.40	75,75,75,75	0
32	MPD	X	3245	8/8	0.76	0.23	128,128,128,128	0
30	MG	X	3086	1/1	0.77	0.25	112,112,112,112	0
30	MG	X	2944	1/1	0.77	0.50	101,101,101,101	0
30	MG	X	3187	1/1	0.77	0.35	120,120,120,120	0
30	MG	X	3116	1/1	0.77	0.47	115,115,115,115	0
30	MG	X	3189	1/1	0.77	0.17	153,153,153,153	0
30	MG	X	3004	1/1	0.77	0.94	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2915	1/1	0.78	0.41	83,83,83,83	0
30	MG	X	3001	1/1	0.78	0.54	128,128,128,128	0
30	MG	X	3221	1/1	0.78	0.46	82,82,82,82	0
30	MG	X	3036	1/1	0.78	0.32	89,89,89,89	0
30	MG	X	2921	1/1	0.78	0.32	97,97,97,97	0
30	MG	Y	217	1/1	0.78	0.24	161,161,161,161	0
30	MG	X	2925	1/1	0.78	0.44	99,99,99,99	0
30	MG	A	303	1/1	0.78	0.49	113,113,113,113	0
30	MG	X	2960	1/1	0.78	0.49	74,74,74,74	0
30	MG	X	3233	1/1	0.78	0.43	68,68,68,68	0
30	MG	X	3005	1/1	0.79	0.43	120,120,120,120	0
30	MG	X	3085	1/1	0.79	0.26	127,127,127,127	0
30	MG	X	3192	1/1	0.79	0.37	88,88,88,88	0
30	MG	X	2913	1/1	0.79	0.36	85,85,85,85	0
30	MG	X	3131	1/1	0.79	0.31	83,83,83,83	0
30	MG	X	3041	1/1	0.79	0.28	88,88,88,88	0
30	MG	X	3216	1/1	0.80	0.20	135,135,135,135	0
30	MG	X	2972	1/1	0.80	0.49	106,106,106,106	0
30	MG	X	3111	1/1	0.80	0.33	100,100,100,100	0
30	MG	X	2923	1/1	0.80	0.48	89,89,89,89	0
30	MG	X	2993	1/1	0.80	0.24	95,95,95,95	0
30	MG	X	3118	1/1	0.80	0.57	98,98,98,98	0
30	MG	X	3008	1/1	0.80	0.32	110,110,110,110	0
30	MG	Y	213	1/1	0.80	0.55	131,131,131,131	0
30	MG	X	2998	1/1	0.80	0.36	84,84,84,84	0
30	MG	X	3207	1/1	0.80	0.47	102,102,102,102	0
30	MG	X	3186	1/1	0.80	0.27	105,105,105,105	0
30	MG	X	3015	1/1	0.80	0.42	72,72,72,72	0
30	MG	I	202	1/1	0.80	0.53	143,143,143,143	0
30	MG	X	3148	1/1	0.80	0.42	88,88,88,88	0
30	MG	X	3048	1/1	0.80	0.39	112,112,112,112	0
30	MG	Y	216	1/1	0.81	0.22	152,152,152,152	0
30	MG	X	3225	1/1	0.81	0.24	132,132,132,132	0
30	MG	X	2962	1/1	0.81	0.46	89,89,89,89	0
30	MG	X	3110	1/1	0.81	0.23	127,127,127,127	0
30	MG	X	2931	1/1	0.81	0.29	93,93,93,93	0
