



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:20 AM UTC

PDB ID : 1K8A / pdb\_00001k8a  
Title : Co-crystal structure of Carbomycin A bound to the 50S ribosomal subunit of *Haloarcula marismortui*  
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.  
Deposited on : 2001-10-23  
Resolution : 3.00 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

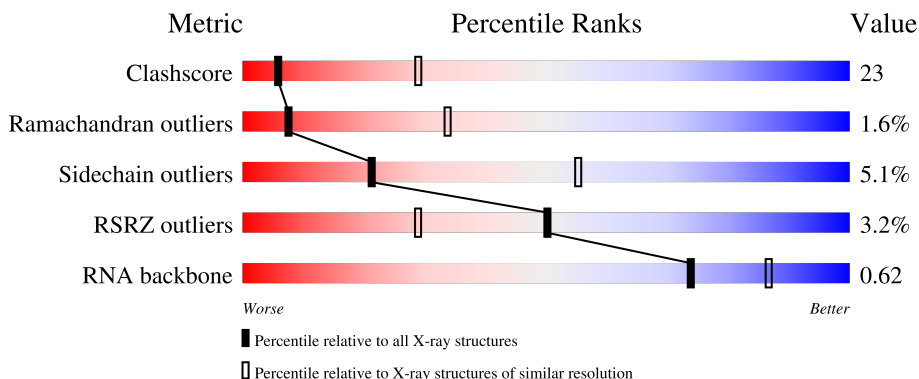
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



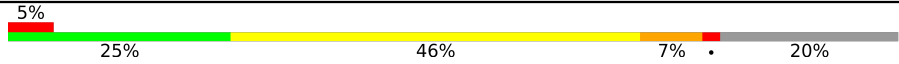

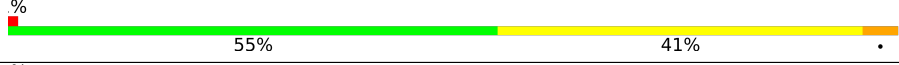
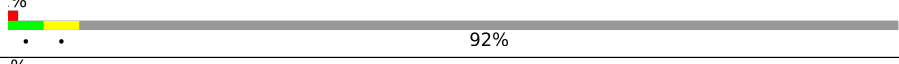
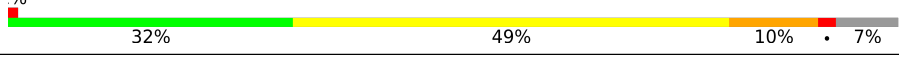
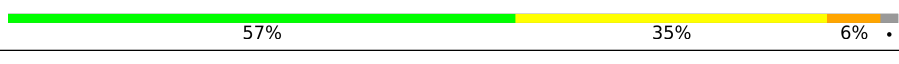
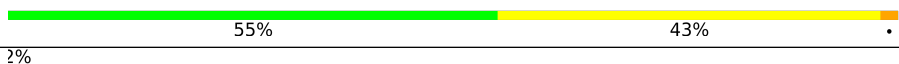
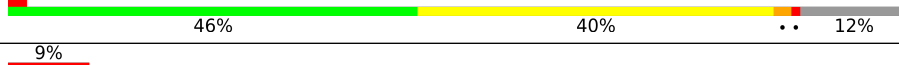
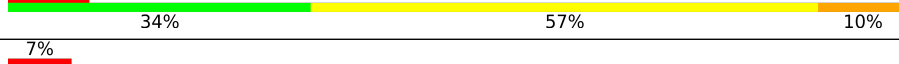
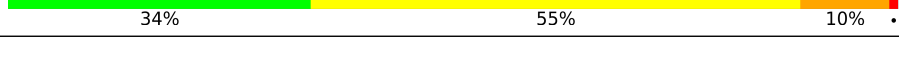

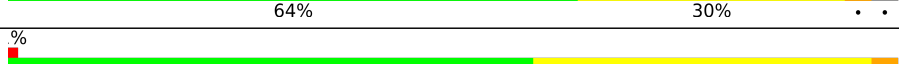
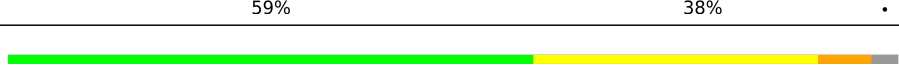
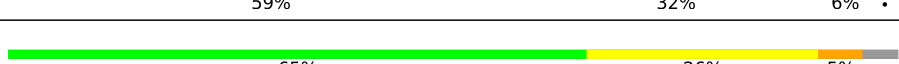

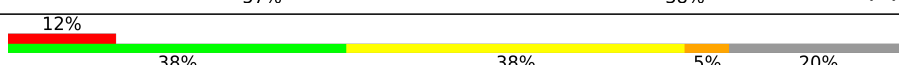


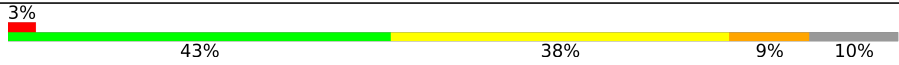
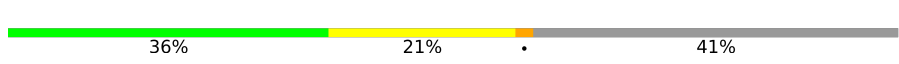

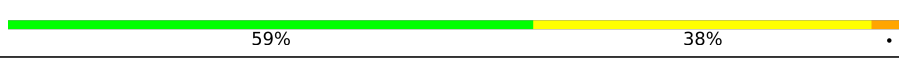
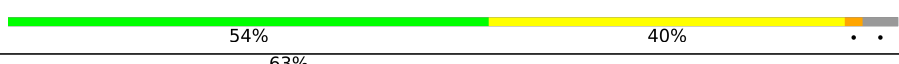


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 46% 39% 8% 6%</p>
2	B	122	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 41%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 41% 45% 11% .</p>
3	C	239	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 43%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 48% 43% 8% .</p>
4	D	337	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">47% 46% 6% .</p>
5	E	246	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">47% 46% 7%</p>

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
33	NA	B	8383	-	-	-	X
34	CL	A	8523	-	-	X	-

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 98560 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	1754	1072	352	325	5	0	0	0

