



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 01:53 PM EDT

PDB ID : 4DV4  
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, A914G  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.65 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

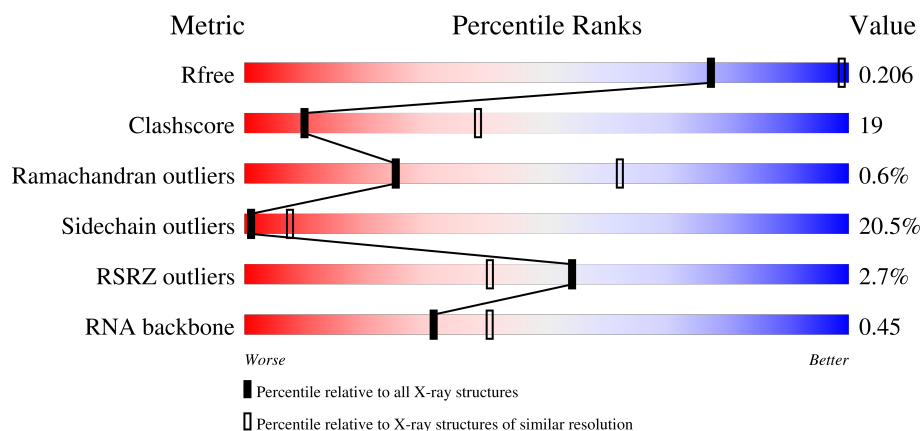
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div>21%</div> <div>42%</div> <div>27%</div> <div>9%</div> </div> </div>
2	B	256	<div> <div>41%</div> <div>37%</div> <div>12%</div> <div>9%</div> </div>
3	C	239	<div> <div>6%</div> <div> <div>43%</div> <div>34%</div> <div>9%</div> <div>14%</div> </div> </div>
4	D	209	<div> <div>2%</div> <div> <div>47%</div> <div>39%</div> <div>13%</div> </div> </div>

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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	

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
22	MG	A	1656	-	-	-	X
22	MG	A	1699	-	-	-	X
22	MG	A	1714	-	-	-	X
22	MG	A	1725	-	-	-	X
22	MG	A	1739	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1777	-	-	-	X
22	MG	A	1813	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1818	-	-	-	X
22	MG	A	1821	-	-	-	X
22	MG	A	1822	-	-	-	X
22	MG	A	1848	-	-	-	X
22	MG	J	201	-	-	-	X

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52434 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32645	14540	6039	10548	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	914	G	A	ENGINEERED MUTATION	GB M26923.1
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 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 ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 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 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 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 ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 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 ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 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 ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	268	Total	Mg	0	0
			268	268		
22	B	2	Total	Mg	0	0
			2	2		
22	C	2	Total	Mg	0	0
			2	2		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	J	2	Total	Mg	0	0
			2	2		
22	M	1	Total	Mg	0	0
			1	1		
22	N	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	3	Total 3	Mg 3	0	0
22	Q	2	Total 2	Mg 2	0	0
22	S	1	Total 1	Mg 1	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

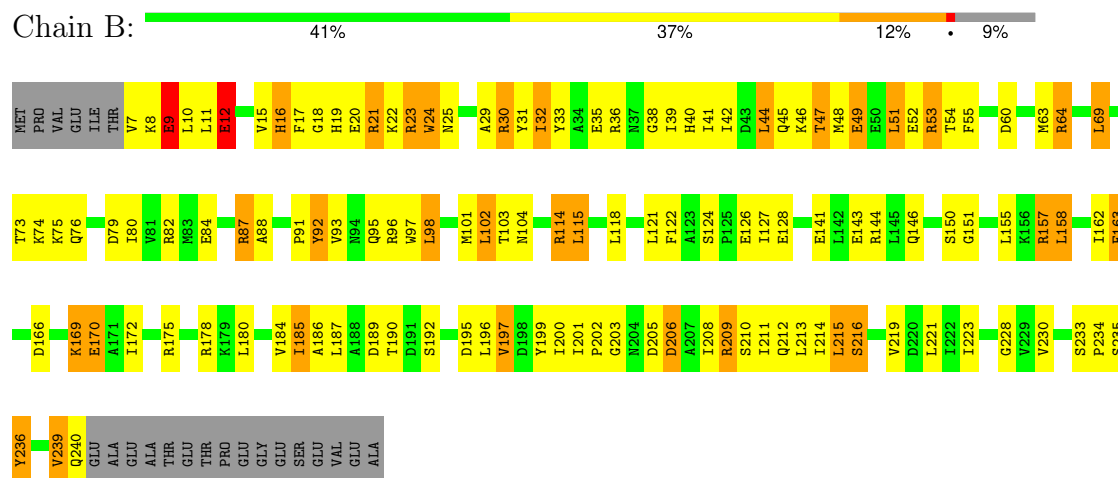
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	383	Total 383	O 383	0	0
24	E	3	Total 3	O 3	0	0
24	G	2	Total 2	O 2	0	0
24	I	1	Total 1	O 1	0	0
24	J	3	Total 3	O 3	0	0
24	L	1	Total 1	O 1	0	0
24	M	7	Total 7	O 7	0	0
24	N	2	Total 2	O 2	0	0
24	P	8	Total 8	O 8	0	0
24	Q	1	Total 1	O 1	0	0
24	T	1	Total 1	O 1	0	0

