



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2019 – 11:59 AM EDT

PDB ID : 3CF5
Title : Thiopeptide antibiotic Thiostrepton bound to the large ribosomal subunit of *Deinococcus radiodurans*
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-02
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

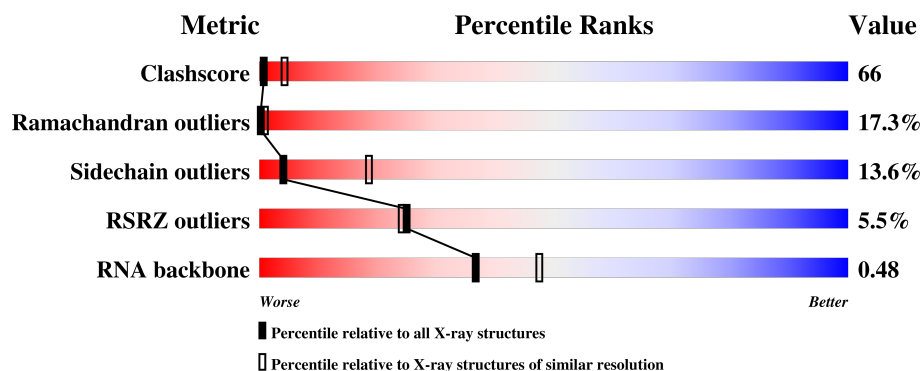
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)
RNA backbone	2636	1009 (3.74-2.86)

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 ≥ 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	1	55	<div> <div>71%</div> <div> <div>96%</div> <div>•</div> </div> </div>
2	2	47	<div> <div>98%</div> <div>98%</div> <div>•</div> </div>
3	3	66	<div> <div>89%</div> <div>94%</div> <div>• 5%</div> </div>
4	4	37	<div> <div>19%</div> <div>8%</div> <div>73%</div> <div>19%</div> </div>
5	5	19	<div> <div>5%</div> <div>68%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
6	A	274	
7	B	211	
8	C	205	
9	D	180	
10	E	185	
11	F	144	
12	G	174	
13	H	134	
14	I	156	
15	J	142	
16	K	116	
17	L	114	
18	M	166	
19	N	118	
20	O	100	
21	P	134	
22	Q	95	
23	R	115	
24	S	237	
25	T	91	
26	U	81	
27	V	67	
28	W	55	
29	X	2880	
30	Y	60	

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Mol	Chain	Length	Quality of chain
31	Z	123	

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
5	BB9	5	13	-	X	-	-
5	BB9	5	15	-	-	-	X
5	DHA	5	16	-	-	-	X
5	DHA	5	3	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 84475 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 protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	1	53	Total C 53 53	0	0	53

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	2	46	Total C 46 46	0	0	46

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	3	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 5 is a protein called THIOSTREPTON.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	19	Total C N O S 114 72 19 18 5	0	0	1

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	A	240	Total C N O S 1826 1137 366 321 2	0	0	0

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	144	Total	C	N	O	S	0	0	0
			1044	663	179	197	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 31 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

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

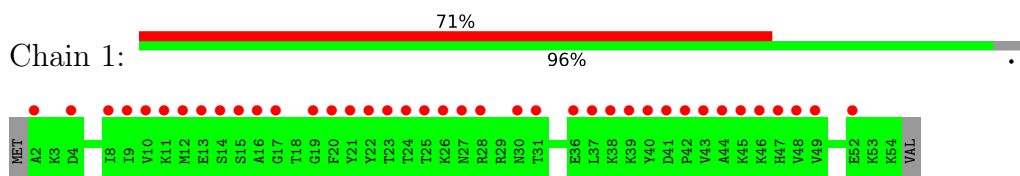
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	30	Total	Mg	0	0
			30	30		
32	Z	5	Total	Mg	0	0
			5	5		
32	M	1	Total	Mg	0	0
			1	1		

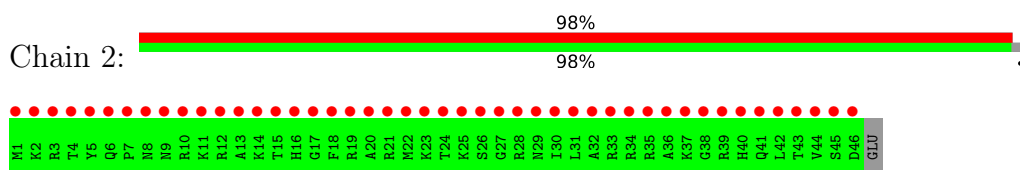
3 Residue-property plots

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

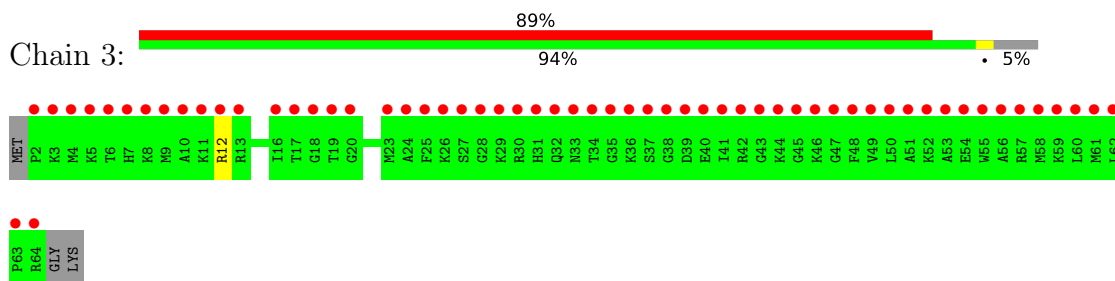
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