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	246	1858	1131	344	382	1	0	0	0

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	119	885	552	141	191	1	0	0	0

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	156	1215	766	233	212	4	0	0	0

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	142	1119	696	199	221	3	0	0	0

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	132	993	609	189	191	4	0	0	0

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	145	1114	668	222	224		0	0	0

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	194	1605	988	346	266	5	0	0	0

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	186	1444	895	262	285	2	0	0	0

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	P	115	864	529	161	174	0	0	0

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	Q	143	1133	680	230	223	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	95	734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	U	119	949	568	180	201	0	0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	X	154	1195	737	209	243	6	0	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Z	142	1130	686	228	216		0	0	0

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	1	73	563	359	111	86	7	0	0	0

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	2	56	430	258	86	82	4	0	0	0

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	3	46	393	238	86	68	1	0	0	0

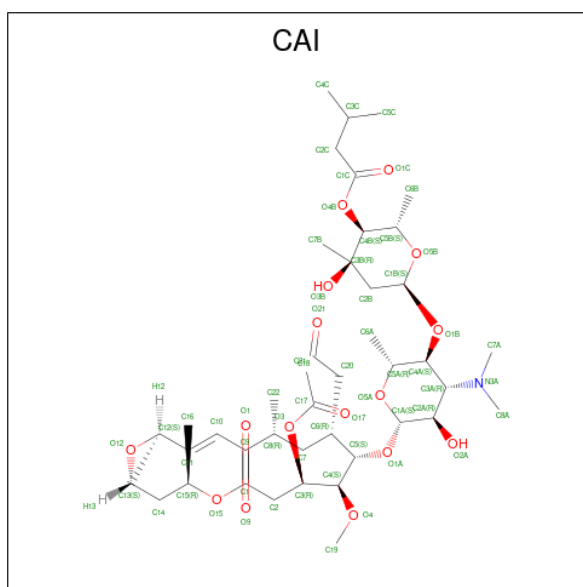
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	4	92	755	458	153	137	7	0	0	0

- Molecule 31 is CARBOMYCIN A (CCD ID: CAI) (formula: C<sub>42</sub>H<sub>67</sub>NO<sub>16</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
31	A	1	59	42	1	16	0	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
32	A	111	111	111	0	0
32	B	1	1	1	0	0
32	C	2	2	2	0	0
32	D	1	1	1	0	0
32	L	1	1	1	0	0
32	U	1	1	1	0	0
32	Z	1	1	1	0	0
32	4	1	1	1	0	0

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	69	Total Na 69 69	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	2	Total Na 2 2	0	0
33	R	1	Total Na 1 1	0	0
33	S	1	Total Na 1 1	0	0
33	T	1	Total Na 1 1	0	0
33	U	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	10	Total Cl 10 10	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Cl 1 1	0	0
34	S	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	4	1	Total Cl 1 1	0	0

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	3	Total K 3 3	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5858	Total O 5858 5858	0	0
37	B	141	Total O 141 141	0	0
37	C	138	Total O 138 138	0	0
37	D	154	Total O 154 154	0	0
37	E	177	Total O 177 177	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	F	49	Total O 49 49	0	0
37	G	44	Total O 44 44	0	0
37	H	26	Total O 26 26	0	0
37	I	21	Total O 21 21	0	0
37	J	79	Total O 79 79	0	0
37	K	53	Total O 53 53	0	0
37	L	59	Total O 59 59	0	0
37	M	87	Total O 87 87	0	0
37	N	130	Total O 130 130	0	0
37	O	69	Total O 69 69	0	0
37	P	44	Total O 44 44	0	0
37	Q	68	Total O 68 68	0	0
37	R	51	Total O 51 51	0	0
37	S	81	Total O 81 81	0	0
37	T	37	Total O 37 37	0	0
37	U	37	Total O 37 37	0	0
37	V	28	Total O 28 28	0	0
37	W	14	Total O 14 14	0	0
37	X	69	Total O 69 69	0	0
37	Y	28	Total O 28 28	0	0
37	Z	100	Total O 100 100	0	0

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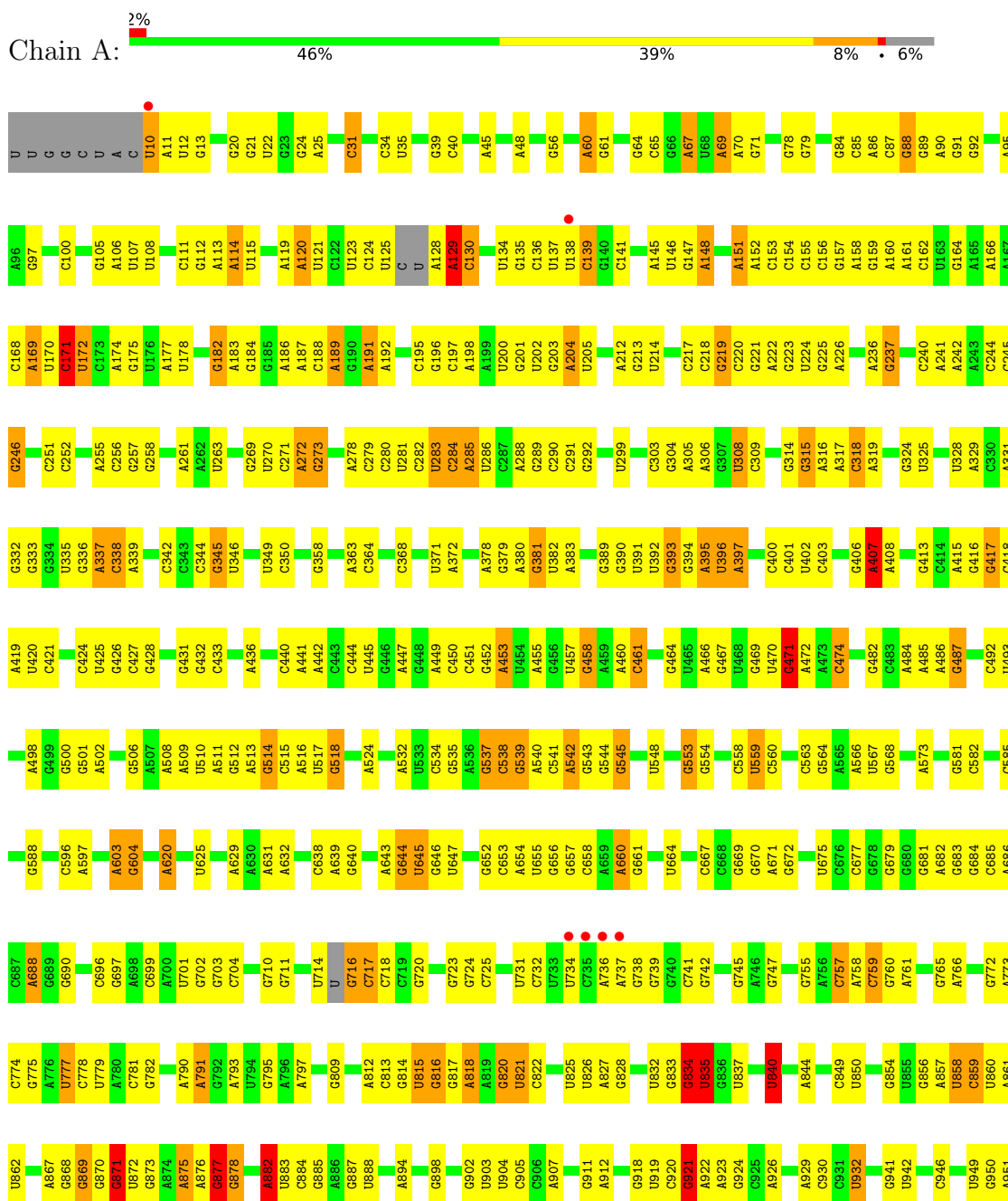
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
37	1	41	Total O 41 41	0	0
37	2	58	Total O 58 58	0	0
37	3	41	Total O 41 41	0	0
37	4	68	Total O 68 68	0	0