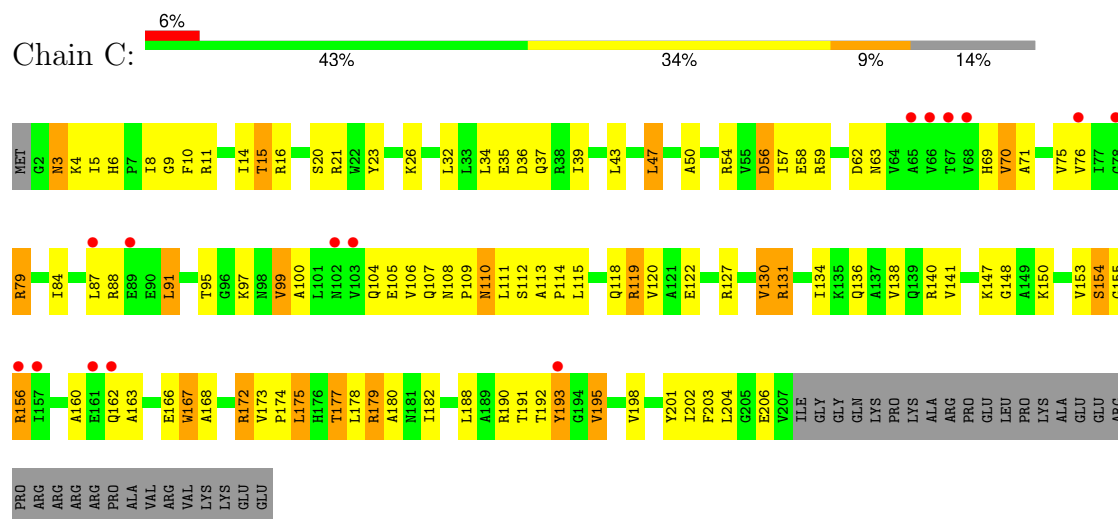


A1503	G1430	G1370	G1310	C1242	A1180	U1049	G989	G925	C862	C795	G731	A665
G1504	A1434	G1371	G1311	C1243	G1181	G1050	C990	G926	U863	C796	C732	G666
G1505	G1435	U1372	G1312	A1244	G1182	G1053	U991	G927	A864	C797	A733	G667
U1506	G1436	G1373	U1313	C1245	A1183	G1054	U992	G928	A865	G798	G734	
A1507	U1437	A1374	C1314	G1248	G1184	C1055	A994		G866	G799		G670
G1508	G1438	A1375	U1315	A1249	G1185	U1056	C995		G867		C738	G671
C1509	G1439	U1376	G1316	C1249	G1186	G1057	C996		A802		C739	U672
U1510	C1440	A1377	G1317	A1250	G1187	G1058	G999		G868		U740	G673
U1511	G1441	G1378	A1318	A1251	G1188	C1059	C999		U870		G741	G674
A1512	G1442	A1379	G1319	A1252	G1189	U1060	U1000		A803		G745	A675
A1513	G1443	U1380	C1320	G1255	G1190	U1062	A1001		C806		C745	A676
C1514	G1444	C1321	G1321	A1256	A1191	G1063	A1002		A807		A746	U677
C1515	G1445	G1382	G1322	U1257	C1192	G1064	G1003		C808		C747	U678
G1516		G1383	G1323	C1258	G1193	U1065	G1003A		C809		C748	C679
A1517	U1450	C1384	G1326	G1259	U1194	U1066	A1004		C810		C749	C680
A1518	A1451	G1385	C1327	C1260	C1195	C1067	A1005		C811		C750	
A1519		G1386	G1328	A1261	G1196	U1068	C942		C812		G751	G683
G1520	G1452	G1387	U1329	G1262	G1197	C1069	U943		U813		G752	A684
G1521	G1453	C1388	A1330	C1263	G1198	C1070	U944		A814		A753	G685
U1522	G1454	C1389	U1331	C1264	U1199	C1071	G945		A815		C754	U686
G1523	G1455	U1390	G1332	G1265	C1200	U1072	G1008		A816		G755	A687
C1524	G1462	U1391	C1333	C1266	A1201	U1073	G1009		C817		C756	G688
G1525	G1463	G1392	A1334	G1267	G1202	G1074	G1010		G883		U757	C689
G1526	G1464	U1393	G1335	C1268	G1203	C1075	U1012		U884		G758	G690
C1527	G1465	A1394	C1336	A1269	A1204	G1076	G1013		G885		U759	G691
U1528	G1466	C1395	C1337	G1270	U1205	G1077	A1014		C886		U760	U692
G1529	G1467	A1396	G1338	G1271	G1206	U1078	A1015		C887		C761	G693
G1530	G1470	C1397	C1339	U1272	G1207	U1079	G1019		C888		C762	A694
A1531	G1471	A1398	A1340	U1273	C1208	G1080	G954		A889		G763	A695
U1532	G1472	C1399	U1341	U1274	G1209	G1081			G890		C764	A696
C1533	G1473	G1400	U1342	U1275	U1212	G1082	U957		U891		G765	U697
C	G1474	C1401	C1343	A1280	A1213	U1083	G1021		A892		A766	G698
A	G1475	C1402	G1344	U1281	C1214	G1084	G1022		C893		C767	C699
C	G1476	A1403	U1345	U1282	G1215	U1085	G1023		G894		A768	G700
U	G1477	C1404	U1346	C1283	G1216	U1086	G1024		G895		C770	A701
C	G1478	G1405	A1347	C1284	U1150	G1087	U1025		G896		C771	A702
C1539	G1479	U1406	G1347	A1285	A1151	G1088	G1026		G897		A772	G703
U1540	G1480	C1407	U1348	A1286	A1152	G1089	C1027		A900		U773	
U1541	U1481	A1408	A1349	U1287	C1153	U1090	C1028		A901		C774	A706
U1542	G1482	C1409	A1350	A1288	G1154	U1091	C1029		C902		G775	C707
C1543	A1483	G1410	U1351	A1289	G1155	A1092	C1030		C903		C776	C708
U1544	C1484	C1411	C1352	G1290	G1156	A1093	G1030A		G906		A777	G709
	U1485	G1412	G1353	G1291	G1224	G1094	C1030B		A907		U778	G710
	G1486	A1413	C1354	U1292	A1225	U1095	G1030C		A908		C779	
	G1487	U1414	G1355	U1293	C1226	C1096	A1030D		A909		C780	G713
	G1488	G1415	G1356	G1294	A1227	C1097	G1031		C910		A781	G714
	G1489	G1416	A1357	G1295	C1228	C1098	G1032		U911		C782	A715
	C1490	G1417	U1358	C1296	A1229	C1099	G1033		C912		A783	A716
	G1491	U1418	C1359	C1297	G1230	G1100	G1034		A913		C784	G717
	A1492	G1419	A1360	C1298	G1231	A1101	A1035		G914		G785	G718
	A1493	C1420	G1361	G1299	U1232	A1102	G1036		A915		C786	C719
	U1494	G1421	C1361A	G1300	U1233	A1103	C1037		G916		G787	C720
	U1495	G1422	C1362	U1301	C1234	G1104	C1038		U917		A788	G721
	C1496	G1423	A1363	U1302	U1235	A1105	C1039		G918		U789	A722
	G1497	C1424	U1364	C1303	G1236	G1106	U981		C856		U790	U723
	U1498	U1425	G1365	C1304	C1237	C1107	U982		U920		C857	G724
	A1499	C1426	C1366	G1305	A1238	A1044	U921		G922		G791	
	A1500	U1427	C1367	A1306	U1239	C1045	G1046		A859		A792	A728
	C1501	A1428	G1368	U1240	U1241	A1047	G1047		A860		A793	A729
	A1502	C1429	C1369	G1309		G1048	G988		G924		A794	G730