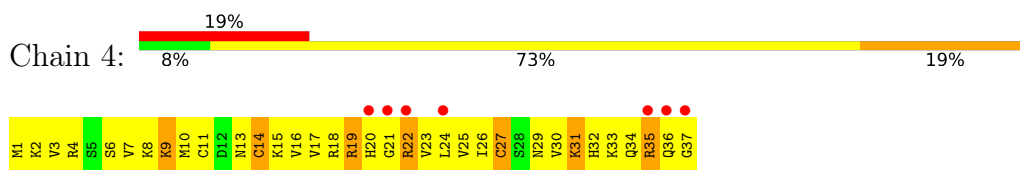
- Molecule 2: 50S RIBOSOMAL PROTEIN L34



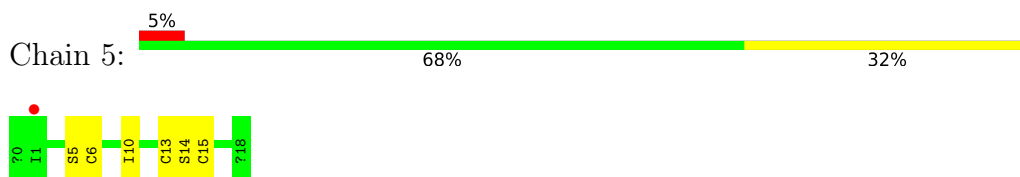
- Molecule 3: 50S RIBOSOMAL PROTEIN L35



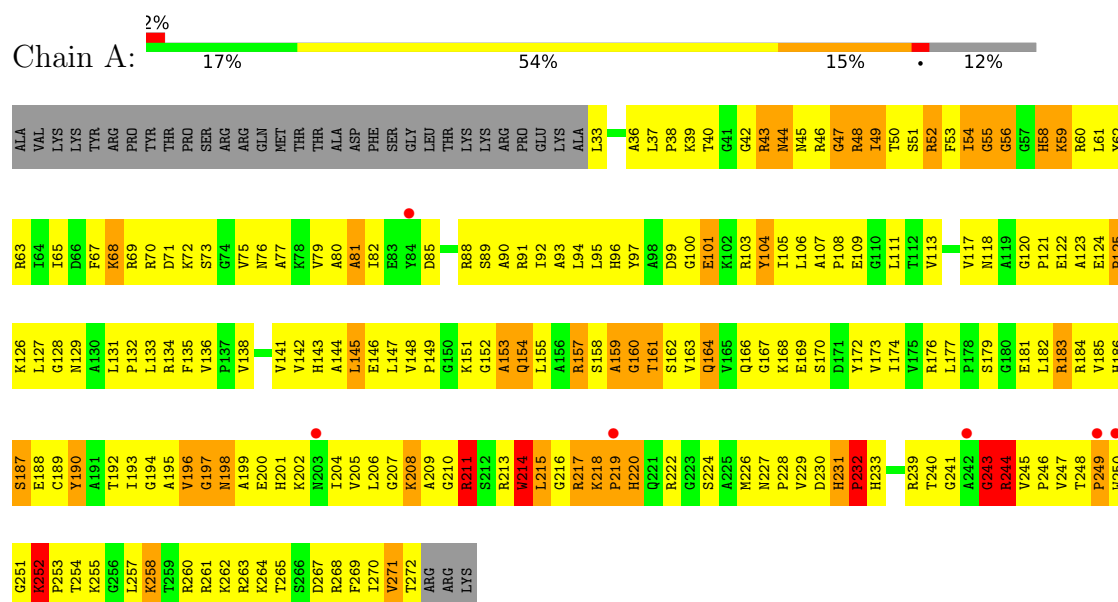
- Molecule 4: 50S RIBOSOMAL PROTEIN L36



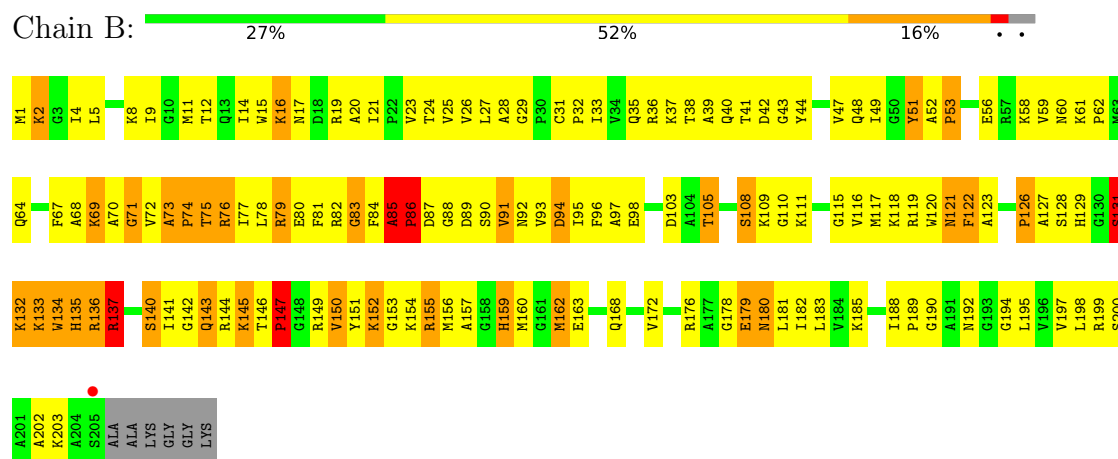
- Molecule 5: THIOSTREPTON



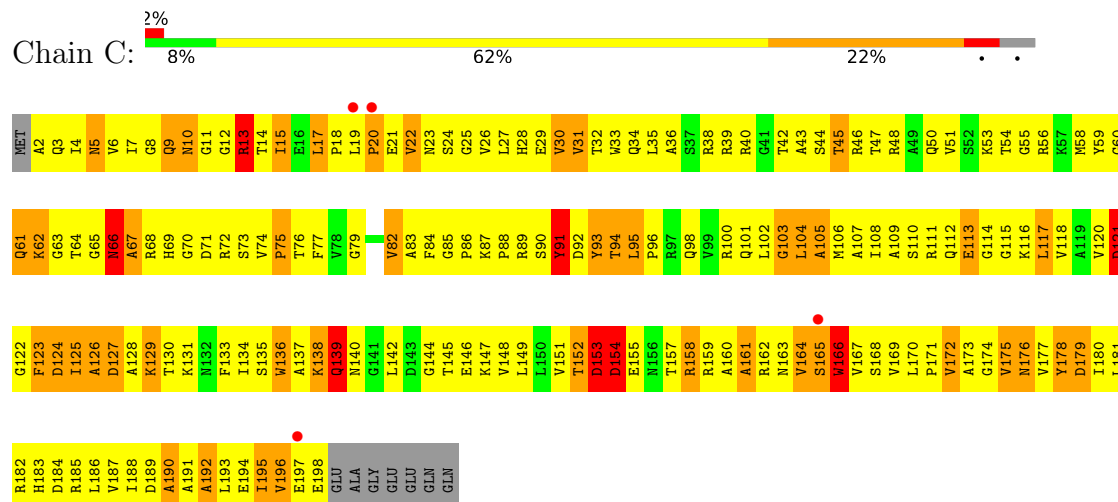
- Molecule 6: 50S RIBOSOMAL PROTEIN L2



• Molecule 7: 50S RIBOSOMAL PROTEIN L3



• Molecule 8: 50S RIBOSOMAL PROTEIN L4

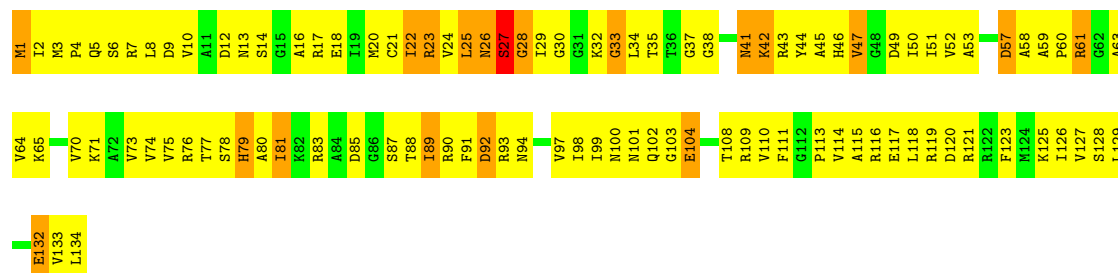