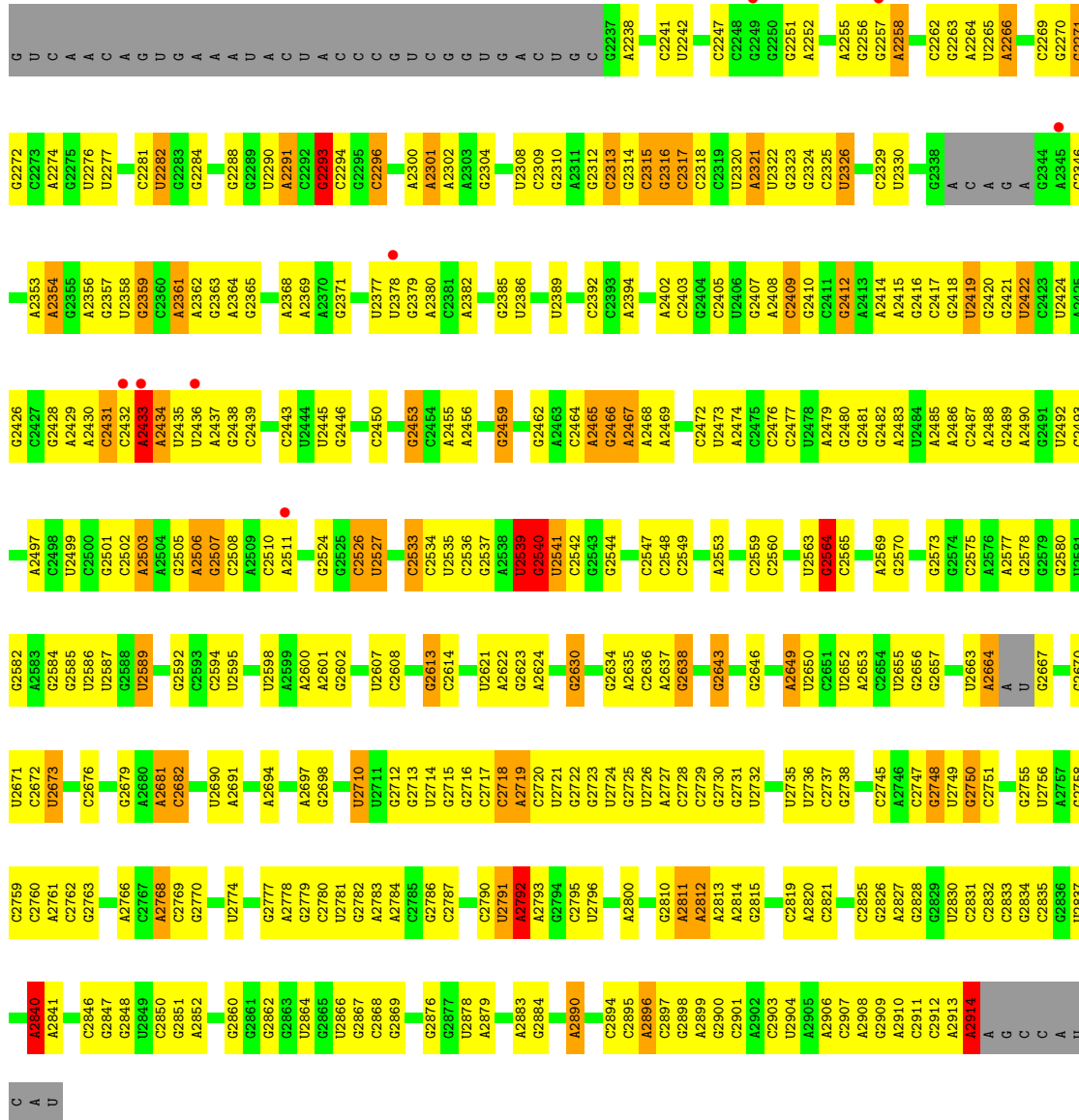
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