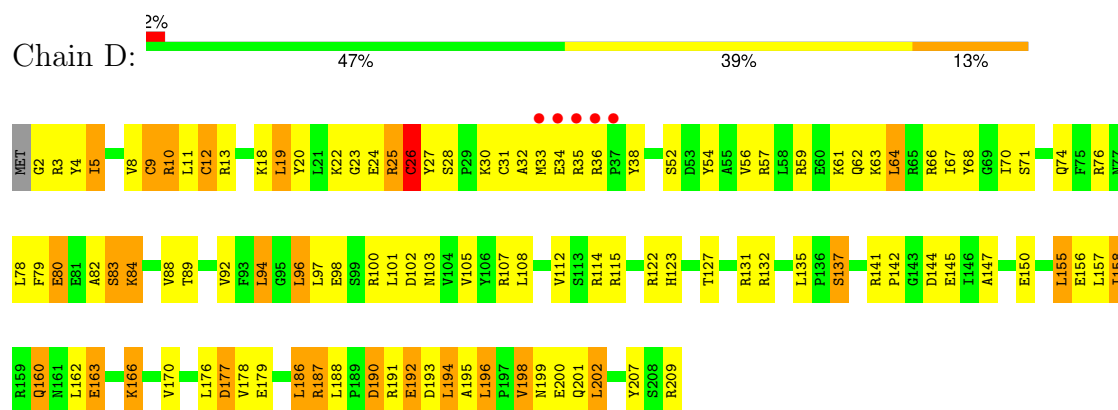
- Molecule 2: ribosomal protein S2



- Molecule 3: ribosomal protein S3

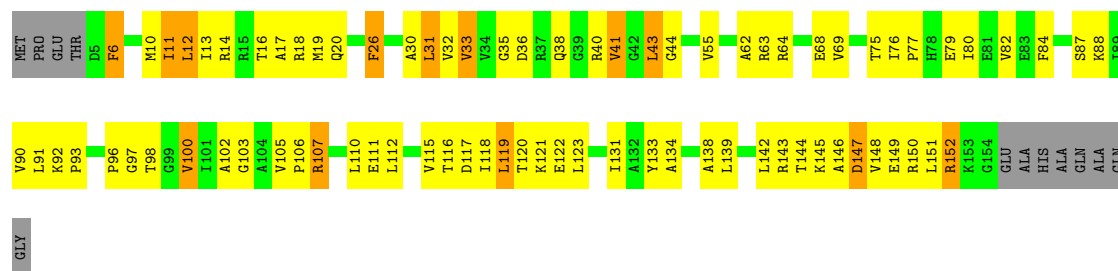


- Molecule 4: ribosomal protein S4



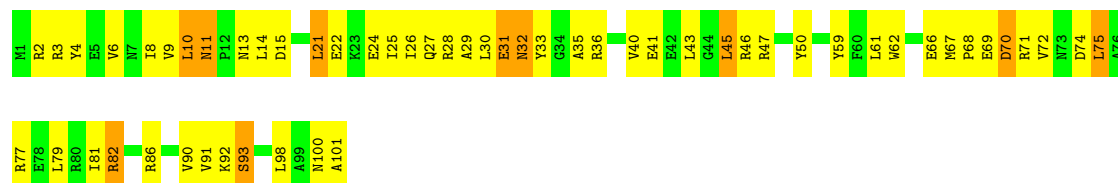
- Molecule 5: ribosomal protein S5





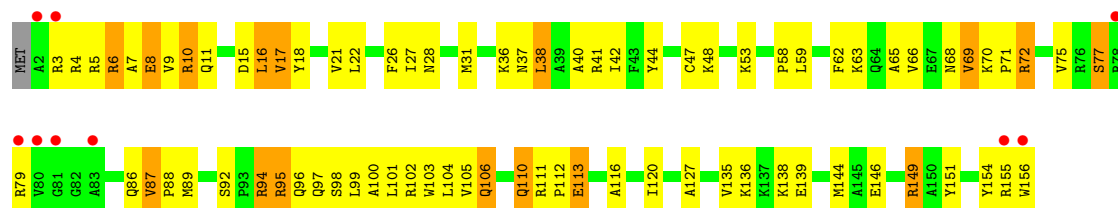
• Molecule 6: ribosomal protein S6

Chain F: 45% 46% 10%



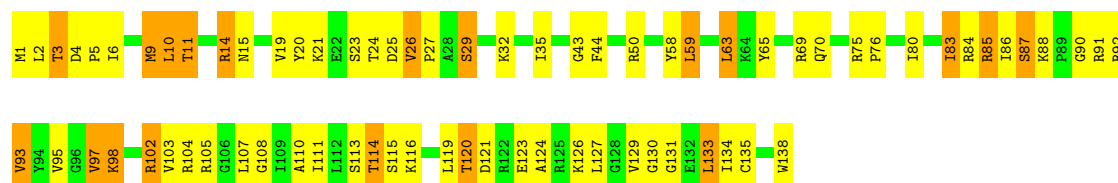
• Molecule 7: ribosomal protein S7

Chain G: 6% 49% 40% 10%



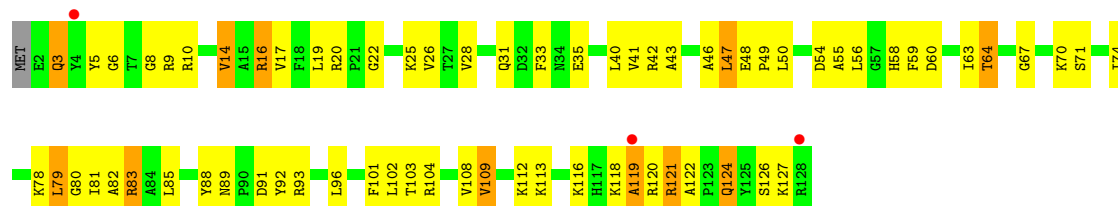
• Molecule 8: ribosomal protein S8

Chain H: 47% 39% 14%

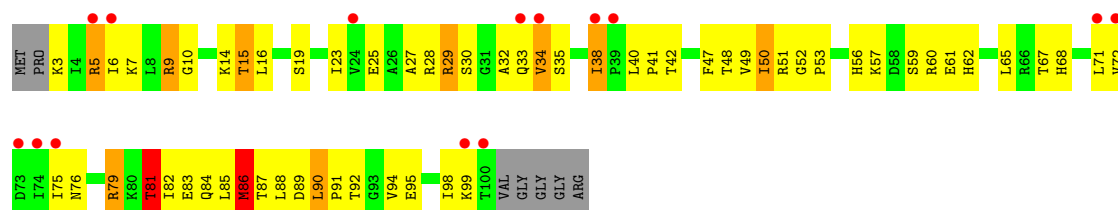


• Molecule 9: ribosomal protein S9

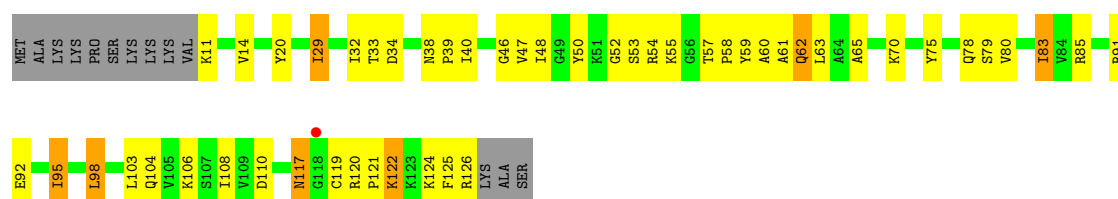
Chain I: 2% 45% 45% 9%



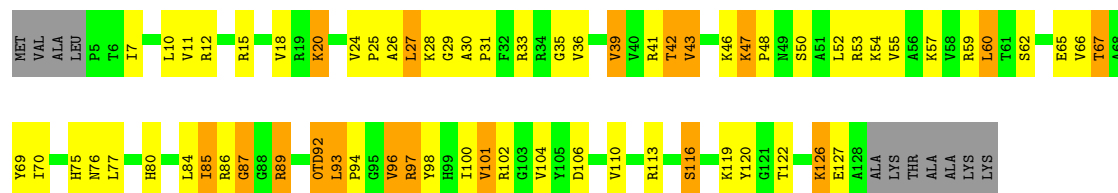
- Molecule 10: ribosomal protein S10



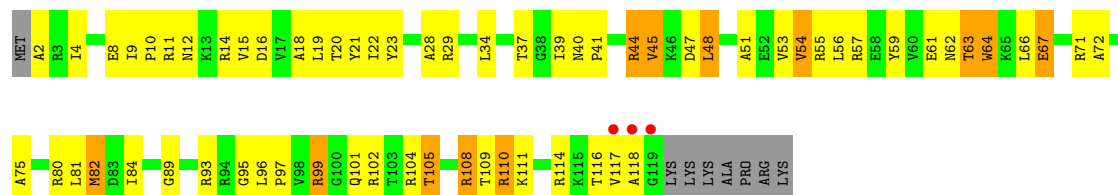
- Molecule 11: ribosomal protein S11



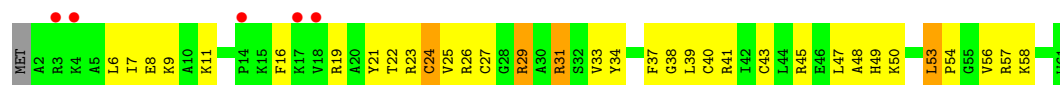
- Molecule 12: ribosomal protein S12



- Molecule 13: ribosomal protein S13

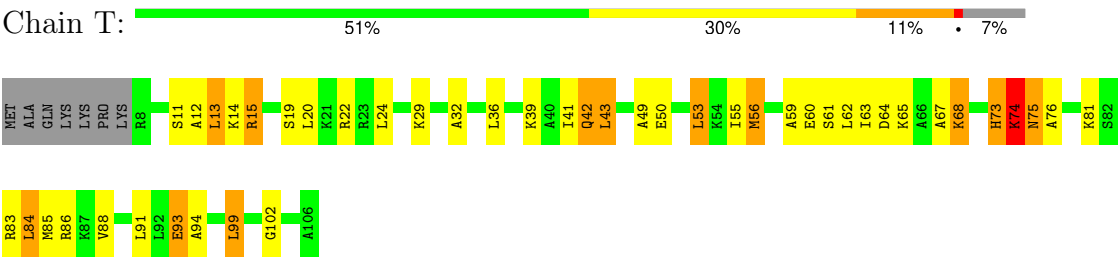


- Molecule 14: ribosomal protein S14



- Chain S:
- 
- | Amino Acid | Percentage |
|------------|------------|
| Met        | 10%        |
| Ala        | 45%        |
| Val        | 29%        |
| Leu        | 10%        |
| Pro        | 14%        |

● Molecule 20: ribosomal protein S20



● Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.64Å 402.64Å 174.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.66 – 3.65 34.66 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.66-3.65) 98.0 (34.66-3.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, $R_{free}$	0.153 , 0.208 0.151 , 0.206	Depositor DCC
$R_{free}$ test set	7745 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	138.2	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 129.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 7MG, 0TD, MA6, PSU, 4OC, M2G, 2MG, UR3, 5MC

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	1.22	174/36140 (0.5%)	1.94	1937/56398 (3.4%)
2	B	0.81	2/1935 (0.1%)	0.96	4/2609 (0.2%)
3	C	0.62	0/1636	0.81	0/2205
4	D	0.77	1/1733 (0.1%)	1.00	5/2318 (0.2%)
5	E	0.97	1/1162 (0.1%)	1.12	5/1564 (0.3%)
6	F	0.69	0/856	0.83	2/1154 (0.2%)
7	G	0.68	0/1276	0.90	1/1709 (0.1%)
8	H	1.03	0/1136	1.12	2/1527 (0.1%)
9	I	0.56	0/1029	0.81	0/1379
10	J	0.63	0/805	0.87	1/1082 (0.1%)
11	K	0.83	1/879 (0.1%)	0.98	2/1187 (0.2%)
12	L	0.82	0/977	1.10	2/1306 (0.2%)
13	M	0.63	0/947	0.83	0/1270
14	N	0.65	0/501	0.87	0/664
15	O	0.81	0/740	1.02	2/987 (0.2%)
16	P	0.88	0/716	1.10	3/963 (0.3%)
17	Q	1.03	0/836	1.15	4/1117 (0.4%)
18	R	0.81	0/579	0.96	0/768
19	S	0.61	0/661	0.81	1/890 (0.1%)
20	T	0.80	0/765	1.07	2/1007 (0.2%)
21	U	0.58	0/212	0.91	0/277
All	All	1.09	179/55521 (0.3%)	1.69	1973/82381 (2.4%)

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
2	B	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
10	J	0	2
12	L	0	2
13	M	0	1
15	O	0	1
18	R	0	1
20	T	0	2
All	All	0	13

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-13.57	1.29	1.37
1	A	300	A	N3-C4	-9.42	1.29	1.34
1	A	1442	G	N9-C4	9.30	1.45	1.38
1	A	301	G	C6-N1	-9.24	1.33	1.39
1	A	822	C	N1-C6	-8.85	1.31	1.37

The worst 5 of 1973 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	G	N1-C6-O6	21.49	132.79	119.90
1	A	758	G	C5-C6-O6	-16.07	118.96	128.60
1	A	1442	G	N3-C4-N9	15.41	135.25	126.00
1	A	722	A	C2-N3-C4	-14.89	103.16	110.60