• Molecule 9: 50S RIBOSOMAL PROTEIN L5



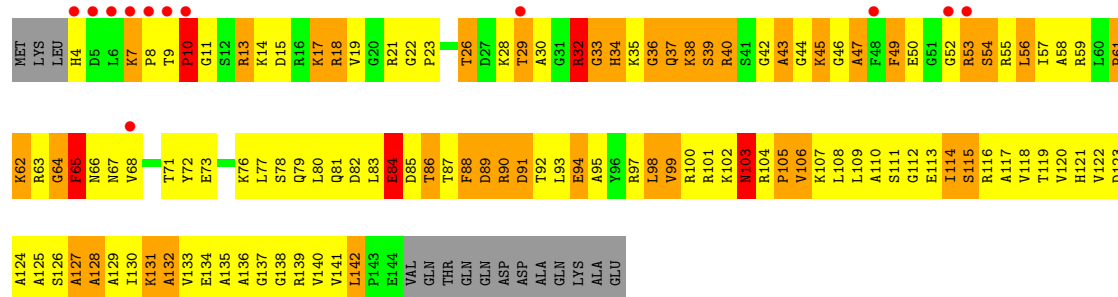
• Molecule 13: 50S RIBOSOMAL PROTEIN L14

Chain H: 22% 63% 13%



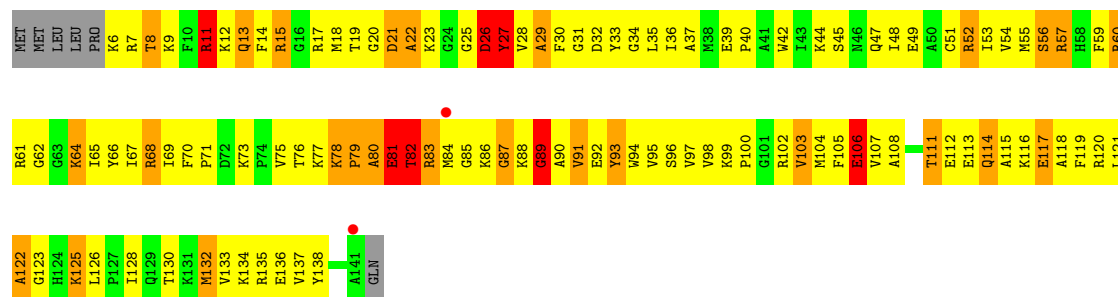
• Molecule 14: 50S RIBOSOMAL PROTEIN L15

Chain I: 8% 13% 49% 26% 10%



• Molecule 15: 50S RIBOSOMAL PROTEIN L16

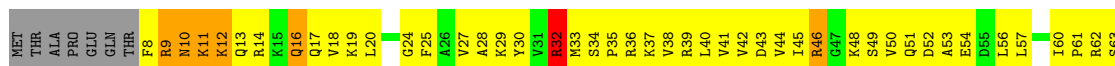
Chain J: 15% 57% 18% 5%

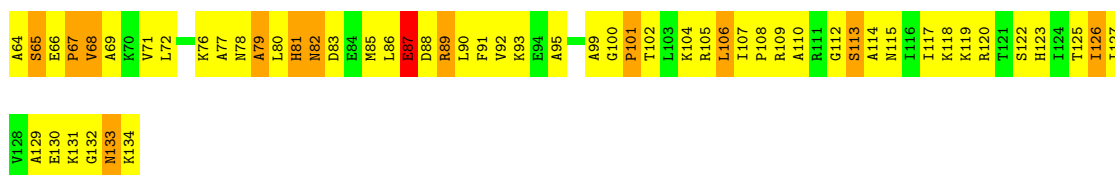


• Molecule 16: 50S RIBOSOMAL PROTEIN L17

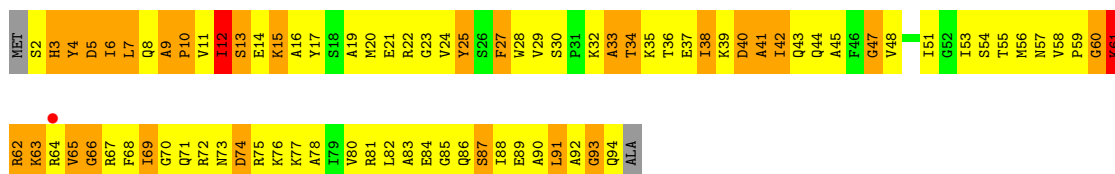
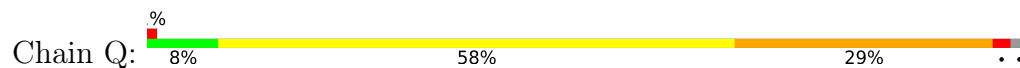
Chain K: 24% 53% 19%