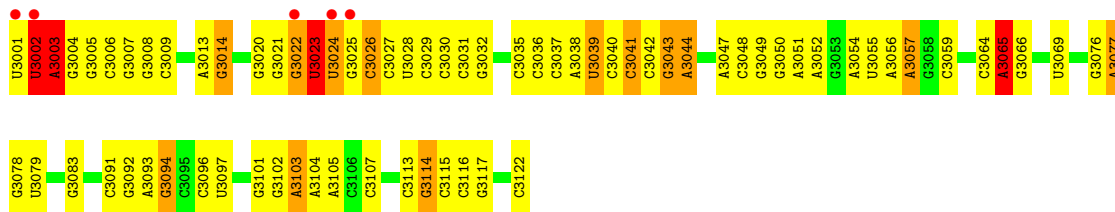
#### • Molecule 1: 23S RRNA



C	G2072	U1980	A1910	G1826	C1731	U1654	C1574	G1484	A1393	G1209	U1130	G1027	G982
G	G2073	A1981	C1911	G1827	A1752	G1655	A1580	A1485	C1594	G1210	G1131	U1028	G983
C	A2074	C1982	A1912	G1828	A1733	A1656	A1580	A1486	G1398	G1211	A1132	U1029	U984
C		C1983		A1829	C1734	A1657	U1583	A1487	A1399	C1212	A1133	U1041	G958
G	G2079	U1992	G1917	C1830	A1735	A1658	G1586	A1488	G1406	C1213	G1134	U1042	C959
U	A2081	C1993	U1918	U1833	A1736	A1659	U1587	A1489	A1307	C1214	G1135	C1043	G960
U	G2082	A1994	A1919	C1834	A1737	G1660	U1588	A1490	U1407	G1215	U1136	C1044	A961
G	A2083	G1995	C1920	U1835	U1741	A1661	G1589	C1495	U1408	G1216	G1137	C1045	C962
C	C2084	U1996	A1922	A1836	A1742	G1666	G1589	G1496	G1409	G1217	U1137	U1045	A962
G	A2085	A1997	G1923	G1837	G1743	A1667	C1592	G1497	U1414	U1218	G1151	G1050	C963
A		G1998	A1924	A1839	A1744	U1668	G1592		A1415	U1219	G1151	G1051	U970
A	C2088	A1999	G1925	A1840	G1751	U1668	C1593	U1500	G1415	U1220	G1152	C1052	U
C	A2089	G2000	G1926	C1841	G1752	G1670	C1594	A1501	G1419	G1221	G1153	G1053	U
A	G2090	G2001			C1753	U1671	U1596	U1502	U1419	C1229	A1161	G1054	U
A	G2091	C2002	A1931	A1845	A1754	A1663	U1596	A1503	U1419		G1162	G1055	U
G	G2092	U2003	G1932	A1846	A1755	A1663	U1597	U1504	A1422	U1234	G1163	U1056	C
A	G2093	U2004	G1933	A1847	A1756	A1663	A1597	A1504	C1423	U1235	U1164	A1057	C
G	G2094	G2005	A1934	U1850	A1759	A1663	A1598	U1505	U1424	U1236	G1165	A1058	C
U	A2095	C1985	C1985	G1851	U1766	C1660	G1601	U1506	A1424	U1237	A1166	C1059	C
A	A2096	U2008	C1986	G1851	U1767	C1661	C1602	G1512	G1430	U1238	A1167	C1060	C
G	A2100	G2009	U1937	C1856	A1767	A1681	A1603	C1513	C1431	G1239	C1168	U1064	U
G	A2101	G1938	C1856	A1857	C1768	A1682	G1604	U1517	U1432	G1240	U1169	U1065	U
G	G2102	U1939	A1857	U1860	C1769	A1683	G1605	U1522	G1433	G1241	U1170	U1066	C
A	A2103	C1940	U1770	C1861	U1771	A1684	A1606	A1525	A1434	U1242	U1171	U1066	C
A	A2104	A1941	U1772	C1861	U1772	C1686	A1607	A1526	U1435	G1243	G1172	A1067	A
C	C2105	C1942	C1772	C1862	G1773	C1687	G1608	A1527	U1440	U1244	A1173	G1068	G
A	C2106	A1943	G1774	C1863	G1774	C1688	G1610	A1528	G1441	C1245	A1174	G1069	A
U	U2107	C1946	G1774	C1863	G1774	C1688	G1610	A1529	G1442	U1246	G1175	G1072	G
U	A2108	C1946	G1777	G1868	U1777	C1692	C1613	A1529	U1442	U1249	G1176	G1072	G
C	U2109	G1947	U1778	A1869	A1778	G1697	G1614	A1529	G1443	U1250	A1177	G1076	A
A	G2110	C1951	U1779	C1870	A1779	U1698	G1618	G1529	G1443	C1251	U1180	G1076	U
A	A2111	U	U1780	C1871	U1780	C1699	U1618	U1530	G1444	G1252	A1181	A1079	C
C	G2112	A	G1785	C1872	C1786	C1700	U1621	U1531	G1445	G1253	C1182	C1080	C
G	G2113	C	C1786	C1873	C1787	A1701	G1622	U1531	G1445	G1254	C1183	C1081	C
G	C2114	C	U1788	U1874	U1788	U1702	C1622	U1531	U1446	C1256	C1183	C1081	C
U	U2115	U	U1789	U1875	U1789	U1702	C1622	U1531	U1447	A1261	C1184	C1084	A
A	C2035	A	G1789	C1877	G1789	G1706	C1622	U1531	U1447	C1262	U1185	G1084	A
C	C2036	U	G1789	C1878	G1789	G1707	U1625	U1543	C1451	C1263	U1186	G1085	A
C	C2037	G	U1791	U1879	C1708	C1708	A1626	U1544	C1451	U1264	U1187	A1086	C
C	A2038	U	A1791	U1879	C1709	C1709	G1627	C1545	C1456	U1265	A1188	G1087	C
C	A2039	U	C1798	C1882	A1710	A1710	A1630	G1546	U1457	U1266	A1189	A1088	C
C	C2040	C	U1804	C1882	A1711	A1711	A1630	G1546	A1458	C1267	G1190	A1088	C
G	G2044	U1964	A1805	A1886	A1712	A1712	A1630	C1549	U1461	C1268	A1191	A1088	C
G	G2045	C1965	G1805	U1887	G1713	G1713	C1633	A1850	C1462	G1269	A1192	G1099	A1006
A	G2046	U1966	C1810	U1890	A1717	A1717	U1636	C1551	C1463	U1270	A1193	G1099	A1007
A	C2047	U1966	C1811	U1890	A1718	A1718	A1637	G1555	U1464	U1271	A1193	C1008	A1007
G	U2128	C	A1815	C1894	G1719	G1719	A1637	G1555	U1464	C1273	A1194	G1110	A1014
G	U2133	A1969	C1816	A1896	C1720	C1720	A1641	U1589	A1470	U1274	A1194	G1110	C1015
G	G2053	G1970	C1817	A1896	C1721	C1721	A1642	U	A1471	A1274	A1194	G1110	U1016
G	A2054	U1971	C1818	A1896	C1722	C1722	C1643	A1589	A1471	C1275	A1199	U1116	C1015
G	A2055	U1972	C1819	A1896	C1723	C1723	C1644	U	A1472	U1276	A1199	A1117	C1015
C	A	A1973	C1819	G1902	G1723	C1643	C1644	C1562	C1473	C1277	A1200	G1118	C1015
C	C	U1903	A1821	U1903	C1724	C1644	U1645	C1562	C1474	A1278	A1201	G1119	A1020
A	U2063	U1974	A1822	U1904	C1725	U1645	U1651	C1564	C1477	U1279	G1204	U1120	G1021
C	C2065	G1976	A1822	U1904	C1725	U1645	U1651	C1564	C1477	U1288	A1123	G1123	A1022
C	U	U1977	G1823	U1907	G1728	C1652	C1652	C1565	U1478	C1289	U1205	G1023	G1023
C	G	A1978	C1824	U1908	G1729	C1652	C1652	C1565	U1478	C1289	U1206	G1024	G1024
A	U	G1979	U1825	A1909	G1730	A1653	A1653	A1572	C1483	A1294	U1207	C1128	C1026