30	MG	X	3176	1/1	0.81	0.29	106,106,106,106	0
30	MG	X	3214	1/1	0.81	0.41	94,94,94,94	0
30	MG	X	3112	1/1	0.82	0.71	128,128,128,128	0
30	MG	X	2963	1/1	0.82	0.38	94,94,94,94	0
30	MG	X	3146	1/1	0.82	0.37	97,97,97,97	0
30	MG	X	2969	1/1	0.82	0.29	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3050	1/1	0.82	0.42	91,91,91,91	0
31	SPD	X	3239	10/10	0.82	0.31	78,78,78,78	0
30	MG	X	2965	1/1	0.82	0.52	99,99,99,99	0
32	MPD	X	3246	8/8	0.82	0.23	93,93,93,93	0
34	EOH	X	3250	3/3	0.82	1.06	88,88,88,88	0
30	MG	X	2934	1/1	0.83	0.44	95,95,95,95	0
30	MG	X	3060	1/1	0.83	0.30	84,84,84,84	0
30	MG	X	2952	1/1	0.83	0.50	78,78,78,78	0
30	MG	X	3135	1/1	0.83	0.12	90,90,90,90	0
30	MG	X	3140	1/1	0.83	0.46	98,98,98,98	0
30	MG	X	3113	1/1	0.83	0.48	86,86,86,86	0
30	MG	X	2930	1/1	0.83	0.34	87,87,87,87	0
30	MG	N	202	1/1	0.83	0.73	95,95,95,95	0
30	MG	X	3203	1/1	0.83	0.34	157,157,157,157	0
30	MG	X	3183	1/1	0.83	0.33	92,92,92,92	0
30	MG	X	2954	1/1	0.83	0.34	115,115,115,115	0
30	MG	X	3153	1/1	0.83	0.37	110,110,110,110	0
30	MG	X	3006	1/1	0.83	0.17	108,108,108,108	0
30	MG	X	2922	1/1	0.84	0.46	95,95,95,95	0
30	MG	X	3072	1/1	0.84	0.63	123,123,123,123	0
30	MG	X	3016	1/1	0.84	0.32	116,116,116,116	0
30	MG	X	3076	1/1	0.84	0.30	108,108,108,108	0
30	MG	X	2991	1/1	0.84	0.32	90,90,90,90	0
30	MG	X	3079	1/1	0.84	0.21	106,106,106,106	0
30	MG	X	3023	1/1	0.84	0.82	91,91,91,91	0
30	MG	X	2966	1/1	0.84	0.50	89,89,89,89	0
30	MG	A	301	1/1	0.84	0.56	105,105,105,105	0
30	MG	X	2932	1/1	0.84	0.16	94,94,94,94	0
30	MG	X	3172	1/1	0.84	0.35	98,98,98,98	0
30	MG	X	3030	1/1	0.84	0.96	83,83,83,83	0
30	MG	X	2956	1/1	0.84	0.29	107,107,107,107	0
30	MG	X	3182	1/1	0.84	0.13	87,87,87,87	0
30	MG	X	3102	1/1	0.84	0.74	98,98,98,98	0
31	SPD	X	3240	10/10	0.84	0.21	75,75,75,75	0
30	MG	X	3211	1/1	0.84	0.35	111,111,111,111	0
30	MG	X	3010	1/1	0.84	0.47	97,97,97,97	0
30	MG	X	3105	1/1	0.84	0.29	105,105,105,105	0
30	MG	X	2903	1/1	0.85	0.30	89,89,89,89	0
