



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2016 – 09:23 PM EST

PDB ID : 5JVG  
Title : The large ribosomal subunit from *Deinococcus radiodurans* in complex with avilamycin  
Authors : Krupkin, M.; Wekselman, I.; Matzov, D.; Eyal, Z.; Diskin Posner, Y.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.  
Deposited on : 2016-05-11  
Resolution : 3.43 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

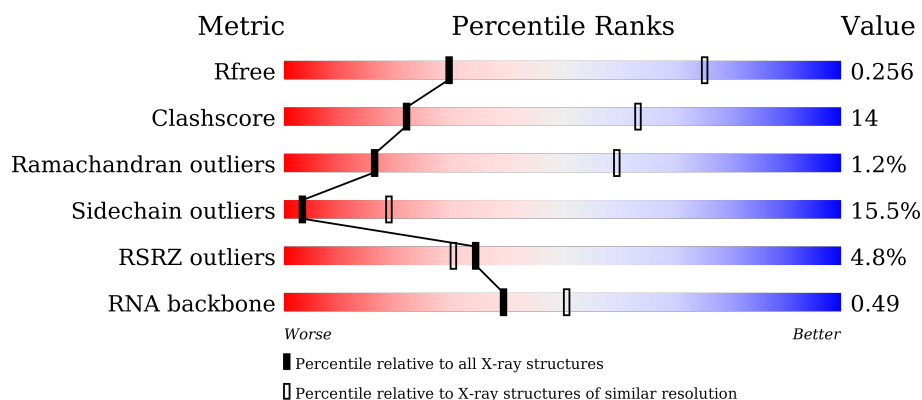
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2877	
2	Y	124	
3	A	275	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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
31	MG	X	2902	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	X	2911	-	-	-	X
31	MG	X	2912	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2925	-	-	-	X
31	MG	X	2931	-	-	-	X
31	MG	X	2932	-	-	-	X
31	MG	X	2937	-	-	-	X
31	MG	X	2938	-	-	-	X
31	MG	X	2940	-	-	-	X
31	MG	X	2944	-	-	-	X
31	MG	X	2949	-	-	-	X
31	MG	X	2958	-	-	-	X
31	MG	X	2962	-	-	-	X
31	MG	X	2964	-	-	-	X
31	MG	X	2977	-	-	-	X
31	MG	X	2987	-	-	-	X
31	MG	X	2988	-	-	-	X
31	MG	X	2997	-	-	-	X
31	MG	X	3000	-	-	-	X
31	MG	X	3011	-	-	-	X
31	MG	X	3029	-	-	-	X
31	MG	X	3030	-	-	-	X
31	MG	X	3036	-	-	-	X
31	MG	X	3042	-	-	-	X
31	MG	X	3045	-	-	-	X
31	MG	X	3082	-	-	-	X
31	MG	X	3096	-	-	-	X
31	MG	X	3099	-	-	-	X
31	MG	X	3101	-	-	-	X
31	MG	X	3114	-	-	-	X
31	MG	X	3124	-	-	-	X
31	MG	X	3127	-	-	-	X
31	MG	X	3134	-	-	-	X
31	MG	X	3161	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	3162	-	-	-	X
31	MG	X	3164	-	-	-	X
31	MG	X	3165	-	-	-	X
31	MG	X	3173	-	-	-	X
31	MG	X	3198	-	-	-	X
31	MG	X	3222	-	-	-	X
31	MG	X	3232	-	-	-	X
31	MG	X	3292	-	-	-	X
31	MG	X	3294	-	-	-	X
31	MG	X	3297	-	-	-	X
31	MG	X	3324	-	-	-	X
31	MG	X	3326	-	-	-	X
31	MG	X	3328	-	-	-	X
31	MG	X	3329	-	-	-	X
31	MG	Y	201	-	-	-	X
32	MPD	X	3316	-	-	X	X
32	MPD	X	3317	-	-	-	X
33	SPD	X	3322	-	-	-	X

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 85766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2710	Total	C	N	O	P	0	1	0
			58191	25957	10742	18782	2710			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	272	Total	C	N	O	S	0	0	0
			2085	1299	416	366	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	195	Total	C	N	O	S	0	0	0
			1489	925	285	276	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1367	869	241	250	7			

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

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	S	0	0	0
			982	601	195	186				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1060	680	192	181	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	115	Total	C	N	O	S	0	0	0
			897	552	183	159	3			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	119	Total	C	N	O	0	0	0
			939	586	185	168			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	97	Total	C	N	O	0	0	0
			759	477	142	140			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	128	Total	C	N	O	S	0	0	0
			1015	640	200	173	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			809	504	153	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25/general stress protein Ctc.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	180	Total	C	N	O	S	0	0	0
			1370	864	241	259	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	74	Total	C	N	O	S	0	0	0
			549	341	111	97				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			444	273	91	75	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

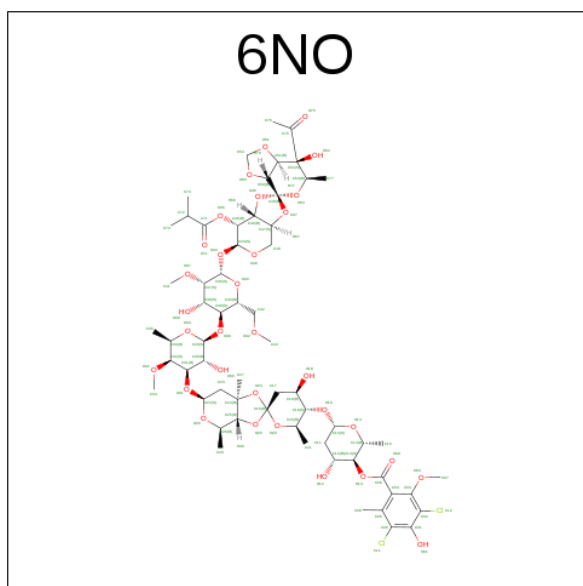
- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			453	285	92	73	3			

- Molecule 30 is Avilamycin (three-letter code: 6NO) (formula:  $C_{61}H_{88}Cl_2O_{32}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	Cl	O	0	0
			95	61	2	32		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

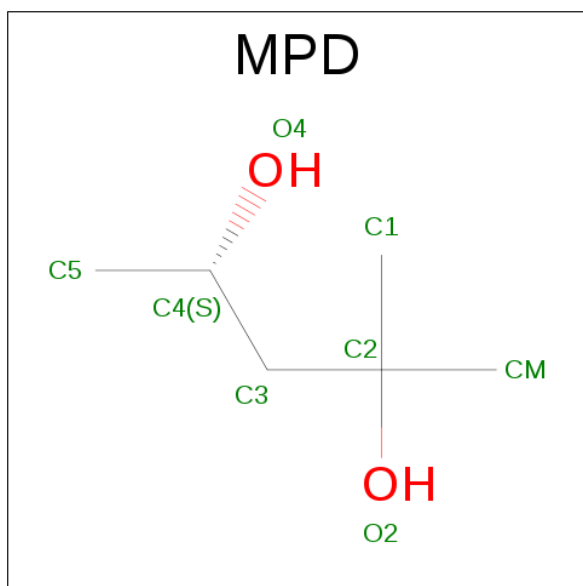
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	J	1	Total	Mg	0	0
			1	1		
31	K	1	Total	Mg	0	0
			1	1		
31	A	1	Total	Mg	0	0
			1	1		
31	T	1	Total	Mg	0	0
			1	1		

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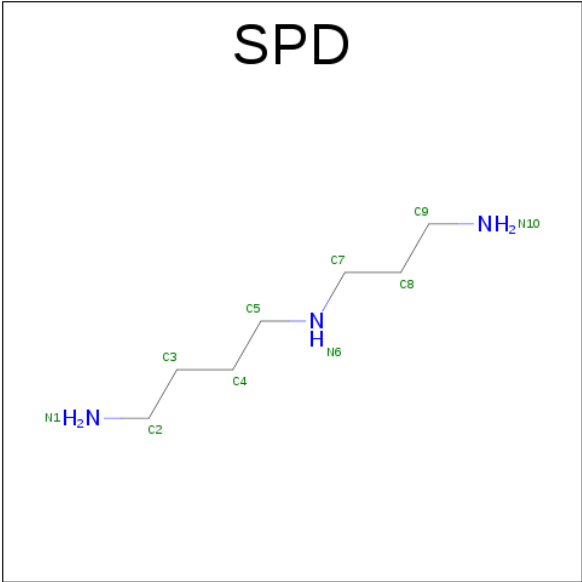
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	N	1	Total 1	Mg 1	0	0
31	X	420	Total 420	Mg 420	0	0
31	Y	19	Total 19	Mg 19	0	0
31	3	1	Total 1	Mg 1	0	0
31	M	1	Total 1	Mg 1	0	0

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).

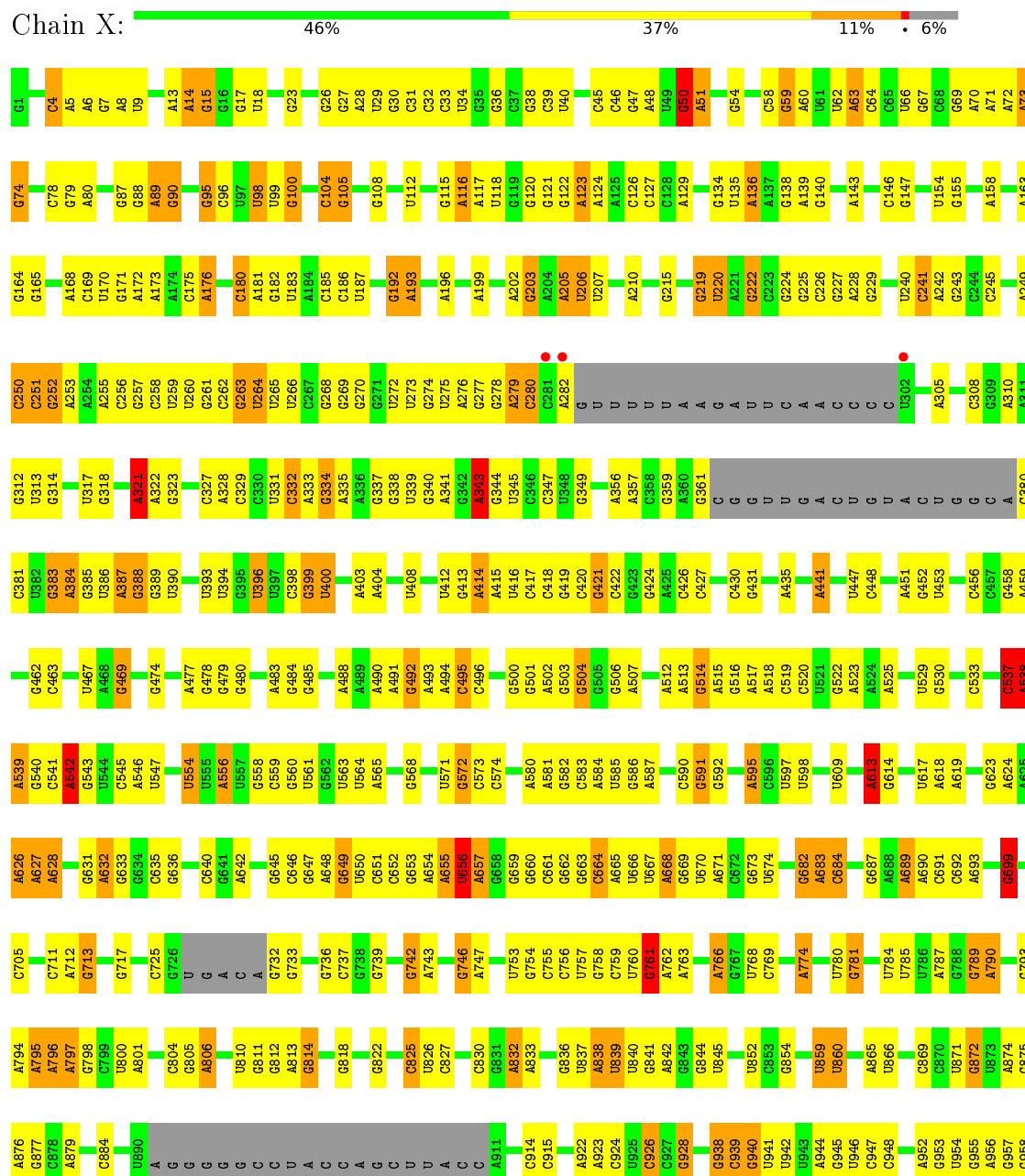


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

### 3 Residue-property plots

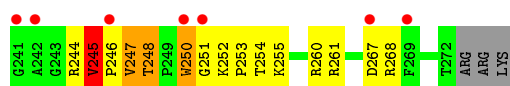
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 23S ribosomal RNA

