



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 08:43 am BST

PDB ID : 3CCE
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.75 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

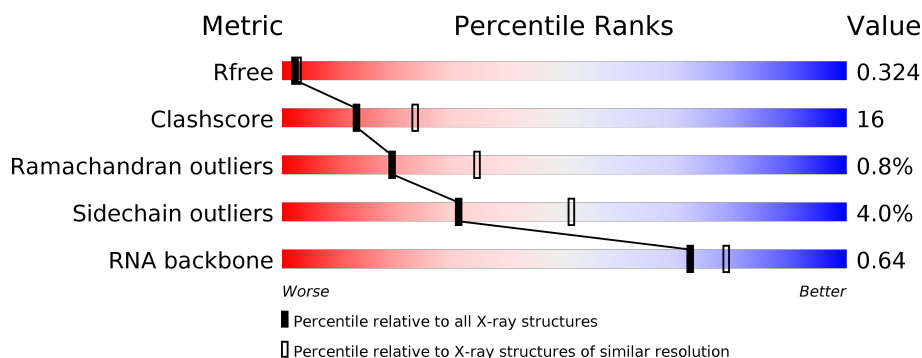
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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

















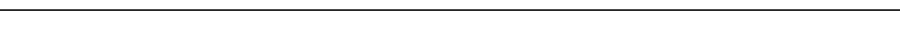




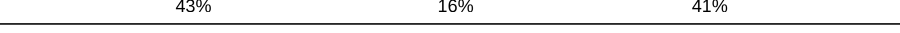
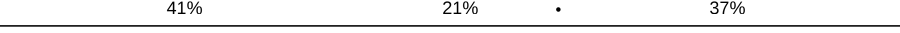




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	240	65% 30% . .
2	B	338	62% 34% .
3	C	246	67% 30% .
4	D	177	41% 37% . 21%
5	E	178	67% 29% .
6	F	120	74% 25% .

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Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

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
33	CL	J	8801	-	-	X	-
33	CL	J	8802	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99124 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 L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59022	26350	10876	19051	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	86	Total	Mg	0	0
			86	86		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	0	0
33	Q	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	92	Total Sr 92 92	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	4	Total Sr 4 4	0	0
34	S	1	Total Sr 1 1	0	0
34	F	1	Total Sr 1 1	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	67	Total 67	Na 67	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	2	Total 2	K 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	118	Total 118	O 118	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	144	Total 144	O 144	0	0
38	C	179	Total 179	O 179	0	0
38	D	46	Total 46	O 46	0	0
38	E	40	Total 40	O 40	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	68	Total 68	O 68	0	0
38	I	5	Total 5	O 5	0	0
38	J	55	Total 55	O 55	0	0
38	K	52	Total 52	O 52	0	0
38	L	84	Total 84	O 84	0	0
38	M	127	Total 127	O 127	0	0
38	N	63	Total 63	O 63	0	0
38	O	40	Total 40	O 40	0	0
38	P	61	Total 61	O 61	0	0
38	Q	43	Total 43	O 43	0	0
38	R	84	Total 84	O 84	0	0
38	S	33	Total 33	O 33	0	0
38	T	33	Total 33	O 33	0	0
38	U	28	Total 28	O 28	0	0
38	V	14	Total 14	O 14	0	0

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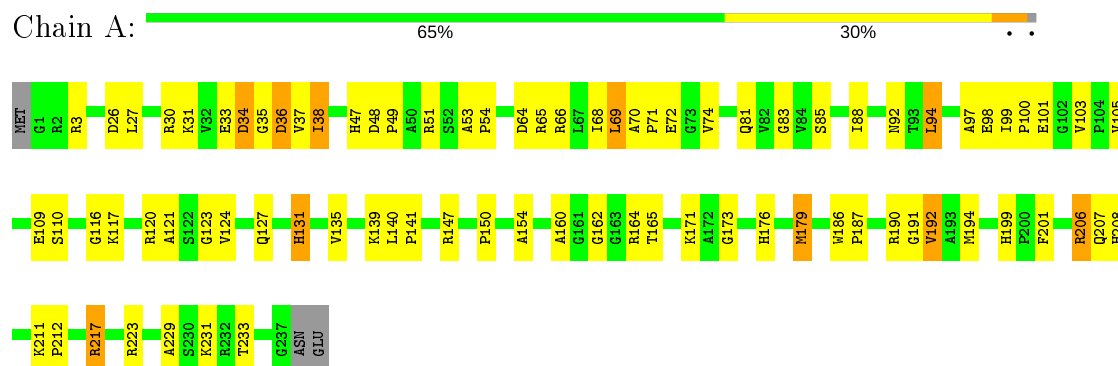
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	67	Total 67	O 67	0	0
38	X	30	Total 30	O 30	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	32	Total 32	O 32	0	0
38	1	55	Total 55	O 55	0	0
38	2	42	Total 42	O 42	0	0
38	3	63	Total 63	O 63	0	0
38	0	5927	Total 5927	O 5927	0	0
38	9	144	Total 144	O 144	0	0