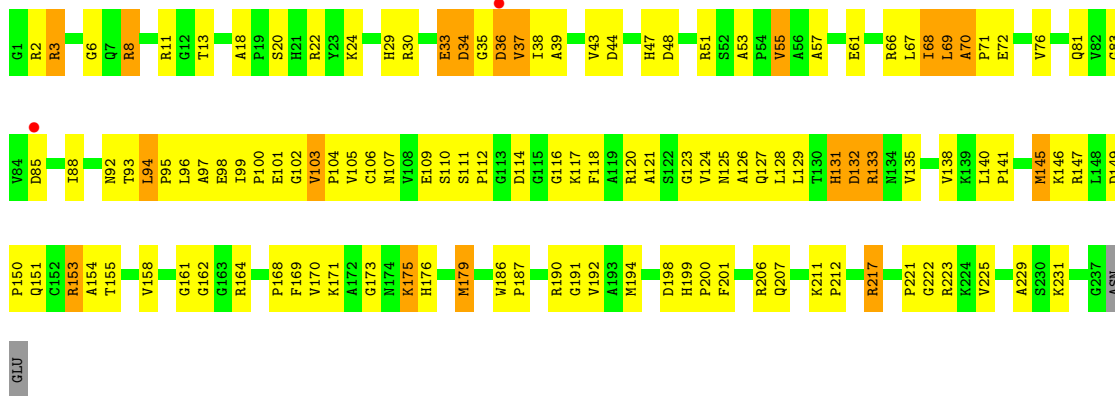


• Molecule 2: 5S RRNA

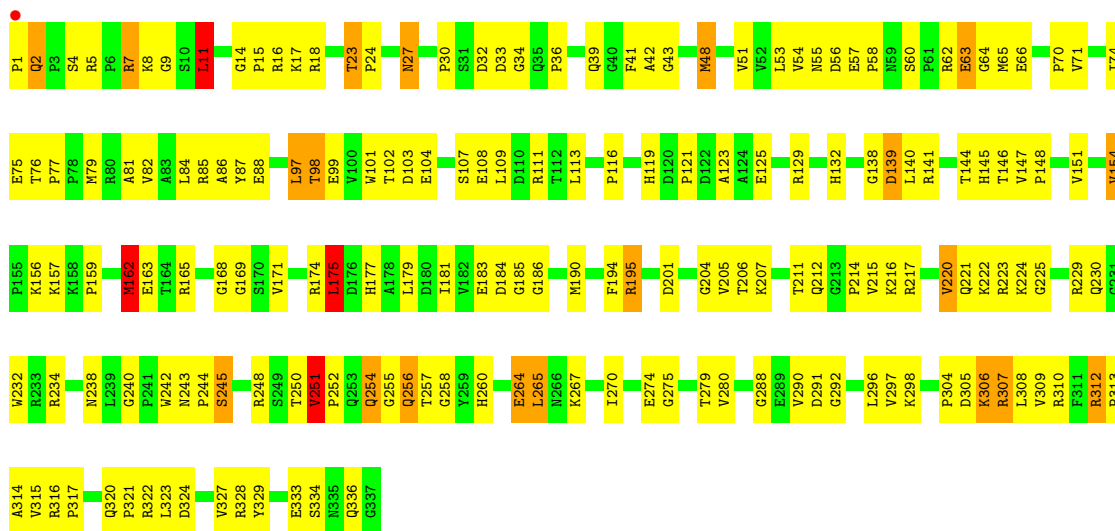


• Molecule 3: RIBOSOMAL PROTEIN L2

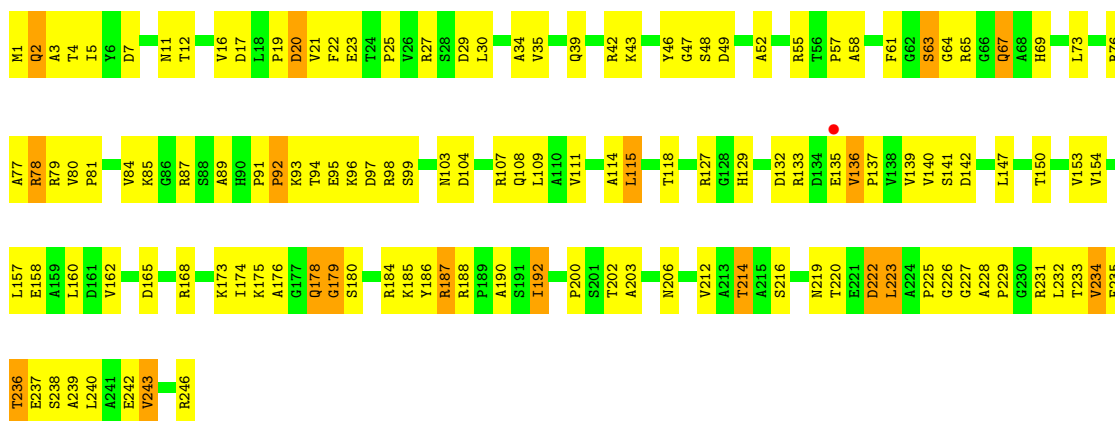




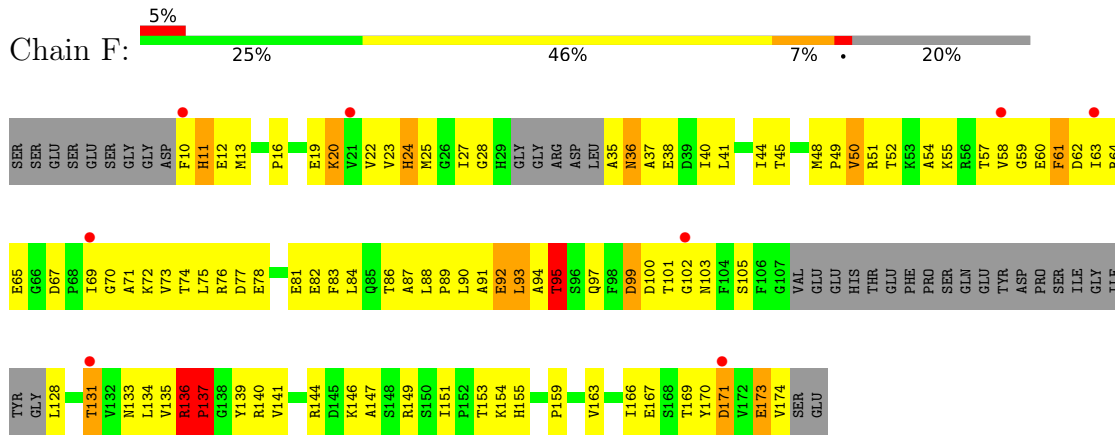
• Molecule 4: RIBOSOMAL PROTEIN L3



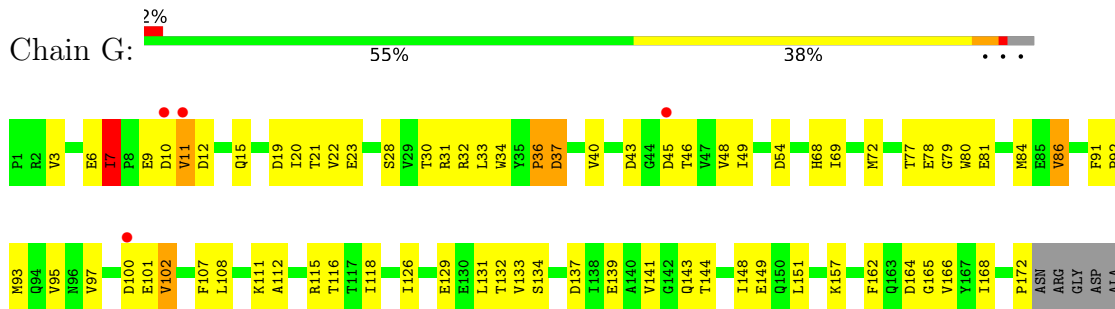
• Molecule 5: RIBOSOMAL PROTEIN L4



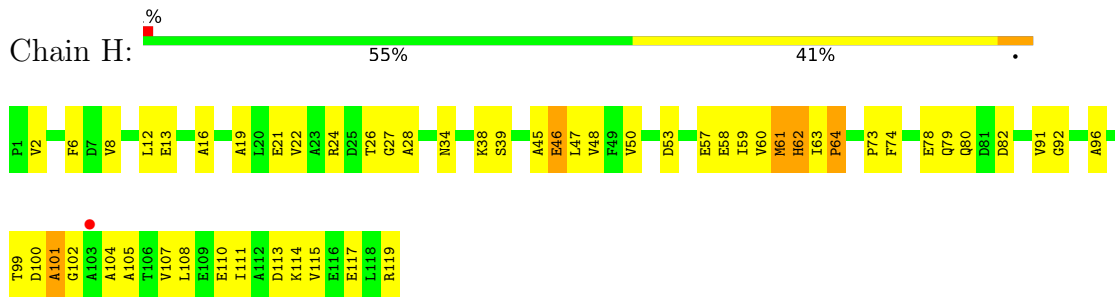
