



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 21, 2026 – 10:11 am BST

PDB ID : 2UUB / pdb_00002uub
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a Valine-ASL with cmo5U in position 34 bound to an mRNA with a GUU-codon in the A-site and paromomycin.
Authors : Weixlbaumer, A.; Murphy, F.V.; Dziergowska, A.; Malkiewicz, A.; Vendeix, F.A.P.; Agris, P.F.; Ramakrishnan, V.
Deposited on : 2007-03-01
Resolution : 2.80 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

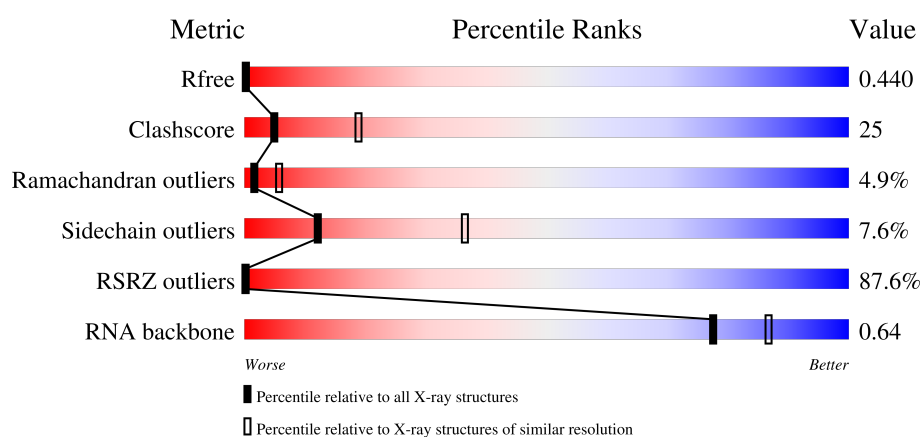
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	A	1522	94% 45% 43% 9% ..
2	B	256	75% 28% 54% 9% 8%
3	C	239	77% 32% 44% 10% 13%
4	D	209	83% 54% 40% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	6	
23	Y	17	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1603	-	-	-	X
25	MG	A	1604	-	-	-	X
25	MG	A	1605	-	-	-	X
25	MG	A	1606	-	-	-	X
25	MG	A	1607	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1610	-	-	-	X
25	MG	A	1612	-	-	-	X
25	MG	A	1618	-	-	-	X
25	MG	A	1622	-	-	-	X
25	MG	A	1625	-	-	-	X
25	MG	A	1628	-	-	-	X
25	MG	A	1630	-	-	-	X
25	MG	A	1631	-	-	-	X
25	MG	A	1632	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	1636	-	-	-	X
25	MG	A	1637	-	-	-	X
25	MG	A	1638	-	-	-	X
25	MG	A	1641	-	-	-	X
25	MG	A	1643	-	-	-	X
25	MG	A	1644	-	-	-	X
25	MG	A	1652	-	-	-	X
25	MG	A	1654	-	-	-	X
25	MG	A	1655	-	-	-	X
25	MG	A	1657	-	-	-	X
25	MG	A	1659	-	-	-	X
25	MG	A	1662	-	-	-	X
25	MG	A	1663	-	-	-	X
25	MG	A	1665	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1669	-	-	-	X
25	MG	A	1671	-	-	-	X
25	MG	A	1673	-	-	-	X
25	MG	A	1676	-	-	-	X
25	MG	A	1678	-	-	-	X
25	MG	A	1680	-	-	-	X
25	MG	A	1681	-	-	-	X
25	MG	A	1683	-	-	-	X
25	MG	A	1684	-	-	-	X
25	MG	A	1685	-	-	-	X
25	MG	A	1686	-	-	-	X
25	MG	A	1687	-	-	-	X
25	MG	A	1688	-	-	-	X
25	MG	A	1692	-	-	-	X
25	MG	A	1694	-	-	-	X
25	MG	A	1696	-	-	-	X
25	MG	A	1701	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1702	-	-	-	X
25	MG	A	1705	-	-	-	X
25	MG	A	1706	-	-	-	X
25	MG	A	1708	-	-	-	X
25	MG	A	1710	-	-	-	X
25	MG	A	1711	-	-	-	X
25	MG	A	1713	-	-	-	X
25	MG	A	1714	-	-	-	X
25	MG	A	1715	-	-	-	X
25	MG	A	1716	-	-	-	X
25	MG	A	1717	-	-	-	X
25	MG	A	1721	-	-	-	X
25	MG	A	1724	-	-	-	X
25	MG	A	1730	-	-	-	X
25	MG	A	1731	-	-	-	X
25	MG	A	1734	-	-	-	X
25	MG	A	1735	-	-	-	X
25	MG	A	1736	-	-	-	X
25	MG	A	1737	-	-	-	X
25	MG	A	1740	-	-	-	X
25	MG	A	1741	-	-	-	X
25	MG	A	1742	-	-	-	X
25	MG	A	1747	-	-	-	X
25	MG	A	1748	-	-	-	X
25	MG	A	1754	-	-	-	X
25	MG	A	1766	-	-	-	X
25	MG	A	1767	-	-	-	X
25	MG	A	1771	-	-	-	X
25	MG	A	1777	-	-	-	X
25	MG	A	1781	-	-	-	X
25	MG	A	1782	-	-	-	X
25	MG	A	1784	-	-	-	X
25	MG	A	1785	-	-	-	X
25	MG	A	1790	-	-	-	X
25	MG	A	1793	-	-	-	X
25	MG	A	1796	-	-	-	X
25	MG	A	1798	-	-	-	X
25	MG	A	1800	-	-	-	X
25	MG	A	1801	-	-	-	X
25	MG	A	1802	-	-	-	X
25	MG	E	201	-	-	-	X
25	MG	N	101	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	K	A	1808	-	-	-	X
26	K	A	1809	-	-	-	X
26	K	A	1811	-	-	-	X
26	K	A	1813	-	-	-	X
26	K	A	1814	-	-	-	X
26	K	A	1816	-	-	-	X
26	K	A	1817	-	-	-	X
26	K	A	1818	-	-	-	X
26	K	A	1822	-	-	-	X
26	K	A	1825	-	-	-	X
26	K	A	1828	-	-	-	X
26	K	A	1829	-	-	-	X
26	K	A	1831	-	-	-	X

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52363 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32489	14462	6011	10505	1511			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

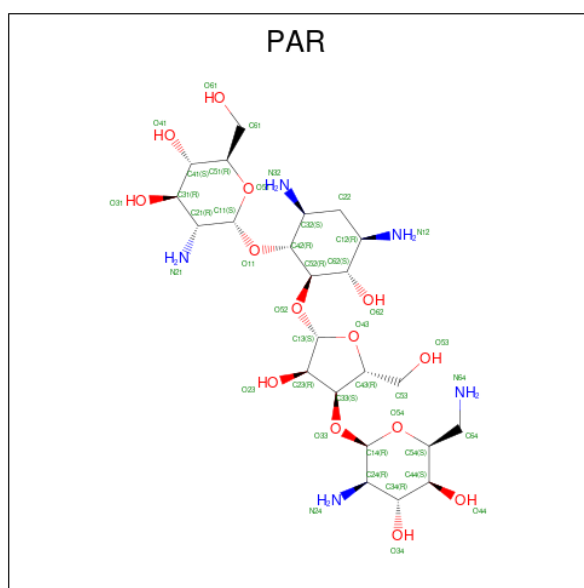
- Molecule 22 is a RNA chain called 5'-R(*GP*UP*UP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

- Molecule 23 is a RNA chain called 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	11	Total	C	N	O	P	0	0	0
			235	107	41	77	10			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	203	Total	Mg	0	0
			203	203		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	1	Total 1	Mg 1	0	0
25	D	1	Total 1	Mg 1	0	0
25	E	2	Total 2	Mg 2	0	0
25	F	1	Total 1	Mg 1	0	0
25	G	1	Total 1	Mg 1	0	0
25	H	1	Total 1	Mg 1	0	0
25	I	1	Total 1	Mg 1	0	0
25	M	1	Total 1	Mg 1	0	0
25	N	1	Total 1	Mg 1	0	0
25	Q	3	Total 3	Mg 3	0	0
25	S	1	Total 1	Mg 1	0	0
25	X	1	Total 1	Mg 1	0	0

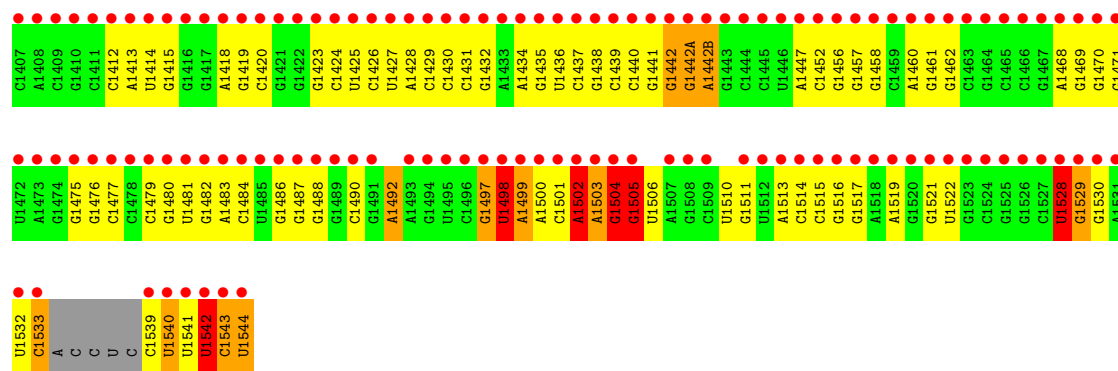
- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	34	Total 34	K 34	0	0
26	E	1	Total 1	K 1	0	0