30	MG	X	3025	1/1	0.85	1.53	109,109,109,109	0
30	MG	X	3139	1/1	0.85	0.22	99,99,99,99	0
30	MG	X	3232	1/1	0.85	0.42	87,87,87,87	0
30	MG	X	3108	1/1	0.85	0.30	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3143	1/1	0.85	0.66	95,95,95,95	0
30	MG	X	2967	1/1	0.85	0.39	97,97,97,97	0
30	MG	X	3013	1/1	0.85	0.31	74,74,74,74	0
30	MG	X	2914	1/1	0.85	0.36	79,79,79,79	0
30	MG	X	2964	1/1	0.85	0.48	85,85,85,85	0
30	MG	X	2943	1/1	0.85	0.24	87,87,87,87	0
30	MG	X	3160	1/1	0.85	0.40	108,108,108,108	0
30	MG	X	3064	1/1	0.85	0.41	82,82,82,82	0
30	MG	X	3045	1/1	0.85	0.26	124,124,124,124	0
30	MG	X	3069	1/1	0.85	0.18	131,131,131,131	0
32	MPD	X	3248	8/8	0.85	0.27	94,94,94,94	0
30	MG	X	2996	1/1	0.85	0.42	71,71,71,71	0
30	MG	X	3062	1/1	0.86	0.43	110,110,110,110	0
30	MG	2	102	1/1	0.86	0.67	116,116,116,116	0
30	MG	X	3106	1/1	0.86	0.26	79,79,79,79	0
30	MG	X	2979	1/1	0.86	0.23	95,95,95,95	0
30	MG	X	3220	1/1	0.86	0.37	88,88,88,88	0
30	MG	X	3114	1/1	0.86	0.62	105,105,105,105	0
30	MG	X	3115	1/1	0.86	0.45	108,108,108,108	0
30	MG	X	2957	1/1	0.86	0.36	72,72,72,72	0
30	MG	X	3017	1/1	0.86	0.29	93,93,93,93	0
30	MG	X	3145	1/1	0.87	0.28	106,106,106,106	0
30	MG	X	3235	1/1	0.87	0.64	80,80,80,80	0
30	MG	X	2976	1/1	0.87	0.25	81,81,81,81	0
30	MG	X	3042	1/1	0.87	0.18	89,89,89,89	0
30	MG	X	3170	1/1	0.87	0.27	127,127,127,127	0
30	MG	X	3150	1/1	0.87	0.23	158,158,158,158	0
30	MG	X	3034	1/1	0.87	0.29	99,99,99,99	0
30	MG	X	3174	1/1	0.87	0.52	115,115,115,115	0
30	MG	3	101	1/1	0.87	0.89	103,103,103,103	0
30	MG	X	3104	1/1	0.87	0.32	97,97,97,97	0
30	MG	X	3155	1/1	0.87	0.32	99,99,99,99	0
30	MG	X	3205	1/1	0.87	0.10	186,186,186,186	0
31	SPD	X	3244	10/10	0.87	0.29	137,137,137,137	0
30	MG	X	2986	1/1	0.87	0.49	101,101,101,101	0
30	MG	X	3075	1/1	0.87	0.30	100,100,100,100	0
30	MG	X	3091	1/1	0.87	0.29	85,85,85,85	0
30	MG	X	3047	1/1	0.87	0.88	100,100,100,100	0
35	CA	X	3251	1/1	0.87	0.17	78,78,78,78	0
30	MG	X	3080	1/1	0.88	0.26	98,98,98,98	0
30	MG	X	3185	1/1	0.88	0.26	92,92,92,92	0