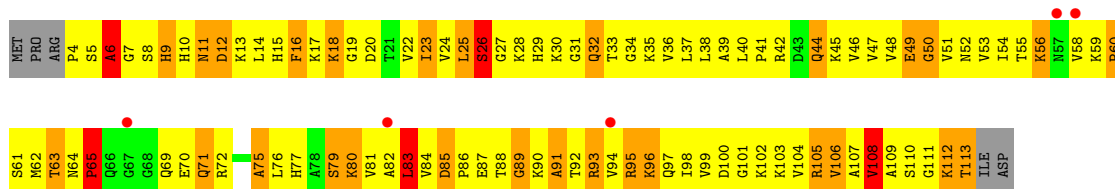
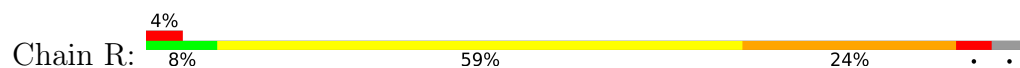




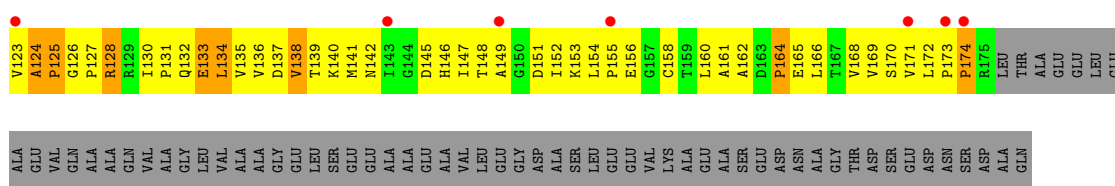
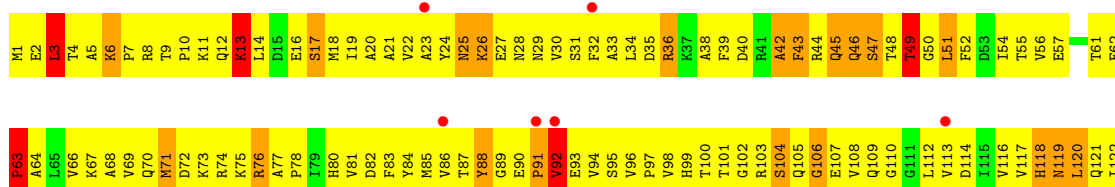
• Molecule 22: 50S RIBOSOMAL PROTEIN L23



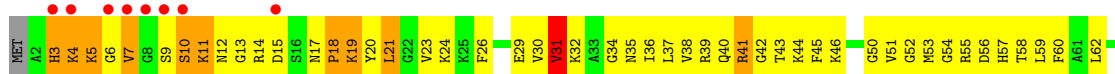
• Molecule 23: 50S RIBOSOMAL PROTEIN L24