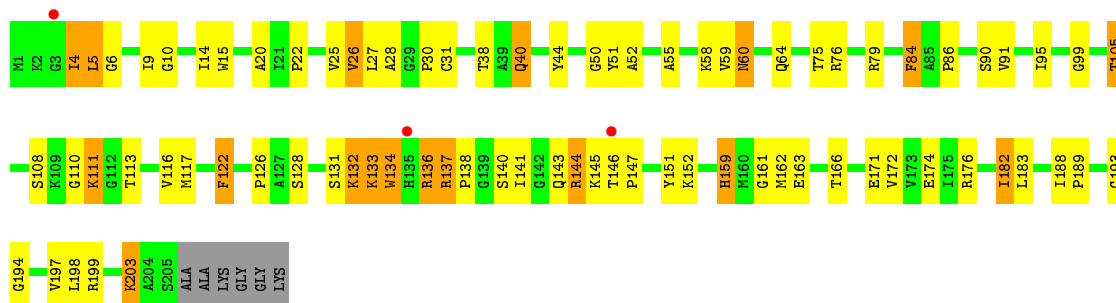


G	G2070	C1991	A	A1821	C1665	C1570	G1479	C1404	U1313	G1222	C1134	G1053	C959
U	G2076	G1992	C	A1750	G1668	G1571	G1480	A1405	A1314	G1223	C1135	C1054	U960
G	G2077	G1993	G	A1751	G1669	C1572	U1482	A1406	A1315	A1224	A1056	A1055	G961
G	G2078	A1996	U	A1752	G1670	C1573	U1483	G1407	A1321	G1225	G1142	A1057	A954
A	G2083	A1997	C	A1753	G1671	C1575	G1488	A1408	G1322			G1058	
G	G2084	A1998	C	A1754	A1671		G1489	U1410	U1325	A1231	C1145	C968	
C	G2085	U1999		G1755	A1672		U1490	C1411	U1326	U1232	C1146	U969	
A	U2000	U2000		G1760	C1673			A1412			G1147	A1060	A970
C	U2006	G2001		C1675	A1582			G1414			G1148	A1061	A971
C	U2007				A1583			G1415			G1149	C972	
C	U2008				A1584			G1416			G1150	G1066	U973
C	U2009				A1585			G1417			U1151	G1067	
C	U2010				A1586			G1418			C1152	A1063	G985
C	U2011				A1587			G1419			A1153	G1069	A994
C	U2012				U1592			G1420			A1154	G1070	
C	U2013				C1593			G1421			G1155	U1071	C998
C	U2014				U1594			G1422			G1156	U1072	A999
C	U2015				A1595			G1423			G1157	G1073	G1000
C	U2016				A1596			G1424				G1074	
C	U2017				A1597			G1425				C1075	
C	U2018				C1598			G1426			U1161	U1076	C1003
C	U2019				A1599			G1427			A1162	U1077	A1004
C	U2020				U1600			G1428			C1163	A1078	U1005
C	U2021				U1601			G1429			C1164	G1079	C1006
C	U2022				G1602			G1430			G1165	A1080	A1007
C	U2023				A1603			U1631			A1166	A1081	
C	U2024				U1604			G1432			A1167	U1082	C1016
C	U2025				C1605			A1433				G1085	U1019
C	U2026				A1606			U1434			U1172	C1086	A1020
C	U2027				U1607			G1435			G1173	A1087	A1021
C	U2028				U1608			G1436			U1174	A1022	
C	U2029				C1614			A1437			U1175	U1023	
C	U2030				A1619			G1438				C1090	U1026
C	U2031				C1623			U1439			C1181	U1092	C1027
C	U2032				A1624			G1440			U1182	U1093	U1028
C	U2033				A1625			A1441			C1183	C1094	G1029
C	U2034				A1626			G1442			U1184	A1095	U1030
C	U2035				U1627			C1443			C1185	A1096	C1031
C	U2036				A1628			G1444			A	A1097	A1032
C	U2037				U1629			A1445			A	A1098	G1033
C	U2038				C1630			U1446			C	A1099	U1034
C	U2039				A1631			G1447			G1191	G1035	
C	U2040				U1632			A1448			U1192	G1036	U1037
C	U2041				C1633			U1449			A1193	A1106	
C	U2042				A1634			G1450			U1194	U1116	A1040
C	U2043				G1635			A1451			G1201	G1041	
C	U2044				U1636			U1452			G1202	G1042	
C	U2045				G1637			G1453			G1121	A1043	
C	U2046				U1638			U1454			A1122	U1044	
C	U2047				G1639			C1455			G1123	G1045	
C	U2048				A1643			G1456			U1124	U1046	
C	U2049				U1644			A1457			G1125		
C	U2050				C1645			U1458			A1126	C1049	
C	U2051				U1646			A1459			G1127	U1050	
C	U2052				G1647			U1460			C1128	G1051	
C	U2053				A1648			A1461			A1129	C1052	
C	U2054				C1649			G1462					
C	U2055				U1650			A1463					
C	U2056				A1651			A1464					
C	U2057				G1652			G1465					
C	U2058				U1653			A1466					
C	U2059				U1654			U1467					
C	U2060				G1664			U1468					
C	U2061							G1470					
C	U2062							U1471					
C	U2063							U1472					
C	U2064							U1473					
C	U2065							U1474					
C	U2066							U1475					
C	U2067							U1476					
C	U2068							U1477					
C	U2069							U1478					

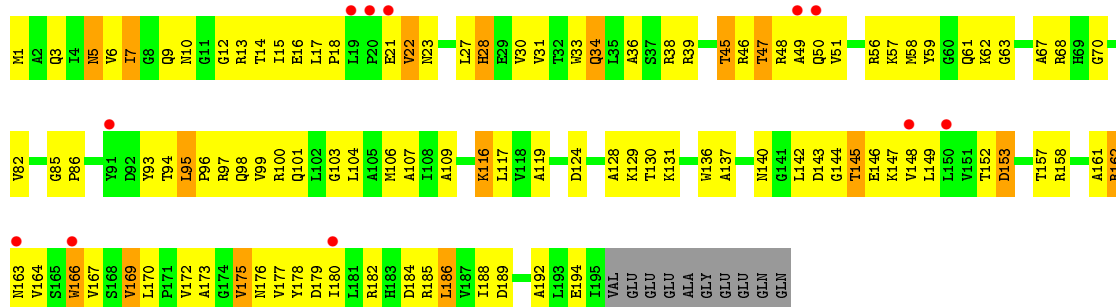




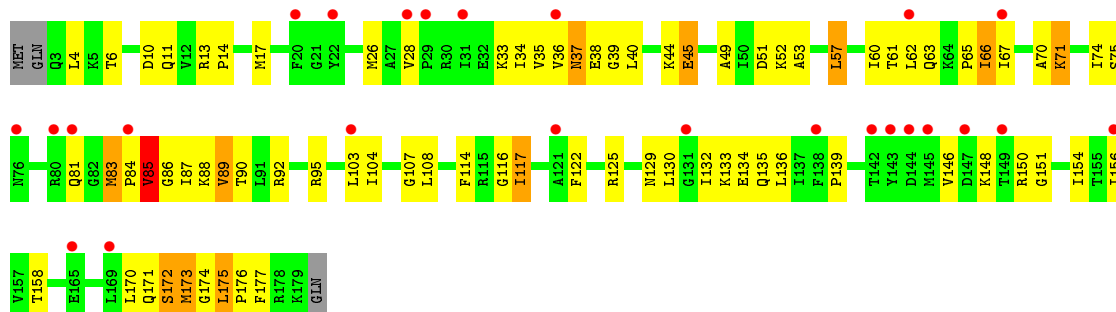
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



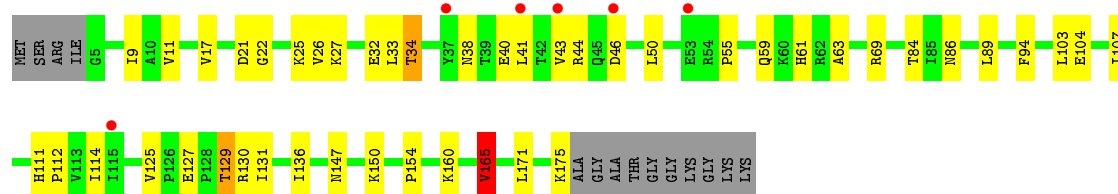
• Molecule 6: 50S ribosomal protein L5



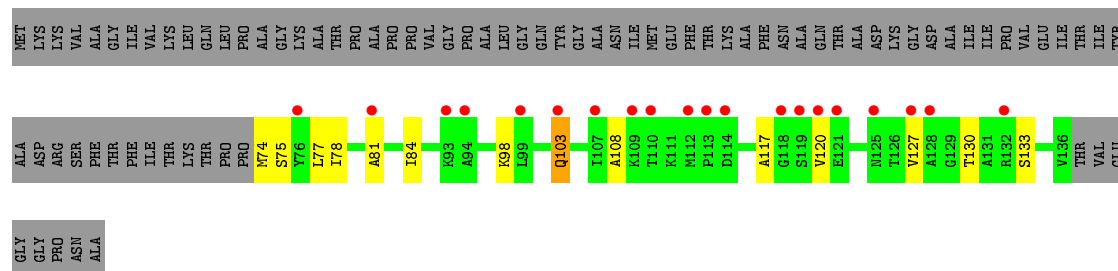
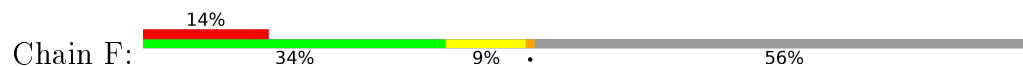
• Molecule 7: 50S ribosomal protein L6



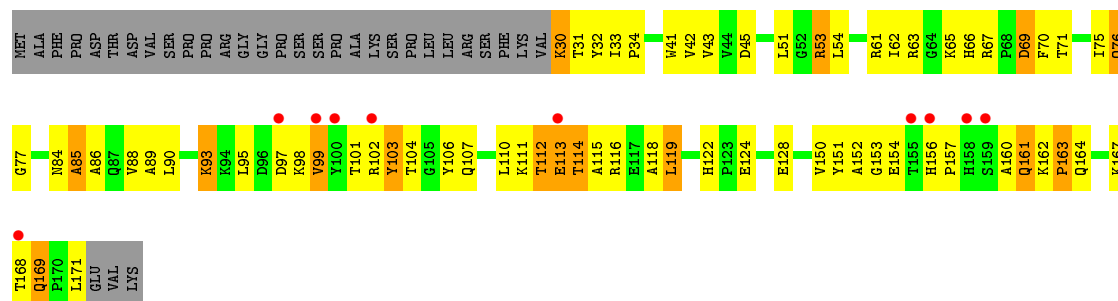
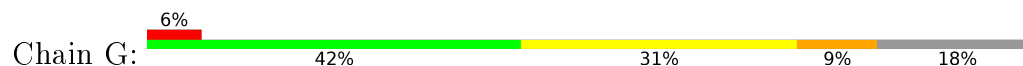