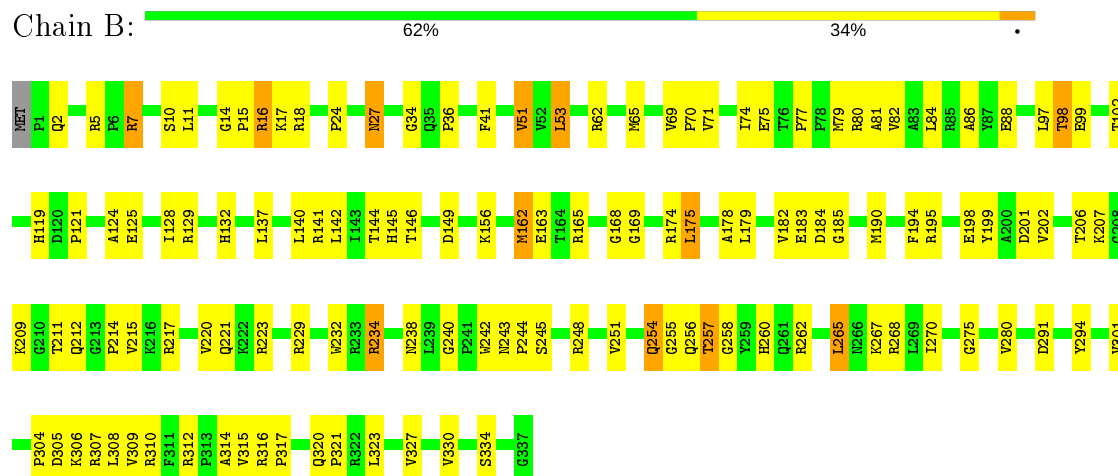
3 Residue-property plots

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. 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. 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.

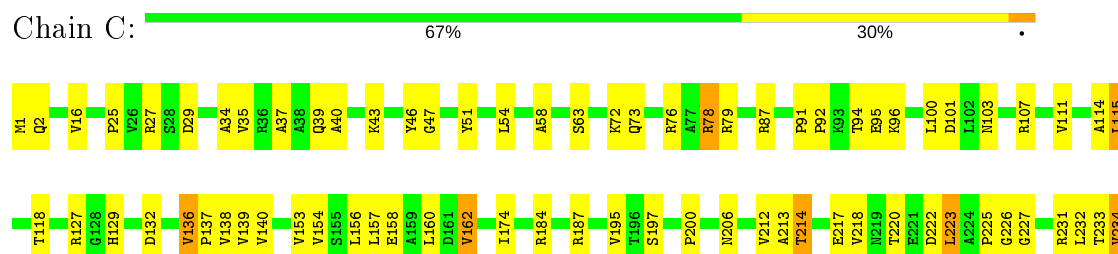
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P



• Molecule 3: 50S ribosomal protein L4P



ASP ASP
SER ASP
THR
ALA
SER
GLU
ASP
ASP
ALA
ASP
ALA
ASP
ASP
ALA
ALA
GLU
GLU
ALA
ASP
ASP
ASP
ASP
ASP
ASP
ASP
GLU
ALA
GLY
ASP
ALA
MET
PHE

• Molecule 8: 50S ribosomal protein L10e

Chain H:  68% 21% 10%

MET SER ASP K4 P6 A6 S7 M8 I12 P15 R19 R20 E21 Y22 T26 P27 G28 S29 K30 K31 K35 Y46 P47 L52 Q59 L60 R61 H62 G63 S64 L70 S71 A72 N73 R74 I77 E82 K87 R91 L98 K102 GLN ALA THR GLY

ALA GLY ALA ASP ARG VAL SER D114 I123 A127 A128 R129 K150 F153 R154 R155 A156 Y157 R165 V168 E169 R170 L174 LEU ILE ALA

• Molecule 9: 50S ribosomal protein L11P

Chain I:  31% 12% 57%

MET ALA GLY THR ILE ILE VAL LEU VAL PRO GLY GLY ALA ASN PRO GLY PRO PRO LEU PRO GLY PRO VAL ASP VAL GLN ALA VAL VAL GLN ASN ASP THR THR ALA ALA PHE ASP GLY THR VAL VAL PRO VAL THR VAL LYS TVR ASP ASP GLY

SER PHE GLU ILE VAL G66 P69 L73 T82 G83 E86 P87 L95 S96 V97 D98 Q99 V100 K101 K107 H108 P109 D110 L111 L112 N118 A119 A120 K121 V124 L130 E135 GLY ASN PRO ARG GLU PHE LYS GLU ARG ILE ASP ALA GLY TTR ASP

ASP VAL PHE ALA ALA GLU ALA GLN ALA

• Molecule 10: 50S ribosomal protein L13P

Chain J:  71% 24% 5%

MET SER VAL A4 E5 I18 M19 V26 V36 V39 N40 A41 V45 I46 Q52 S53 V54 V55 I63 Y69 F70 R74 P75 D76 G77 I78 F79 K80 R81 T82 P88 H89 K90 K93 V101 L105 G106 M107 P108 Y109 I127 K128 F129 V130 T131 L132 G133

E134 I135 S136 E137 T138 R145

• Molecule 11: 50S ribosomal protein L14P

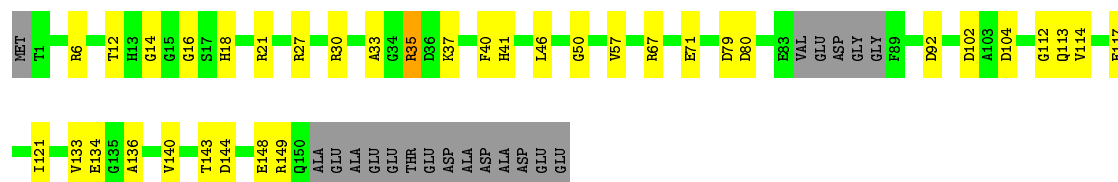
Chain K:  70% 30%

K1 L4 V8 Q10 G11 L12 E13 K14 I18 T19 C20 A21 D22 L29 I32 S33 V34 G39 T40 K41 N42 P45 K46 A47 V55 S56 E63 M64 Q67 V74 K78 P79 I80 R81 R82 R87 N93 V98 E102 I113 A114 R115