30	MG	X	2941	1/1	0.88	0.39	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3051	1/1	0.88	0.22	79,79,79,79	0
30	MG	X	3229	1/1	0.88	0.21	112,112,112,112	0
30	MG	X	3132	1/1	0.88	0.55	75,75,75,75	0
30	MG	X	3020	1/1	0.88	0.23	85,85,85,85	0
30	MG	X	3089	1/1	0.88	0.43	89,89,89,89	0
31	SPD	X	3243	10/10	0.88	0.26	96,96,96,96	0
30	MG	X	3157	1/1	0.88	0.49	97,97,97,97	0
30	MG	X	2916	1/1	0.88	0.24	80,80,80,80	0
30	MG	X	3195	1/1	0.88	0.45	91,91,91,91	0
30	MG	X	3012	1/1	0.88	0.36	101,101,101,101	0
30	MG	X	3181	1/1	0.88	0.12	91,91,91,91	0
30	MG	X	3049	1/1	0.88	0.57	106,106,106,106	0
30	MG	N	203	1/1	0.89	0.32	98,98,98,98	0
30	MG	X	3028	1/1	0.89	0.35	101,101,101,101	0
30	MG	X	3021	1/1	0.89	0.41	90,90,90,90	0
30	MG	X	2905	1/1	0.89	0.40	84,84,84,84	0
30	MG	X	3194	1/1	0.89	0.24	85,85,85,85	0
30	MG	X	2949	1/1	0.89	0.27	91,91,91,91	0
30	MG	X	3228	1/1	0.89	0.30	109,109,109,109	0
30	MG	X	3142	1/1	0.89	0.30	94,94,94,94	0
30	MG	X	3156	1/1	0.89	0.27	121,121,121,121	0
30	MG	X	2984	1/1	0.89	0.33	88,88,88,88	0
30	MG	I	201	1/1	0.89	0.59	105,105,105,105	0
30	MG	X	3018	1/1	0.89	0.13	89,89,89,89	0
30	MG	X	3002	1/1	0.89	0.43	107,107,107,107	0
30	MG	X	3151	1/1	0.90	0.50	157,157,157,157	0
30	MG	X	3215	1/1	0.90	0.13	105,105,105,105	0
30	MG	X	2924	1/1	0.90	0.48	78,78,78,78	0
30	MG	X	2959	1/1	0.90	0.50	79,79,79,79	0
30	MG	X	2929	1/1	0.90	0.23	79,79,79,79	0
30	MG	X	3127	1/1	0.90	0.40	83,83,83,83	0
30	MG	Y	215	1/1	0.90	0.39	130,130,130,130	0
30	MG	X	3222	1/1	0.90	0.22	109,109,109,109	0
30	MG	X	2902	1/1	0.90	0.53	105,105,105,105	0
30	MG	X	3063	1/1	0.90	0.40	88,88,88,88	0
30	MG	X	3081	1/1	0.90	0.20	123,123,123,123	0
30	MG	X	3226	1/1	0.90	0.43	79,79,79,79	0
30	MG	X	3134	1/1	0.90	0.26	82,82,82,82	0
30	MG	X	2945	1/1	0.90	0.23	96,96,96,96	0
30	MG	X	3136	1/1	0.90	0.38	77,77,77,77	0
30	MG	X	3137	1/1	0.90	0.26	78,78,78,78	0
30	MG	X	3200	1/1	0.90	0.19	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3065	1/1	0.90	0.37	102,102,102,102	0