1	A	232	G	N1-C6-O6	14.78	128.76	119.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	GLU	Peptide
4	D	195	ALA	Peptide
7	G	154	TYR	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	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	A	32645	0	16507	767	0
2	B	1900	0	1951	95	0
3	C	1612	0	1677	92	0
4	D	1703	0	1763	97	0
5	E	1146	0	1207	71	0
6	F	843	0	857	43	0
7	G	1257	0	1296	63	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	67	0
10	J	792	0	835	62	0
11	K	864	0	881	40	0
12	L	972	0	1058	57	0
13	M	937	0	995	50	0
14	N	492	0	529	29	0
15	O	729	0	768	46	0
16	P	700	0	720	37	0
17	Q	823	0	893	47	0
18	R	574	0	644	37	0
19	S	647	0	673	28	0
20	T	763	0	861	29	0
21	U	208	0	221	12	0
22	A	268	0	0	0	0
22	B	2	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	J	2	0	0	0	0
22	M	1	0	0	0	0
22	N	1	0	0	0	0
22	P	3	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	383	0	0	11	0
24	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	G	2	0	0	2	0
24	I	1	0	0	1	0
24	J	3	0	0	3	0
24	L	1	0	0	0	0
24	M	7	0	0	1	0
24	N	2	0	0	0	0
24	P	8	0	0	1	0
24	Q	1	0	0	0	0
24	T	1	0	0	0	0
All	All	52434	0	36550	1661	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 19.

The worst 5 of 1661 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)
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.46	0.98
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.41	0.98
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.53	0.90
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.54	0.88
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.07	0.87

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	232/256 (91%)	201 (87%)	28 (12%)	3 (1%)	12	47
3	C	204/239 (85%)	173 (85%)	31 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
5	E	148/162 (91%)	139 (94%)	9 (6%)	0	100	100
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	56
10	J	96/105 (91%)	76 (79%)	17 (18%)	3 (3%)	4	32
11	K	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	54
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	19	56
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	17	54
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
18	R	68/88 (77%)	58 (85%)	9 (13%)	1 (2%)	10	44
19	S	78/93 (84%)	73 (94%)	4 (5%)	1 (1%)	12	47
20	T	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	7	38
21	U	22/27 (82%)	21 (96%)	0	1 (4%)	2	23
All	All	2336/2541 (92%)	2086 (89%)	235 (10%)	15 (1%)	25	62

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
20	T	99	LEU
9	I	119	ALA
10	J	86	MET

### 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%)	152 (75%)	50 (25%)	0	5
3	C	160/188 (85%)	127 (79%)	33 (21%)	1	7
4	D	180/181 (99%)	142 (79%)	38 (21%)	1	7
5	E	115/123 (94%)	90 (78%)	25 (22%)	1	7
6	F	90/90 (100%)	71 (79%)	19 (21%)	1	7
7	G	126/127 (99%)	101 (80%)	25 (20%)	1	8
8	H	119/119 (100%)	95 (80%)	24 (20%)	1	8
9	I	98/99 (99%)	79 (81%)	19 (19%)	1	9
10	J	87/92 (95%)	75 (86%)	12 (14%)	3	20
11	K	88/99 (89%)	76 (86%)	12 (14%)	3	21
12	L	103/110 (94%)	77 (75%)	26 (25%)	0	4
13	M	94/101 (93%)	75 (80%)	19 (20%)	1	8
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	7
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	9
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	10
17	Q	94/97 (97%)	78 (83%)	16 (17%)	2	13
18	R	61/77 (79%)	49 (80%)	12 (20%)	1	8
19	S	71/80 (89%)	54 (76%)	17 (24%)	0	5
20	T	76/82 (93%)	58 (76%)	18 (24%)	1	5
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	7
All	All	1983/2111 (94%)	1576 (80%)	407 (20%)	1	7