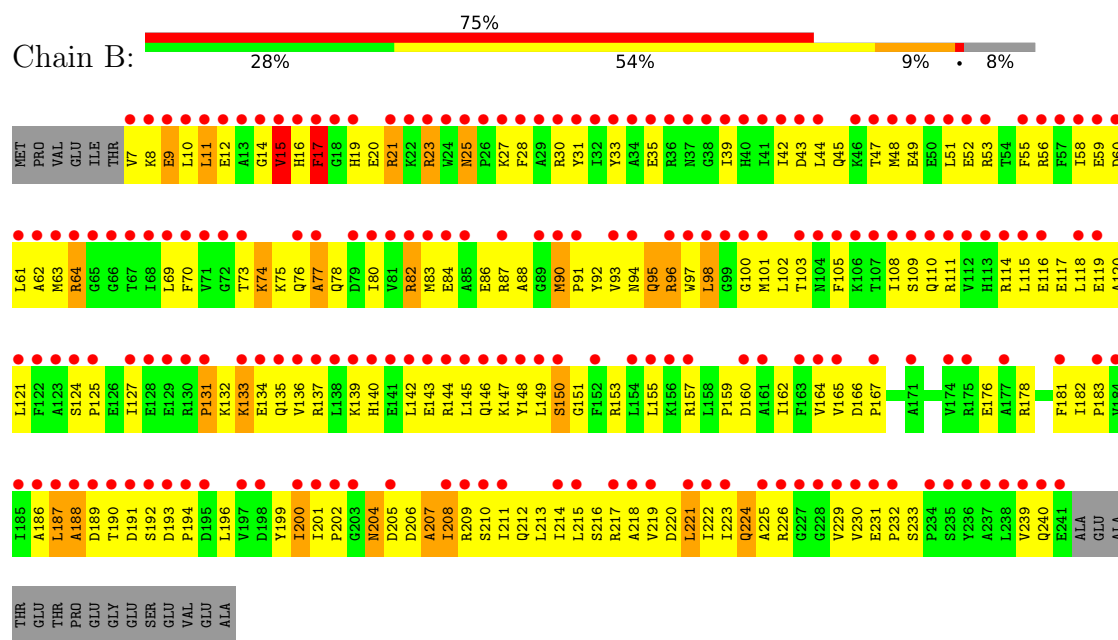
- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total 1	Zn 1	0	0
27	N	1	Total 1	Zn 1	0	0

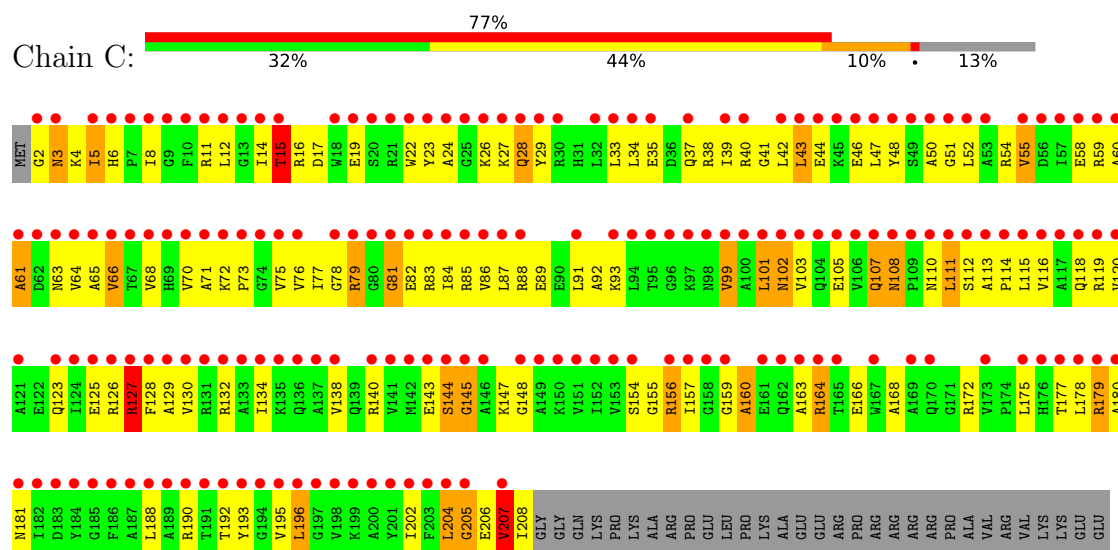
G1347	A1287	A1227	G1166	G1106	A1046	C991	U871	U804	C744	A684	C624
U1348	A1288	C1228	A1168	C1107	G1047	C992	A872	C805	C745	G685	G625
A1349	A1289	A1229	A1169	G1108	U1048	G993	A873	C806	A746	U686	U626
A1350	G1290	C1230	A1170	C1109	C1049	A994	G874	A807	C747	A687	G627
U1351	G1291	G1231	G1171	A1110	G1050	C995	A875	C808	C748	G688	G628
C1352	U1292	U1232	G1172	A1111	C1051	A996	G876	G809	C749	C689	G629
G1353	G1293	G1233	G1173	C1112	U1052	U997	C877	C810	G750	G690	G630
C1354	G1294	G1234	G1174	C1113	U1053	G998	C878	C811	U751	G691	G631
G1355	G1295	U1235	G1175	C1114	C1054	C999	C879	C812	G752	U692	A632
A1356	C1296	A1236	C1115	C1115	U1055	C900	G880	U813	A753	G693	G633
G1357	C1297	C1237	A1176	C1116	U1056	A1001	G881	U814	C754	A694	C634
U1358	A1298	A1238	G1178	G1117	G1057	G1001A	C882	A815	G755	A695	G635
C1359	C1299	U1239	A1179	C1118	U1058	U943	C883	A816	C756	U696	U636
A1360	A1300	U1240	A1180	C1119	C1059	G944	U884	C817	U757	G697	G637
G1361	U1301	G1241	G1181	G1120	U1060	G945	G885	G818	G758	G698	G638
C1362	G1302	C1242	G1182	U1121	G1061	A1005	A886	A819	A759	G699	G639
G1363	C1303	C1243	A1183	U1122	U1062	G947	G887	U820	G760	G700	A640
A1363A	G1304	C1244	G1184	A1123	C1063	C948	G888	G821	G761	C701	U641
U1364	G1305	A1245	G1185	G1124	U1064	A949	A889	C822	C762	A702	A642
G1365	A1306	G1246	G1186	U1125	U1065	U950	G890	G823	G763	G703	C643
C1366	U1307	U1247	G1187	U1126	C1066	G951	G891	G824	G764	A704	G644
G1367	U1308	A1248	A1188	G1127	A1067	U952	A892	G825	G765	U705	G645
C1368	G1309	C1249	C1189	U1128	U1068	G953	C893	C826	A766	A706	U646
G1369	G1310	A1250	G1190	C1129	C1069	G954	G894	U827	A767	C707	C647
U1370	G1311	A1251	A1191	A1130	U1070	U955	G895	A828	A768	C708	A648
G1371	G1312	A1252	C1192	G1131	C1071	U956	C896	C829	G769	G709	G649
U1372	U1313	G1253	G1193	C1132	U1072	U957	G897	G830	C770	G710	G650
G1373	C1314	C1254	U1194	G1133	U1073	A958	G898	U831	G771	G711	C651
A1374	U1315	G1255	G1195	G1134	G1074	A959	C899	U832	U772	G712	U652
C1375	G1316	A1256	U1196	U1135	C1075	U960	A900	U833	G773	G713	A653
U1376	C1317	U1257	U1197	U1136	G1076	U961	A901	C834	G774	G714	G654
A1377	G1318	G1258	G1198	C1137	U1077	C962	G902	U835	G775	A715	A655
C1378	A1319	C1259	U1199	U1138	U1078	G963	G903	G836	G776	A716	C656
G1379	C1320	C1260	C1200	G1139	G1079	A964	C904	G837	A777	C717	G657
U1380	C1321	A1261	A1201	C1140	A1080	A965	U905	U838	C778	G718	G658
C1381	C1322	C1262	G1202	G1141	U1081	G966	A907	C840	A780	C719	G659
G1382	G1323	C1263	C1203	G1142	G1082	C967	G908	U841	U781	G721	G661
A1383	A1324	G1264	A1204	G1143	U1083	A968	A909	C842	A782	A722	A662
C1384	C1325	G1265	U1205	C1144	G1084	A969	C910	C843	C783	U723	A663
G1385	G1326	G1266	G1206	C1145	U1085	C970	U911	U850	G784	G724	G664
C1386	C1327	G1267	G1207	A1146	U1086	G971	C912	G851	G785	G725	A665
G1387	C1328	A1268	C1208	G1147	G1087	C972	A913	G852	G786	C726	G666
A1388	A1329	U1269	C1209	U1148	U1088	G973	A914	G853	A787	G727	G667
C1389	U1330	C1270	C1210	G1149	G1089	A974	A915	G854	U788	A728	G668
U1390	G1331	G1271	U1211	U1150	U1090	A975	A916	G855	U789	A729	U669
C1391	A1332	C1272	U1212	A1151	A1091	G976	G917	A790	A790	G730	G670
G1392	A1333	G1273	A1213	G1152	A1092	A977	A918	A859	G791	G731	U671
U1393	G1334	G1274	C1153	G1153	G1093	A978	A919	G860	A792	C732	U672
A1394	C1335	A1275	G1214	G1154	U1094	C979	U920	G861	U793	A733	G673
C1395	G1336	G1276	G1215	G1155	U1095	C980	U921	G862	A794	G734	G674
A1396	C1337	C1277	C1216	G1156	C1096	U981	G922	C863	C795	A675	G675
C1397	G1338	U1278	C1217	A1157	C1097	U982	A923	U864	C796	C736	A676
U1398	A1339	A1279	U1218	C1158	G1098	A983	C924	A865	A797	U677	U677
G1401	A1340	U1280	G1220	U1159	G1099	A984	G925	A866	G798	C738	U678
C1402	C1341	U1281	G1221	G1160	U1040	C985	G926	A867	G799	G739	C679
G1403	G1342	G1282	G1222	C1161	A1041	A986	C927	G868	G800	U740	C680
C1404	C1343	G1283	C1223	C1162	A102	G987	G928	C869	U801	G741	G681
G1405	U1344	C1284	G1224	C1163	G1104	C988	G929	C870	A802	G742	G682
U1406	A1346	A1286	C1226	C1165	A1105	C990	C930	U870	G803	U743	G683