30	MG	X	3169	1/1	0.90	0.50	112,112,112,112	0
30	MG	X	2918	1/1	0.90	0.27	97,97,97,97	0
30	MG	X	3088	1/1	0.90	0.36	87,87,87,87	0
30	MG	X	2912	1/1	0.90	0.48	80,80,80,80	0
30	MG	Y	203	1/1	0.90	0.51	101,101,101,101	0
30	MG	X	2975	1/1	0.90	0.70	79,79,79,79	0
30	MG	X	3094	1/1	0.90	0.20	84,84,84,84	0
30	MG	X	3096	1/1	0.90	0.35	90,90,90,90	0
30	MG	X	3149	1/1	0.90	0.26	100,100,100,100	0
30	MG	X	3014	1/1	0.90	0.15	96,96,96,96	0
30	MG	X	3212	1/1	0.91	0.27	95,95,95,95	0
30	MG	X	3179	1/1	0.91	0.29	75,75,75,75	0
30	MG	X	2935	1/1	0.91	0.26	76,76,76,76	0
30	MG	X	3044	1/1	0.91	0.55	82,82,82,82	0
30	MG	X	3087	1/1	0.91	0.38	82,82,82,82	0
30	MG	X	2994	1/1	0.91	0.16	86,86,86,86	0
30	MG	X	3219	1/1	0.91	0.71	103,103,103,103	0
30	MG	X	3046	1/1	0.91	0.26	94,94,94,94	0
30	MG	X	2977	1/1	0.91	0.48	82,82,82,82	0
30	MG	X	2997	1/1	0.91	0.34	97,97,97,97	0
30	MG	X	3095	1/1	0.91	0.41	106,106,106,106	0
30	MG	X	3126	1/1	0.91	0.22	107,107,107,107	0
30	MG	X	3029	1/1	0.91	0.21	87,87,87,87	0
30	MG	X	3128	1/1	0.91	0.11	92,92,92,92	0
30	MG	X	2988	1/1	0.91	0.38	100,100,100,100	0
30	MG	K	201	1/1	0.91	0.12	89,89,89,89	0
30	MG	N	201	1/1	0.91	0.25	108,108,108,108	0
30	MG	X	3000	1/1	0.91	0.48	98,98,98,98	0
30	MG	X	3074	1/1	0.91	0.49	106,106,106,106	0
30	MG	X	3011	1/1	0.91	0.41	87,87,87,87	0
30	MG	X	3054	1/1	0.91	0.48	93,93,93,93	0
31	SPD	X	3237	10/10	0.91	0.26	82,82,82,82	0
30	MG	X	3055	1/1	0.91	0.30	111,111,111,111	0
30	MG	X	3037	1/1	0.91	0.63	95,95,95,95	0
30	MG	X	3040	1/1	0.91	0.09	143,143,143,143	0
31	SPD	X	3242	10/10	0.91	0.29	95,95,95,95	0
30	MG	X	2970	1/1	0.91	0.51	88,88,88,88	0
30	MG	X	3206	1/1	0.91	0.21	102,102,102,102	0
30	MG	X	3171	1/1	0.91	0.28	116,116,116,116	0
30	MG	X	3141	1/1	0.91	0.23	87,87,87,87	0
30	MG	X	3082	1/1	0.91	0.31	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2946	1/1	0.91	0.43	75,75,75,75	0
30	MG	X	3144	1/1	0.91	0.72	108,108,108,108	0