• Molecule 6: RIBOSOMAL PROTEIN L5



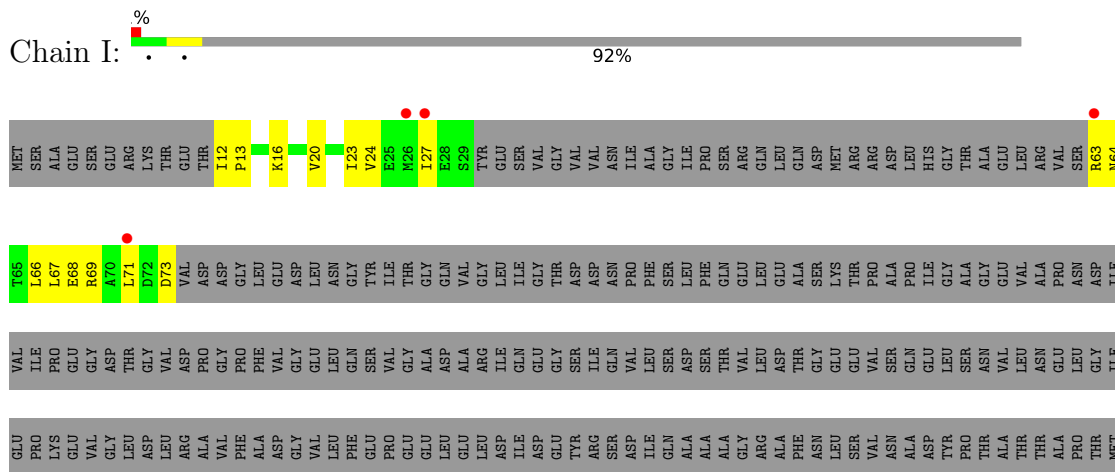
• Molecule 7: RIBOSOMAL PROTEIN L6



• Molecule 8: RIBOSOMAL PROTEIN L7AE



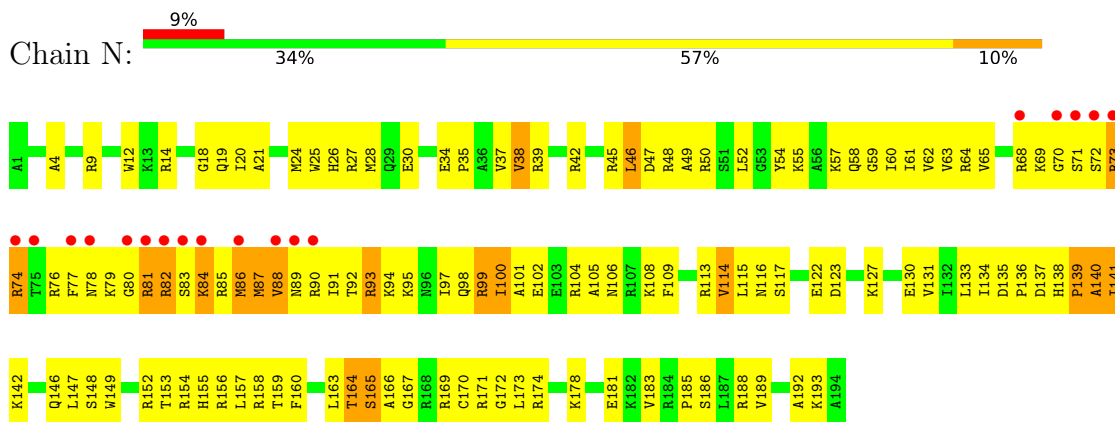
• Molecule 9: RIBOSOMAL PROTEIN L10



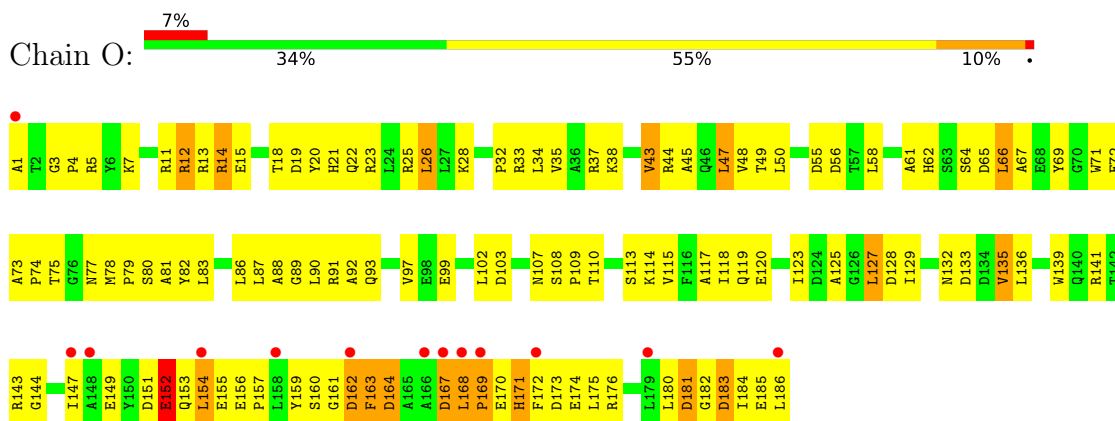


ASP  
ALA  
ASP  
ALA  
ASP  
GLU  
GLU

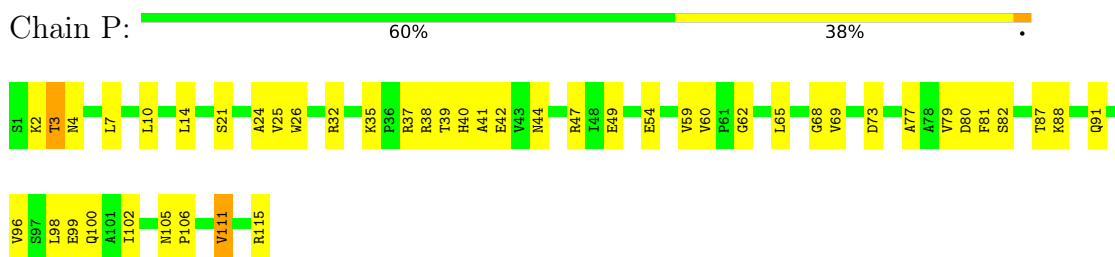