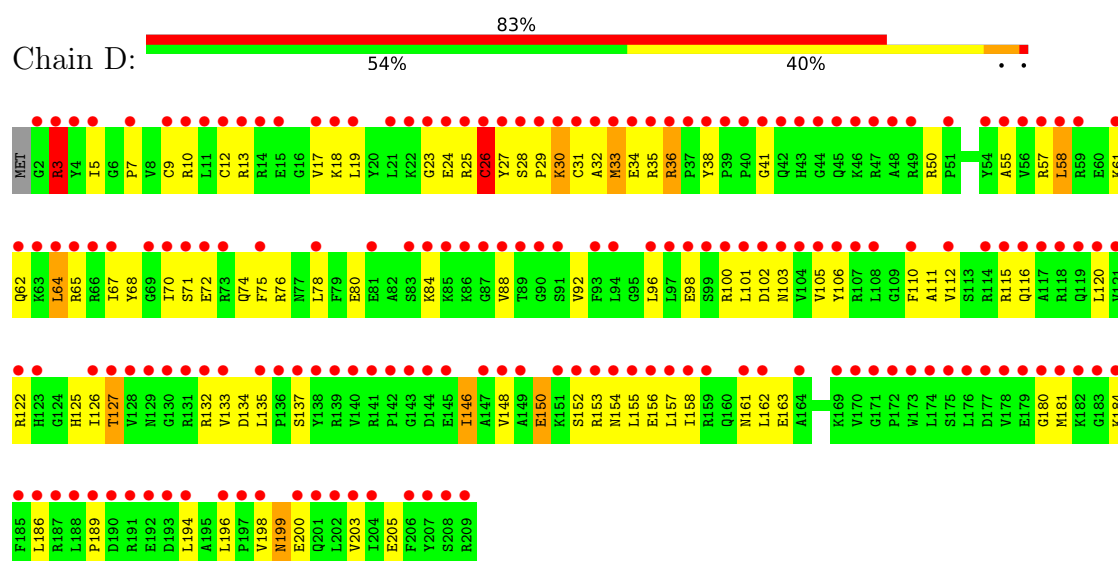
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



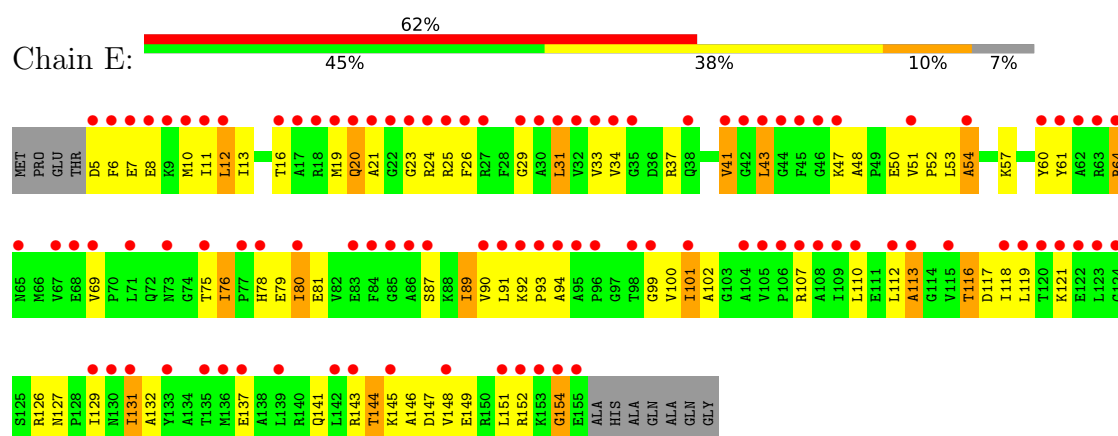
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

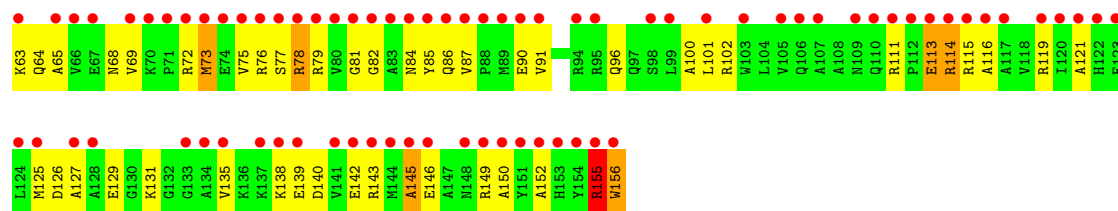


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

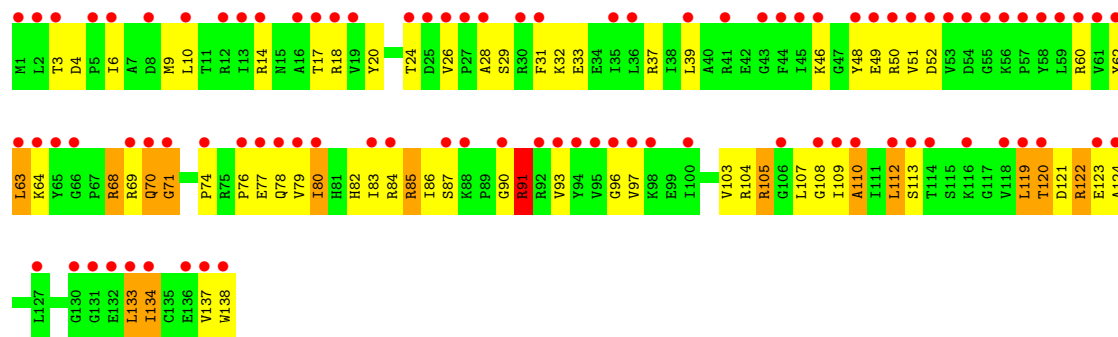


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

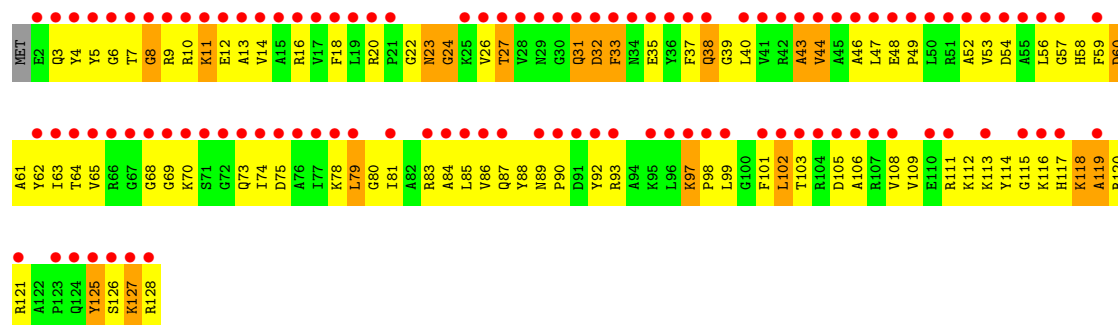
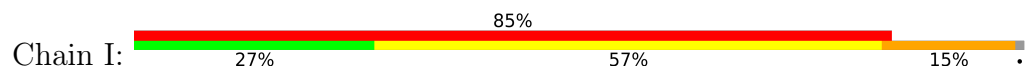




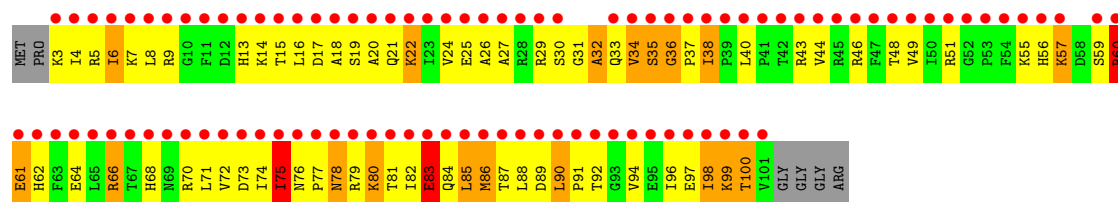
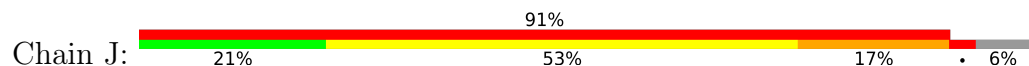
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



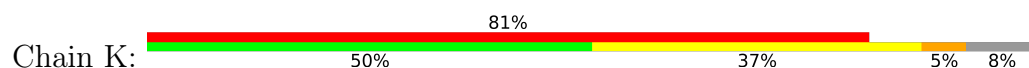
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



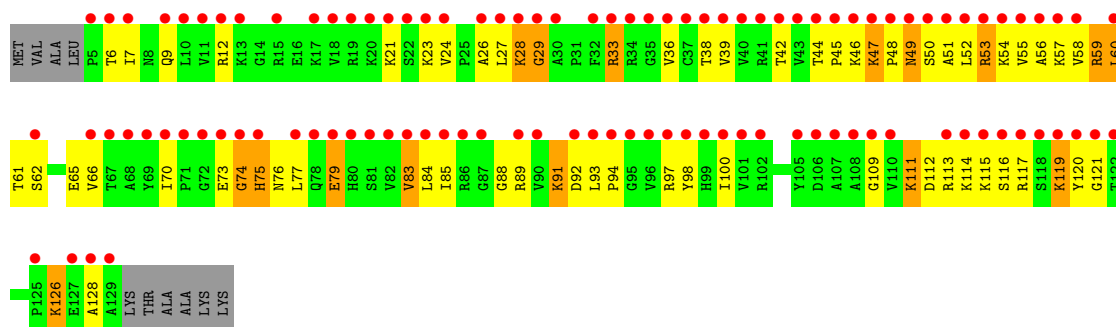
• Molecule 11: 30S RIBOSOMAL PROTEIN S11