E116 V117 A118 A125 A128 T129 M130 I131 V132

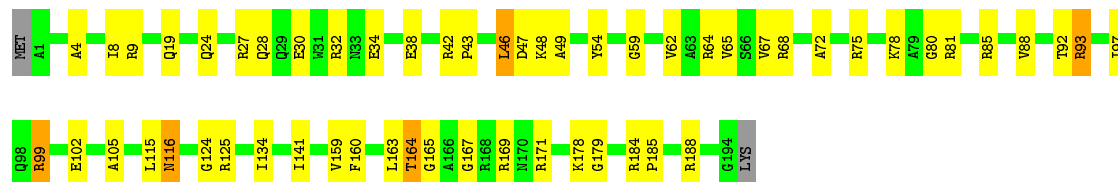
• Molecule 12: 50S ribosomal protein L15P

Chain L:  66% 21% 12%



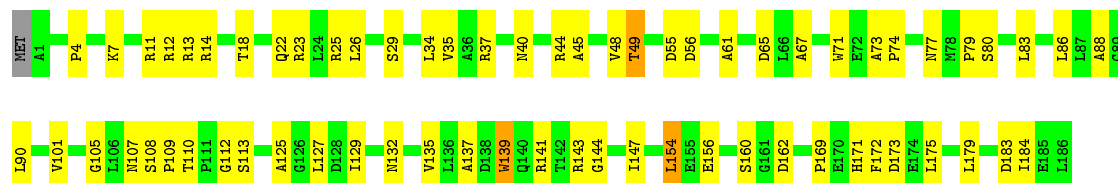
- Molecule 13: 50S ribosomal protein L15e

Chain M: 70% 26% ..



- Molecule 14: 50S ribosomal protein L18P

Chain N: 64% 34% ..



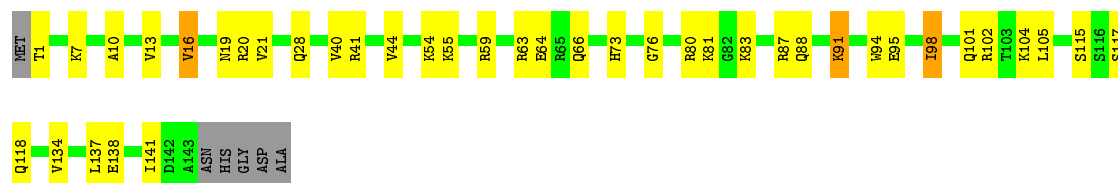
- Molecule 15: 50S ribosomal protein L18e

Chain O: 85% 14% .



- Molecule 16: 50S ribosomal protein L19e

Chain P: 69% 25% ..

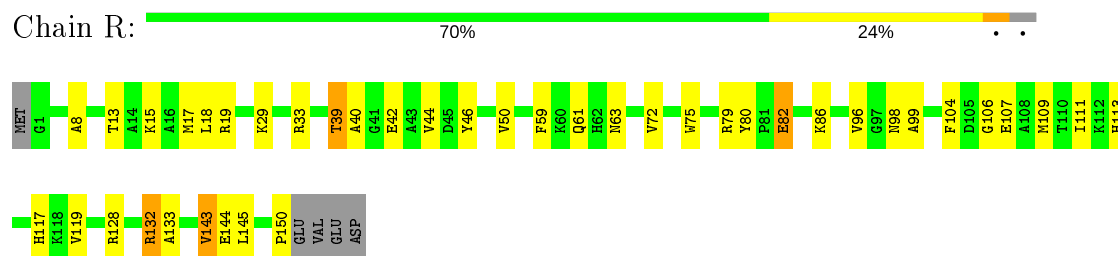


- Molecule 17: 50S ribosomal protein L21e

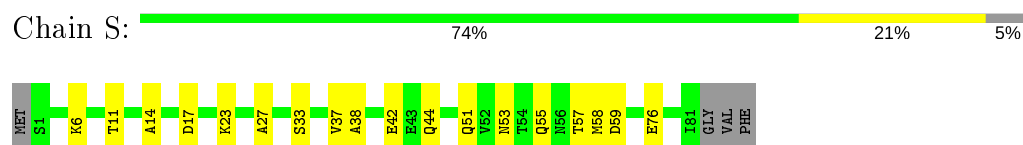
Chain Q: 73% 25% ..



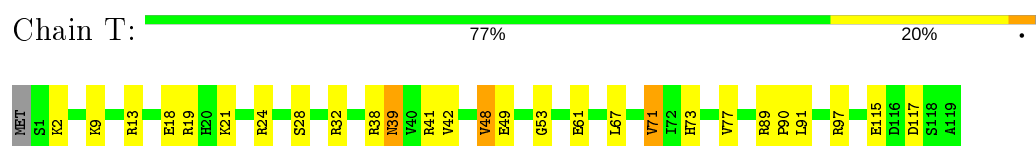
- Molecule 18: 50S ribosomal protein L22P