● Molecule 14: RIBOSOMAL PROTEIN L15E



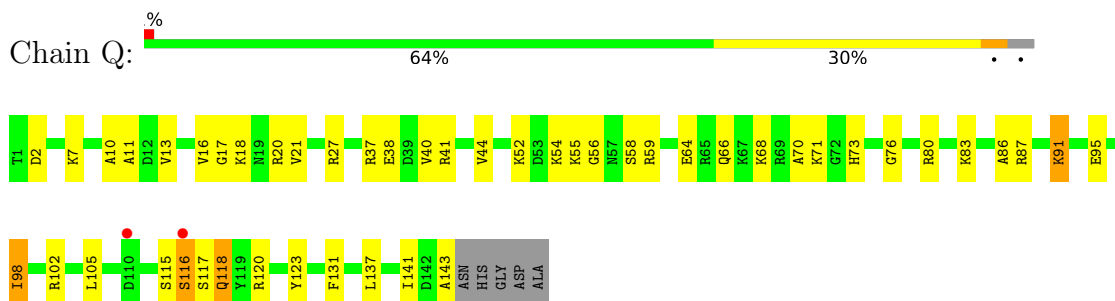
● Molecule 15: RIBOSOMAL PROTEIN L18



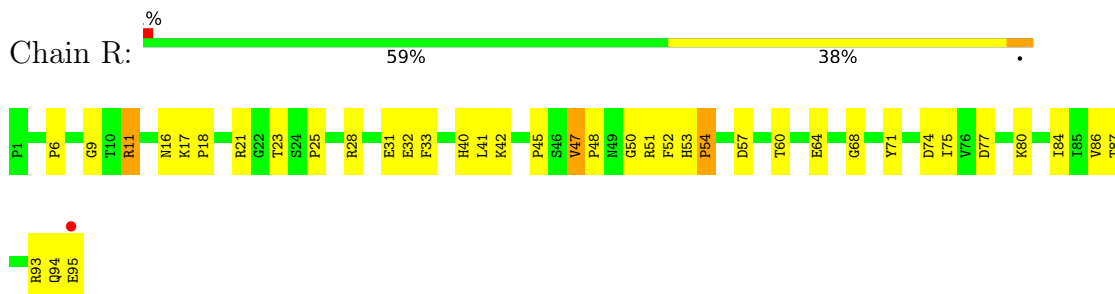
● Molecule 16: RIBOSOMAL PROTEIN L18E



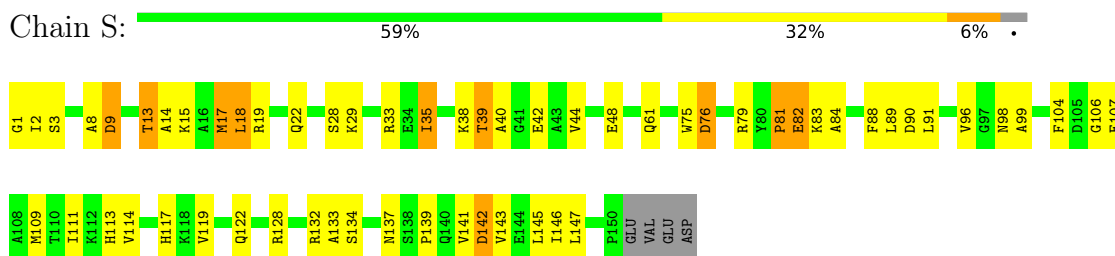
● Molecule 17: RIBOSOMAL PROTEIN L19E



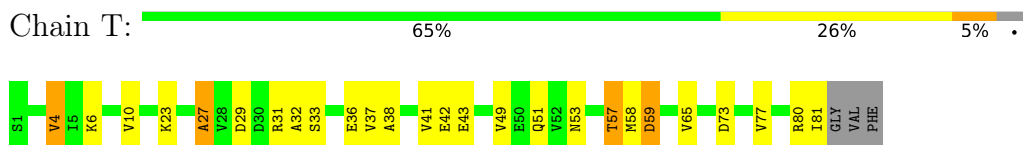
- Molecule 18: RIBOSOMAL PROTEIN L21E