• Molecule 24: 50S RIBOSOMAL PROTEIN L25

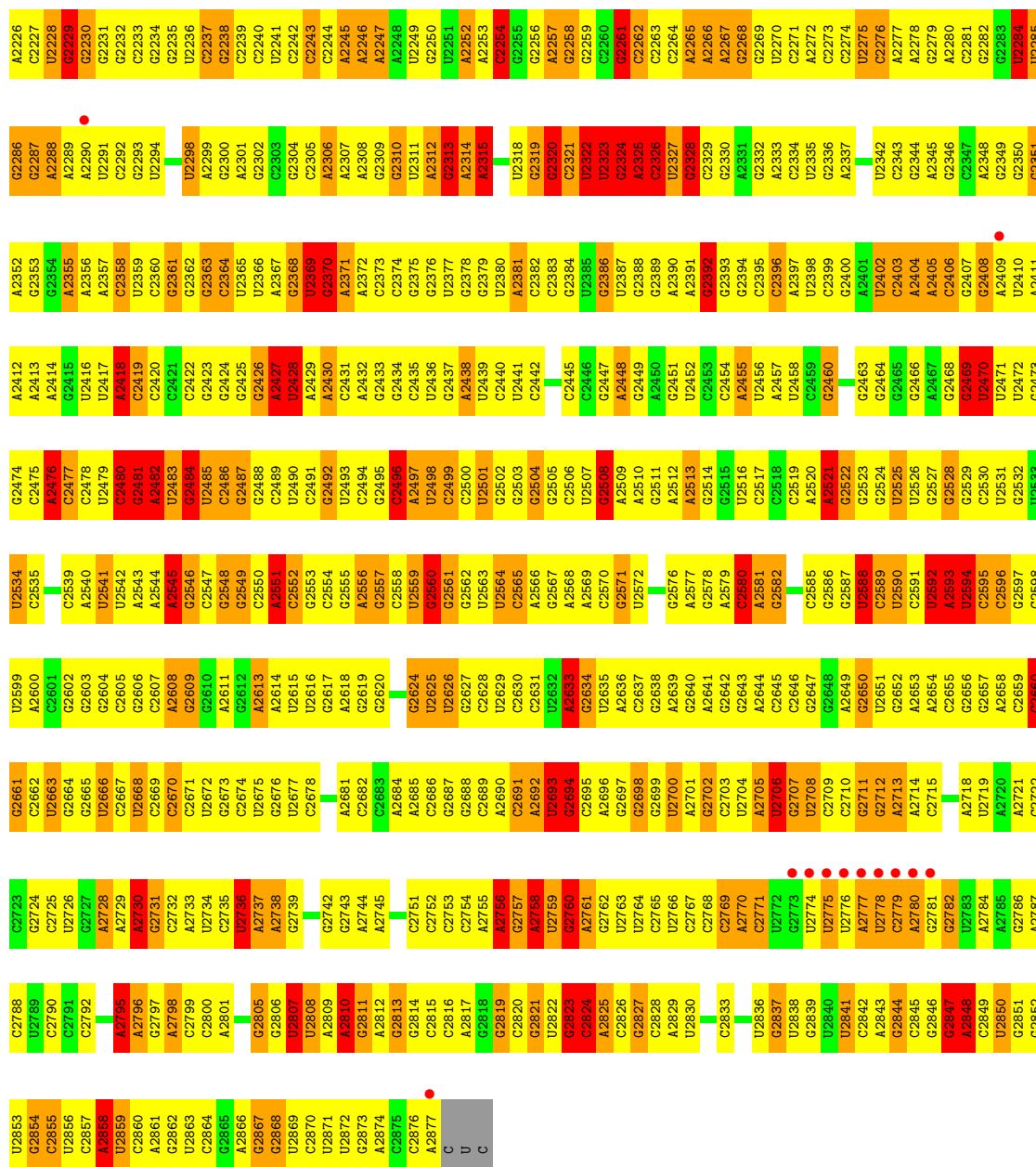


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

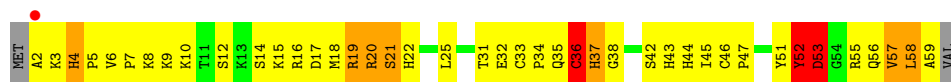


A1239	G1240	G1241	A1242	G1243	U1244	G1245	G1246	U1247	G1248	G1249	A1250	G1251	C1252	C1253	G1254	A1255	C1256	U1257	G1258	A1259	A1260	G1261	U1262	C1263	G1264	G1265	G1266	A1267	U1268	G1269	C1270	G1273	C1274	A1275	U1276	G1277	A1278	G1279	U1280	A1281	A1282	C1283	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	A1292	A1293	A1294	U1295	G1296	A1297	G1298	A1299																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C1178	G1117	U1056	U1057	U1058	U1059	C1060	A1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	U1072	G1073	G1074	C1075	U1076	U1077	A1078	G1079	C1080	A1081	C1082	C1083	A1084	G1085	C1086	U1087	A1088	C1089	C1090	C1091	C1092	U1093	C1094	A1095	A1096	A1097	C1098	A1099	G1100	U1101	G1102	C1103	G1104	U1105	A1106	A1107	U1108	A1109	U1110	U1111	C1112	C1113	A1114	C1115	U1116	U1117	A1118	C1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	C1132	G1133	C1134	C1135	G1136	A1137	U1138	A1139	A1140	A1141	G1142	A1143	U1144	G1145	G1146	G1147	U1148	G1149	C1150	C1151	C1152	A1153	A1154	G1155	U1156	U1157	U1158	U1159	C1160	U1161	A1162	C1163	C1164	G1165	G1166	A1167	G1168	C1169	U1170	A1171	U1172	G1173	G1174	A1175	U1176	U1177	A1178	C1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	U1194	A1195	U1196	U1197	A1198	U1199	A1200	A1201	U1202	A1203	G1204	G1205	G1206	G1207	A1208	A1209	C1210	G1211	U1212	U1213	C1214	A1215	G1216	U1217	C1218	C1219	G1220	U1221	U1222	A1223	G1224	A1225	G1226	A1227	G1228	C1229	C1230	A1231	U1232	A1233	C1234	G1235	A1236	U1237	A1238	A1239																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
U	A	C	U	G	G	C	A	C	C	U	G	A	G	U	A	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U

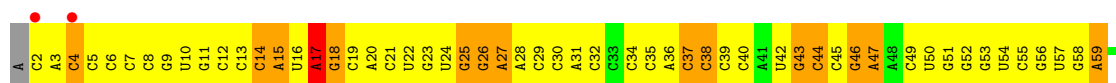




• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: RRNA-5S RIBOSOMAL RNA



C62	A63	C64	A65	G66	C67	A68	G69	C70	G71	C72	C73	A74	A75	U76	G77	A78	U79	A80	C81	U82	C83	G84	G85	G88	G94	U95	C96	C97	G100	A101	A102	A103	U106	C107	G108	G109	U110	C111	A112	G113	C114	G115	C116	G117	G118	G119	G120	G121	U122	U123
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.76 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-3.30) 93.2 (29.76-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.318 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	84475	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DCY, DHA, QUA, BB9, NH2, MH6, DBU, TS9

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	$\# Z > 5$
4	4	0.46	0/298	0.67	0/390
5	5	1.46	0/31	1.18	0/38
6	A	0.55	0/1862	0.85	2/2510 (0.1%)
7	B	0.77	0/1567	1.04	4/2105 (0.2%)
8	C	0.63	0/1529	0.91	0/2070
9	D	0.48	0/1419	0.71	0/1903
10	E	0.48	0/1308	0.80	1/1771 (0.1%)
11	F	0.50	0/1063	0.71	0/1440
12	G	0.69	0/1138	1.00	3/1539 (0.2%)
13	H	0.79	0/1007	0.96	1/1352 (0.1%)
14	I	0.65	0/1081	0.94	3/1448 (0.2%)
15	J	0.67	0/1113	0.91	2/1486 (0.1%)
16	K	0.87	0/886	1.06	2/1188 (0.2%)
17	L	0.52	0/785	0.86	0/1048
18	M	0.73	0/884	1.20	6/1186 (0.5%)
19	N	0.63	0/994	0.89	0/1323
20	O	0.61	0/750	0.90	0/1000
21	P	0.77	0/1027	0.93	1/1373 (0.1%)
22	Q	0.67	0/737	0.98	4/988 (0.4%)
23	R	0.55	0/835	0.95	2/1121 (0.2%)
24	S	0.50	0/1370	0.75	0/1862
25	T	0.56	0/633	0.83	1/838 (0.1%)
26	U	0.58	0/556	0.95	1/741 (0.1%)
27	V	0.44	0/537	0.67	0/714
28	W	0.56	0/426	0.84	0/568
29	X	0.88	59/64561 (0.1%)	1.05	497/100708 (0.5%)
30	Y	0.70	0/469	1.11	2/629 (0.3%)
31	Z	0.55	0/2904	0.76	0/4525
All	All	0.81	59/91770 (0.1%)	1.01	532/137864 (0.4%)