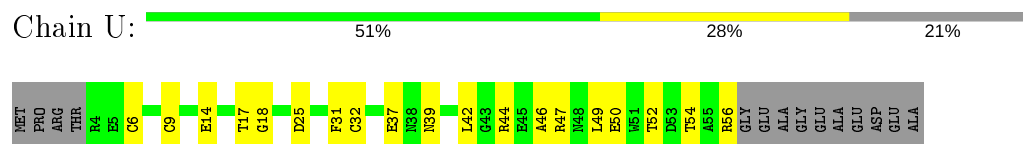
- Molecule 19: 50S ribosomal protein L23P



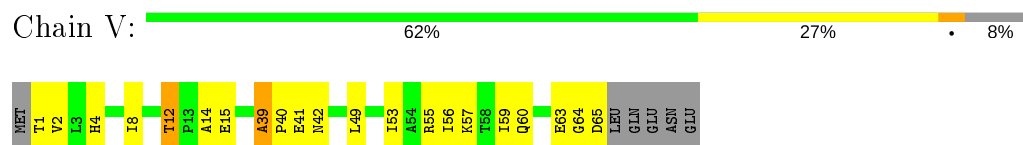
- Molecule 20: 50S ribosomal protein L24P



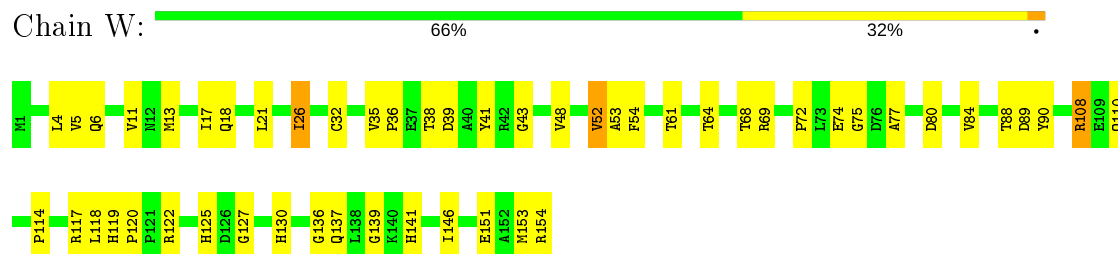
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P



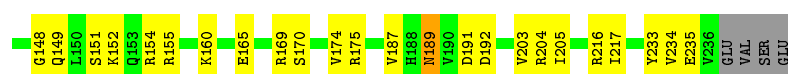
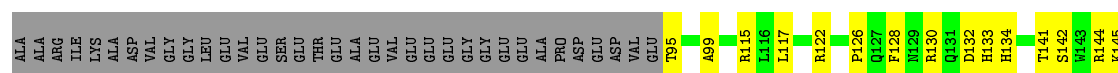
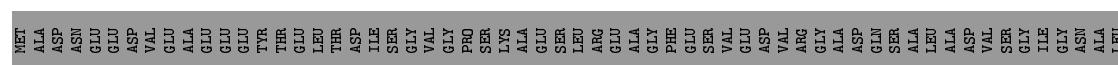
- Molecule 24: 50S ribosomal protein L31e

Chain X: 



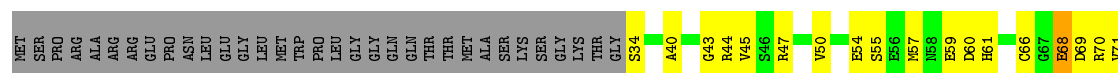
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



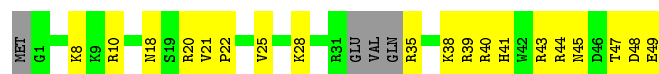
- Molecule 27: 50S ribosomal protein L37e

Chain 1: 




- Molecule 28: 50S ribosomal protein L39e

Chain 2: 