5 of 407 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	121	ARG
13	M	47	ASP
20	T	84	LEU
10	J	33	GLN
12	L	36	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	28	GLN
16	P	82	GLN
18	R	36	ASN
17	Q	45	HIS
4	D	161	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	358 (23%)	45 (2%)

5 of 358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	21	G
1	A	22	G
1	A	31	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1004	A
1	A	1201	A
1	A	1049	U
1	A	1145	C
1	A	1257	U

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

17 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
1	2MG	A	1207	1	18,26,27	1.77	3 (16%)	16,38,41	1.60	3 (18%)
1	7MG	A	527	22,1	23,26,27	4.56	8 (34%)	27,39,42	2.76	9 (33%)
1	5MC	A	1404	1	19,22,23	1.48	3 (15%)	26,32,35	1.56	4 (15%)
1	UR3	A	1498	1	19,22,23	1.14	2 (10%)	26,32,35	1.52	3 (11%)
1	MA6	A	1518[B]	1	19,26,27	1.13	1 (5%)	18,38,41	0.80	0
1	5MC	A	1407	1	19,22,23	1.44	3 (15%)	26,32,35	1.37	3 (11%)
1	5MC	A	967	1	19,22,23	1.52	5 (26%)	26,32,35	0.82	0
1	PSU	A	1540	1	18,21,22	1.18	1 (5%)	21,30,33	1.45	3 (14%)
1	MA6	A	1519[A]	1	19,26,27	1.24	2 (10%)	18,38,41	0.88	0
1	4OC	A	1402	1	20,23,24	1.29	1 (5%)	25,32,35	0.74	0
12	0TD	L	92	12	8,9,10	2.13	1 (12%)	6,11,13	3.25	5 (83%)
1	5MC	A	1400	1	19,22,23	1.61	4 (21%)	26,32,35	1.03	2 (7%)
1	MA6	A	1519[B]	1	19,26,27	1.64	4 (21%)	18,38,41	0.64	0
1	PSU	A	516	22,1	18,21,22	1.31	1 (5%)	21,30,33	1.46	4 (19%)
1	MA6	A	1518[A]	1	19,26,27	1.24	2 (10%)	18,38,41	0.95	1 (5%)
1	M2G	A	966	1	20,27,28	1.38	3 (15%)	19,40,43	1.30	2 (10%)
1	PSU	A	1541	1	18,21,22	1.04	1 (5%)	21,30,33	1.70	4 (19%)

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
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	7MG	A	527	22,1	-	2/7/37/38	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	1/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	4/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	2/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
12	0TD	L	92	12	-	4/7/12/14	-
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519[B]	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	22,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-20.19	1.32	1.45
1	A	1404	5MC	C5-C4	5.39	1.48	1.44
12	L	92	0TD	CB-CA	5.36	1.56	1.54
1	A	1207	2MG	C6-N1	4.95	1.45	1.37
1	A	516	PSU	C6-C5	4.51	1.40	1.35

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.87	123.04	110.94
1	A	527	7MG	N9-C4-N3	6.49	134.96	125.46
12	L	92	0TD	CSB-SB-CB	-5.97	91.63	102.36
1	A	527	7MG	C5-C4-N3	-5.29	118.21	128.13
1	A	527	7MG	C2-N3-C4	4.88	120.70	112.30

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	5	0
1	A	1518[B]	MA6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1407	5MC	2	0
1	A	967	5MC	3	0
1	A	1519[A]	MA6	4	0
1	A	1402	4OC	3	0
12	L	92	0TD	2	0
1	A	1400	5MC	1	0
1	A	1519[B]	MA6	3	0
1	A	516	PSU	1	0
1	A	1518[A]	MA6	3	0
1	A	966	M2G	3	0
1	A	1541	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 289 ligands modelled in this entry, 289 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1498/1522 (98%)	-0.30	33 (2%) 62 48	88, 150, 286, 387	0
2	B	234/256 (91%)	-0.54	0 100 100	110, 168, 268, 286	0
3	C	206/239 (86%)	0.12	15 (7%) 15 10	162, 213, 261, 290	0
4	D	208/209 (99%)	-0.39	5 (2%) 59 45	108, 155, 199, 234	0
5	E	150/162 (92%)	-0.59	0 100 100	86, 126, 170, 198	0
6	F	101/101 (100%)	-0.59	0 100 100	121, 179, 212, 250	0
7	G	155/156 (99%)	-0.27	9 (5%) 23 15	143, 190, 248, 259	0
8	H	138/138 (100%)	-0.59	0 100 100	82, 115, 151, 197	0
9	I	127/128 (99%)	-0.11	3 (2%) 59 45	157, 217, 260, 283	0
10	J	98/105 (93%)	0.61	14 (14%) 2 2	188, 246, 325, 368	0
11	K	116/129 (89%)	-0.30	1 (0%) 84 74	116, 151, 201, 215	0
12	L	123/135 (91%)	-0.36	0 100 100	95, 157, 200, 225	0
13	M	118/126 (93%)	-0.09	3 (2%) 57 43	151, 183, 216, 272	0
14	N	60/61 (98%)	0.22	5 (8%) 11 8	166, 205, 258, 282	0
15	O	87/89 (97%)	-0.35	1 (1%) 80 70	94, 140, 184, 196	0
16	P	83/88 (94%)	-0.44	0 100 100	103, 146, 190, 220	0
17	Q	99/105 (94%)	-0.57	0 100 100	84, 126, 176, 199	0
18	R	70/88 (79%)	-0.48	1 (1%) 75 63	106, 150, 201, 227	0
19	S	80/93 (86%)	0.34	9 (11%) 5 3	185, 234, 275, 291	0
20	T	99/106 (93%)	-0.55	0 100 100	115, 152, 198, 234	0
21	U	24/27 (88%)	1.25	7 (29%) 0 0	165, 177, 208, 219	0
All	All	3874/4063 (95%)	-0.28	106 (2%) 54 40	82, 163, 261, 387	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	7.0
1	A	993	G	6.8
1	A	1037	C	5.4
21	U	18	TYR	5.2
10	J	39	PRO	4.7