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
6	A	0	1
19	N	0	2
22	Q	0	1
29	X	2	257
30	Y	0	1
31	Z	0	4
All	All	2	266

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	1856	U	C4'-C3'	-9.30	1.43	1.53
29	X	1856	U	O3'-P	-8.64	1.50	1.61
29	X	1056	U	P-O5'	8.52	1.68	1.59
29	X	1855	G	O3'-P	-8.11	1.51	1.61
29	X	551	A	O3'-P	-8.05	1.51	1.61

The worst 5 of 532 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
29	X	2324	G	N9-C1'-C2'	22.22	142.88	114.00
29	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
29	X	417	C	N1-C1'-C2'	18.73	138.35	114.00
18	M	28	ARG	C-N-CD	-18.52	79.85	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	X	1278	A	C1'
29	X	2592	U	C1'

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	104	TYR	Sidechain
19	N	32	TYR	Sidechain
19	N	76	TYR	Sidechain
22	Q	25	TYR	Sidechain

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Mol	Chain	Res	Type	Group
29	X	12	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	53	0	0	0	0
2	2	46	0	0	0	0
3	3	63	0	0	1	0
4	4	297	0	330	62	0
5	5	114	0	79	5	0
6	A	1826	0	1885	451	0
7	B	1539	0	1600	303	0
8	C	1506	0	1525	371	0
9	D	1400	0	1481	373	0
10	E	1286	0	1336	264	0
11	F	1044	0	1088	176	0
12	G	1114	0	1144	310	0
13	H	997	0	1046	194	0
14	I	1067	0	1103	301	0
15	J	1090	0	1125	273	0
16	K	878	0	930	135	0
17	L	779	0	820	231	0
18	M	871	0	894	208	0
19	N	978	0	1020	239	0
20	O	741	0	756	186	0
21	P	1014	0	1096	181	0
22	Q	726	0	753	150	0
23	R	825	0	881	266	0
24	S	1345	0	1372	303	0
25	T	625	0	655	111	0
26	U	552	0	604	207	0
27	V	533	0	558	109	0
28	W	424	0	470	83	0
29	X	57651	0	29049	4301	0
30	Y	457	0	462	86	0
31	Z	2598	0	1328	185	0
32	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	30	0	0	0	0
32	Z	5	0	0	0	0
All	All	84475	0	55390	9214	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 66.

The worst 5 of 9214 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)
7:B:116:VAL:N	7:B:136:ARG:HE	1.23	1.30
29:X:1053:G:H2'	29:X:1054:C:C6	1.70	1.26
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23
29:X:2736:U:O2'	29:X:2737:A:H5''	1.36	1.21
29:X:2496:C:O2'	29:X:2497:A:H3'	1.40	1.19

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	
4	4	35/37 (95%)	20 (57%)	10 (29%)	5 (14%)	0	1
5	5	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
6	A	238/274 (87%)	154 (65%)	50 (21%)	34 (14%)	0	1
7	B	203/211 (96%)	148 (73%)	32 (16%)	23 (11%)	0	3
8	C	195/205 (95%)	97 (50%)	54 (28%)	44 (23%)	0	0
9	D	175/180 (97%)	95 (54%)	48 (27%)	32 (18%)	0	1
10	E	169/185 (91%)	100 (59%)	38 (22%)	31 (18%)	0	1
11	F	142/144 (99%)	94 (66%)	29 (20%)	19 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	1
13	H	132/134 (98%)	105 (80%)	18 (14%)	9 (7%)	1	9
14	I	139/156 (89%)	59 (42%)	45 (32%)	35 (25%)	0	0
15	J	134/142 (94%)	82 (61%)	31 (23%)	21 (16%)	0	1
16	K	111/116 (96%)	74 (67%)	25 (22%)	12 (11%)	0	3
17	L	102/114 (90%)	59 (58%)	19 (19%)	24 (24%)	0	0
18	M	106/166 (64%)	70 (66%)	23 (22%)	13 (12%)	0	2
19	N	115/118 (98%)	57 (50%)	40 (35%)	18 (16%)	0	1
20	O	92/100 (92%)	57 (62%)	10 (11%)	25 (27%)	0	0
21	P	125/134 (93%)	89 (71%)	21 (17%)	15 (12%)	0	2
22	Q	91/95 (96%)	39 (43%)	28 (31%)	24 (26%)	0	0
23	R	108/115 (94%)	62 (57%)	27 (25%)	19 (18%)	0	1
24	S	173/237 (73%)	93 (54%)	46 (27%)	34 (20%)	0	1
25	T	82/91 (90%)	47 (57%)	19 (23%)	16 (20%)	0	1
26	U	70/81 (86%)	35 (50%)	16 (23%)	19 (27%)	0	0
27	V	64/67 (96%)	35 (55%)	16 (25%)	13 (20%)	0	1
28	W	53/55 (96%)	38 (72%)	9 (17%)	6 (11%)	0	3
30	Y	56/60 (93%)	40 (71%)	9 (16%)	7 (12%)	0	2
All	All	3055/3410 (90%)	1829 (60%)	698 (23%)	528 (17%)	0	1

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	59	LYS
6	A	145	LEU
6	A	168	LYS
6	A	217	ARG
6	A	220	HIS