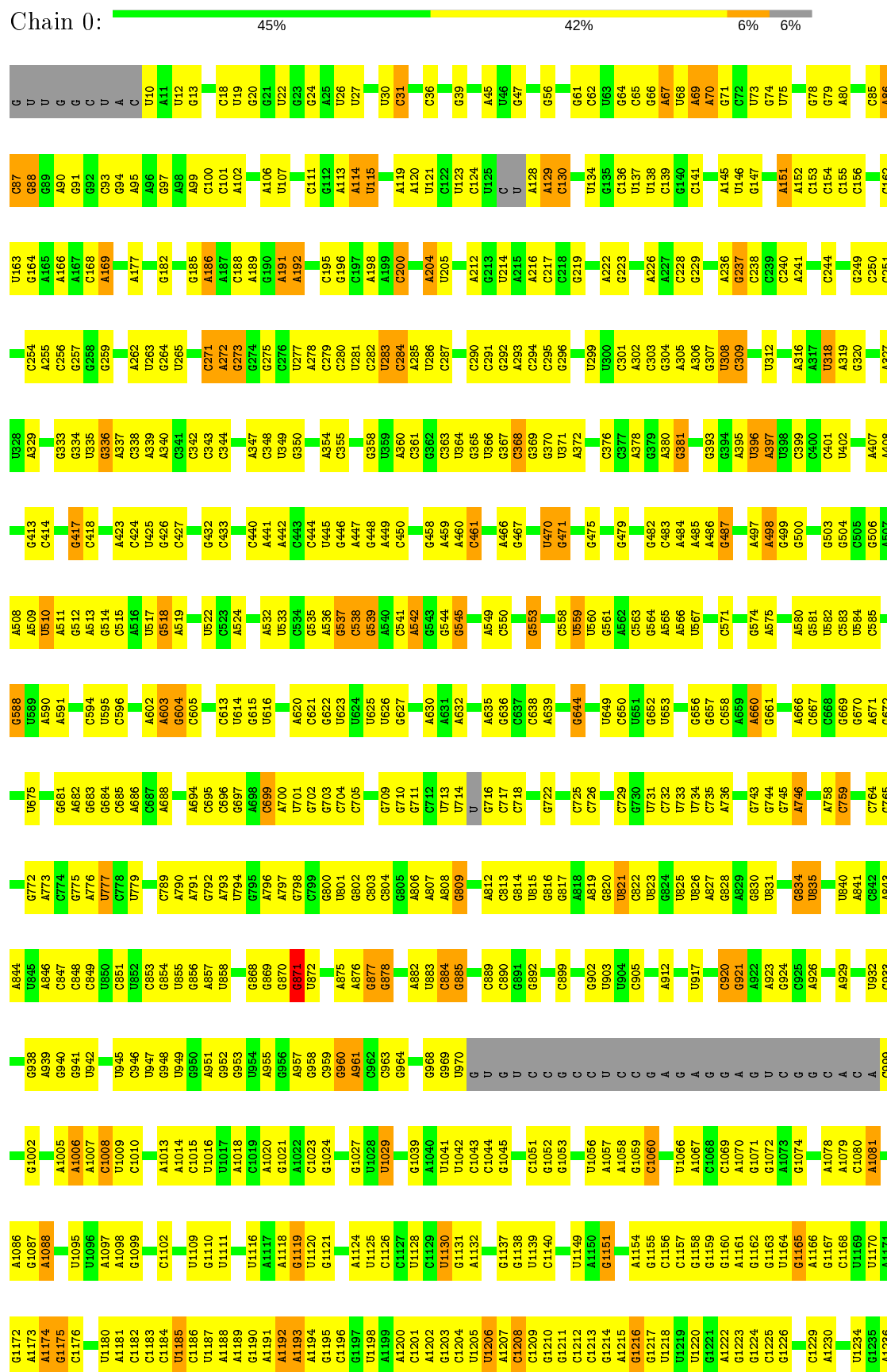


- Molecule 29: 50S ribosomal protein L44E

Chain 3: 