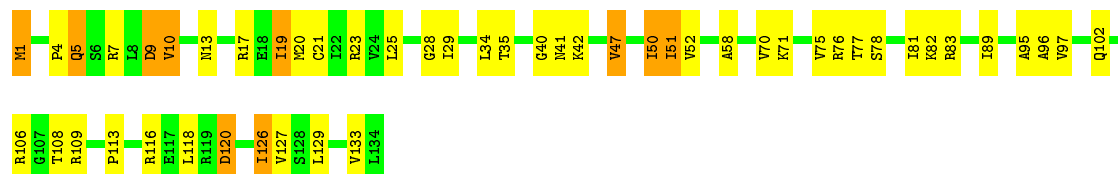
- Molecule 8: 50S ribosomal protein L11



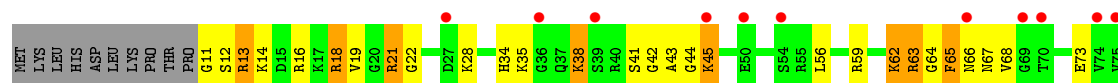
- Molecule 9: 50S ribosomal protein L13

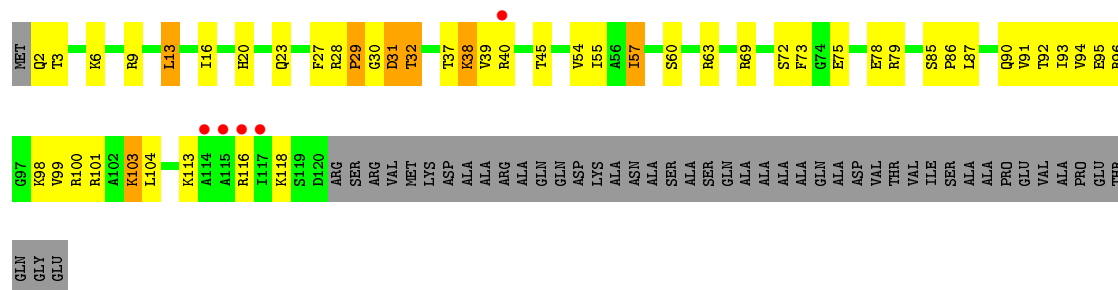
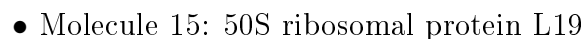
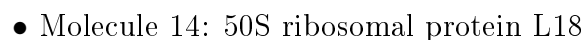
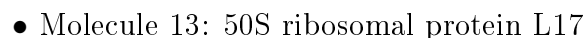
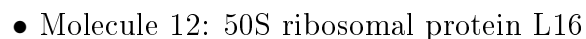


- Molecule 10: 50S ribosomal protein L14

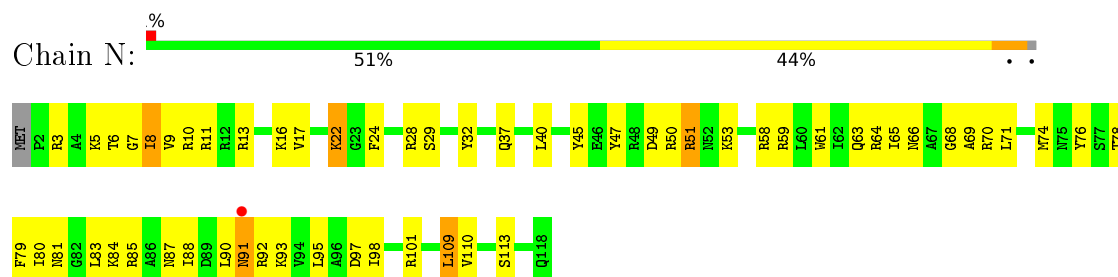


- Molecule 11: 50S ribosomal protein L15

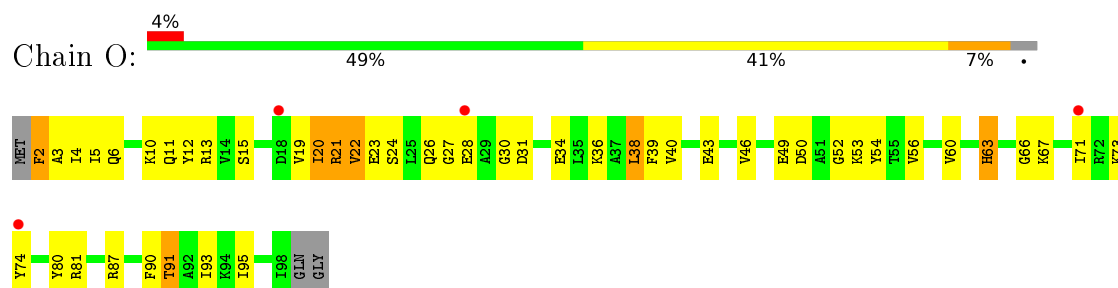




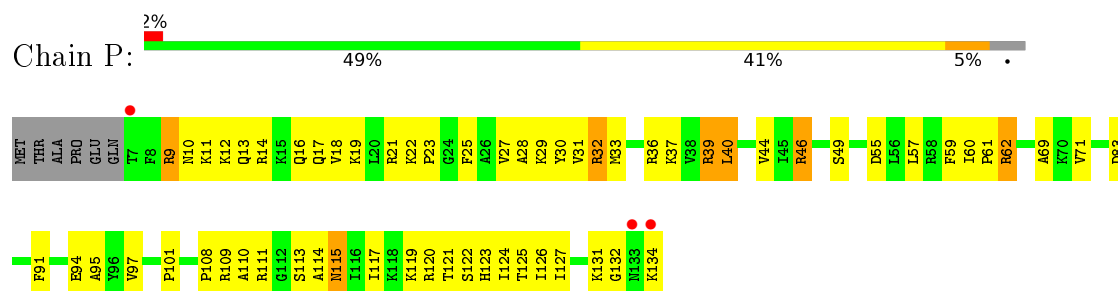
- Molecule 16: 50S ribosomal protein L20



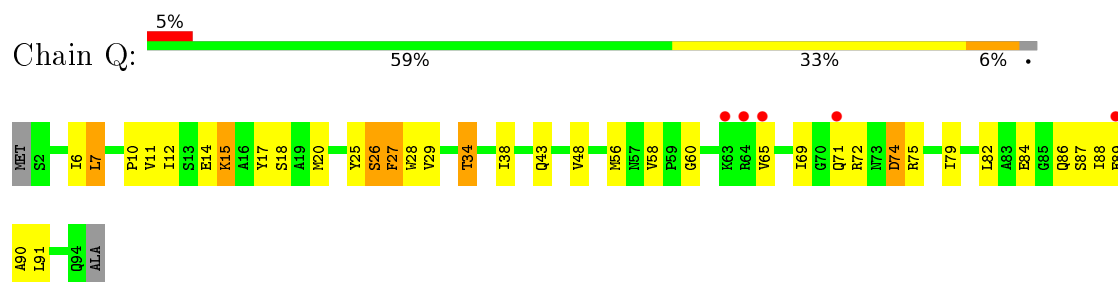
- Molecule 17: 50S ribosomal protein L21



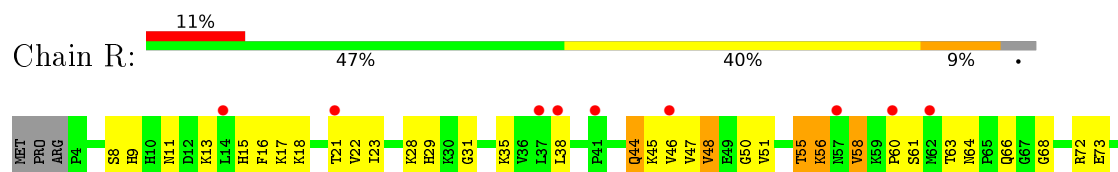
- Molecule 18: 50S ribosomal protein L22

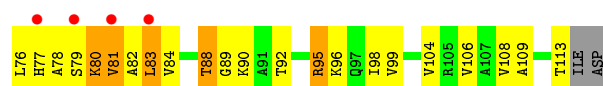


- Molecule 19: 50S ribosomal protein L23

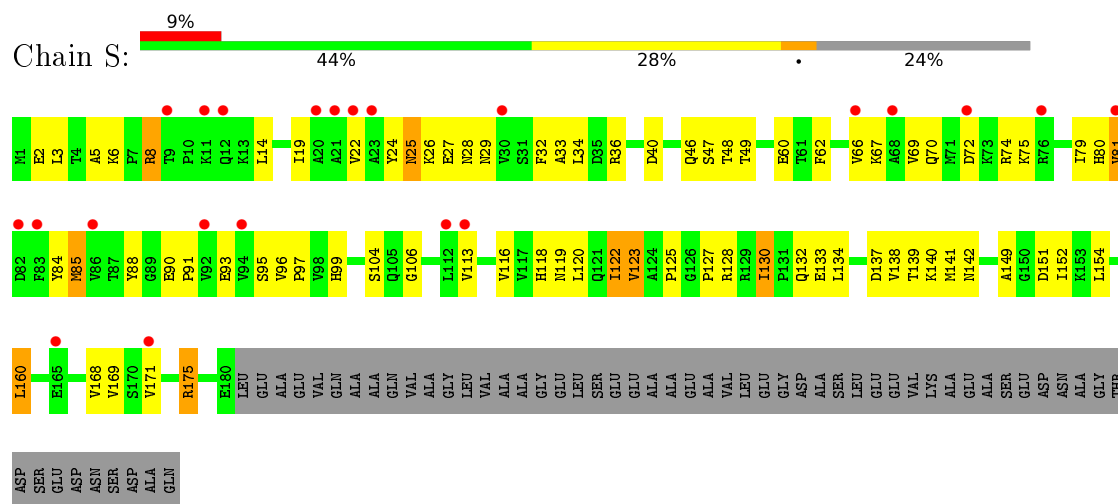


- Molecule 20: 50S ribosomal protein L24

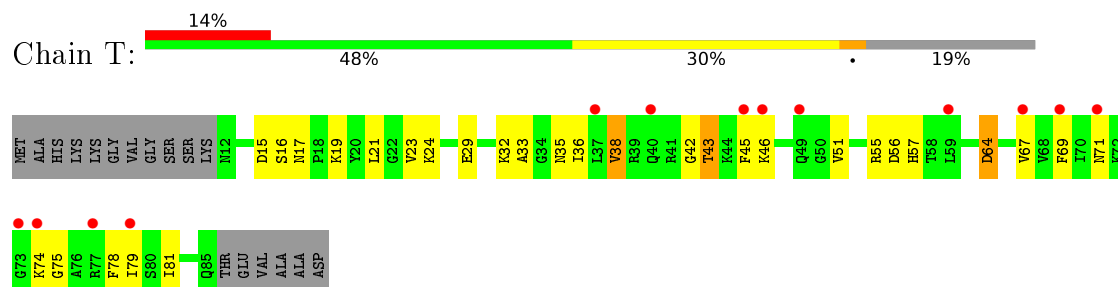




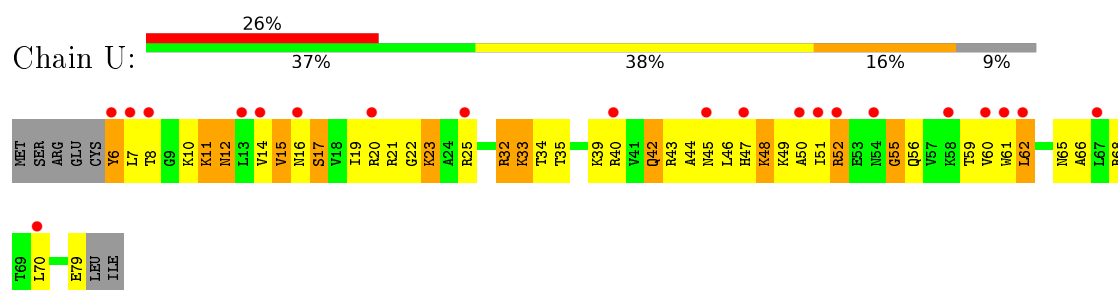
- Molecule 21: 50S ribosomal protein L25/general stress protein Ctc