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PSU	A	1540	20/21	0.87	0.41	212,224,250,256	0
1	PSU	A	1541	20/21	0.89	0.24	220,227,234,235	0
1	PSU	A	516	20/21	0.92	0.14	130,162,189,195	0
1	5MC	A	1404	21/22	0.94	0.17	127,137,174,177	0
1	5MC	A	1407	21/22	0.94	0.21	155,176,182,195	0
1	7MG	A	527	24/25	0.94	0.17	125,139,158,159	0
1	2MG	A	1207	24/25	0.94	0.14	201,225,261,267	0
1	MA6	A	1518[A]	24/25	0.95	0.39	121,138,144,149	24
1	MA6	A	1518[B]	24/25	0.95	0.39	123,140,152,155	24
1	M2G	A	966	25/26	0.95	0.20	167,195,202,204	0
1	5MC	A	1400	21/22	0.95	0.18	117,141,147,151	0
1	MA6	A	1519[A]	24/25	0.96	0.32	114,123,128,180	24
1	MA6	A	1519[B]	24/25	0.96	0.32	115,125,129,130	24
1	5MC	A	967	21/22	0.96	0.16	158,165,199,200	0
1	UR3	A	1498	21/22	0.96	0.26	132,143,155,163	0
1	4OC	A	1402	22/23	0.97	0.19	130,141,155,213	0
12	0TD	L	92	10/11	0.97	0.58	144,153,175,322	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1822	1/1	0.38	1.20	147,147,147,147	0
22	MG	A	1821	1/1	0.39	0.73	119,119,119,119	0
22	MG	A	1818	1/1	0.48	0.90	126,126,126,126	0
22	MG	P	102	1/1	0.54	0.37	141,141,141,141	0
22	MG	A	1689	1/1	0.60	0.39	124,124,124,124	0
22	MG	A	1656	1/1	0.65	0.55	110,110,110,110	0
22	MG	A	1777	1/1	0.68	0.74	144,144,144,144	0
22	MG	A	1725	1/1	0.70	0.88	126,126,126,126	0
22	MG	Q	201	1/1	0.71	0.18	136,136,136,136	0
22	MG	A	1767	1/1	0.72	0.46	167,167,167,167	0
22	MG	A	1858	1/1	0.72	0.38	115,115,115,115	0
22	MG	A	1714	1/1	0.73	0.49	124,124,124,124	0
22	MG	A	1739	1/1	0.73	0.69	132,132,132,132	0
22	MG	A	1853	1/1	0.74	0.40	161,161,161,161	0
22	MG	A	1699	1/1	0.74	0.49	171,171,171,171	0
22	MG	A	1761	1/1	0.74	0.16	157,157,157,157	0
22	MG	A	1816	1/1	0.74	0.31	422,422,422,422	0
22	MG	A	1686	1/1	0.75	0.16	166,166,166,166	0
22	MG	Q	202	1/1	0.75	0.34	146,146,146,146	0
22	MG	A	1866	1/1	0.76	0.18	123,123,123,123	0
22	MG	A	1817	1/1	0.76	0.34	144,144,144,144	0
22	MG	P	103	1/1	0.76	0.38	132,132,132,132	0
22	MG	A	1813	1/1	0.76	0.40	105,105,105,105	0
22	MG	A	1754	1/1	0.76	0.32	134,134,134,134	0
22	MG	A	1841	1/1	0.78	0.16	149,149,149,149	0
22	MG	A	1628	1/1	0.78	0.36	110,110,110,110	0
22	MG	A	1747	1/1	0.78	0.24	118,118,118,118	0
22	MG	A	1799	1/1	0.78	0.24	466,466,466,466	0
22	MG	A	1780	1/1	0.79	0.36	154,154,154,154	0
22	MG	A	1717	1/1	0.80	0.34	120,120,120,120	0
22	MG	A	1773	1/1	0.80	0.27	142,142,142,142	0
22	MG	A	1848	1/1	0.80	0.44	144,144,144,144	0
22	MG	J	201	1/1	0.80	0.74	127,127,127,127	0
22	MG	A	1652	1/1	0.81	0.26	150,150,150,150	0
22	MG	A	1728	1/1	0.81	0.29	128,128,128,128	0
22	MG	A	1709	1/1	0.81	0.43	118,118,118,118	0
22	MG	A	1776	1/1	0.82	0.45	135,135,135,135	0
22	MG	A	1712	1/1	0.82	0.43	151,151,151,151	0
22	MG	D	304	1/1	0.82	0.16	111,111,111,111	0
22	MG	A	1737	1/1	0.82	0.51	133,133,133,133	0
22	MG	A	1722	1/1	0.82	0.30	115,115,115,115	0
22	MG	A	1809	1/1	0.82	0.29	466,466,466,466	0
22	MG	A	1772	1/1	0.82	0.20	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1621	1/1	0.82	0.80	111,111,111,111	0
22	MG	A	1746	1/1	0.83	0.42	181,181,181,181	0
22	MG	A	1863	1/1	0.83	0.87	121,121,121,121	0
22	MG	A	1854	1/1	0.83	0.42	112,112,112,112	0
22	MG	A	1674	1/1	0.84	0.29	171,171,171,171	0
22	MG	A	1834	1/1	0.84	0.26	157,157,157,157	0
22	MG	A	1840	1/1	0.84	0.67	136,136,136,136	0
22	MG	A	1788	1/1	0.84	0.17	420,420,420,420	0
22	MG	A	1845	1/1	0.84	0.81	157,157,157,157	0
22	MG	A	1791	1/1	0.84	0.27	244,244,244,244	0
22	MG	A	1738	1/1	0.84	0.22	115,115,115,115	0
22	MG	A	1675	1/1	0.84	0.43	123,123,123,123	0
22	MG	A	1855	1/1	0.84	0.19	114,114,114,114	0
22	MG	A	1778	1/1	0.85	0.72	132,132,132,132	0
22	MG	A	1659	1/1	0.85	0.27	148,148,148,148	0
22	MG	A	1787	1/1	0.85	0.30	175,175,175,175	0
22	MG	A	1758	1/1	0.85	0.22	150,150,150,150	0
22	MG	A	1601	1/1	0.85	0.36	122,122,122,122	0
22	MG	A	1637	1/1	0.85	0.25	127,127,127,127	0
22	MG	A	1836	1/1	0.86	0.46	98,98,98,98	0
22	MG	A	1837	1/1	0.86	0.36	150,150,150,150	0
22	MG	A	1607	1/1	0.86	0.10	183,183,183,183	0
22	MG	A	1682	1/1	0.86	0.30	126,126,126,126	0
22	MG	A	1830	1/1	0.86	0.42	512,512,512,512	0
22	MG	A	1710	1/1	0.86	0.59	111,111,111,111	0
22	MG	A	1745	1/1	0.87	0.79	155,155,155,155	0
22	MG	A	1625	1/1	0.87	0.27	124,124,124,124	0
22	MG	A	1640	1/1	0.87	0.33	145,145,145,145	0
22	MG	A	1666	1/1	0.87	0.16	118,118,118,118	0
22	MG	A	1755	1/1	0.87	0.33	118,118,118,118	0
22	MG	A	1820	1/1	0.87	0.22	459,459,459,459	0
22	MG	A	1619	1/1	0.87	0.63	178,178,178,178	0
22	MG	S	101	1/1	0.87	0.84	156,156,156,156	0
22	MG	A	1653	1/1	0.88	0.27	127,127,127,127	0
22	MG	A	1751	1/1	0.88	0.40	139,139,139,139	0
22	MG	A	1859	1/1	0.89	0.48	143,143,143,143	0
22	MG	A	1713	1/1	0.89	0.35	92,92,92,92	0
22	MG	A	1687	1/1	0.89	0.20	162,162,162,162	0
22	MG	A	1789	1/1	0.89	0.14	215,215,215,215	0
22	MG	A	1729	1/1	0.89	0.33	105,105,105,105	0
22	MG	N	102	1/1	0.89	0.17	184,184,184,184	0