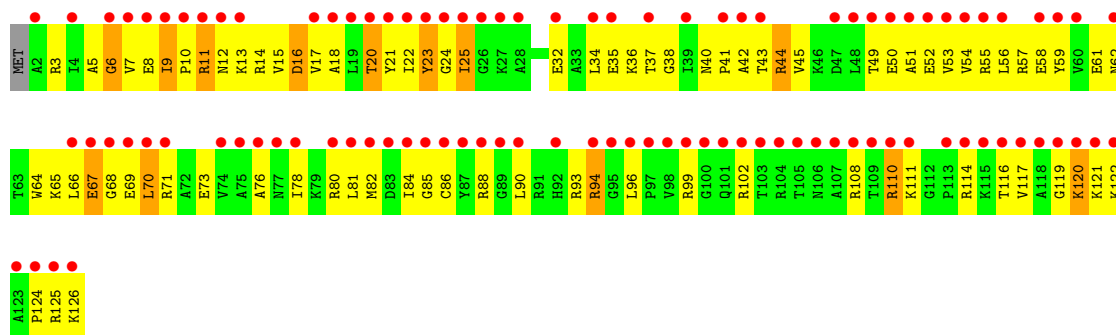
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 41% 78% 39% 12% 7%



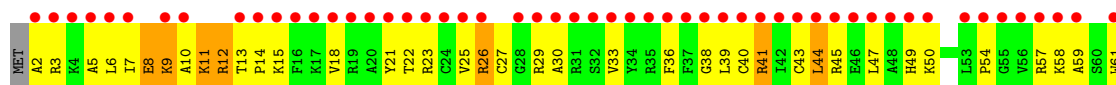
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 33% 79% 56% 10%



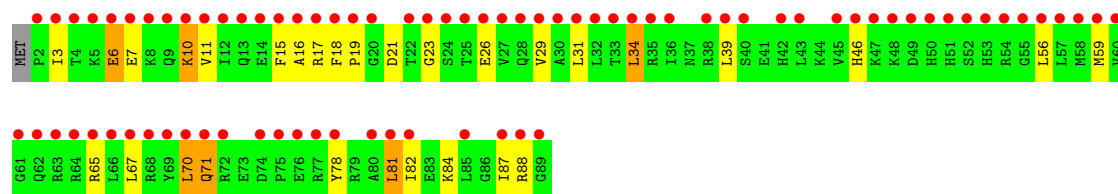
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 34% 87% 52% 11%

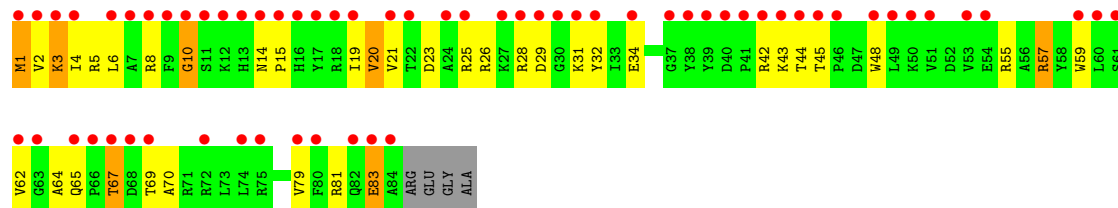


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

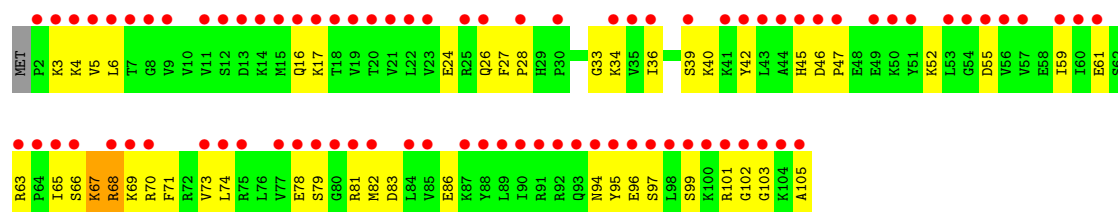
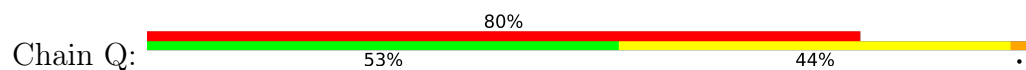
Chain O: 65% 89% 27% 7%



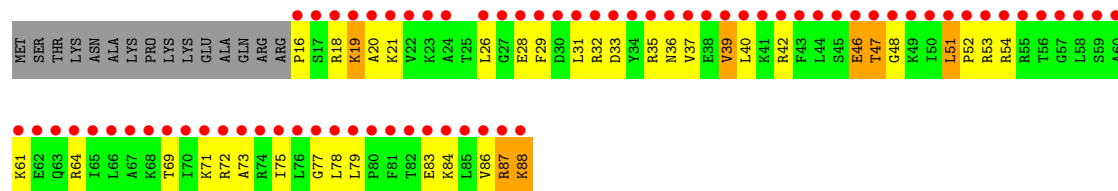
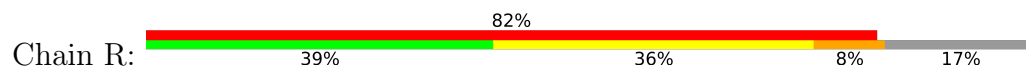
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



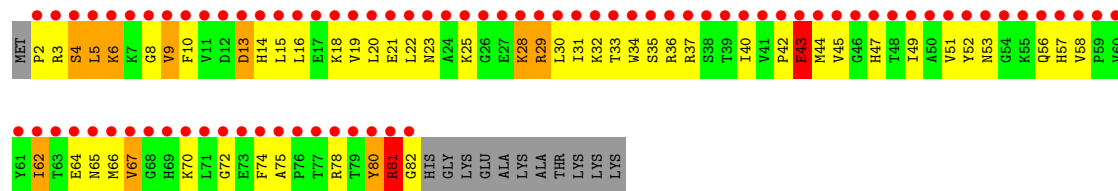
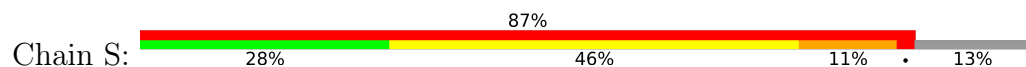
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



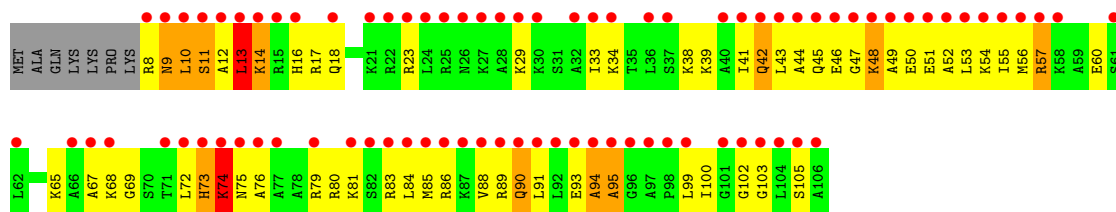
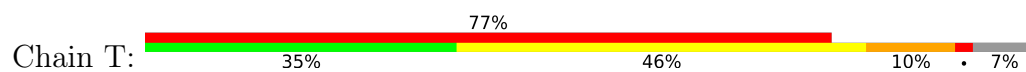
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



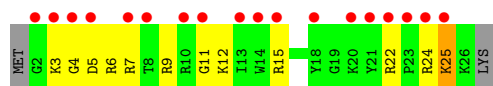
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



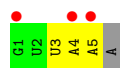
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



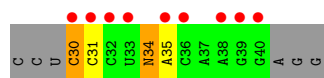
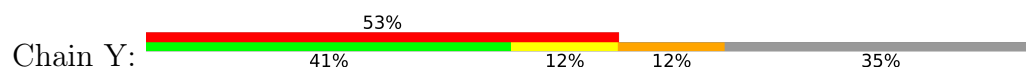
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: 5'-R(*GP*UP*UP*AP*AP*AP)-3'



• Molecule 23: 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP *GP*GP*AP*GP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.44Å 400.44Å 173.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.80 29.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.99-2.80) 97.5 (29.99-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.243 0.439 , 0.440	Depositor DCC
R_{free} test set	24813 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.3	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	0.71	EDS
Total number of atoms	52363	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: PAR, K, 6MZ, ZN, MG, CM0