- Molecule 30: 23S RIBOSOMAL RNA



A2425	G2337	G2254	C2132	A2039	G1951	C1872	U1784	G1695	G1512	A1406	G1323	U1237
G2426	G2338	A2285	U2133	C2040	U	G1873	G1785	U1696	C1513	A1407	G1324	C1238
A2430	A	G2256	A2134	A	A	U1874	C1786	G1604	C1514	U1408	G1325	G1239
A2433	C	G2257	A2135	G2044	A	A1875	C1787	G1605	A1515	G1409		
A2434	A	A2258	G2136	A	C	C1876	U1788	A1606	U1516	G1410	A1328	A1242
U2435	G	U2265	A	G2050	U	G1877	G1789	A1607	C1517	A1413	U1333	C1243
U2436	C	A2286	C	A2054	U	G1878	C1790	U1702	G1520	A1414	C1334	U1244
G2237	G	C	C	C	A	U1879	U1791		G1521	A1415	U1245	U1245
A2344	C	U	U	U	G	C1880	G1795	C1705	C1522	A1416	A1246	
A2345	C	C	C	U2059	C	C1881	A1881	G1706	A1523	G1417	G1340	U1249
A2346	C	C	G	A2060	C	C1882	A1796	G1707	G1524	A1418	A1341	C1250
G2237	C	C	U	C2061	C	U1883	C1797	A1616	U1525	U1419	C1342	C1251
G2238	A	G	C	A2062	C	G1884	C1798	A1617	G1526	C1420	G1343	
C2281	A	A	G	U2063	U1964	A1885	G1799	A1710	A1527	A1421	A1345	A1285
C2282	C	C	C	U2064	C1965	A1886	G1800	A1711	A1528	U1422	A1346	
G2235	C	C	C	C2065	U1966	U1887	G1801	A1712	G1529	C1423	U1347	G1260
A2354	A	A	G	C2066	U1967	C1888	A1804	A1717	G1535	C1426	U1350	U1266
A2355	C	A	U	A1968	A1969	C1889	G1805	G1718	C1536	G1441	G1351	C1267
A2361	A	G	U	C2071	G1970	U1890	C1810	C1721	G1543	A1442	G1352	G1269
A2362	U	U	G	G2072	U1971	C1894	A1815	U1722	U1544	G1445	A1355	C1273
A2363	G	G	G	A2074	A1972	G1902	G1816	G1723	C1545	U1446	C1360	A1278
A2364	A	A	A	G2075	A1973	U1903	U1817	U1724	G1546	C1451	G1364	G1284
G2365	A	A	C	U2076	C1974	A1904	C1826	C1734		C1452	C1365	U1285
A2366	A	A	C	A2081	G1975	U1905	C1838	C1735		C1453	C1366	A1286
A2367	U	U	C	C	G1976	U1906	A1839	A1736	U	C1454	A1367	U1287
A2368	A	A	C	C	U1977	C1907	A1840	A1737	U1561	U1461	U1368	U1288
A2369	C	C	U	C2087	A1978	A1909	G1820	C1738	C1562	U1462	A1372	U1289
A2370	U	U	A	G2073	U1979	A1910	U1825	A1732	G1568	U1463	A1375	G1290
A2371	A	C	G	A2088	U1980	A1911	U1836	A1733	U1569	C1464	G1376	A1294
A2372	C	C	G	C2090	G1981	U1915	A1837	A1734	A1573	A1471	C1377	G1295
A2373	C	C	U	G2091	U1982	C1916	G1837	A1754	C1574	C1472	G1378	U1297
A2374	C	C	U	C2092	C1983	A1919	A1838	A1755	A1575	U1473	A1381	U1298
A2375	C	C	G	G2093	U1984	C1920	A1839	G1756	U1577	C1474	G1382	G1299
U2308	U	U	G	A2096	G1985	A1921	A1841	U1757	C1578	U1477	U1383	G1300
C2309	C	C	A	C	U1995	A1922	A1845	C1762	U1583	A1482	G1384	C1305
G2310	G	G	A	U2107	U1996	A1923	U1846	U1766	C1584	C1483	G1385	U1306
A2311	G	U	U	A2100	A1997	A1924	U1846	A1767	C1585	G1484	G1386	A1307
G2314	G	U	C	A2101	C2002	G1925	A1836	C1752	G1586	A1501	C1395	U1308
G2315	G	C	G	G2102	U2003	G1926	A1837	C1753	A1592	A1502	G1396	G1312
G2316	A	C	U	A2103	U2004	A1927	U1850	A1754	C1593	U1503	C1397	G1315
G2317	C	C	U	C2104	G2005	C1928	G1851	C1768	G1595	U1504	G1398	G1316
C2317	U	U	A	C2105	C2006	G1929	A1852	U1770	U1596	U1505	A1399	
U2320	C	C	C	C2106	A2067	A1930	C1853	U1771	A1597	U1506	G1401	
A2321	C	C	A	U2107	U2008	A1931	G1854	C1772	U1598	G1497		
A2322	A	A	G	A2108	G2009	G1932	G1855	U1772	C1599	A1501		
A2323	A	A	A	U2109	A2010	G1933	A1856	G1773	C1603	A1502		
A2324	G	U	G	G2110	A2011	A1934	A1857	G1774	C1604	U1503		
A2325	G	G	G	G2111	U2012	C1935	A1858	G1775	C1605	U1504		
A2326	U	U	U	A2112	G2013	C1936	A1859	G1776	C1606	U1505		
A2327	A	A	A	G2113	G2014	C1937	A1860	G1777	C1607	U1506		
A2328	C	C	C	G2114	G2015	C1938	A1861	A1778	C1608	U1507		
A2329	C	C	C	A2015	U1939	U1939	A1862	A1779	C1609	U1508		
A2330	C	C	C	U2016	A1942	A1942	A1863	A1780	C1610	U1509		
A2331	C	C	C	A2022	A2022	A2022	A1864	A1781	C1611	U1510		
A2332	G	G	G	U2023	U2023	U2023	A1865	A1782	C1612	U1511		
A2333	C	C	C	G2121	U2024	G1947	A1866	A1783	C1613	U1512		
A2334	C	C	C	C2122	U2025	G1948	A1867	A1784	C1614	U1513		
A2335	C	C	C	G2123	U2026	G1949	A1868	A1785	C1615	U1514		
A2336	U	U	U	G2124	U2027	G1950	A1869	A1786	C1616	U1515		
A2337	A	A	A	A	U2028	G1951	A1870	A1787	C1617	U1516		
A2338	C	C	C	G2125	U2029	G1952	A1871	A1788	C1618	U1517		
A2339	C	C	C	G2126	U2030	G1953	A1872	A1789	C1619	U1518		
A2340	C	C	C	G2127	U2031	G1954	A1873	A1790	C1620	U1519		
A2341	C	C	C	G2128	U2032	G1955	A1874	A1791	C1621	U1520		
A2342	C	C	C	G2129	U2033	G1956	A1875	A1792	C1622	U1521		
A2343	C	C	C	G2130	U2034	G1957	A1876	A1793	C1623	U1522		
A2344	C	C	C	G2131	U2035	G1958	A1877	A1794	C1624	U1523		
A2345	C	C	C	G2132	U2036	G1959	A1878	A1795	C1625	U1524		
A2346	C	C	C	G2133	U2037	G1960	A1879	A1796	C1626	U1525		
A2347	C	C	C	G2134	U2038	G1961	A1880	A1797	C1627	U1526		
A2348	C	C	C	G2135	U2039	G1962	A1881	A1798	C1628	U1527		
A2349	C	C	C	G2136	U2040	G1963	A1882	A1799	C1629	U1528		
A2350	C	C	C	G2137	U2041	G1964	A1883	A1800	C1630	U1529		
A2351	C	C	C	G2138	U2042	G1965	A1884	A1801	C1631	U1530		
A2352	C	C	C	G2139	U2043	G1966	A1885	A1802	C1632	U1531		
A2353	C	C	C	G2140	U2044	G1967	A1886	A1803	C1633	U1532		
A2354	C	C	C	G2141	U2045	G1968	A1887	A1804	C1634	U1533		
A2355	C	C	C	G2142	U2046	G1969	A1888	A1805	C1635	U1534		
A2356	C	C	C	G2143	U2047	G1970	A1889	A1806	C1636	U1535		
A2357	C	C	C	G2144	U2048	G1971	A1890	A1807	C1637	U1536		
A2358	C	C	C	G2145	U2049	G1972	A1891	A1808	C1638	U1537		
A2359	C	C	C	G2146	U2050	G1973	A1892	A1809	C1639	U1538		
A2360	C	C	C	G2147	U2051	G1974	A1893	A1810	C1640	U1539		
A2361	C	C	C	G2148	U2052	G1975	A1894	A1811	C1641	U1540		
A2362	C	C	C	G2149	U2053	G1976	A1895	A1812	C1642	U1541		
A2363	C	C	C	G2150	U2054	G1977	A1896	A1813	C1643	U1542		
A2364	C	C	C	G2151	U2055	G1978	A1897	A1814	C1644	U1543		
A2365	C	C	C	G2152	U2056	G1979	A1898	A1815	C1645	U1544		
A2366	C	C	C	G2153	U2057	G1980	A1899	A1816	C1646	U1545		
A2367	C	C	C	G2154	U2058	G1981	A1900	A1817	C1647	U1546		
A2368	C	C	C	G2155	U2059	G1982	A1901	A1818	C1648	U1547		
A2369	C	C	C	G2156	U2060	G1983	A1902	A1819	C1649	U1548		
A2370	C	C	C	G2157	U2061	G1984	A1903	A1820	C1650	U1549		
A2371	C	C	C	G2158	U2062	G1985	A1904	A1821	C1651	U1550		
A2372	C	C	C	G2159	U2063	G1986	A1905	A1822	C1652	U1551		
A2373	C	C	C	G2160	U2064	G1987	A1906	A1823	C1653	U1552		
A2374	C	C	C	G2161	U2065	G1988	A1907	A1824	C1654	U1553		
A2375	C	C	C	G2162	U2066	G1989	A1908	A1825	C1655	U1554		
A2376	C	C	C	G2163	U2067	G1990	A1909	A1826	C1656	U1555		
A2377	C	C	C	G2164	U2068	G1991	A1910	A1827	C1657	U1556		
A2378	C	C	C	G2165	U2069	G1992	A1911	A1828	C1658	U1557		
A2379	C	C	C	G2166	U2070	G1993	A1912	A1829	C1659	U1558		
A2380	C	C	C	G2167	U2071	G1994	A1913	A1830	C1660	U1559		
A2381	C	C	C	G2168	U2072	G1995	A1914	A1831	C1661	U1560		
A2382	C	C	C	G2169	U2073	G1996	A1915	A1832	C1662	U1561		
A2383	C	C	C	G2170	U2074	G1997	A1916	A1833	C1663	U1562		
A2384	C	C	C	G2171	U2075	G1998	A1917	A1834	C1664	U1563		
A2385	C	C	C	G2172	U2076	G1999	A1918	A1835	C1665	U1564		
A2386	C	C	C	G2173	U2077	G2000	A1919	A1836	C1666	U1565		
A2387	C	C	C	G2174	U2078	G2001	A1920	A1837	C1667	U1566		
A2388	C	C	C	G2175	U2079	G2002	A1921	A1838	C1668	U1567		
A2389	C	C	C	G2176	U2080	G2003	A1922	A1839	C1669	U1568		
A2390	C	C	C	G2177	U2081	G2004	A1923	A1840	C1670	U1569		
A2391	C	C	C	G2178	U2082	G2005	A1924	A1841	C1671	U1570		
A2392	C	C	C	G2179	U2083	G2006	A1925	A1842	C1672	U1571		
A2393	C											