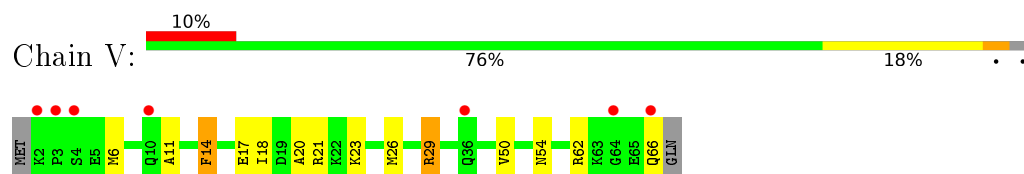
- Molecule 22: 50S ribosomal protein L27



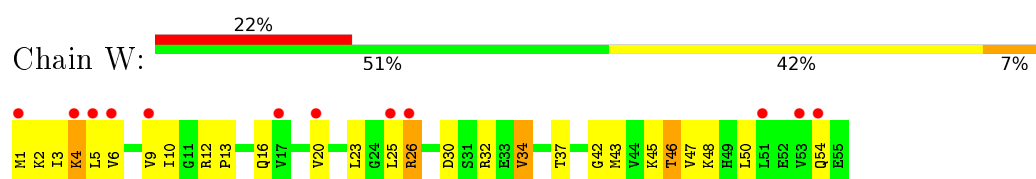
- Molecule 23: 50S ribosomal protein L28



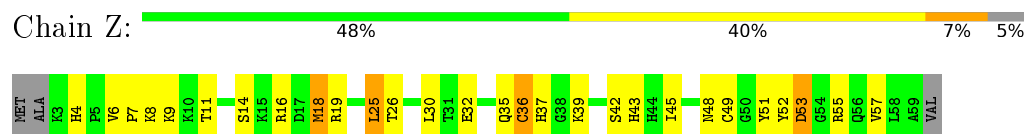
- Molecule 24: 50S ribosomal protein L29



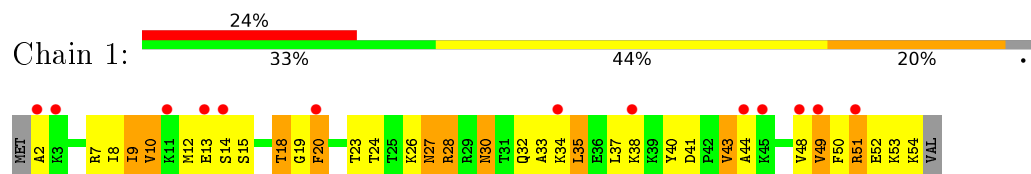
- Molecule 25: 50S ribosomal protein L30



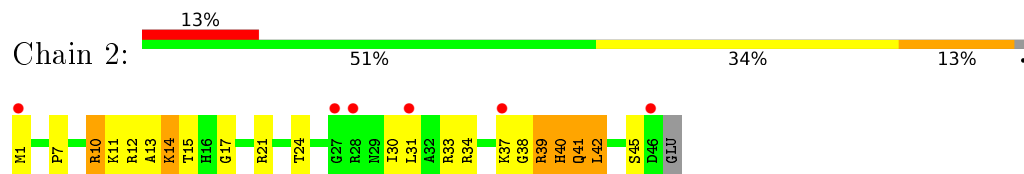
- Molecule 26: 50S ribosomal protein L32



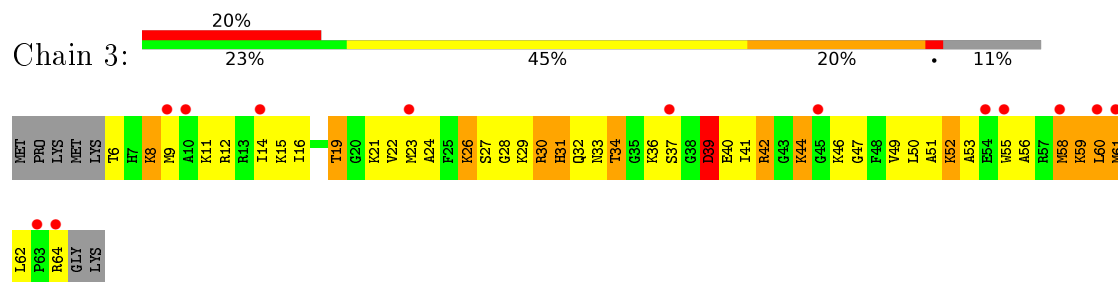
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.03Å 412.63Å 698.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.43 51.02 – 3.43	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.55-3.43) 88.9 (51.02-3.43)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.253 0.217 , 0.256	Depositor DCC
$R_{free}$ test set	14626 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.1	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	85766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 6NO, MG, SPD, MPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	X	0.45	3/65161 (0.0%)	0.98	120/101636 (0.1%)
2	Y	0.32	0/2863	0.82	2/4461 (0.0%)
3	A	0.34	0/2127	0.66	3/2864 (0.1%)
4	B	0.41	0/1567	0.69	0/2105
5	C	0.34	0/1512	0.61	0/2046
6	D	0.25	0/1385	0.54	0/1862
7	E	0.25	0/1308	0.47	0/1771
8	F	0.24	0/455	0.48	0/611
9	G	0.39	0/1138	0.70	0/1539
10	H	0.40	0/1007	0.68	0/1352
11	I	0.39	0/991	0.69	0/1328
12	J	0.41	0/1083	0.64	0/1451
13	K	0.43	0/905	0.68	0/1212
14	L	0.35	0/785	0.64	0/1048
15	M	0.45	0/952	0.72	1/1277 (0.1%)
16	N	0.36	0/994	0.58	0/1323
17	O	0.35	0/768	0.66	1/1025 (0.1%)
18	P	0.43	0/1028	0.65	0/1375
19	Q	0.35	0/737	0.60	0/988
20	R	0.37	0/819	0.71	0/1103
21	S	0.27	0/1395	0.57	0/1897
22	T	0.37	0/563	0.66	0/747
23	U	0.36	0/553	0.73	0/741
24	V	0.25	0/529	0.48	0/704
25	W	0.32	0/426	0.52	0/568
26	Z	0.38	0/456	0.64	0/613
27	1	0.37	0/434	0.76	1/579 (0.2%)
28	2	0.37	0/387	0.72	0/509
29	3	0.40	0/459	0.72	0/604
All	All	0.43	3/92787 (0.0%)	0.90	128/139339 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	D	0	2
9	G	0	2
11	I	0	2
14	L	0	2
15	M	0	1
21	S	0	1
22	T	0	1
23	U	0	3
27	1	0	1
28	2	0	1
29	3	0	3
All	All	0	19

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	N9-C4	7.85	1.42	1.37
1	X	774	A	N7-C5	6.14	1.43	1.39
1	X	774	A	C6-N1	-5.13	1.31	1.35

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1670	G	N1-C6-O6	-12.98	112.11	119.90
1	X	774	A	N1-C6-N6	-12.65	111.01	118.60
1	X	1675	C	O5'-P-OP1	-12.45	94.49	105.70
1	X	1670	G	C5-C6-O6	9.99	134.60	128.60
1	X	1670	G	C6-C5-N7	9.02	135.81	130.40

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	81	GLN	Peptide
6	D	83	MET	Peptide
9	G	107	GLN	Peptide
9	G	113	GLU	Peptide
11	I	38	LYS	Peptide



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58191	0	29325	975	0
2	Y	2561	0	1306	46	0
3	A	2085	0	2158	110	0
4	B	1539	0	1600	84	0
5	C	1489	0	1516	87	0
6	D	1367	0	1408	59	0
7	E	1286	0	1336	25	0
8	F	451	0	474	9	0
9	G	1114	0	1144	69	0
10	H	997	0	1046	34	0
11	I	982	0	1002	54	0
12	J	1060	0	1073	40	0
13	K	897	0	955	48	0
14	L	779	0	820	62	0
15	M	939	0	964	38	0
16	N	978	0	1020	55	0
17	O	759	0	774	38	0
18	P	1015	0	1094	47	0
19	Q	726	0	753	22	0
20	R	809	0	848	45	0
21	S	1370	0	1385	41	0
22	T	556	0	579	18	0
23	U	549	0	584	40	0
24	V	525	0	546	7	0
25	W	424	0	470	17	0
26	Z	444	0	440	28	0
27	1	427	0	445	33	0
28	2	383	0	414	21	0
29	3	453	0	488	37	0
30	X	95	0	0	2	0
31	3	1	0	0	0	0
31	A	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	X	420	0	0	0	0
31	Y	19	0	0	0	0
32	X	40	0	70	15	0
33	X	30	0	57	7	0
All	All	85766	0	56094	1909	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 14.

The worst 5 of 1909 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1277:G:OP1	26:Z:19:ARG:NH2	1.99	0.95
1:X:1669:A:OP2	13:K:9:LYS:NZ	2.00	0.95
1:X:2757:G:H5''	1:X:2758:A:H5'	1.49	0.94
1:X:2015:G:N7	32:X:3316:MPD:O4	2.00	0.93
10:H:28:GLY:HA2	10:H:50:ILE:HD11	1.52	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	270/275 (98%)	226 (84%)	44 (16%)	0	100	100
4	B	203/211 (96%)	189 (93%)	13 (6%)	1 (0%)	34	75
5	C	193/205 (94%)	163 (84%)	27 (14%)	3 (2%)	12	53
6	D	175/180 (97%)	145 (83%)	27 (15%)	3 (2%)	11	52
7	E	169/185 (91%)	160 (95%)	8 (5%)	1 (1%)	30	73
8	F	61/144 (42%)	54 (88%)	6 (10%)	1 (2%)	12	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	140/174 (80%)	120 (86%)	16 (11%)	4 (3%)	6	41
10	H	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
11	I	132/156 (85%)	103 (78%)	27 (20%)	2 (2%)	13	55
12	J	134/141 (95%)	111 (83%)	23 (17%)	0	100	100
13	K	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
14	L	102/114 (90%)	79 (78%)	20 (20%)	3 (3%)	6	41
15	M	117/166 (70%)	109 (93%)	6 (5%)	2 (2%)	11	52
16	N	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	21	66
17	O	95/100 (95%)	83 (87%)	12 (13%)	0	100	100
18	P	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
19	Q	91/95 (96%)	74 (81%)	15 (16%)	2 (2%)	8	47
20	R	108/115 (94%)	87 (81%)	20 (18%)	1 (1%)	21	66
21	S	178/237 (75%)	153 (86%)	21 (12%)	4 (2%)	8	47
22	T	72/91 (79%)	62 (86%)	10 (14%)	0	100	100
23	U	72/81 (89%)	52 (72%)	15 (21%)	5 (7%)	1	17
24	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
25	W	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
26	Z	55/60 (92%)	52 (94%)	3 (6%)	0	100	100
27	1	51/55 (93%)	33 (65%)	15 (29%)	3 (6%)	2	21
28	2	44/47 (94%)	36 (82%)	7 (16%)	1 (2%)	8	46
29	3	57/66 (86%)	42 (74%)	13 (23%)	2 (4%)	4	36
All	All	3121/3522 (89%)	2696 (86%)	386 (12%)	39 (1%)	16	60