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	A	0.47	1/36365 (0.0%)	0.67	65/56754 (0.1%)
2	B	0.45	1/1936 (0.1%)	1.04	9/2611 (0.3%)
3	C	0.47	1/1637 (0.1%)	0.98	8/2207 (0.4%)
4	D	0.46	0/1733	0.97	5/2318 (0.2%)
5	E	0.58	1/1163 (0.1%)	1.09	7/1566 (0.4%)
6	F	0.38	0/856	0.90	1/1154 (0.1%)
7	G	0.45	0/1276	0.93	2/1709 (0.1%)
8	H	0.57	0/1136	1.16	11/1527 (0.7%)
9	I	0.42	0/1029	1.01	3/1379 (0.2%)
10	J	0.48	1/806 (0.1%)	0.99	3/1084 (0.3%)
11	K	0.51	0/900	1.08	5/1213 (0.4%)
12	L	0.56	1/987 (0.1%)	1.24	10/1322 (0.8%)
13	M	0.44	0/1008	0.93	2/1347 (0.1%)
14	N	0.45	0/501	0.90	1/664 (0.2%)
15	O	0.44	0/745	0.85	0/992
16	P	0.56	1/717 (0.1%)	1.02	3/965 (0.3%)
17	Q	0.53	0/870	1.12	3/1159 (0.3%)
18	R	0.43	0/604	1.01	4/801 (0.5%)
19	S	0.44	1/662 (0.2%)	1.06	3/892 (0.3%)
20	T	0.55	0/765	1.12	4/1007 (0.4%)
21	U	0.64	1/213 (0.5%)	0.85	0/279
22	X	0.51	0/116	0.76	0/179
23	Y	0.46	0/206	0.81	1/314 (0.3%)
All	All	0.48	9/56231 (0.0%)	0.80	150/83443 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	34

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	U	O3'-P	-9.56	1.46	1.61
3	C	207	VAL	C-N	-5.89	1.25	1.33
10	J	100	THR	C-N	-5.66	1.25	1.33
2	B	240	GLN	C-N	-5.50	1.25	1.33
12	L	128	ALA	C-N	-5.46	1.25	1.33

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	14.97	131.96	109.50
1	A	1503	A	C2'-C3'-O3'	13.84	130.27	109.50
1	A	484	G	C2'-C3'-O3'	13.32	129.47	109.50
1	A	366	C	C2'-C3'-O3'	13.26	129.38	109.50
1	A	115	G	C2'-C3'-O3'	13.13	129.19	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	366	C	C3'
1	A	1503	A	C3'

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	145	G	Sidechain
1	A	195	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain

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	A	32489	0	16399	795	0
2	B	1901	0	1951	219	0
3	C	1613	0	1677	163	0
4	D	1703	0	1765	116	0
5	E	1147	0	1207	75	0
6	F	843	0	857	67	0
7	G	1257	0	1296	99	0
8	H	1116	0	1177	61	0
9	I	1010	0	1036	109	0
10	J	793	0	835	142	0
11	K	885	0	904	51	0
12	L	971	0	1057	80	0
13	M	997	0	1072	90	0
14	N	492	0	530	60	0
15	O	734	0	771	38	0
16	P	701	0	720	45	0
17	Q	857	0	928	53	0
18	R	598	0	670	49	0
19	S	648	0	673	65	0
20	T	763	0	861	71	0
21	U	209	0	221	17	0
22	X	104	0	55	4	0
23	Y	235	0	124	7	0
24	A	42	0	45	1	0
25	A	203	0	0	0	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	2	0	0	0	0
25	F	1	0	0	0	0
25	G	1	0	0	0	0
25	H	1	0	0	0	0
25	I	1	0	0	0	0
25	M	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	3	0	0	0	0
25	S	1	0	0	0	0
25	X	1	0	0	0	0
26	A	34	0	0	0	0
26	E	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	1	0
All	All	52363	0	36831	2241	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 25.

The worst 5 of 2241 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:C:O5'	7:G:82:GLY:CA	1.86	1.22
1:A:1532:U:C2'	1:A:1533:C:H5''	1.68	1.22
1:A:402:G:H2'	1:A:403:C:H5''	1.20	1.18
10:J:99:LYS:HD3	10:J:100:THR:H	1.06	1.18
1:A:1539:C:O5'	7:G:82:GLY:HA2	1.42	1.15

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	
2	B	233/256 (91%)	173 (74%)	48 (21%)	12 (5%)	1	5
3	C	205/239 (86%)	153 (75%)	36 (18%)	16 (8%)	1	2
4	D	206/209 (99%)	179 (87%)	22 (11%)	5 (2%)	4	17
5	E	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	18	47
6	F	99/101 (98%)	84 (85%)	13 (13%)	2 (2%)	6	21
7	G	153/156 (98%)	130 (85%)	20 (13%)	3 (2%)	6	21
8	H	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	5	19
9	I	125/128 (98%)	103 (82%)	10 (8%)	12 (10%)	0	1
10	J	97/105 (92%)	68 (70%)	15 (16%)	14 (14%)	0	0
11	K	117/129 (91%)	102 (87%)	11 (9%)	4 (3%)	3	11
12	L	123/135 (91%)	103 (84%)	14 (11%)	6 (5%)	1	6
13	M	123/126 (98%)	89 (72%)	23 (19%)	11 (9%)	0	1
14	N	58/61 (95%)	47 (81%)	8 (14%)	3 (5%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	P	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	10	34
17	Q	102/105 (97%)	91 (89%)	10 (10%)	1 (1%)	12	38
18	R	71/88 (81%)	61 (86%)	8 (11%)	2 (3%)	4	14
19	S	79/93 (85%)	62 (78%)	8 (10%)	9 (11%)	0	1
20	T	97/106 (92%)	80 (82%)	9 (9%)	8 (8%)	0	1
21	U	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	0	1
All	All	2364/2541 (93%)	1962 (83%)	287 (12%)	115 (5%)	1	6

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	207	ALA
3	C	15	THR
3	C	61	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	188 (93%)	14 (7%)	14	41
3	C	160/188 (85%)	146 (91%)	14 (9%)	9	29
4	D	180/181 (99%)	171 (95%)	9 (5%)	22	54
5	E	115/123 (94%)	101 (88%)	14 (12%)	5	16
6	F	90/90 (100%)	83 (92%)	7 (8%)	11	35
7	G	126/127 (99%)	119 (94%)	7 (6%)	19	50
8	H	119/119 (100%)	105 (88%)	14 (12%)	5	17
9	I	98/99 (99%)	90 (92%)	8 (8%)	10	33
10	J	87/92 (95%)	79 (91%)	8 (9%)	8	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	90/99 (91%)	86 (96%)	4 (4%)	25	59
12	L	104/111 (94%)	97 (93%)	7 (7%)	15	42
13	M	100/101 (99%)	90 (90%)	10 (10%)	7	24
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	23
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	29
16	P	72/74 (97%)	66 (92%)	6 (8%)	10	32
17	Q	96/97 (99%)	92 (96%)	4 (4%)	26	61
18	R	64/77 (83%)	62 (97%)	2 (3%)	35	70
19	S	71/80 (89%)	67 (94%)	4 (6%)	19	50
20	T	76/82 (93%)	68 (90%)	8 (10%)	6	22
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1845 (92%)	152 (8%)	12	36

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	110	ARG
19	S	65	ASN
14	N	41	ARG
16	P	8	ARG
20	T	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	62	ASN
19	S	57	HIS
15	O	13	GLN
16	P	65	GLN
4	D	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	191 (12%)	58 (3%)
22	X	4/6 (66%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	Y	10/17 (58%)	0	0
All	All	1524/1545 (98%)	191 (12%)	58 (3%)

5 of 191 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	793	U
1	A	1505	G
1	A	1049	U
1	A	1504	G
1	A	1397	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	6MZ	Y	37	23	22,25,26	0.56	0	30,36,39	0.59	0
23	CM0	Y	34	23	22,26,27	1.47	3 (13%)	28,37,40	2.99	3 (10%)

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
23	6MZ	Y	37	23	-	0/9/27/28	0/3/3/3
23	CM0	Y	34	23	-	5/12/30/31	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	CM0	O9-C8	4.31	1.36	1.22
23	Y	34	CM0	O5-C7	3.91	1.53	1.44
23	Y	34	CM0	O8-C8	-2.30	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	CM0	C7-O5-C5	14.37	136.39	117.58
23	Y	34	CM0	O5-C7-C8	5.34	122.47	110.88
23	Y	34	CM0	O4-C4-N3	-2.26	115.79	120.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	34	CM0	C4-C5-O5-C7
23	Y	34	CM0	C6-C5-O5-C7
23	Y	34	CM0	C8-C7-O5-C5
23	Y	34	CM0	O5-C7-C8-O8
23	Y	34	CM0	O5-C7-C8-O9

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	CM0	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 255 are monoatomic - leaving 1 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$
24	PAR	A	1601	-	45,45,45	1.56	10 (22%)	64,67,67	1.25	8 (12%)

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
24	PAR	A	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C64-C54	4.49	1.58	1.52
24	A	1601	PAR	O54-C14	3.43	1.50	1.41
24	A	1601	PAR	C52-C42	3.05	1.58	1.52
24	A	1601	PAR	C31-C21	2.76	1.57	1.53
24	A	1601	PAR	C11-C21	2.43	1.57	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	4.26	115.56	108.22
24	A	1601	PAR	O54-C54-C64	3.73	112.95	106.01
24	A	1601	PAR	C14-O54-C54	3.44	120.44	113.69
24	A	1601	PAR	O52-C13-C23	2.63	113.41	107.96
24	A	1601	PAR	O11-C11-C21	2.39	112.34	108.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64

Continued on next page...

Continued from previous page...