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 2.75 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	81.3 (49.33-2.75) 81.1 (85.81-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.183 , 0.232 0.311 , 0.324	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	99124	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.55	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.57	0/1224
7	G	0.30	0/241	0.50	0/324
8	H	0.35	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.34	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.66	0/1351
12	L	0.31	0/1130	0.64	0/1509
13	M	0.34	0/1582	0.63	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.60	0/1181
16	P	0.32	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	0.35	0/1172	0.64	0/1578
19	S	0.35	0/648	0.59	0/875
20	T	0.33	0/958	0.62	0/1289
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.49	0/675
23	W	0.34	0/1219	0.61	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.58	0/781
27	1	0.40	0/438	0.63	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.37	0/65960	0.68	6/102872 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.36	0/98704	0.66	7/147591 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1
30	0	0	26
All	All	0	27

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C5'-C4'-C3'	6.12	125.79	116.00
30	0	871	G	C5'-C4'-O4'	-6.04	101.86	109.10
30	0	1504	A	C1'-O4'-C4'	-5.84	105.22	109.90
30	0	1504	A	N9-C1'-C2'	5.53	121.18	114.00
30	0	841	A	C1'-O4'-C4'	-5.34	105.63	109.90

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	22	U	Sidechain
30	0	26	U	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	80	0
2	B	2625	0	2533	110	0
3	C	1860	0	1813	73	0
4	D	1094	0	1085	56	0
5	E	1357	0	1266	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	890	0	843	23	0
7	G	240	0	231	7	0
8	H	1282	0	1292	33	0
9	I	519	0	500	24	0
10	J	1120	0	1098	36	0
11	K	994	0	1027	37	0
12	L	1118	0	1076	30	0
13	M	1558	0	1573	48	0
14	N	1445	0	1401	61	0
15	O	865	0	873	22	0
16	P	1136	0	1123	36	0
17	Q	735	0	729	20	0
18	R	1149	0	1122	33	0
19	S	641	0	605	13	0
20	T	950	0	924	21	0
21	U	410	0	364	16	0
22	V	499	0	511	16	0
23	W	1196	0	1137	58	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	41	0
26	Z	573	0	531	18	0
27	1	431	0	426	25	0
28	2	396	0	413	21	0
29	3	755	0	729	15	0
30	0	59022	0	29809	1550	0
31	9	2599	0	1325	114	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	5	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	4	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5927	0	0	235	0
38	1	55	0	0	3	0
38	2	42	0	0	3	0
38	3	63	0	0	3	0
38	9	144	0	0	10	0
38	A	118	0	0	7	0
38	B	144	0	0	11	0
38	C	179	0	0	19	0
38	D	46	0	0	4	0
38	E	40	0	0	2	0
38	F	27	0	0	1	0
38	G	19	0	0	0	0
38	H	68	0	0	5	0
38	I	5	0	0	1	0
38	J	55	0	0	2	0
38	K	52	0	0	2	0
38	L	84	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	127	0	0	5	0
38	N	63	0	0	4	0
38	O	40	0	0	2	0
38	P	61	0	0	1	0
38	Q	43	0	0	1	0
38	R	84	0	0	5	0
38	S	33	0	0	2	0
38	T	33	0	0	2	0
38	U	28	0	0	2	0
38	V	14	0	0	1	0
38	W	67	0	0	5	0
38	X	30	0	0	0	0
38	Y	100	0	0	10	0
38	Z	32	0	0	0	0
All	All	99124	0	59911	2446	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 16.