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	85	VAL
6	D	173	MET
9	G	85	ALA
28	2	39	ARG
29	3	40	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	212/216 (98%)	175 (82%)	37 (18%)	2	13
4	B	155/157 (99%)	134 (86%)	21 (14%)	5	25
5	C	155/163 (95%)	134 (86%)	21 (14%)	5	25
6	D	143/156 (92%)	126 (88%)	17 (12%)	6	30
7	E	136/144 (94%)	129 (95%)	7 (5%)	29	69
8	F	46/107 (43%)	44 (96%)	2 (4%)	35	74
9	G	118/146 (81%)	100 (85%)	18 (15%)	3	20
10	H	103/103 (100%)	84 (82%)	19 (18%)	2	10
11	I	96/121 (79%)	74 (77%)	22 (23%)	1	4
12	J	104/115 (90%)	81 (78%)	23 (22%)	1	5
13	K	92/93 (99%)	80 (87%)	12 (13%)	5	26
14	L	74/82 (90%)	49 (66%)	25 (34%)	0	2
15	M	99/134 (74%)	86 (87%)	13 (13%)	5	26
16	N	96/97 (99%)	87 (91%)	9 (9%)	11	43
17	O	76/79 (96%)	64 (84%)	12 (16%)	3	18
18	P	108/115 (94%)	95 (88%)	13 (12%)	6	30
19	Q	75/76 (99%)	64 (85%)	11 (15%)	4	21
20	R	88/96 (92%)	72 (82%)	16 (18%)	2	11
21	S	149/192 (78%)	130 (87%)	19 (13%)	5	27
22	T	55/67 (82%)	50 (91%)	5 (9%)	12	45
23	U	55/66 (83%)	45 (82%)	10 (18%)	2	11
24	V	53/55 (96%)	50 (94%)	3 (6%)	25	66
25	W	48/48 (100%)	40 (83%)	8 (17%)	3	15
26	Z	49/53 (92%)	39 (80%)	10 (20%)	1	7
27	1	45/48 (94%)	34 (76%)	11 (24%)	1	4
28	2	39/40 (98%)	30 (77%)	9 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	3	44/52 (85%)	28 (64%)	16 (36%)	0 2
All	All	2513/2821 (89%)	2124 (84%)	389 (16%)	3 19

5 of 389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	94	TRP
14	L	82	LYS
27	1	40	TYR
12	J	128	ILE
13	K	99	ARG

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

Mol	Chain	Res	Type
18	P	10	ASN
26	Z	35	GLN
19	Q	43	GLN
8	F	103	GLN
24	V	54	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2700/2877 (93%)	584 (21%)	42 (1%)
2	Y	119/124 (95%)	25 (21%)	1 (0%)
All	All	2819/3001 (93%)	609 (21%)	43 (1%)

5 of 609 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1313	U
1	X	1607	A
1	X	2736	U
1	X	1391	A
1	X	1441	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 455 ligands modelled in this entry, 446 are monoatomic - leaving 9 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	$\# Z  > 2$
30	6NO	X	2901	-	98,105,105	1.52	13 (13%)	127,164,164	1.66	24 (18%)
32	MPD	X	3315	-	6,7,7	0.20	0	6,10,10	0.35	0
32	MPD	X	3316	-	6,7,7	0.38	0	6,10,10	0.77	0
32	MPD	X	3317	-	6,7,7	0.33	0	6,10,10	0.17	0
32	MPD	X	3318	-	6,7,7	0.34	0	6,10,10	0.30	0
32	MPD	X	3319	-	6,7,7	0.33	0	6,10,10	0.13	0
33	SPD	X	3320	-	9,9,9	0.33	0	8,8,8	1.12	1 (12%)
33	SPD	X	3321	-	9,9,9	0.31	0	8,8,8	0.94	1 (12%)
33	SPD	X	3322	-	9,9,9	0.35	0	8,8,8	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	6NO	X	2901	-	-	0/47/211/211	0/11/11/11
32	MPD	X	3315	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3316	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3317	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3318	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3319	-	-	0/5/5/5	0/0/0/0
33	SPD	X	3320	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3321	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3322	-	-	0/7/7/7	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2901	6NO	C08-C05	-6.18	1.39	1.51
30	X	2901	6NO	C04-C09	-4.02	1.40	1.50
30	X	2901	6NO	C51-C50	-3.85	1.47	1.54
30	X	2901	6NO	O26-C22	2.10	1.47	1.42
30	X	2901	6NO	O19-C10	2.10	1.47	1.41

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2901	6NO	C44-O44-C36	-6.56	104.11	114.40
30	X	2901	6NO	O47-C47-C46	-4.09	96.54	103.48
30	X	2901	6NO	O46-C46-C47	-3.61	98.90	103.51
30	X	2901	6NO	C24-C23-C22	-3.47	108.98	115.04
30	X	2901	6NO	C01-C06-C05	-3.43	119.54	122.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2901	6NO	2	0
32	X	3315	MPD	3	0
32	X	3316	MPD	11	0
32	X	3319	MPD	1	0
33	X	3320	SPD	1	0
33	X	3321	SPD	3	0
33	X	3322	SPD	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	X	2710/2877 (94%)	-0.65	11 (0%) 93 91	35, 91, 200, 334	0
2	Y	120/124 (96%)	-0.72	1 (0%) 87 82	97, 137, 188, 213	0
3	A	272/275 (98%)	0.30	16 (5%) 26 23	53, 112, 177, 240	0
4	B	205/211 (97%)	-0.14	3 (1%) 76 71	28, 66, 136, 250	0
5	C	195/205 (95%)	0.12	11 (5%) 28 25	56, 103, 204, 281	0
6	D	177/180 (98%)	0.65	25 (14%) 4 4	120, 178, 253, 296	0
7	E	171/185 (92%)	0.17	6 (3%) 48 42	69, 137, 216, 268	0
8	F	63/144 (43%)	1.89	20 (31%) 1 1	142, 200, 295, 418	0
9	G	142/174 (81%)	0.29	10 (7%) 19 18	48, 89, 188, 342	0
10	H	134/134 (100%)	-0.37	0 100 100	29, 61, 104, 144	0
11	I	134/156 (85%)	0.62	17 (12%) 5 6	51, 120, 206, 280	0
12	J	136/141 (96%)	0.28	9 (6%) 22 19	58, 99, 176, 252	0
13	K	115/116 (99%)	-0.19	1 (0%) 85 80	25, 47, 100, 192	0
14	L	104/114 (91%)	1.07	21 (20%) 1 2	65, 124, 188, 298	0
15	M	119/166 (71%)	-0.20	5 (4%) 40 35	40, 62, 136, 200	0
16	N	117/118 (99%)	-0.21	1 (0%) 85 80	51, 82, 127, 243	0
17	O	97/100 (97%)	0.02	4 (4%) 41 36	63, 107, 193, 284	0
18	P	128/134 (95%)	-0.12	3 (2%) 64 58	17, 64, 110, 190	0
19	Q	93/95 (97%)	0.26	5 (5%) 29 26	57, 103, 159, 219	0
20	R	110/115 (95%)	0.69	13 (11%) 6 7	65, 110, 221, 253	0
21	S	180/237 (75%)	0.54	22 (12%) 5 6	95, 152, 223, 265	0
22	T	74/91 (81%)	0.90	13 (17%) 2 2	66, 101, 148, 193	0
23	U	74/81 (91%)	1.42	21 (28%) 1 1	62, 127, 214, 239	0
24	V	65/67 (97%)	0.39	7 (10%) 8 8	84, 131, 191, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	1.10	12 (21%) 1 1	57, 93, 139, 184	0
26	Z	57/60 (95%)	-0.46	0 100 100	28, 55, 117, 149	0
27	1	53/55 (96%)	1.23	13 (24%) 1 1	82, 147, 236, 292	0
28	2	46/47 (97%)	0.61	6 (13%) 5 5	56, 78, 116, 190	0
29	3	59/66 (89%)	1.04	13 (22%) 1 1	59, 106, 166, 333	0
All	All	6005/6523 (92%)	-0.13	289 (4%) 34 30	17, 100, 205, 418	0

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	G	155	THR	10.6
8	F	114	ASP	8.8
8	F	110	THR	8.5
8	F	127	VAL	7.9
14	L	52	ALA	7.7