22	MG	A	1734	1/1	0.89	0.23	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1802	1/1	0.89	0.08	250,250,250,250	0
22	MG	A	1806	1/1	0.89	0.26	242,242,242,242	0
22	MG	A	1769	1/1	0.89	0.13	134,134,134,134	0
22	MG	A	1770	1/1	0.89	0.20	99,99,99,99	0
22	MG	A	1833	1/1	0.90	0.26	230,230,230,230	0
22	MG	A	1850	1/1	0.90	1.04	150,150,150,150	0
22	MG	A	1851	1/1	0.90	0.42	136,136,136,136	0
22	MG	A	1662	1/1	0.90	0.18	128,128,128,128	0
22	MG	A	1783	1/1	0.90	1.09	179,179,179,179	0
22	MG	A	1622	1/1	0.90	0.83	67,67,67,67	0
22	MG	A	1655	1/1	0.90	0.23	113,113,113,113	0
22	MG	A	1702	1/1	0.90	0.51	124,124,124,124	0
22	MG	A	1756	1/1	0.90	0.25	127,127,127,127	0
22	MG	A	1864	1/1	0.91	0.26	129,129,129,129	0
22	MG	A	1706	1/1	0.91	0.17	207,207,207,207	0
22	MG	A	1792	1/1	0.91	0.32	145,145,145,145	0
22	MG	A	1798	1/1	0.91	0.22	212,212,212,212	0
22	MG	A	1735	1/1	0.91	0.31	122,122,122,122	0
22	MG	P	101	1/1	0.91	0.43	90,90,90,90	0
22	MG	A	1708	1/1	0.91	0.42	127,127,127,127	0
22	MG	A	1685	1/1	0.91	0.81	109,109,109,109	0
22	MG	A	1807	1/1	0.91	0.48	254,254,254,254	0
22	MG	A	1860	1/1	0.91	0.09	167,167,167,167	0
22	MG	A	1757	1/1	0.91	0.22	105,105,105,105	0
22	MG	A	1763	1/1	0.92	0.22	362,362,362,362	0
22	MG	A	1868	1/1	0.92	0.20	144,144,144,144	0
22	MG	A	1723	1/1	0.92	0.08	151,151,151,151	0
22	MG	E	201	1/1	0.92	0.44	163,163,163,163	0
22	MG	A	1724	1/1	0.92	0.38	133,133,133,133	0
22	MG	A	1670	1/1	0.92	0.34	109,109,109,109	0
22	MG	A	1814	1/1	0.92	0.36	113,113,113,113	0
22	MG	A	1793	1/1	0.92	0.27	134,134,134,134	0
22	MG	A	1794	1/1	0.92	0.23	211,211,211,211	0
22	MG	A	1782	1/1	0.92	0.28	244,244,244,244	0
22	MG	A	1638	1/1	0.92	0.37	95,95,95,95	0
22	MG	A	1705	1/1	0.92	0.08	156,156,156,156	0
22	MG	A	1857	1/1	0.93	0.17	141,141,141,141	0
22	MG	A	1796	1/1	0.93	0.47	168,168,168,168	0
22	MG	A	1603	1/1	0.93	0.18	117,117,117,117	0
22	MG	A	1630	1/1	0.93	0.11	139,139,139,139	0
22	MG	A	1801	1/1	0.93	0.26	135,135,135,135	0
22	MG	A	1779	1/1	0.93	0.30	374,374,374,374	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1646	1/1	0.93	0.29	134,134,134,134	0
22	MG	A	1743	1/1	0.93	0.58	112,112,112,112	0
22	MG	A	1744	1/1	0.93	0.14	150,150,150,150	0
22	MG	A	1844	1/1	0.93	0.18	123,123,123,123	0
22	MG	F	201	1/1	0.93	0.35	144,144,144,144	0
22	MG	A	1765	1/1	0.93	0.24	127,127,127,127	0
22	MG	A	1649	1/1	0.93	0.19	130,130,130,130	0
22	MG	A	1663	1/1	0.93	0.09	102,102,102,102	0
22	MG	A	1633	1/1	0.93	0.24	113,113,113,113	0
22	MG	A	1669	1/1	0.93	0.27	144,144,144,144	0
22	MG	A	1696	1/1	0.93	0.37	399,399,399,399	0
22	MG	A	1609	1/1	0.93	0.26	115,115,115,115	0
22	MG	A	1856	1/1	0.93	0.18	136,136,136,136	0
22	MG	A	1797	1/1	0.94	0.12	176,176,176,176	0
22	MG	A	1766	1/1	0.94	0.18	131,131,131,131	0
22	MG	A	1826	1/1	0.94	0.25	225,225,225,225	0
22	MG	A	1781	1/1	0.94	0.07	174,174,174,174	0
22	MG	A	1752	1/1	0.94	0.20	108,108,108,108	0
22	MG	A	1861	1/1	0.94	0.14	163,163,163,163	0
22	MG	A	1605	1/1	0.94	0.31	105,105,105,105	0
22	MG	A	1785	1/1	0.94	0.09	364,364,364,364	0
22	MG	A	1711	1/1	0.94	0.50	139,139,139,139	0
22	MG	A	1771	1/1	0.94	0.10	114,114,114,114	0
22	MG	A	1810	1/1	0.94	0.70	386,386,386,386	0
22	MG	A	1843	1/1	0.94	0.16	186,186,186,186	0
22	MG	A	1812	1/1	0.94	0.09	429,429,429,429	0
22	MG	A	1733	1/1	0.94	0.21	102,102,102,102	0
22	MG	A	1626	1/1	0.94	0.21	112,112,112,112	0
22	MG	A	1815	1/1	0.94	0.37	286,286,286,286	0
22	MG	A	1700	1/1	0.94	0.40	110,110,110,110	0
22	MG	A	1852	1/1	0.94	0.18	102,102,102,102	0
22	MG	A	1608	1/1	0.94	0.29	99,99,99,99	0
22	MG	A	1748	1/1	0.94	0.36	136,136,136,136	0
22	MG	A	1726	1/1	0.94	0.20	130,130,130,130	0
22	MG	A	1849	1/1	0.95	0.14	133,133,133,133	0
22	MG	A	1623	1/1	0.95	0.08	148,148,148,148	0
22	MG	A	1831	1/1	0.95	0.16	244,244,244,244	0
22	MG	B	301	1/1	0.95	0.35	138,138,138,138	0
22	MG	A	1731	1/1	0.95	0.25	109,109,109,109	0
22	MG	A	1803	1/1	0.95	0.36	386,386,386,386	0
22	MG	A	1805	1/1	0.95	0.14	162,162,162,162	0
22	MG	A	1643	1/1	0.95	0.13	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1740	1/1	0.95	0.15	129,129,129,129	0
22	MG	A	1819	1/1	0.95	0.19	294,294,294,294	0
22	MG	A	1842	1/1	0.95	0.20	161,161,161,161	0
22	MG	A	1808	1/1	0.95	0.49	265,265,265,265	0
22	MG	A	1749	1/1	0.95	0.14	114,114,114,114	0
22	MG	A	1677	1/1	0.95	0.11	130,130,130,130	0
22	MG	A	1657	1/1	0.95	0.16	136,136,136,136	0
22	MG	A	1618	1/1	0.96	0.35	147,147,147,147	0
22	MG	A	1688	1/1	0.96	0.19	121,121,121,121	0
22	MG	A	1671	1/1	0.96	0.39	120,120,120,120	0
22	MG	A	1838	1/1	0.96	0.14	187,187,187,187	0
22	MG	A	1862	1/1	0.96	0.27	155,155,155,155	0
22	MG	A	1750	1/1	0.96	0.08	102,102,102,102	0
22	MG	A	1602	1/1	0.96	0.50	145,145,145,145	0
22	MG	A	1736	1/1	0.96	0.20	156,156,156,156	0
22	MG	A	1624	1/1	0.96	0.49	113,113,113,113	0
22	MG	A	1676	1/1	0.96	0.44	151,151,151,151	0
22	MG	A	1642	1/1	0.96	0.28	158,158,158,158	0