The worst 5 of 2446 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)
14:N:37:ARG:NH1	31:9:6:C:H5''	1.60	1.15
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.11
13:M:171:ARG:HD3	30:0:156:C:H5''	1.32	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.12	1.11
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11

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	
1	A	235/240 (98%)	211 (90%)	22 (9%)	2 (1%)	17	31
2	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	10	18
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	110 (82%)	22 (16%)	2 (2%)	10	18
5	E	170/178 (96%)	160 (94%)	9 (5%)	1 (1%)	25	42
6	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	16
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	141 (90%)	14 (9%)	1 (1%)	25	42
9	I	68/162 (42%)	53 (78%)	13 (19%)	2 (3%)	4	6
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	22	39
11	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
12	L	141/165 (86%)	125 (89%)	13 (9%)	3 (2%)	7	12
13	M	192/196 (98%)	181 (94%)	10 (5%)	1 (0%)	29	47
14	N	184/187 (98%)	164 (89%)	16 (9%)	4 (2%)	6	11
15	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
16	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	25
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
20	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17	31
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	9	16
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	5	9
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3432 (93%)	244 (7%)	29 (1%)	19	34

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
8	H	19	ARG
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP

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	
1	A	179/182 (98%)	166 (93%)	13 (7%)	14	25
2	B	282/283 (100%)	264 (94%)	18 (6%)	17	31
3	C	193/193 (100%)	179 (93%)	14 (7%)	14	25
4	D	117/148 (79%)	113 (97%)	4 (3%)	37	58
5	E	152/156 (97%)	150 (99%)	2 (1%)	69	81
6	F	93/94 (99%)	92 (99%)	1 (1%)	73	84
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	24
8	H	134/145 (92%)	129 (96%)	5 (4%)	34	54
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	112 (95%)	6 (5%)	24	41
11	K	106/106 (100%)	105 (99%)	1 (1%)	78	87
12	L	113/127 (89%)	107 (95%)	6 (5%)	22	38
13	M	158/160 (99%)	152 (96%)	6 (4%)	33	53
14	N	149/150 (99%)	142 (95%)	7 (5%)	26	45
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	110 (97%)	3 (3%)	44	65
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	41
18	R	117/122 (96%)	111 (95%)	6 (5%)	24	41
19	S	71/74 (96%)	70 (99%)	1 (1%)	67	79
20	T	105/106 (99%)	98 (93%)	7 (7%)	16	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	50 (98%)	1 (2%)	55	72
23	W	130/130 (100%)	126 (97%)	4 (3%)	40	60
24	X	66/74 (89%)	62 (94%)	4 (6%)	18	33
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	58
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	76
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	70
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
29	3	79/79 (100%)	76 (96%)	3 (4%)	33	53
All	All	3095/3646 (85%)	2970 (96%)	125 (4%)	31	51

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	87	LYS
12	L	104	ASP
25	Y	95	THR
8	H	157	TYR
10	J	93	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	137	ASN
16	P	73	HIS
28	2	18	ASN
13	M	143	ASN
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	18 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	248 (8%)	19 (0%)

5 of 248 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1506	U
30	0	2718	C
30	0	1237	U
30	0	2726	U

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

5 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	$\# Z > 2$
30	1MA	0	628	30,35	15,25,26	0.74	0	15,37,40	1.34	1 (6%)
30	OMU	0	2587	30	14,22,23	0.98	1 (7%)	14,31,34	1.17	1 (7%)
30	OMG	0	2588	30	18,26,27	1.10	2 (11%)	20,38,41	2.57	5 (25%)
30	UR3	0	2619	30	14,22,23	0.72	0	15,32,35	0.60	0
30	PSU	0	2621	30	17,21,22	1.70	3 (17%)	20,30,33	5.46	4 (20%)

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	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.35	1.47	1.52
30	0	2588	OMG	C6-N1	3.51	1.39	1.33
30	0	2621	PSU	C4-N3	2.92	1.38	1.33
30	0	2621	PSU	C2-N1	2.65	1.43	1.38
30	0	2587	OMU	C4-N3	2.64	1.37	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.55	114.48	128.43
30	0	2621	PSU	C4-N3-C2	14.23	127.16	115.14
30	0	2588	OMG	C5-C6-N1	-8.54	111.74	123.43
30	0	2621	PSU	C5-C4-N3	-8.09	114.94	125.36
30	0	2588	OMG	C6-N1-C2	5.80	125.14	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.