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	3000	1/1	0.43	1.83	138.33	82,82,82,82	0
31	MG	X	3127	1/1	0.89	1.49	61.40	52,52,52,52	0
31	MG	X	2988	1/1	0.94	0.51	41.58	48,48,48,48	0
31	MG	X	3134	1/1	0.92	0.59	25.81	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2932	1/1	0.97	0.46	24.95	31,31,31,31	0
31	MG	X	2987	1/1	0.97	0.63	20.21	32,32,32,32	0
31	MG	X	2907	1/1	0.97	0.47	18.93	18,18,18,18	0
31	MG	X	2920	1/1	0.95	0.62	18.49	19,19,19,19	0
31	MG	X	2925	1/1	0.93	0.52	17.38	9,9,9,9	0
31	MG	X	3165	1/1	0.94	0.32	17.14	8,8,8,8	0
31	MG	X	2949	1/1	0.94	0.41	16.22	16,16,16,16	0
31	MG	X	2958	1/1	0.76	0.54	15.44	38,38,38,38	0
31	MG	X	2997	1/1	0.91	0.39	15.26	47,47,47,47	0
32	MPD	X	3317	8/8	0.94	0.35	13.97	73,73,73,73	0
31	MG	X	3164	1/1	0.96	0.48	13.04	16,16,16,16	0
31	MG	X	3011	1/1	0.92	0.34	11.54	33,33,33,33	0
31	MG	X	3099	1/1	0.99	0.32	10.78	46,46,46,46	0
31	MG	X	3161	1/1	0.96	0.33	10.68	25,25,25,25	0
32	MPD	X	3316	8/8	0.89	0.39	10.17	62,62,62,62	0
31	MG	X	3082	1/1	0.85	0.29	10.14	51,51,51,51	0
31	MG	X	3114	1/1	0.89	0.27	9.58	70,70,70,70	0
31	MG	X	3045	1/1	0.89	0.61	9.58	30,30,30,30	0
31	MG	X	3162	1/1	0.98	0.31	9.36	20,20,20,20	0
31	MG	X	2912	1/1	0.98	0.38	9.33	3,3,3,3	0
31	MG	X	2903	1/1	0.97	0.32	8.62	11,11,11,11	0
31	MG	Y	201	1/1	0.93	0.41	8.05	57,57,57,57	0
31	MG	X	3328	1/1	0.90	0.32	8.02	33,33,33,33	0
31	MG	X	3036	1/1	0.90	0.27	7.33	41,41,41,41	0
31	MG	X	2911	1/1	0.96	0.34	7.08	11,11,11,11	0
31	MG	X	3292	1/1	0.91	0.36	6.98	28,28,28,28	0
31	MG	X	2940	1/1	0.97	0.26	6.87	32,32,32,32	0
31	MG	X	2906	1/1	0.99	0.30	6.71	35,35,35,35	0
31	MG	X	3329	1/1	0.92	0.57	6.39	95,95,95,95	0
31	MG	X	2962	1/1	0.90	0.32	5.87	84,84,84,84	0
33	SPD	X	3322	10/10	0.86	0.23	5.30	90,90,90,90	0
31	MG	X	3096	1/1	0.93	0.24	4.80	50,50,50,50	0
31	MG	X	2938	1/1	0.99	0.27	4.77	8,8,8,8	0
31	MG	X	2964	1/1	0.98	0.34	4.66	9,9,9,9	0
31	MG	X	3029	1/1	0.96	0.22	4.40	48,48,48,48	0
31	MG	X	3232	1/1	0.96	0.33	4.16	8,8,8,8	0
31	MG	X	2931	1/1	0.96	0.43	4.16	25,25,25,25	0
31	MG	X	3222	1/1	0.94	0.21	4.13	21,21,21,21	0
31	MG	X	2937	1/1	0.88	0.22	3.99	31,31,31,31	0
31	MG	X	2908	1/1	0.93	0.36	3.96	15,15,15,15	0
31	MG	X	2977	1/1	0.98	0.21	3.44	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2922	1/1	0.98	0.24	3.28	12,12,12,12	0
31	MG	X	3324	1/1	0.96	0.52	3.27	26,26,26,26	0
31	MG	X	2944	1/1	0.98	0.25	3.14	1,1,1,1	0
31	MG	X	3173	1/1	0.88	0.46	2.91	82,82,82,82	0
31	MG	X	2902	1/1	0.96	0.31	2.86	27,27,27,27	0
31	MG	X	3198	1/1	0.87	0.22	2.78	66,66,66,66	0
31	MG	X	3326	1/1	0.94	0.44	2.76	55,55,55,55	0
31	MG	X	3297	1/1	0.95	0.26	2.66	25,25,25,25	0
31	MG	X	3042	1/1	0.94	0.22	2.65	42,42,42,42	0
31	MG	X	3101	1/1	0.92	0.22	2.59	52,52,52,52	0
31	MG	X	3030	1/1	0.99	0.27	2.51	0,0,0,0	0
31	MG	X	3124	1/1	0.94	0.20	2.24	47,47,47,47	0
31	MG	X	3294	1/1	0.95	0.23	2.01	78,78,78,78	0
30	6NO	X	2901	95/95	0.93	0.19	1.98	114,114,114,114	0
31	MG	X	2918	1/1	0.97	0.39	1.87	6,6,6,6	0
31	MG	X	3115	1/1	0.81	0.19	1.80	75,75,75,75	0
31	MG	X	3019	1/1	0.95	0.24	1.67	44,44,44,44	0
31	MG	X	2909	1/1	0.98	0.21	1.42	24,24,24,24	0
33	SPD	X	3321	10/10	0.91	0.27	1.40	88,88,88,88	0
32	MPD	X	3319	8/8	0.93	0.15	1.38	91,91,91,91	0
33	SPD	X	3320	10/10	0.94	0.28	1.27	44,44,44,44	0
31	MG	X	2934	1/1	0.95	0.20	1.24	64,64,64,64	0
31	MG	X	2910	1/1	0.96	0.19	1.22	25,25,25,25	0
31	MG	X	3149	1/1	0.89	0.27	1.05	24,24,24,24	0
31	MG	X	2945	1/1	0.98	0.19	0.99	32,32,32,32	0
32	MPD	X	3315	8/8	0.97	0.14	0.94	62,62,62,62	0
31	MG	J	201	1/1	0.94	0.26	0.40	55,55,55,55	0
31	MG	X	3063	1/1	0.94	0.27	0.38	52,52,52,52	0
31	MG	X	3327	1/1	0.92	0.20	0.24	66,66,66,66	0
31	MG	X	3220	1/1	0.92	0.16	0.11	66,66,66,66	0
31	MG	X	3148	1/1	0.95	0.15	0.09	29,29,29,29	0
31	MG	X	3121	1/1	0.98	0.18	0.01	30,30,30,30	0
31	MG	X	3205	1/1	0.96	0.15	-0.02	55,55,55,55	0
31	MG	N	201	1/1	0.95	0.20	-0.06	44,44,44,44	0
31	MG	X	3323	1/1	0.93	0.20	-0.29	22,22,22,22	0
31	MG	X	3271	1/1	0.74	0.11	-0.49	78,78,78,78	0
31	MG	X	3018	1/1	0.99	0.19	-0.55	35,35,35,35	0
31	MG	X	3052	1/1	0.97	0.13	-0.71	21,21,21,21	0
31	MG	X	3244	1/1	0.94	0.07	-1.09	61,61,61,61	0
31	MG	X	3046	1/1	0.88	0.13	-1.10	64,64,64,64	0
31	MG	X	3305	1/1	0.73	0.05	-1.78	125,125,125,125	0
31	MG	X	3081	1/1	0.97	0.09	-2.27	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3035	1/1	0.98	0.11	-3.28	31,31,31,31	0
31	MG	X	3069	1/1	0.76	0.27	-	49,49,49,49	0
31	MG	X	3264	1/1	0.95	0.30	-	47,47,47,47	0
31	MG	Y	211	1/1	0.92	0.07	-	59,59,59,59	0
31	MG	X	3184	1/1	0.91	0.62	-	131,131,131,131	0
31	MG	X	3193	1/1	0.95	0.08	-	63,63,63,63	0
31	MG	X	3177	1/1	0.78	0.29	-	75,75,75,75	0
31	MG	X	3302	1/1	0.90	0.13	-	100,100,100,100	0
31	MG	X	3211	1/1	0.95	0.22	-	32,32,32,32	0
31	MG	Y	217	1/1	0.97	0.05	-	65,65,65,65	0
31	MG	X	3024	1/1	0.94	0.25	-	27,27,27,27	0
31	MG	X	3131	1/1	0.94	0.22	-	36,36,36,36	0
31	MG	X	3110	1/1	0.91	0.26	-	55,55,55,55	0
31	MG	X	3209	1/1	0.93	0.32	-	52,52,52,52	0
31	MG	X	3093	1/1	0.86	0.66	-	44,44,44,44	0
31	MG	X	3299	1/1	0.97	0.20	-	89,89,89,89	0
31	MG	X	3137	1/1	0.81	0.60	-	57,57,57,57	0
31	MG	X	2946	1/1	0.97	0.28	-	11,11,11,11	0
31	MG	X	3290	1/1	0.91	0.15	-	71,71,71,71	0
31	MG	X	3120	1/1	0.88	0.38	-	56,56,56,56	0
31	MG	X	3014	1/1	0.93	0.56	-	28,28,28,28	0
31	MG	X	3288	1/1	0.96	0.18	-	54,54,54,54	0
31	MG	X	3116	1/1	0.96	0.22	-	61,61,61,61	0
31	MG	X	3017	1/1	0.93	0.34	-	30,30,30,30	0
31	MG	X	3178	1/1	0.79	0.21	-	60,60,60,60	0
31	MG	X	3226	1/1	0.98	0.20	-	145,145,145,145	0
31	MG	X	3073	1/1	0.73	0.81	-	94,94,94,94	0
31	MG	Y	203	1/1	0.88	0.45	-	30,30,30,30	0
31	MG	X	2919	1/1	0.96	0.49	-	40,40,40,40	0
31	MG	X	3133	1/1	0.86	0.30	-	73,73,73,73	0
31	MG	X	2994	1/1	0.90	0.68	-	58,58,58,58	0
31	MG	X	3129	1/1	0.93	0.15	-	21,21,21,21	0
31	MG	X	3268	1/1	0.88	0.10	-	115,115,115,115	0
31	MG	X	2980	1/1	0.98	0.13	-	23,23,23,23	0
31	MG	Y	218	1/1	0.70	0.14	-	83,83,83,83	0
31	MG	X	3228	1/1	0.92	0.84	-	85,85,85,85	0
31	MG	Y	210	1/1	0.83	0.31	-	64,64,64,64	0
31	MG	X	3219	1/1	0.73	0.49	-	85,85,85,85	0
31	MG	X	3199	1/1	0.97	0.18	-	53,53,53,53	0
31	MG	X	2973	1/1	0.91	0.34	-	23,23,23,23	0
31	MG	X	3157	1/1	0.97	0.14	-	77,77,77,77	0
31	MG	X	3233	1/1	0.95	0.65	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3008	1/1	0.95	0.72	-	39,39,39,39	0
31	MG	X	3225	1/1	0.64	0.56	-	79,79,79,79	0
31	MG	Y	206	1/1	0.83	0.19	-	70,70,70,70	0
31	MG	X	3040	1/1	0.93	0.70	-	70,70,70,70	0
31	MG	X	2904	1/1	0.79	0.39	-	64,64,64,64	0
31	MG	X	2951	1/1	0.98	0.21	-	15,15,15,15	0
31	MG	X	2992	1/1	0.98	0.15	-	25,25,25,25	0
31	MG	X	2981	1/1	0.89	0.40	-	52,52,52,52	0
31	MG	X	3242	1/1	0.97	0.25	-	72,72,72,72	0
31	MG	X	3309	1/1	0.74	0.30	-	87,87,87,87	0
31	MG	X	3284	1/1	0.97	0.07	-	56,56,56,56	0
31	MG	X	3192	1/1	0.96	0.51	-	55,55,55,55	0
31	MG	X	3003	1/1	0.91	0.47	-	49,49,49,49	0
31	MG	3	101	1/1	0.79	0.65	-	31,31,31,31	0
31	MG	X	3070	1/1	0.92	0.20	-	39,39,39,39	0
31	MG	X	3080	1/1	0.78	0.38	-	29,29,29,29	0
31	MG	X	2923	1/1	0.94	0.48	-	13,13,13,13	0