30	MG	X	3100	1/1	0.92	0.32	88,88,88,88	0
30	MG	X	2999	1/1	0.92	0.18	105,105,105,105	0
30	MG	X	3007	1/1	0.92	0.37	100,100,100,100	0
29	QU2	X	2901	50/50	0.92	0.19	80,80,80,80	0
30	MG	X	2958	1/1	0.92	0.52	79,79,79,79	0
30	MG	X	2910	1/1	0.92	0.34	70,70,70,70	0
30	MG	X	2937	1/1	0.92	0.28	80,80,80,80	0
30	MG	X	3196	1/1	0.92	0.55	86,86,86,86	0
30	MG	X	3019	1/1	0.92	0.41	82,82,82,82	0
30	MG	X	3167	1/1	0.92	0.06	117,117,117,117	0
30	MG	X	2947	1/1	0.92	0.41	89,89,89,89	0
30	MG	X	3201	1/1	0.92	0.29	104,104,104,104	0
30	MG	X	3061	1/1	0.92	0.28	82,82,82,82	0
30	MG	X	3098	1/1	0.92	0.38	69,69,69,69	0
30	MG	X	2995	1/1	0.93	0.40	76,76,76,76	0
30	MG	X	2955	1/1	0.93	0.34	80,80,80,80	0
30	MG	X	2904	1/1	0.93	0.28	62,62,62,62	0
30	MG	X	3099	1/1	0.93	0.38	101,101,101,101	0
30	MG	X	3003	1/1	0.93	0.26	82,82,82,82	0
30	MG	X	2973	1/1	0.93	0.19	107,107,107,107	0
30	MG	X	2936	1/1	0.93	0.23	87,87,87,87	0
30	MG	X	3122	1/1	0.93	0.15	97,97,97,97	0
30	MG	X	3123	1/1	0.93	0.10	104,104,104,104	0
30	MG	X	3180	1/1	0.93	0.13	76,76,76,76	0
30	MG	X	3124	1/1	0.93	0.12	95,95,95,95	0
32	MPD	X	3247	8/8	0.93	0.23	103,103,103,103	0
30	MG	X	3032	1/1	0.93	0.43	56,56,56,56	0
30	MG	X	3236	1/1	0.93	0.39	88,88,88,88	0
30	MG	2	101	1/1	0.93	0.65	103,103,103,103	0
30	MG	X	3121	1/1	0.94	0.40	103,103,103,103	0
30	MG	B	301	1/1	0.94	0.17	72,72,72,72	0
30	MG	X	3078	1/1	0.94	0.55	86,86,86,86	0
30	MG	X	2990	1/1	0.94	0.51	89,89,89,89	0
30	MG	X	3066	1/1	0.94	0.22	94,94,94,94	0
30	MG	X	3035	1/1	0.94	0.22	80,80,80,80	0
30	MG	X	3193	1/1	0.94	0.39	68,68,68,68	0
30	MG	X	2982	1/1	0.94	0.44	83,83,83,83	0
30	MG	X	3090	1/1	0.94	0.21	78,78,78,78	0
30	MG	X	3033	1/1	0.94	0.29	119,119,119,119	0
33	NA	X	3249	1/1	0.94	0.20	91,91,91,91	0

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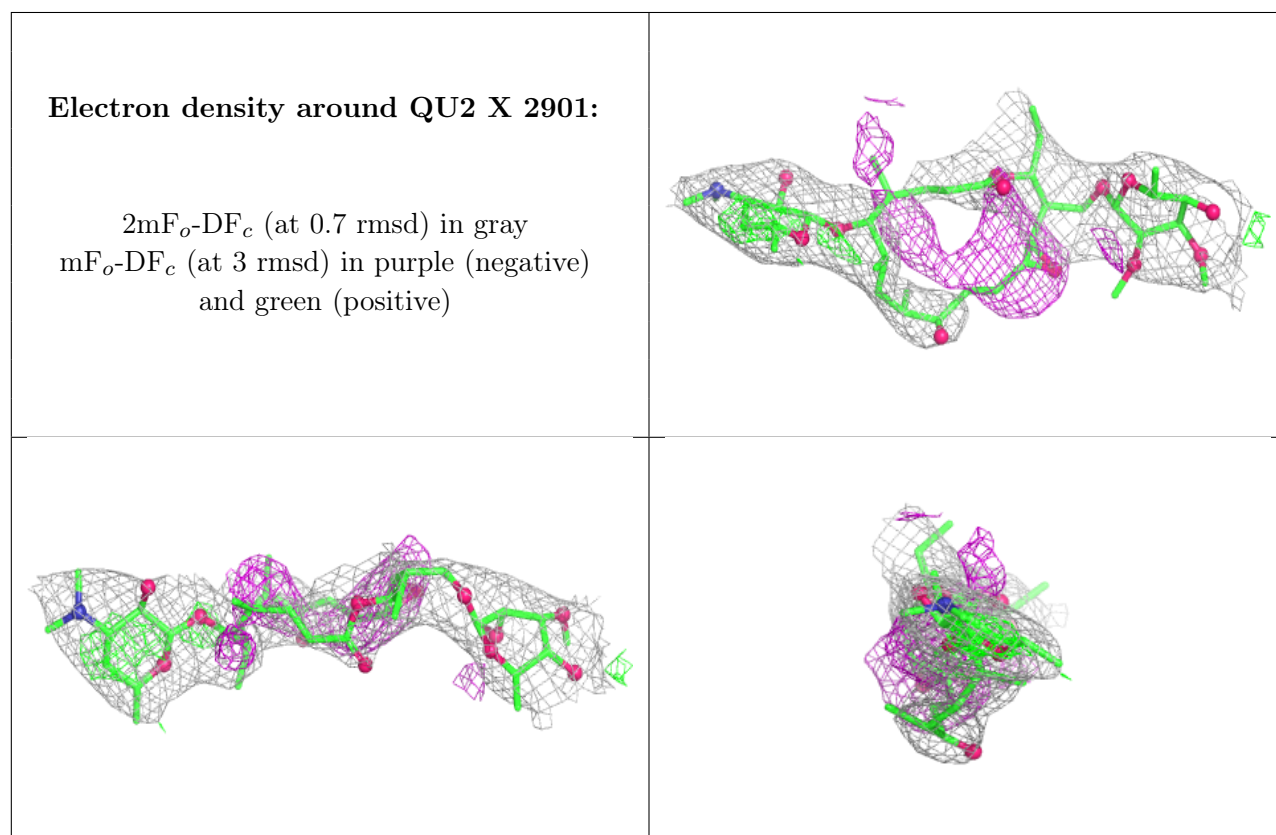
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3197	1/1	0.94	0.13	94,94,94,94	0
30	MG	X	3084	1/1	0.94	0.13	128,128,128,128	0