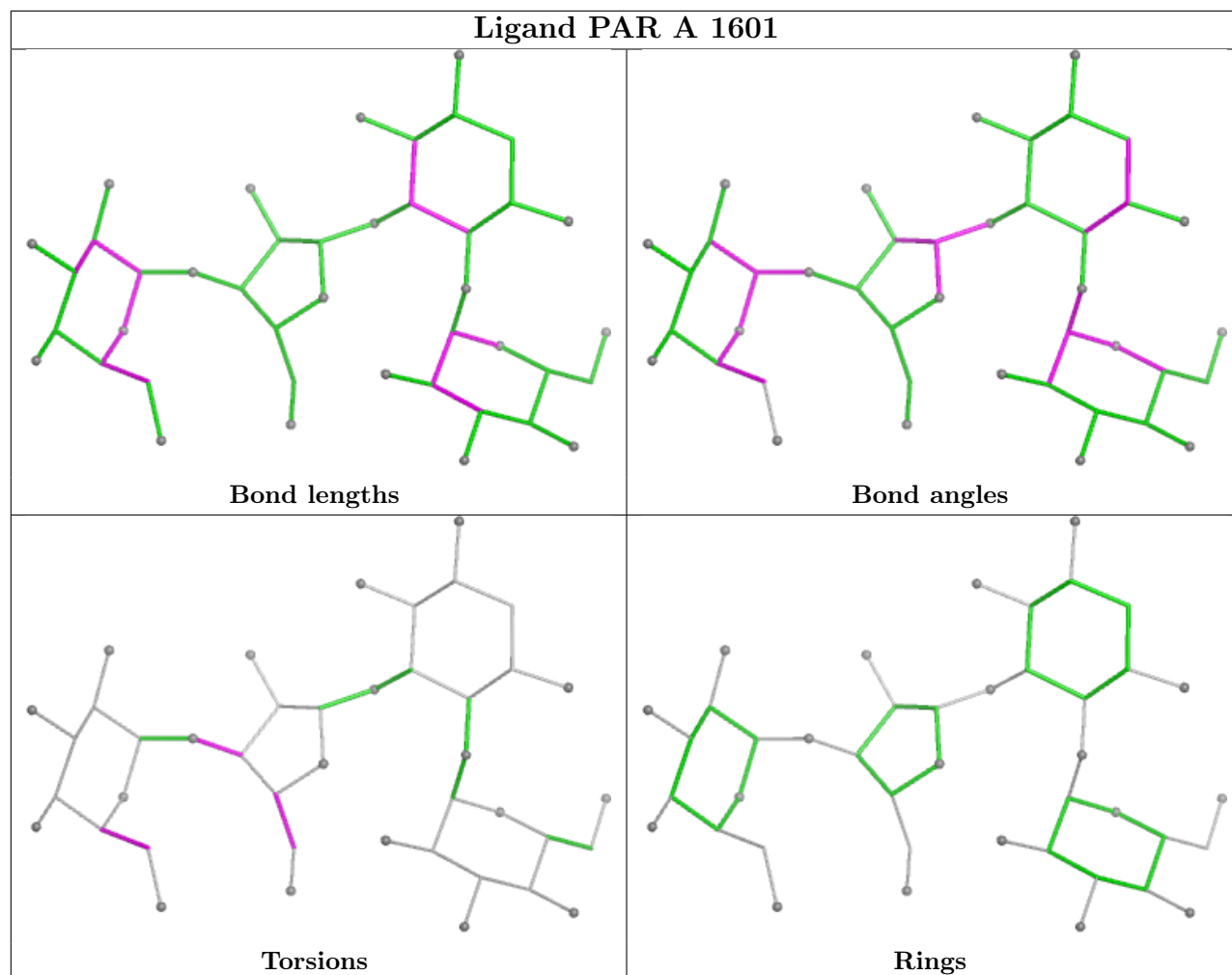
Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C33-C43-C53-O53
24	A	1601	PAR	O43-C43-C53-O53
24	A	1601	PAR	O54-C54-C64-N64
24	A	1601	PAR	C43-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1522 (99%)	3.77	1427 (94%) 0 0	29, 55, 119, 166	0
2	B	235/256 (91%)	3.43	193 (82%) 0 0	47, 82, 126, 148	0
3	C	207/239 (86%)	3.68	183 (88%) 0 0	47, 75, 110, 117	0
4	D	208/209 (99%)	3.43	174 (83%) 0 0	45, 60, 82, 89	0
5	E	151/162 (93%)	2.77	101 (66%) 0 0	30, 46, 63, 85	0
6	F	101/101 (100%)	4.06	92 (91%) 0 0	56, 79, 92, 101	0
7	G	155/156 (99%)	2.94	121 (78%) 0 0	52, 72, 110, 127	0
8	H	138/138 (100%)	2.82	92 (66%) 0 0	29, 44, 63, 68	0
9	I	127/128 (99%)	3.40	109 (85%) 0 0	43, 82, 101, 104	0
10	J	99/105 (94%)	4.17	96 (96%) 0 0	44, 103, 140, 145	0
11	K	119/129 (92%)	3.81	105 (88%) 0 0	33, 59, 80, 103	0
12	L	125/135 (92%)	3.37	105 (84%) 0 0	22, 51, 72, 108	0
13	M	125/126 (99%)	3.52	99 (79%) 0 0	47, 69, 125, 159	0
14	N	60/61 (98%)	4.07	53 (88%) 0 0	49, 66, 90, 98	0
15	O	88/89 (98%)	3.97	79 (89%) 0 0	40, 60, 79, 104	0
16	P	84/88 (95%)	2.92	63 (75%) 0 0	36, 48, 59, 91	0
17	Q	104/105 (99%)	3.65	84 (80%) 0 0	32, 53, 98, 127	0
18	R	73/88 (82%)	4.18	72 (98%) 0 0	49, 66, 103, 132	0
19	S	81/93 (87%)	4.38	81 (100%) 0 0	63, 85, 107, 116	0
20	T	99/106 (93%)	3.38	82 (82%) 0 0	35, 53, 80, 85	0
21	U	25/27 (92%)	2.93	18 (72%) 0 0	44, 56, 81, 87	0
22	X	5/6 (83%)	2.36	3 (60%) 0 0	51, 52, 85, 109	0
23	Y	9/17 (52%)	3.32	9 (100%) 0 0	57, 78, 113, 120	0
All	All	3930/4086 (96%)	3.60	3441 (87%) 0 0	22, 60, 113, 166	0

The worst 5 of 3441 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	13.9
3	C	103	VAL	12.3
3	C	101	LEU	12.0
19	S	4	SER	11.8
4	D	32	ALA	11.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
23	CM0	Y	34	25/26	0.59	0.20	64,69,71,72	0
23	6MZ	Y	37	23/24	0.82	0.17	60,64,65,66	0