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	
4	4	35/35 (100%)	32 (91%)	3 (9%)	11	39
5	5	3/4 (75%)	3 (100%)	0	100	100
6	A	185/215 (86%)	161 (87%)	24 (13%)	4	20
7	B	155/157 (99%)	132 (85%)	23 (15%)	3	16
8	C	157/163 (96%)	131 (83%)	26 (17%)	2	12
9	D	153/156 (98%)	138 (90%)	15 (10%)	9	32
10	E	136/144 (94%)	128 (94%)	8 (6%)	21	55
11	F	107/107 (100%)	100 (94%)	7 (6%)	19	51
12	G	118/146 (81%)	96 (81%)	22 (19%)	2	8
13	H	103/103 (100%)	88 (85%)	15 (15%)	3	16
14	I	108/121 (89%)	91 (84%)	17 (16%)	3	14
15	J	110/116 (95%)	89 (81%)	21 (19%)	1	7
16	K	90/93 (97%)	76 (84%)	14 (16%)	3	14
17	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
18	M	94/134 (70%)	72 (77%)	22 (23%)	1	3
19	N	96/97 (99%)	83 (86%)	13 (14%)	4	18
20	O	75/79 (95%)	70 (93%)	5 (7%)	18	50
21	P	109/115 (95%)	100 (92%)	9 (8%)	12	40
22	Q	75/76 (99%)	67 (89%)	8 (11%)	7	28
23	R	91/96 (95%)	72 (79%)	19 (21%)	1	5
24	S	149/192 (78%)	137 (92%)	12 (8%)	13	41
25	T	62/67 (92%)	57 (92%)	5 (8%)	13	41
26	U	57/66 (86%)	44 (77%)	13 (23%)	1	3
27	V	54/55 (98%)	48 (89%)	6 (11%)	7	26
28	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
30	Y	51/53 (96%)	48 (94%)	3 (6%)	21	55
All	All	2495/2720 (92%)	2155 (86%)	340 (14%)	4	18

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	I	65	PHE

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Mol	Chain	Res	Type
16	K	83	VAL
26	U	47	HIS
14	I	103	ASN
15	J	82	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
13	H	41	ASN
16	K	13	ASN
27	V	45	GLN
13	H	79	HIS
14	I	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	688 (25%)	313 (11%)
31	Z	121/123 (98%)	24 (19%)	1 (0%)
All	All	2801/3003 (93%)	712 (25%)	314 (11%)

5 of 712 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	2	G
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G

5 of 314 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1261	G
29	X	1552	C
29	X	2660	C
29	X	1278	A
29	X	1345	G

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

11 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
5	TS9	5	10	5	6,8,10	0.88	0	5,12,15	1.15	0
5	BB9	5	11	5	3,5,6	1.29	0	1,5,7	2.51	1 (100%)
5	BB9	5	13	5	2,4,6	1.64	1 (50%)	3,4,7	2.68	3 (100%)
5	MH6	5	14	5	3,3,6	1.51	0	1,3,7	0.43	0
5	BB9	5	15	5	3,5,6	3.75	1 (33%)	1,5,7	3.97	1 (100%)
5	DHA	5	16	5	4,4,5	4.23	2 (50%)	2,4,6	5.61	1 (50%)
5	DHA	5	17	5	4,4,5	1.84	1 (25%)	2,4,6	2.56	1 (50%)
5	DHA	5	3	5	4,4,5	2.02	2 (50%)	2,4,6	1.81	1 (50%)
5	BB9	5	6	5	3,5,6	1.85	1 (33%)	1,5,7	2.53	1 (100%)
5	DBU	5	8	5	4,4,6	3.10	2 (50%)	4,4,7	1.52	1 (25%)

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
5	TS9	5	10	5	-	0/9/12/16	-
5	BB9	5	11	5	-	0/0/4/6	-
5	BB9	5	13	5	-	0/0/2/6	-
5	BB9	5	15	5	-	0/0/4/6	-
5	DHA	5	16	5	-	0/0/2/4	-
5	DHA	5	17	5	-	0/0/2/4	-
5	DHA	5	3	5	-	0/0/2/4	-
5	BB9	5	6	5	-	0/0/4/6	-
5	DBU	5	8	5	-	0/1/2/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	16	DHA	CA-N	8.02	1.55	1.35
5	5	15	BB9	O-C	-6.45	1.07	1.22
5	5	8	DBU	CA-N	5.73	1.47	1.33
5	5	17	DHA	CA-N	3.16	1.43	1.35
5	5	6	BB9	O-C	2.91	1.28	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	16	DHA	O-C-CA	-7.91	111.08	125.47
5	5	15	BB9	O-C-CA	3.97	130.46	125.39
5	5	17	DHA	O-C-CA	-3.05	119.92	125.47
5	5	13	BB9	C-CA-CB	2.88	126.66	121.36
5	5	8	DBU	CB-CA-N	2.75	124.53	122.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	10	TS9	1	0
5	5	13	BB9	1	0
5	5	15	BB9	1	0
5	5	6	BB9	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 36 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	53/55 (96%)	3.45	39 (73%) 0 0	48, 56, 77, 82	0
2	2	46/47 (97%)	5.52	46 (100%) 0 0	9, 29, 38, 40	0
3	3	63/66 (95%)	5.06	59 (93%) 0 0	23, 41, 51, 57	0
4	4	37/37 (100%)	1.16	7 (18%) 1 1	60, 69, 77, 81	0
5	5	6/19 (31%)	1.08	1 (16%) 1 1	79, 83, 86, 86	0
6	A	240/274 (87%)	-0.11	6 (2%) 57 55	25, 63, 77, 84	0
7	B	205/211 (97%)	-0.69	1 (0%) 90 90	3, 22, 49, 63	0
8	C	197/205 (96%)	-0.30	4 (2%) 65 64	8, 51, 73, 83	0
9	D	177/180 (98%)	0.03	10 (5%) 24 23	60, 75, 85, 91	0
10	E	171/185 (92%)	-0.34	3 (1%) 68 67	44, 66, 79, 88	0
11	F	144/144 (100%)	1.48	41 (28%) 0 0	74, 89, 98, 102	0
12	G	142/174 (81%)	-0.29	3 (2%) 63 62	22, 43, 67, 72	0
13	H	134/134 (100%)	-0.78	0 100 100	3, 16, 37, 45	0
14	I	141/156 (90%)	0.25	12 (8%) 11 11	22, 62, 77, 85	0
15	J	136/142 (95%)	-0.33	2 (1%) 73 71	27, 51, 73, 80	0
16	K	113/116 (97%)	-0.83	0 100 100	3, 9, 24, 34	0
17	L	104/114 (91%)	-0.06	4 (3%) 40 38	43, 62, 72, 75	0
18	M	108/166 (65%)	-0.74	0 100 100	4, 19, 43, 64	0
19	N	117/118 (99%)	-0.57	0 100 100	4, 40, 62, 73	0
20	O	94/100 (94%)	-0.43	0 100 100	18, 53, 71, 81	0
21	P	127/134 (94%)	-0.72	0 100 100	4, 18, 53, 76	0
22	Q	93/95 (97%)	-0.41	1 (1%) 80 81	32, 50, 69, 80	0
23	R	110/115 (95%)	-0.15	5 (4%) 33 33	36, 54, 80, 87	0
24	S	175/237 (73%)	0.23	13 (7%) 14 16	61, 71, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	0.02	8 (9%) 8 9	35, 51, 80, 90	0
26	U	72/81 (88%)	0.09	3 (4%) 36 35	45, 61, 72, 78	0
27	V	66/67 (98%)	-0.49	0 100 100	49, 61, 81, 88	0
28	W	55/55 (100%)	-0.42	0 100 100	23, 41, 61, 78	0
29	X	2686/2880 (93%)	-0.37	60 (2%) 62 61	4, 41, 116, 151	0
30	Y	58/60 (96%)	-0.52	1 (1%) 70 68	4, 17, 44, 52	0
31	Z	122/123 (99%)	-0.11	3 (2%) 57 55	30, 75, 102, 129	0
All	All	6076/6581 (92%)	-0.15	332 (5%) 25 24	3, 49, 95, 151	0