30	MG	X	3070	1/1	0.95	0.26	105,105,105,105	0
30	MG	X	3133	1/1	0.95	0.65	70,70,70,70	0
30	MG	X	3227	1/1	0.95	0.44	98,98,98,98	0
30	MG	X	3071	1/1	0.95	0.06	155,155,155,155	0
31	SPD	X	3241	10/10	0.95	0.24	160,160,160,160	0
30	MG	X	3158	1/1	0.95	0.48	67,67,67,67	0
30	MG	X	3125	1/1	0.95	0.12	94,94,94,94	0
30	MG	X	3147	1/1	0.95	0.10	93,93,93,93	0
30	MG	X	2961	1/1	0.95	0.33	70,70,70,70	0
30	MG	X	3178	1/1	0.95	0.26	95,95,95,95	0
30	MG	X	3031	1/1	0.95	0.56	69,69,69,69	0
30	MG	X	3038	1/1	0.95	0.26	80,80,80,80	0
30	MG	X	3129	1/1	0.95	0.25	76,76,76,76	0
30	MG	X	3068	1/1	0.95	0.36	83,83,83,83	0
30	MG	X	3039	1/1	0.95	0.32	76,76,76,76	0
35	CA	X	3252	1/1	0.95	0.19	100,100,100,100	0
35	CA	X	3253	1/1	0.95	0.17	72,72,72,72	0
30	MG	X	2909	1/1	0.96	0.21	68,68,68,68	0
30	MG	X	2980	1/1	0.96	0.20	92,92,92,92	0
30	MG	X	3027	1/1	0.96	0.09	107,107,107,107	0
30	MG	X	2907	1/1	0.96	0.31	75,75,75,75	0
30	MG	X	2992	1/1	0.96	0.30	91,91,91,91	0
30	MG	X	2920	1/1	0.96	0.40	67,67,67,67	0
30	MG	X	2911	1/1	0.96	0.48	59,59,59,59	0
30	MG	X	3177	1/1	0.96	0.15	97,97,97,97	0
30	MG	X	3053	1/1	0.96	0.07	110,110,110,110	0
30	MG	M	201	1/1	0.96	0.12	90,90,90,90	0
30	MG	X	3138	1/1	0.96	0.20	85,85,85,85	0
35	CA	X	3255	1/1	0.96	0.06	78,78,78,78	0
30	MG	X	3154	1/1	0.97	0.06	106,106,106,106	0
30	MG	X	2933	1/1	0.97	0.19	81,81,81,81	0
30	MG	X	3109	1/1	0.97	0.50	77,77,77,77	0
30	MG	J	201	1/1	0.97	0.11	134,134,134,134	0
30	MG	X	3092	1/1	0.97	0.15	91,91,91,91	0
30	MG	X	3162	1/1	0.97	0.07	112,112,112,112	0
36	K	X	3256	1/1	0.97	0.05	89,89,89,89	0
30	MG	X	3175	1/1	0.98	0.07	89,89,89,89	0
35	CA	X	3254	1/1	0.98	0.07	82,82,82,82	0
30	MG	X	3093	1/1	0.98	0.13	89,89,89,89	0
30	MG	X	2908	1/1	0.98	0.35	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3184	1/1	0.99	0.05	75,75,75,75	0
30	MG	X	3218	1/1	0.99	0.09	88,88,88,88	0
30	MG	X	3119	1/1	0.99	0.06	102,102,102,102	0
30	MG	X	3163	1/1	0.99	0.19	71,71,71,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.