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
25	MG	A	1643	1/1	-0.20	0.68	66,66,66,66	0
25	MG	A	1631	1/1	-0.14	0.42	59,59,59,59	0
25	MG	A	1721	1/1	-0.14	0.89	68,68,68,68	0
25	MG	A	1608	1/1	-0.12	0.36	74,74,74,74	0
25	MG	A	1731	1/1	-0.09	1.18	82,82,82,82	0
25	MG	A	1736	1/1	-0.03	1.39	72,72,72,72	0
25	MG	A	1630	1/1	0.00	0.66	90,90,90,90	0
25	MG	A	1747	1/1	0.01	0.70	55,55,55,55	0
25	MG	A	1742	1/1	0.04	0.41	78,78,78,78	0
25	MG	A	1710	1/1	0.04	0.97	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	N	101	1/1	0.08	0.77	104,104,104,104	0
26	K	E	203	1/1	0.09	0.28	93,93,93,93	0
25	MG	F	201	1/1	0.12	0.25	49,49,49,49	0
26	K	A	1808	1/1	0.13	0.70	81,81,81,81	0
25	MG	A	1714	1/1	0.13	0.73	60,60,60,60	0
26	K	A	1810	1/1	0.14	0.30	102,102,102,102	0
25	MG	A	1753	1/1	0.14	0.26	35,35,35,35	0
25	MG	A	1673	1/1	0.16	0.47	67,67,67,67	0
25	MG	A	1637	1/1	0.16	0.83	68,68,68,68	0
26	K	A	1820	1/1	0.17	0.33	85,85,85,85	0
25	MG	A	1684	1/1	0.20	1.03	92,92,92,92	0
25	MG	A	1622	1/1	0.20	0.76	78,78,78,78	0
26	K	A	1809	1/1	0.20	0.77	92,92,92,92	0
26	K	A	1828	1/1	0.21	0.70	99,99,99,99	0
25	MG	A	1789	1/1	0.21	0.28	51,51,51,51	0
25	MG	A	1661	1/1	0.23	0.33	44,44,44,44	0
25	MG	A	1785	1/1	0.24	1.02	81,81,81,81	0
25	MG	A	1611	1/1	0.24	0.18	13,13,13,13	0
25	MG	A	1612	1/1	0.25	0.49	48,48,48,48	0
25	MG	A	1625	1/1	0.25	0.58	49,49,49,49	0
25	MG	A	1655	1/1	0.25	0.50	64,64,64,64	0
25	MG	A	1605	1/1	0.26	0.93	70,70,70,70	0
25	MG	A	1614	1/1	0.26	0.40	91,91,91,91	0
25	MG	A	1652	1/1	0.27	0.51	60,60,60,60	0
25	MG	A	1717	1/1	0.28	0.57	79,79,79,79	0
25	MG	A	1775	1/1	0.28	0.19	33,33,33,33	0
25	MG	A	1748	1/1	0.28	0.77	70,70,70,70	0
25	MG	A	1696	1/1	0.30	0.70	96,96,96,96	0
25	MG	A	1606	1/1	0.30	0.68	54,54,54,54	0
25	MG	A	1711	1/1	0.31	0.56	57,57,57,57	0
25	MG	A	1800	1/1	0.32	0.46	42,42,42,42	0
26	K	A	1821	1/1	0.32	0.40	90,90,90,90	0
25	MG	A	1685	1/1	0.33	0.79	81,81,81,81	0
26	K	A	1816	1/1	0.33	0.46	120,120,120,120	0
25	MG	A	1656	1/1	0.34	0.34	69,69,69,69	0
26	K	A	1817	1/1	0.34	0.77	108,108,108,108	0
25	MG	A	1724	1/1	0.34	0.61	55,55,55,55	0
25	MG	A	1793	1/1	0.34	0.42	45,45,45,45	0
25	MG	A	1634	1/1	0.34	0.53	30,30,30,30	0
25	MG	A	1802	1/1	0.34	0.93	82,82,82,82	0
25	MG	A	1638	1/1	0.35	0.44	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1692	1/1	0.36	0.42	51,51,51,51	0
25	MG	A	1657	1/1	0.37	0.50	74,74,74,74	0
25	MG	A	1787	1/1	0.37	0.34	48,48,48,48	0
26	K	A	1832	1/1	0.37	0.30	103,103,103,103	0
25	MG	Q	202	1/1	0.37	0.15	39,39,39,39	0
26	K	A	1818	1/1	0.38	0.45	110,110,110,110	0
25	MG	A	1766	1/1	0.38	0.49	65,65,65,65	0
25	MG	A	1782	1/1	0.39	0.58	49,49,49,49	0
25	MG	A	1737	1/1	0.40	0.61	56,56,56,56	0
25	MG	A	1705	1/1	0.40	0.48	50,50,50,50	0
25	MG	A	1607	1/1	0.41	0.72	91,91,91,91	0
25	MG	A	1798	1/1	0.41	0.41	52,52,52,52	0
25	MG	A	1688	1/1	0.41	0.61	76,76,76,76	0
25	MG	A	1759	1/1	0.42	0.30	44,44,44,44	0
25	MG	A	1629	1/1	0.43	0.31	56,56,56,56	0
25	MG	A	1761	1/1	0.43	0.24	48,48,48,48	0
25	MG	A	1735	1/1	0.43	0.67	96,96,96,96	0
25	MG	S	101	1/1	0.43	0.30	45,45,45,45	0
25	MG	A	1754	1/1	0.43	0.42	51,51,51,51	0
25	MG	A	1633	1/1	0.44	0.38	69,69,69,69	0
26	K	A	1814	1/1	0.44	0.46	95,95,95,95	0
25	MG	A	1642	1/1	0.45	0.33	48,48,48,48	0
25	MG	A	1723	1/1	0.45	0.30	47,47,47,47	0
25	MG	A	1677	1/1	0.45	0.17	89,89,89,89	0
25	MG	A	1666	1/1	0.45	0.37	57,57,57,57	0
25	MG	A	1790	1/1	0.46	0.43	45,45,45,45	0
25	MG	A	1715	1/1	0.46	0.61	68,68,68,68	0
25	MG	A	1681	1/1	0.46	0.73	82,82,82,82	0
26	K	A	1811	1/1	0.46	0.54	86,86,86,86	0
26	K	A	1819	1/1	0.46	0.39	96,96,96,96	0
25	MG	A	1718	1/1	0.47	0.30	51,51,51,51	0
25	MG	A	1610	1/1	0.47	0.79	50,50,50,50	0
25	MG	A	1621	1/1	0.47	0.31	59,59,59,59	0
25	MG	A	1686	1/1	0.47	0.75	34,34,34,34	0
25	MG	A	1730	1/1	0.47	0.73	84,84,84,84	0
26	K	A	1807	1/1	0.48	0.33	76,76,76,76	0
25	MG	A	1751	1/1	0.48	0.35	61,61,61,61	0
26	K	A	1833	1/1	0.48	0.32	99,99,99,99	0
26	K	A	1805	1/1	0.48	0.14	68,68,68,68	0
25	MG	A	1767	1/1	0.49	0.40	61,61,61,61	0
26	K	A	1815	1/1	0.49	0.28	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1665	1/1	0.50	0.49	49,49,49,49	0
25	MG	A	1741	1/1	0.50	0.50	74,74,74,74	0
25	MG	A	1623	1/1	0.51	0.36	54,54,54,54	0
26	K	A	1830	1/1	0.51	0.36	97,97,97,97	0
25	MG	A	1784	1/1	0.51	0.80	79,79,79,79	0
25	MG	A	1771	1/1	0.51	0.60	58,58,58,58	0
26	K	A	1835	1/1	0.51	0.36	114,114,114,114	0
25	MG	A	1618	1/1	0.51	0.69	60,60,60,60	0
25	MG	A	1794	1/1	0.52	0.36	47,47,47,47	0
26	K	A	1822	1/1	0.52	0.42	100,100,100,100	0
25	MG	A	1702	1/1	0.52	0.63	50,50,50,50	0
25	MG	A	1667	1/1	0.52	0.54	47,47,47,47	0
25	MG	A	1716	1/1	0.53	0.77	66,66,66,66	0
25	MG	A	1709	1/1	0.53	0.39	46,46,46,46	0
26	K	A	1829	1/1	0.54	0.42	94,94,94,94	0
25	MG	A	1680	1/1	0.54	0.42	39,39,39,39	0
25	MG	A	1635	1/1	0.54	0.23	43,43,43,43	0
25	MG	A	1763	1/1	0.55	0.19	47,47,47,47	0
26	K	A	1834	1/1	0.55	0.23	91,91,91,91	0
26	K	A	1806	1/1	0.56	0.21	72,72,72,72	0
25	MG	A	1620	1/1	0.56	0.36	51,51,51,51	0
25	MG	A	1792	1/1	0.56	0.12	54,54,54,54	0
26	K	A	1825	1/1	0.56	0.55	107,107,107,107	0
26	K	A	1831	1/1	0.57	0.48	95,95,95,95	0
25	MG	A	1801	1/1	0.57	0.47	56,56,56,56	0
26	K	A	1838	1/1	0.57	0.35	120,120,120,120	0
25	MG	A	1617	1/1	0.57	0.26	25,25,25,25	0
25	MG	A	1693	1/1	0.58	0.37	43,43,43,43	0
25	MG	A	1669	1/1	0.58	0.81	74,74,74,74	0
25	MG	A	1627	1/1	0.58	0.16	39,39,39,39	0
25	MG	A	1760	1/1	0.59	0.22	41,41,41,41	0
25	MG	A	1728	1/1	0.59	0.40	47,47,47,47	0
25	MG	A	1745	1/1	0.59	0.13	29,29,29,29	0
25	MG	A	1641	1/1	0.60	0.47	38,38,38,38	0
25	MG	A	1632	1/1	0.60	0.48	72,72,72,72	0
25	MG	A	1624	1/1	0.60	0.37	74,74,74,74	0
25	MG	A	1602	1/1	0.60	0.12	45,45,45,45	0
26	K	A	1836	1/1	0.60	0.36	92,92,92,92	0
25	MG	A	1701	1/1	0.60	0.51	65,65,65,65	0
25	MG	A	1654	1/1	0.60	0.52	48,48,48,48	0
25	MG	A	1678	1/1	0.61	0.59	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1676	1/1	0.62	0.50	45,45,45,45	0
25	MG	A	1671	1/1	0.62	0.50	74,74,74,74	0
25	MG	A	1628	1/1	0.62	0.81	51,51,51,51	0
25	MG	A	1796	1/1	0.63	0.44	46,46,46,46	0
25	MG	A	1640	1/1	0.63	0.27	46,46,46,46	0
26	K	A	1812	1/1	0.63	0.21	91,91,91,91	0
25	MG	A	1780	1/1	0.63	0.23	38,38,38,38	0
25	MG	A	1749	1/1	0.63	0.19	34,34,34,34	0
25	MG	A	1694	1/1	0.63	0.56	50,50,50,50	0
25	MG	A	1662	1/1	0.63	0.64	61,61,61,61	0
25	MG	A	1786	1/1	0.63	0.24	63,63,63,63	0
25	MG	I	201	1/1	0.64	0.35	67,67,67,67	0
25	MG	A	1695	1/1	0.64	0.38	43,43,43,43	0
25	MG	A	1648	1/1	0.64	0.35	46,46,46,46	0
25	MG	A	1604	1/1	0.65	0.62	49,49,49,49	0
25	MG	A	1603	1/1	0.65	0.64	75,75,75,75	0
26	K	A	1824	1/1	0.65	0.16	83,83,83,83	0
25	MG	A	1663	1/1	0.65	0.59	55,55,55,55	0
25	MG	A	1644	1/1	0.65	0.46	73,73,73,73	0
25	MG	A	1791	1/1	0.66	0.23	56,56,56,56	0
25	MG	A	1697	1/1	0.66	0.35	51,51,51,51	0
25	MG	A	1664	1/1	0.66	0.37	35,35,35,35	0
25	MG	A	1706	1/1	0.66	0.52	56,56,56,56	0
25	MG	D	302	1/1	0.67	0.16	41,41,41,41	0
25	MG	A	1740	1/1	0.67	0.56	51,51,51,51	0
25	MG	A	1729	1/1	0.67	0.25	68,68,68,68	0
25	MG	A	1777	1/1	0.67	0.60	69,69,69,69	0
25	MG	A	1659	1/1	0.67	0.56	50,50,50,50	0
25	MG	A	1636	1/1	0.67	0.40	32,32,32,32	0
25	MG	A	1739	1/1	0.68	0.40	53,53,53,53	0
26	K	A	1813	1/1	0.68	0.47	88,88,88,88	0
25	MG	A	1613	1/1	0.68	0.21	44,44,44,44	0
25	MG	A	1762	1/1	0.68	0.29	38,38,38,38	0
25	MG	A	1682	1/1	0.69	0.26	51,51,51,51	0
25	MG	A	1757	1/1	0.69	0.13	32,32,32,32	0
25	MG	A	1750	1/1	0.70	0.23	65,65,65,65	0
25	MG	A	1722	1/1	0.70	0.26	57,57,57,57	0
25	MG	A	1660	1/1	0.70	0.38	43,43,43,43	0
25	MG	A	1626	1/1	0.70	0.18	44,44,44,44	0
25	MG	A	1755	1/1	0.70	0.23	56,56,56,56	0
26	K	A	1826	1/1	0.71	0.21	83,83,83,83	0
25	MG	A	1781	1/1	0.71	0.41	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1647	1/1	0.71	0.35	41,41,41,41	0
25	MG	Q	203	1/1	0.71	0.27	63,63,63,63	0
25	MG	A	1774	1/1	0.72	0.21	14,14,14,14	0
25	MG	A	1704	1/1	0.72	0.38	57,57,57,57	0
25	MG	A	1734	1/1	0.72	0.42	40,40,40,40	0
25	MG	A	1779	1/1	0.72	0.26	37,37,37,37	0
25	MG	A	1768	1/1	0.72	0.37	45,45,45,45	0
25	MG	A	1788	1/1	0.72	0.11	19,19,19,19	0
25	MG	A	1698	1/1	0.72	0.25	16,16,16,16	0
25	MG	A	1776	1/1	0.73	0.33	31,31,31,31	0
25	MG	A	1799	1/1	0.73	0.25	69,69,69,69	0
25	MG	A	1674	1/1	0.73	0.19	39,39,39,39	0
25	MG	A	1645	1/1	0.73	0.24	35,35,35,35	0
25	MG	A	1619	1/1	0.73	0.13	44,44,44,44	0
25	MG	A	1765	1/1	0.73	0.17	34,34,34,34	0
25	MG	E	201	1/1	0.73	0.48	50,50,50,50	0
25	MG	A	1732	1/1	0.73	0.35	34,34,34,34	0
25	MG	A	1797	1/1	0.73	0.09	74,74,74,74	0
24	PAR	A	1601	42/42	0.74	0.27	43,47,64,68	0
25	MG	A	1720	1/1	0.74	0.14	38,38,38,38	0
25	MG	A	1713	1/1	0.74	0.76	56,56,56,56	0
26	K	A	1827	1/1	0.75	0.15	85,85,85,85	0
25	MG	A	1700	1/1	0.75	0.25	37,37,37,37	0
25	MG	A	1803	1/1	0.76	0.19	44,44,44,44	0
26	K	A	1837	1/1	0.76	0.30	93,93,93,93	0
25	MG	A	1699	1/1	0.76	0.15	32,32,32,32	0
25	MG	A	1687	1/1	0.76	0.73	62,62,62,62	0
25	MG	A	1725	1/1	0.77	0.15	29,29,29,29	0
25	MG	A	1707	1/1	0.77	0.11	20,20,20,20	0
25	MG	A	1764	1/1	0.77	0.21	27,27,27,27	0
25	MG	A	1708	1/1	0.77	0.47	46,46,46,46	0
25	MG	A	1683	1/1	0.77	0.47	48,48,48,48	0
25	MG	A	1743	1/1	0.77	0.25	38,38,38,38	0
25	MG	A	1670	1/1	0.77	0.26	45,45,45,45	0
25	MG	A	1783	1/1	0.78	0.36	57,57,57,57	0
25	MG	A	1773	1/1	0.78	0.25	30,30,30,30	0
25	MG	A	1769	1/1	0.78	0.18	32,32,32,32	0
25	MG	A	1726	1/1	0.78	0.19	35,35,35,35	0
25	MG	A	1795	1/1	0.78	0.11	41,41,41,41	0
27	ZN	D	301	1/1	0.78	0.22	81,81,81,81	0
25	MG	M	201	1/1	0.79	0.15	35,35,35,35	0
25	MG	A	1738	1/1	0.79	0.24	34,34,34,34	0