The worst 5 of 332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	39	ASP	15.9
2	2	26	SER	9.7
1	1	2	ALA	9.6
3	3	31	HIS	9.6
2	2	4	THR	9.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DHA	5	16	5/6	0.52	0.55	83,83,85,86	0
5	DHA	5	17	5/6	0.55	0.39	76,77,78,80	2
5	DHA	5	3	5/6	0.76	0.47	82,83,84,85	0
5	BB9	5	15	6/7	0.78	0.48	88,88,88,88	0
5	DCY	5	9	6/7	0.81	0.18	87,87,87,87	0
5	BB9	5	13	5/7	0.83	0.22	85,86,86,87	0
5	MH6	5	14	4/7	0.85	0.30	86,86,87,87	0
5	BB9	5	11	6/7	0.86	0.23	85,87,87,88	0
5	TS9	5	10	9/11	0.87	0.38	87,88,89,89	0
5	BB9	5	6	6/7	0.88	0.18	82,84,85,86	0
5	DBU	5	8	5/7	0.93	0.16	85,86,87,87	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	X	2884	1/1	0.82	0.79	55,55,55,55	0
32	MG	X	2910	1/1	0.90	0.38	19,19,19,19	0
32	MG	X	2898	1/1	0.90	0.54	19,19,19,19	0
32	MG	X	2890	1/1	0.91	0.34	49,49,49,49	0
32	MG	X	2886	1/1	0.91	0.26	41,41,41,41	0
32	MG	X	2885	1/1	0.93	0.41	56,56,56,56	0
32	MG	Z	124	1/1	0.95	0.31	26,26,26,26	0
32	MG	Z	126	1/1	0.95	0.34	25,25,25,25	0
32	MG	X	2903	1/1	0.95	0.30	3,3,3,3	0
32	MG	X	2896	1/1	0.95	0.26	3,3,3,3	0
32	MG	X	2889	1/1	0.95	0.77	3,3,3,3	0
32	MG	X	2881	1/1	0.95	0.24	59,59,59,59	0
32	MG	Z	127	1/1	0.95	0.17	12,12,12,12	0
32	MG	X	2892	1/1	0.95	0.16	22,22,22,22	0
32	MG	X	2888	1/1	0.95	0.30	3,3,3,3	0
32	MG	X	2893	1/1	0.96	0.15	13,13,13,13	0
32	MG	X	2905	1/1	0.96	0.50	13,13,13,13	0
32	MG	X	2907	1/1	0.96	0.73	17,17,17,17	0
32	MG	X	2900	1/1	0.96	0.26	3,3,3,3	0
32	MG	X	2902	1/1	0.96	0.39	24,24,24,24	0
32	MG	Z	128	1/1	0.96	0.09	41,41,41,41	0
32	MG	X	2882	1/1	0.97	0.36	12,12,12,12	0
32	MG	X	2909	1/1	0.97	0.21	3,3,3,3	0
32	MG	X	2904	1/1	0.97	0.32	6,6,6,6	0
32	MG	X	2908	1/1	0.97	0.11	3,3,3,3	0
32	MG	X	2897	1/1	0.98	0.47	3,3,3,3	0
32	MG	M	167	1/1	0.98	0.54	3,3,3,3	0
32	MG	X	2895	1/1	0.98	0.25	3,3,3,3	0
32	MG	X	2887	1/1	0.98	0.18	3,3,3,3	0
32	MG	X	2901	1/1	0.98	0.09	60,60,60,60	0
32	MG	X	2906	1/1	0.98	0.19	58,58,58,58	0
32	MG	Z	125	1/1	0.98	0.29	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	X	2894	1/1	0.99	0.40	15,15,15,15	0
32	MG	X	2883	1/1	0.99	0.10	49,49,49,49	0
32	MG	X	2891	1/1	0.99	0.41	12,12,12,12	0
32	MG	X	2899	1/1	0.99	0.53	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.