31	MG	X	3041	1/1	0.97	0.27	-	30,30,30,30	0
31	MG	X	2979	1/1	0.89	0.17	-	37,37,37,37	0
31	MG	X	2970	1/1	0.97	0.54	-	30,30,30,30	0
31	MG	X	2941	1/1	0.96	0.19	-	40,40,40,40	0
31	MG	X	3240	1/1	0.89	0.51	-	82,82,82,82	0
31	MG	X	3298	1/1	0.89	0.39	-	20,20,20,20	0
31	MG	X	3037	1/1	0.97	0.52	-	60,60,60,60	0
31	MG	X	3039	1/1	0.73	0.54	-	51,51,51,51	0
31	MG	X	3142	1/1	0.94	0.45	-	57,57,57,57	0
31	MG	X	3188	1/1	0.95	0.23	-	68,68,68,68	0
31	MG	X	3182	1/1	0.86	0.31	-	75,75,75,75	0
31	MG	X	3267	1/1	0.84	0.45	-	50,50,50,50	0
31	MG	X	3100	1/1	0.97	0.29	-	69,69,69,69	0
31	MG	X	3230	1/1	0.84	0.36	-	99,99,99,99	0
31	MG	T	101	1/1	0.86	0.40	-	30,30,30,30	0
31	MG	X	3276	1/1	0.91	0.51	-	114,114,114,114	0
31	MG	X	2915	1/1	0.83	0.56	-	39,39,39,39	0
31	MG	X	3183	1/1	0.96	0.17	-	40,40,40,40	0
31	MG	X	2966	1/1	0.98	0.38	-	32,32,32,32	0
31	MG	X	3236	1/1	0.95	0.27	-	56,56,56,56	0
31	MG	X	3313	1/1	0.92	0.15	-	74,74,74,74	0
31	MG	X	2953	1/1	0.98	0.29	-	53,53,53,53	0
31	MG	X	3218	1/1	0.80	0.31	-	78,78,78,78	0
31	MG	X	3307	1/1	0.91	0.38	-	25,25,25,25	0
31	MG	X	3089	1/1	0.58	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2955	1/1	0.96	0.36	-	14,14,14,14	0
31	MG	X	3263	1/1	0.89	0.36	-	59,59,59,59	0
31	MG	X	3094	1/1	0.92	0.37	-	76,76,76,76	0
31	MG	X	2961	1/1	0.81	0.60	-	35,35,35,35	0
31	MG	X	2948	1/1	0.95	0.41	-	32,32,32,32	0
31	MG	X	2943	1/1	0.97	0.22	-	35,35,35,35	0
31	MG	X	2972	1/1	0.91	0.17	-	33,33,33,33	0
31	MG	X	3076	1/1	0.93	0.53	-	90,90,90,90	0
31	MG	X	2984	1/1	0.96	0.24	-	22,22,22,22	0
31	MG	X	3057	1/1	0.94	0.33	-	36,36,36,36	0
31	MG	X	2976	1/1	0.93	0.23	-	29,29,29,29	0
31	MG	X	3251	1/1	0.85	0.29	-	85,85,85,85	0
31	MG	X	3007	1/1	0.91	0.41	-	30,30,30,30	0
31	MG	X	3132	1/1	0.77	0.40	-	70,70,70,70	0
31	MG	X	3255	1/1	0.75	0.16	-	69,69,69,69	0
31	MG	X	2914	1/1	0.97	0.38	-	4,4,4,4	0
31	MG	X	3176	1/1	0.74	0.22	-	47,47,47,47	0
31	MG	X	3170	1/1	0.68	0.61	-	105,105,105,105	0
31	MG	X	3071	1/1	0.97	0.16	-	46,46,46,46	0
31	MG	X	3214	1/1	0.90	0.56	-	71,71,71,71	0
31	MG	X	3270	1/1	0.94	0.16	-	85,85,85,85	0
31	MG	X	3107	1/1	0.93	0.22	-	67,67,67,67	0
31	MG	X	3145	1/1	0.84	0.24	-	83,83,83,83	0
31	MG	X	3204	1/1	0.91	0.31	-	51,51,51,51	0
31	MG	X	2967	1/1	0.93	0.29	-	14,14,14,14	0
31	MG	X	3180	1/1	0.64	0.39	-	115,115,115,115	0
31	MG	X	2928	1/1	0.96	0.26	-	10,10,10,10	0
31	MG	X	3091	1/1	0.75	0.40	-	49,49,49,49	0
31	MG	Y	204	1/1	0.91	0.65	-	60,60,60,60	0
31	MG	X	3031	1/1	0.94	0.21	-	64,64,64,64	0
31	MG	X	3259	1/1	0.96	0.46	-	69,69,69,69	0
31	MG	X	3087	1/1	0.72	0.37	-	54,54,54,54	0
31	MG	Y	219	1/1	0.73	0.34	-	81,81,81,81	0
31	MG	X	2913	1/1	0.97	0.52	-	0,0,0,0	0
31	MG	X	3090	1/1	0.97	0.20	-	11,11,11,11	0
31	MG	X	3250	1/1	0.75	0.78	-	73,73,73,73	0
31	MG	X	3231	1/1	0.75	1.06	-	96,96,96,96	0
31	MG	X	3012	1/1	0.88	0.53	-	49,49,49,49	0
31	MG	K	201	1/1	0.84	0.54	-	48,48,48,48	0
31	MG	Y	213	1/1	0.85	0.40	-	83,83,83,83	0
31	MG	X	3061	1/1	0.94	0.25	-	38,38,38,38	0
31	MG	X	3154	1/1	0.96	0.26	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2986	1/1	0.97	0.49	-	42,42,42,42	0
31	MG	Y	214	1/1	0.94	0.38	-	64,64,64,64	0
31	MG	X	2975	1/1	0.94	0.50	-	38,38,38,38	0
31	MG	X	3196	1/1	0.91	0.37	-	95,95,95,95	0
31	MG	X	3235	1/1	0.91	0.32	-	79,79,79,79	0
31	MG	X	3243	1/1	0.97	0.15	-	83,83,83,83	0
31	MG	X	3215	1/1	0.76	0.40	-	54,54,54,54	0
31	MG	X	3287	1/1	0.98	0.41	-	65,65,65,65	0
31	MG	X	3195	1/1	0.83	0.29	-	90,90,90,90	0
31	MG	X	2974	1/1	0.92	0.40	-	45,45,45,45	0
31	MG	X	3212	1/1	0.86	0.29	-	53,53,53,53	0
31	MG	X	3085	1/1	0.95	0.35	-	45,45,45,45	0
31	MG	Y	209	1/1	0.67	0.40	-	81,81,81,81	0
31	MG	X	3092	1/1	0.94	0.17	-	53,53,53,53	0
31	MG	X	3118	1/1	0.92	0.16	-	113,113,113,113	0
31	MG	X	3261	1/1	0.45	0.59	-	78,78,78,78	0
31	MG	X	3272	1/1	0.95	0.13	-	105,105,105,105	0
31	MG	X	3109	1/1	0.96	0.24	-	74,74,74,74	0
31	MG	X	2947	1/1	0.97	0.09	-	33,33,33,33	0
31	MG	X	3043	1/1	0.96	0.29	-	33,33,33,33	0
31	MG	X	3310	1/1	0.94	0.29	-	63,63,63,63	0
31	MG	X	3027	1/1	0.98	0.31	-	14,14,14,14	0
31	MG	X	3044	1/1	0.96	0.12	-	10,10,10,10	0
31	MG	X	3201	1/1	0.91	0.56	-	69,69,69,69	0
31	MG	X	3075	1/1	0.90	0.63	-	52,52,52,52	0
31	MG	X	3241	1/1	0.74	0.32	-	85,85,85,85	0
31	MG	X	3223	1/1	0.95	0.26	-	34,34,34,34	0
31	MG	X	3009	1/1	0.99	0.72	-	31,31,31,31	0
31	MG	X	3077	1/1	0.90	0.28	-	61,61,61,61	0
31	MG	X	2965	1/1	0.92	0.42	-	52,52,52,52	0
31	MG	X	2995	1/1	0.97	0.40	-	41,41,41,41	0
31	MG	X	3049	1/1	0.79	0.37	-	70,70,70,70	0
31	MG	X	2927	1/1	0.97	0.30	-	9,9,9,9	0
31	MG	X	3275	1/1	0.84	0.40	-	70,70,70,70	0
31	MG	X	3258	1/1	0.92	0.65	-	56,56,56,56	0
31	MG	X	3113	1/1	0.83	0.31	-	38,38,38,38	0
31	MG	X	3281	1/1	0.88	0.62	-	54,54,54,54	0
31	MG	X	3248	1/1	0.57	0.51	-	87,87,87,87	0
31	MG	Y	205	1/1	0.91	0.35	-	44,44,44,44	0
31	MG	X	3139	1/1	0.98	0.34	-	29,29,29,29	0
31	MG	X	3147	1/1	0.99	0.10	-	82,82,82,82	0
31	MG	X	3279	1/1	0.89	0.29	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3249	1/1	0.82	0.33	-	103,103,103,103	0
31	MG	Y	208	1/1	0.89	0.20	-	72,72,72,72	0
31	MG	X	2993	1/1	0.94	0.64	-	26,26,26,26	0
31	MG	X	3001	1/1	0.95	0.54	-	57,57,57,57	0
31	MG	X	3103	1/1	0.70	0.43	-	84,84,84,84	0
31	MG	X	2960	1/1	0.98	0.55	-	30,30,30,30	0
31	MG	X	3186	1/1	0.96	0.11	-	45,45,45,45	0
31	MG	X	3155	1/1	0.88	0.25	-	68,68,68,68	0
31	MG	X	3185	1/1	0.94	0.20	-	87,87,87,87	0
31	MG	X	3286	1/1	0.96	0.15	-	47,47,47,47	0
31	MG	X	3034	1/1	0.87	0.46	-	35,35,35,35	0
31	MG	X	2939	1/1	0.94	0.42	-	24,24,24,24	0
31	MG	X	3303	1/1	0.89	0.23	-	67,67,67,67	0
31	MG	X	3010	1/1	0.77	0.88	-	72,72,72,72	0
31	MG	X	3050	1/1	0.97	0.23	-	41,41,41,41	0
31	MG	X	3059	1/1	0.78	0.34	-	51,51,51,51	0
31	MG	X	3048	1/1	0.94	0.43	-	0,0,0,0	0
31	MG	A	301	1/1	0.90	0.40	-	46,46,46,46	0
31	MG	Y	216	1/1	0.72	0.36	-	70,70,70,70	0
31	MG	X	3028	1/1	0.92	0.19	-	3,3,3,3	0
31	MG	X	2916	1/1	0.90	0.53	-	0,0,0,0	0
31	MG	X	3239	1/1	0.23	0.76	-	84,84,84,84	0
31	MG	X	3006	1/1	0.97	0.16	-	29,29,29,29	0
31	MG	X	2924	1/1	0.94	0.22	-	26,26,26,26	0
31	MG	X	3143	1/1	0.92	0.46	-	56,56,56,56	0
31	MG	X	3159	1/1	0.89	0.66	-	31,31,31,31	0
31	MG	X	2990	1/1	0.86	0.36	-	60,60,60,60	0
31	MG	X	3067	1/1	0.90	0.40	-	60,60,60,60	0
31	MG	X	3053	1/1	0.90	0.20	-	64,64,64,64	0
31	MG	X	3237	1/1	0.94	0.35	-	88,88,88,88	0
31	MG	X	3111	1/1	0.86	0.60	-	49,49,49,49	0
31	MG	X	2999	1/1	0.91	0.31	-	29,29,29,29	0
31	MG	X	3002	1/1	0.96	0.24	-	34,34,34,34	0
31	MG	X	3112	1/1	0.83	0.63	-	42,42,42,42	0
31	MG	X	2971	1/1	0.96	0.78	-	38,38,38,38	0
31	MG	X	3125	1/1	0.98	0.31	-	37,37,37,37	0
31	MG	X	3221	1/1	0.87	0.30	-	49,49,49,49	0
31	MG	X	3306	1/1	0.92	0.09	-	116,116,116,116	0
31	MG	X	3189	1/1	0.75	0.47	-	61,61,61,61	0
31	MG	X	3257	1/1	0.81	0.55	-	77,77,77,77	0
31	MG	X	3136	1/1	0.88	0.10	-	43,43,43,43	0
31	MG	X	2954	1/1	0.97	0.23	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3130	1/1	0.91	0.53	-	62,62,62,62	0
31	MG	X	3169	1/1	0.49	0.19	-	77,77,77,77	0
31	MG	X	3190	1/1	0.83	0.64	-	56,56,56,56	0
31	MG	X	3277	1/1	0.91	0.39	-	39,39,39,39	0