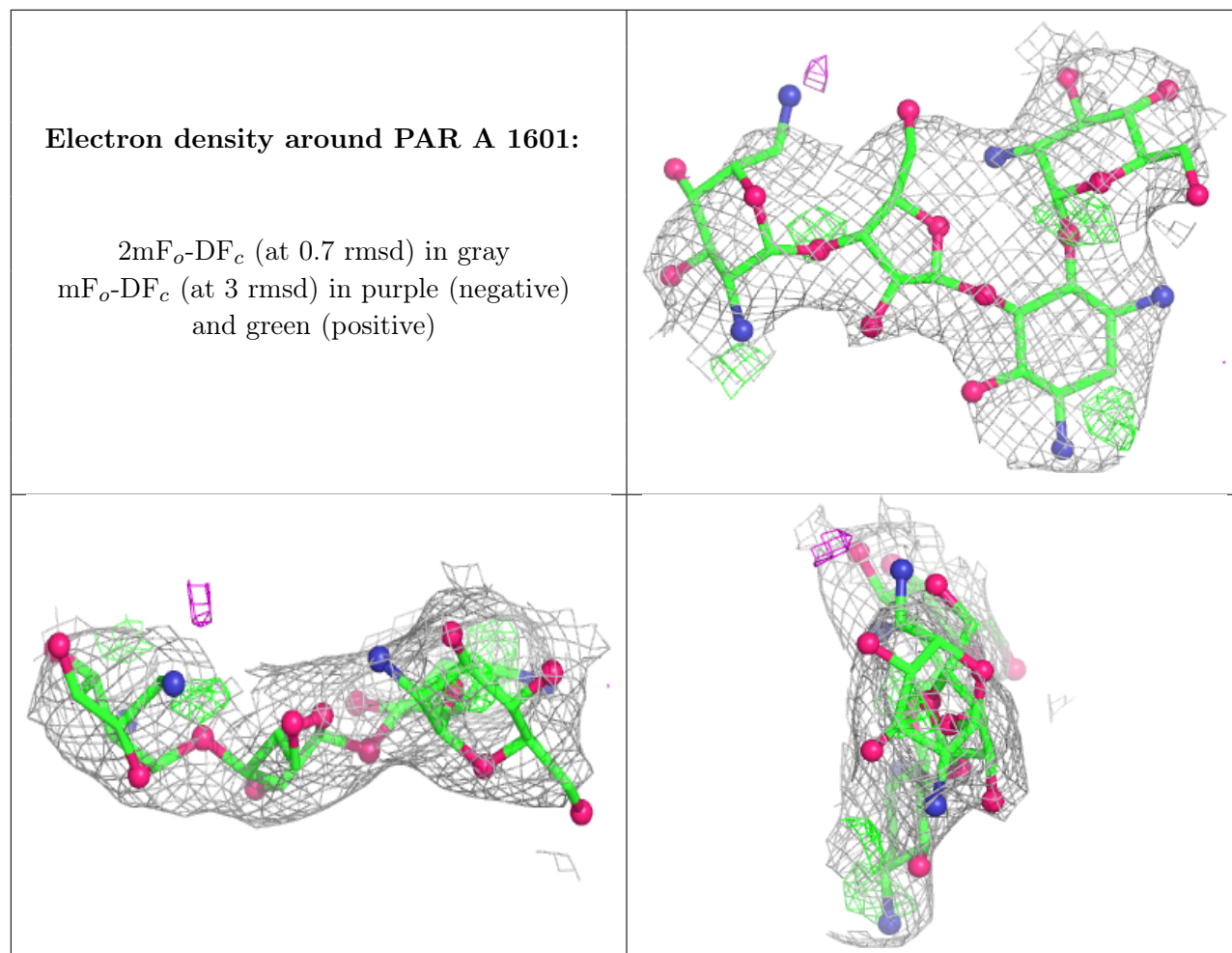
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	G	201	1/1	0.79	0.29	58,58,58,58	0
25	MG	A	1733	1/1	0.79	0.23	40,40,40,40	0
25	MG	A	1770	1/1	0.80	0.19	11,11,11,11	0
25	MG	A	1675	1/1	0.80	0.17	36,36,36,36	0
25	MG	A	1772	1/1	0.80	0.12	24,24,24,24	0
25	MG	X	101	1/1	0.81	0.16	27,27,27,27	0
25	MG	A	1615	1/1	0.81	0.13	42,42,42,42	0
25	MG	A	1639	1/1	0.81	0.43	48,48,48,48	0
25	MG	H	201	1/1	0.82	0.12	37,37,37,37	0
25	MG	A	1746	1/1	0.83	0.14	31,31,31,31	0
25	MG	A	1703	1/1	0.83	0.22	31,31,31,31	0
25	MG	Q	201	1/1	0.83	0.32	52,52,52,52	0
26	K	A	1823	1/1	0.84	0.34	85,85,85,85	0
25	MG	A	1668	1/1	0.84	0.63	106,106,106,106	0
25	MG	A	1756	1/1	0.84	0.16	43,43,43,43	0
25	MG	A	1804	1/1	0.84	0.21	88,88,88,88	0
25	MG	B	301	1/1	0.84	0.11	36,36,36,36	0
25	MG	A	1712	1/1	0.84	0.13	16,16,16,16	0
25	MG	A	1758	1/1	0.85	0.07	20,20,20,20	0
25	MG	A	1719	1/1	0.85	0.36	42,42,42,42	0
25	MG	A	1650	1/1	0.86	0.16	47,47,47,47	0
25	MG	A	1672	1/1	0.86	0.26	27,27,27,27	0
25	MG	A	1679	1/1	0.86	0.24	27,27,27,27	0
25	MG	A	1690	1/1	0.87	0.25	43,43,43,43	0
25	MG	A	1658	1/1	0.87	0.11	18,18,18,18	0
25	MG	A	1744	1/1	0.87	0.10	26,26,26,26	0
25	MG	A	1727	1/1	0.88	0.18	27,27,27,27	0
25	MG	A	1609	1/1	0.88	0.49	37,37,37,37	0
25	MG	E	202	1/1	0.89	0.16	52,52,52,52	0
25	MG	A	1616	1/1	0.89	0.26	30,30,30,30	0
25	MG	A	1689	1/1	0.89	0.14	34,34,34,34	0
25	MG	A	1646	1/1	0.89	0.42	48,48,48,48	0
25	MG	A	1653	1/1	0.90	0.12	1,1,1,1	0
25	MG	A	1649	1/1	0.90	0.33	50,50,50,50	0
27	ZN	N	102	1/1	0.90	0.07	69,69,69,69	0
25	MG	A	1778	1/1	0.91	0.09	44,44,44,44	0
25	MG	A	1651	1/1	0.92	0.34	34,34,34,34	0
25	MG	A	1691	1/1	0.93	0.22	28,28,28,28	0
25	MG	A	1752	1/1	0.93	0.18	42,42,42,42	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.