22	MG	A	1679	1/1	0.96	0.30	150,150,150,150	0
22	MG	A	1664	1/1	0.96	0.08	129,129,129,129	0
22	MG	A	1683	1/1	0.96	0.13	175,175,175,175	0
22	MG	A	1762	1/1	0.96	0.17	184,184,184,184	0
22	MG	A	1611	1/1	0.96	0.19	171,171,171,171	0
22	MG	A	1804	1/1	0.96	0.67	366,366,366,366	0
22	MG	A	1828	1/1	0.96	0.11	351,351,351,351	0
22	MG	A	1764	1/1	0.96	0.24	220,220,220,220	0
22	MG	A	1644	1/1	0.96	0.19	126,126,126,126	0
22	MG	A	1786	1/1	0.96	0.20	179,179,179,179	0
22	MG	A	1716	1/1	0.97	0.44	139,139,139,139	0
22	MG	A	1615	1/1	0.97	0.21	87,87,87,87	0
22	MG	A	1790	1/1	0.97	0.18	356,356,356,356	0
22	MG	A	1753	1/1	0.97	0.19	128,128,128,128	0
22	MG	A	1719	1/1	0.97	0.16	108,108,108,108	0
22	MG	A	1839	1/1	0.97	0.29	170,170,170,170	0
22	MG	A	1635	1/1	0.97	0.13	101,101,101,101	0
22	MG	A	1775	1/1	0.97	0.18	110,110,110,110	0
22	MG	A	1665	1/1	0.97	0.09	271,271,271,271	0
22	MG	A	1707	1/1	0.97	0.13	83,83,83,83	0
22	MG	A	1651	1/1	0.97	0.23	184,184,184,184	0
22	MG	B	302	1/1	0.97	0.27	147,147,147,147	0
22	MG	D	302	1/1	0.97	0.65	122,122,122,122	0
22	MG	A	1616	1/1	0.97	0.25	195,195,195,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1846	1/1	0.97	0.10	150,150,150,150	0
22	MG	A	1690	1/1	0.97	0.14	387,387,387,387	0
22	MG	A	1693	1/1	0.97	0.31	150,150,150,150	0
22	MG	J	202	1/1	0.97	0.39	344,344,344,344	0
22	MG	M	201	1/1	0.97	0.20	375,375,375,375	0
22	MG	A	1680	1/1	0.97	0.10	128,128,128,128	0
22	MG	A	1825	1/1	0.97	0.17	470,470,470,470	0
22	MG	A	1732	1/1	0.97	0.18	81,81,81,81	0
22	MG	A	1661	1/1	0.97	0.12	141,141,141,141	0
22	MG	A	1613	1/1	0.97	0.13	160,160,160,160	0
22	MG	A	1768	1/1	0.97	0.29	112,112,112,112	0
22	MG	A	1832	1/1	0.97	0.15	390,390,390,390	0
23	ZN	N	101	1/1	0.97	0.17	233,233,233,233	0
22	MG	A	1811	1/1	0.98	0.18	255,255,255,255	0
22	MG	A	1715	1/1	0.98	0.35	88,88,88,88	0
22	MG	A	1691	1/1	0.98	0.11	128,128,128,128	0
22	MG	A	1692	1/1	0.98	0.08	175,175,175,175	0
22	MG	A	1718	1/1	0.98	0.11	103,103,103,103	0
22	MG	A	1672	1/1	0.98	0.07	166,166,166,166	0
22	MG	A	1721	1/1	0.98	0.18	127,127,127,127	0
22	MG	A	1695	1/1	0.98	0.19	134,134,134,134	0
22	MG	A	1645	1/1	0.98	0.22	76,76,76,76	0
22	MG	A	1697	1/1	0.98	0.39	335,335,335,335	0
22	MG	A	1698	1/1	0.98	0.10	218,218,218,218	0
22	MG	A	1612	1/1	0.98	0.04	174,174,174,174	0
22	MG	A	1824	1/1	0.98	0.89	407,407,407,407	0
22	MG	A	1727	1/1	0.98	0.12	91,91,91,91	0
22	MG	A	1660	1/1	0.98	0.07	116,116,116,116	0
22	MG	A	1760	1/1	0.98	0.12	147,147,147,147	0
22	MG	A	1829	1/1	0.98	0.26	202,202,202,202	0
22	MG	A	1867	1/1	0.98	0.19	139,139,139,139	0
22	MG	A	1701	1/1	0.98	0.13	146,146,146,146	0
22	MG	A	1648	1/1	0.98	0.25	176,176,176,176	0
22	MG	A	1795	1/1	0.98	0.27	247,247,247,247	0
22	MG	C	302	1/1	0.98	0.16	181,181,181,181	0
22	MG	A	1703	1/1	0.98	0.13	142,142,142,142	0
22	MG	D	303	1/1	0.98	0.10	119,119,119,119	0
22	MG	A	1704	1/1	0.98	0.18	95,95,95,95	0
22	MG	A	1639	1/1	0.98	0.13	163,163,163,163	0
22	MG	A	1650	1/1	0.98	0.11	112,112,112,112	0
22	MG	A	1614	1/1	0.98	0.08	144,144,144,144	0
22	MG	A	1641	1/1	0.98	0.31	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1627	1/1	0.98	0.10	110,110,110,110	0
22	MG	A	1667	1/1	0.98	0.09	123,123,123,123	0
22	MG	A	1668	1/1	0.98	0.29	271,271,271,271	0
22	MG	A	1741	1/1	0.98	0.38	118,118,118,118	0
22	MG	A	1742	1/1	0.98	0.12	129,129,129,129	0
22	MG	A	1654	1/1	0.98	0.10	121,121,121,121	0
22	MG	A	1636	1/1	0.98	0.27	127,127,127,127	0
22	MG	A	1847	1/1	0.98	0.11	155,155,155,155	0
22	MG	A	1617	1/1	0.98	0.22	113,113,113,113	0
22	MG	A	1865	1/1	0.99	0.18	180,180,180,180	0
22	MG	A	1720	1/1	0.99	0.08	114,114,114,114	0
22	MG	A	1784	1/1	0.99	0.08	153,153,153,153	0
22	MG	A	1823	1/1	0.99	0.07	276,276,276,276	0
22	MG	A	1694	1/1	0.99	0.34	194,194,194,194	0
22	MG	A	1604	1/1	0.99	0.26	151,151,151,151	0
22	MG	C	301	1/1	0.99	0.33	165,165,165,165	0
22	MG	A	1629	1/1	0.99	0.50	147,147,147,147	0
22	MG	A	1827	1/1	0.99	0.24	304,304,304,304	0
22	MG	A	1684	1/1	0.99	0.15	158,158,158,158	0
22	MG	A	1673	1/1	0.99	0.06	211,211,211,211	0
22	MG	A	1610	1/1	0.99	0.21	119,119,119,119	0
22	MG	A	1658	1/1	0.99	0.19	111,111,111,111	0
22	MG	A	1774	1/1	0.99	0.05	142,142,142,142	0
22	MG	A	1632	1/1	0.99	0.40	90,90,90,90	0
22	MG	A	1759	1/1	0.99	0.11	155,155,155,155	0
22	MG	A	1835	1/1	0.99	0.15	349,349,349,349	0
22	MG	A	1606	1/1	0.99	0.09	113,113,113,113	0
22	MG	A	1730	1/1	0.99	0.12	129,129,129,129	0
22	MG	A	1678	1/1	0.99	0.13	182,182,182,182	0
22	MG	A	1634	1/1	0.99	0.28	290,290,290,290	0
22	MG	A	1647	1/1	0.99	0.25	138,138,138,138	0
22	MG	A	1800	1/1	0.99	0.13	62,62,62,62	0
23	ZN	D	301	1/1	0.99	0.34	117,117,117,117	0
22	MG	A	1681	1/1	0.99	0.13	152,152,152,152	0
22	MG	A	1620	1/1	1.00	0.13	116,116,116,116	0
22	MG	A	1631	1/1	1.00	0.14	93,93,93,93	0

## 6.5 Other polymers

There are no such residues in this entry.