31	MG	X	3098	1/1	0.98	0.39	-	23,23,23,23	0
31	MG	Y	207	1/1	0.94	0.49	-	93,93,93,93	0
31	MG	X	3181	1/1	0.87	0.46	-	51,51,51,51	0
31	MG	X	3254	1/1	0.88	0.63	-	19,19,19,19	0
31	MG	X	3213	1/1	0.90	0.16	-	34,34,34,34	0
31	MG	X	3055	1/1	0.92	0.29	-	49,49,49,49	0
32	MPD	X	3318	8/8	0.90	0.18	-	79,79,79,79	0
31	MG	X	3253	1/1	0.95	0.14	-	25,25,25,25	0
31	MG	X	3060	1/1	0.71	0.21	-	47,47,47,47	0
31	MG	X	3308	1/1	0.96	0.18	-	46,46,46,46	0
31	MG	X	3079	1/1	0.97	0.12	-	62,62,62,62	0
31	MG	X	3229	1/1	0.74	0.40	-	71,71,71,71	0
31	MG	X	3167	1/1	0.99	0.06	-	7,7,7,7	0
31	MG	X	3138	1/1	0.91	1.02	-	44,44,44,44	0
31	MG	X	3104	1/1	0.74	0.94	-	70,70,70,70	0
31	MG	X	3238	1/1	0.88	0.28	-	50,50,50,50	0
31	MG	X	3032	1/1	0.91	0.36	-	39,39,39,39	0
31	MG	X	3283	1/1	0.88	0.39	-	50,50,50,50	0
31	MG	X	3072	1/1	0.64	0.65	-	73,73,73,73	0
31	MG	X	3217	1/1	0.91	0.56	-	48,48,48,48	0
31	MG	X	3260	1/1	0.96	0.19	-	63,63,63,63	0
31	MG	X	3066	1/1	0.94	0.41	-	48,48,48,48	0
31	MG	X	3291	1/1	0.96	0.09	-	116,116,116,116	0
31	MG	X	3200	1/1	0.92	0.30	-	64,64,64,64	0
31	MG	X	2952	1/1	0.97	0.22	-	31,31,31,31	0
31	MG	X	3210	1/1	0.92	0.15	-	62,62,62,62	0
31	MG	X	3020	1/1	0.94	0.35	-	47,47,47,47	0
31	MG	X	3141	1/1	0.82	0.30	-	62,62,62,62	0
31	MG	X	3150	1/1	0.90	0.43	-	65,65,65,65	0
31	MG	X	3207	1/1	0.85	0.29	-	75,75,75,75	0
31	MG	X	2933	1/1	0.92	0.74	-	32,32,32,32	0
31	MG	X	3156	1/1	0.84	0.31	-	72,72,72,72	0
31	MG	X	3278	1/1	0.92	0.16	-	50,50,50,50	0
31	MG	X	2982	1/1	0.97	0.46	-	40,40,40,40	0
31	MG	X	2935	1/1	0.95	0.20	-	15,15,15,15	0
31	MG	X	3202	1/1	0.87	0.22	-	64,64,64,64	0
31	MG	X	3022	1/1	0.97	0.16	-	53,53,53,53	0
31	MG	X	3033	1/1	0.76	0.46	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3126	1/1	0.78	0.25	-	42,42,42,42	0
31	MG	X	3168	1/1	0.93	0.53	-	76,76,76,76	0
31	MG	X	3056	1/1	0.86	0.31	-	66,66,66,66	0
31	MG	X	3174	1/1	0.94	0.40	-	52,52,52,52	0
31	MG	X	3054	1/1	0.72	0.51	-	72,72,72,72	0
31	MG	X	3051	1/1	0.89	0.24	-	29,29,29,29	0
31	MG	X	3256	1/1	0.97	0.23	-	48,48,48,48	0
31	MG	X	3314	1/1	0.73	0.87	-	62,62,62,62	0
31	MG	X	3311	1/1	0.90	0.27	-	59,59,59,59	0
31	MG	X	3252	1/1	0.28	0.42	-	111,111,111,111	0
31	MG	X	3068	1/1	0.94	0.65	-	48,48,48,48	0
31	MG	X	3224	1/1	0.85	0.21	-	32,32,32,32	0
31	MG	X	3285	1/1	0.93	0.23	-	84,84,84,84	0
31	MG	X	2929	1/1	0.99	0.24	-	21,21,21,21	0
31	MG	X	3191	1/1	0.79	0.31	-	32,32,32,32	0
31	MG	X	3312	1/1	0.82	0.14	-	71,71,71,71	0
31	MG	X	3023	1/1	0.95	0.30	-	50,50,50,50	0
31	MG	X	3016	1/1	0.86	0.44	-	60,60,60,60	0
31	MG	X	2905	1/1	0.97	0.36	-	13,13,13,13	0
31	MG	X	3074	1/1	0.52	0.39	-	61,61,61,61	0
31	MG	X	3095	1/1	0.88	0.66	-	65,65,65,65	0
31	MG	X	2983	1/1	0.98	0.20	-	27,27,27,27	0
31	MG	X	2959	1/1	0.99	0.21	-	39,39,39,39	0
31	MG	X	3160	1/1	0.71	0.46	-	92,92,92,92	0
31	MG	X	2991	1/1	0.97	0.20	-	22,22,22,22	0
31	MG	X	2917	1/1	0.93	0.45	-	6,6,6,6	0
31	MG	X	2926	1/1	0.97	0.63	-	23,23,23,23	0
31	MG	X	3062	1/1	0.82	0.72	-	49,49,49,49	0
31	MG	X	2921	1/1	0.95	0.27	-	7,7,7,7	0
31	MG	X	3216	1/1	0.92	0.14	-	70,70,70,70	0
31	MG	X	3172	1/1	0.91	0.32	-	60,60,60,60	0
31	MG	X	3265	1/1	0.88	0.27	-	74,74,74,74	0
31	MG	X	3295	1/1	0.97	0.17	-	59,59,59,59	0
31	MG	X	3234	1/1	0.61	0.54	-	83,83,83,83	0
31	MG	X	3117	1/1	0.97	0.14	-	64,64,64,64	0
31	MG	X	3282	1/1	0.91	0.38	-	58,58,58,58	0
31	MG	X	3194	1/1	0.94	0.18	-	70,70,70,70	0
31	MG	X	3106	1/1	0.89	0.26	-	57,57,57,57	0
31	MG	X	2957	1/1	0.98	0.24	-	26,26,26,26	0
31	MG	X	3301	1/1	0.62	1.15	-	80,80,80,80	0
31	MG	X	3083	1/1	0.84	0.29	-	50,50,50,50	0
31	MG	X	3245	1/1	0.45	0.39	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3179	1/1	0.84	0.42	-	62,62,62,62	0
31	MG	X	2998	1/1	0.95	0.45	-	50,50,50,50	0
31	MG	X	3203	1/1	0.99	0.04	-	42,42,42,42	0
31	MG	X	3304	1/1	0.95	0.15	-	88,88,88,88	0
31	MG	X	3171	1/1	0.96	0.25	-	39,39,39,39	0
31	MG	Y	212	1/1	0.87	0.41	-	78,78,78,78	0
31	MG	X	3119	1/1	0.90	0.38	-	62,62,62,62	0
31	MG	X	3175	1/1	0.89	0.24	-	72,72,72,72	0
31	MG	X	2985	1/1	0.95	0.42	-	29,29,29,29	0
31	MG	X	3105	1/1	0.84	0.30	-	80,80,80,80	0
31	MG	X	3274	1/1	0.94	0.23	-	74,74,74,74	0
31	MG	X	3088	1/1	0.86	0.29	-	51,51,51,51	0
31	MG	X	3064	1/1	0.72	1.13	-	76,76,76,76	0
31	MG	X	3140	1/1	0.98	0.32	-	27,27,27,27	0
31	MG	X	3152	1/1	0.84	0.20	-	74,74,74,74	0
31	MG	X	3015	1/1	0.95	0.29	-	46,46,46,46	0
31	MG	X	3108	1/1	0.98	0.07	-	74,74,74,74	0
31	MG	X	3325	1/1	0.92	0.66	-	104,104,104,104	0
31	MG	X	3065	1/1	0.83	0.76	-	57,57,57,57	0
31	MG	X	3013	1/1	0.94	0.10	-	42,42,42,42	0
31	MG	X	3151	1/1	0.96	0.14	-	79,79,79,79	0
31	MG	X	3293	1/1	0.95	0.40	-	71,71,71,71	0
31	MG	X	2936	1/1	0.98	0.43	-	21,21,21,21	0
31	MG	X	3247	1/1	0.94	0.20	-	101,101,101,101	0
31	MG	X	3289	1/1	0.92	0.28	-	74,74,74,74	0
31	MG	X	3296	1/1	0.95	0.23	-	56,56,56,56	0
31	MG	X	3047	1/1	0.90	0.61	-	23,23,23,23	0
31	MG	X	3163	1/1	0.99	0.47	-	0,0,0,0	0
31	MG	X	3187	1/1	0.89	0.25	-	57,57,57,57	0
31	MG	X	3123	1/1	0.90	0.47	-	18,18,18,18	0
31	MG	X	3135	1/1	0.88	0.27	-	67,67,67,67	0
31	MG	X	3280	1/1	0.95	0.08	-	84,84,84,84	0
31	MG	X	3084	1/1	0.96	0.17	-	37,37,37,37	0
31	MG	X	3128	1/1	0.95	0.24	-	73,73,73,73	0
31	MG	X	3005	1/1	0.92	0.46	-	45,45,45,45	0
31	MG	X	3208	1/1	0.88	0.23	-	61,61,61,61	0
31	MG	X	3269	1/1	0.97	0.14	-	62,62,62,62	0
31	MG	X	3146	1/1	0.94	0.35	-	46,46,46,46	0
31	MG	Y	202	1/1	0.88	0.28	-	52,52,52,52	0
31	MG	X	3273	1/1	0.60	0.28	-	70,70,70,70	0
31	MG	X	2969	1/1	0.98	0.23	-	8,8,8,8	0
31	MG	X	3246	1/1	0.91	0.40	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3025	1/1	0.94	0.18	-	33,33,33,33	0
31	MG	X	3097	1/1	0.94	0.77	-	63,63,63,63	0
31	MG	X	2963	1/1	0.96	0.29	-	29,29,29,29	0
31	MG	X	3021	1/1	0.96	0.45	-	48,48,48,48	0
31	MG	Y	215	1/1	0.81	0.57	-	81,81,81,81	0
31	MG	X	2956	1/1	0.88	0.40	-	31,31,31,31	0
31	MG	X	3038	1/1	0.90	0.65	-	32,32,32,32	0
31	MG	X	3166	1/1	0.96	0.35	-	18,18,18,18	0
31	MG	X	3122	1/1	0.94	0.31	-	52,52,52,52	0
31	MG	X	3300	1/1	0.68	0.66	-	67,67,67,67	0
31	MG	X	2942	1/1	0.94	0.17	-	19,19,19,19	0
31	MG	X	3227	1/1	0.98	0.13	-	44,44,44,44	0
31	MG	X	3026	1/1	0.96	0.54	-	35,35,35,35	0
31	MG	X	3266	1/1	0.42	0.76	-	56,56,56,56	0
31	MG	X	3004	1/1	0.79	0.28	-	43,43,43,43	0
31	MG	X	2989	1/1	0.97	0.20	-	45,45,45,45	0
31	MG	X	3078	1/1	0.96	0.47	-	82,82,82,82	0
31	MG	X	2930	1/1	0.96	0.38	-	26,26,26,26	0
31	MG	X	3102	1/1	0.72	0.54	-	46,46,46,46	0
31	MG	X	3262	1/1	0.75	0.28	-	113,113,113,113	0
31	MG	X	2968	1/1	0.94	0.58	-	34,34,34,34	0
31	MG	X	3058	1/1	0.95	0.35	-	35,35,35,35	0
31	MG	X	3197	1/1	0.95	0.26	-	49,49,49,49	0
31	MG	X	2978	1/1	0.97	0.52	-	42,42,42,42	0
31	MG	M	201	1/1	0.97	0.57	-	7,7,7,7	0
31	MG	X	3158	1/1	0.96	0.19	-	118,118,118,118	0
31	MG	X	3153	1/1	0.84	0.62	-	58,58,58,58	0
31	MG	X	3144	1/1	0.46	0.28	-	76,76,76,76	0
31	MG	X	3206	1/1	0.94	0.22	-	57,57,57,57	0
31	MG	X	2996	1/1	0.89	0.27	-	41,41,41,41	0
31	MG	X	3086	1/1	0.82	0.30	-	41,41,41,41	0
31	MG	X	2950	1/1	0.98	0.55	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.