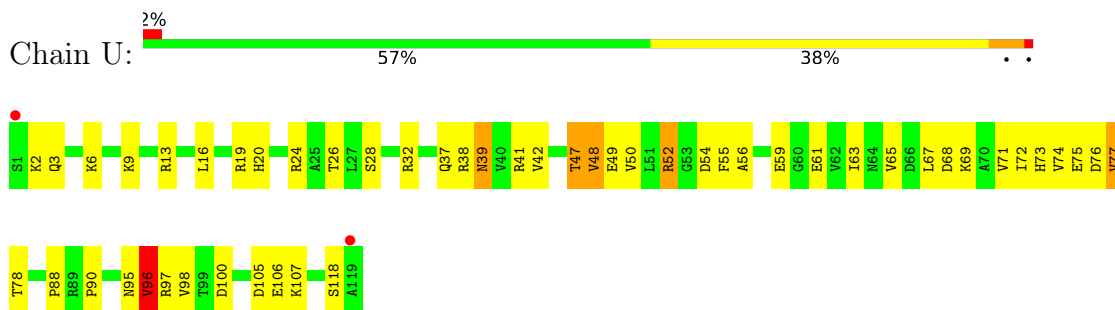
- Molecule 19: RIBOSOMAL PROTEIN L22



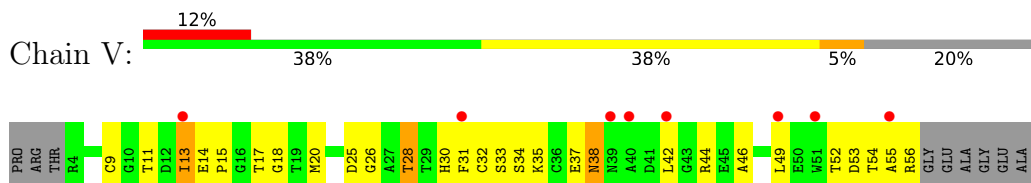
- Molecule 20: RIBOSOMAL PROTEIN L23



- Molecule 21: RIBOSOMAL PROTEIN L24

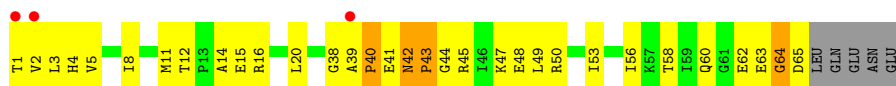


- Molecule 22: RIBOSOMAL PROTEIN L24E



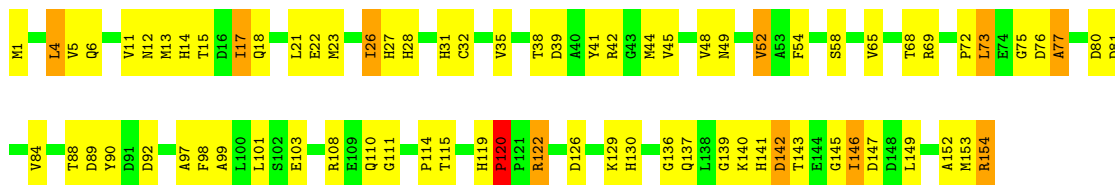
- Molecule 23: RIBOSOMAL PROTEIN L29





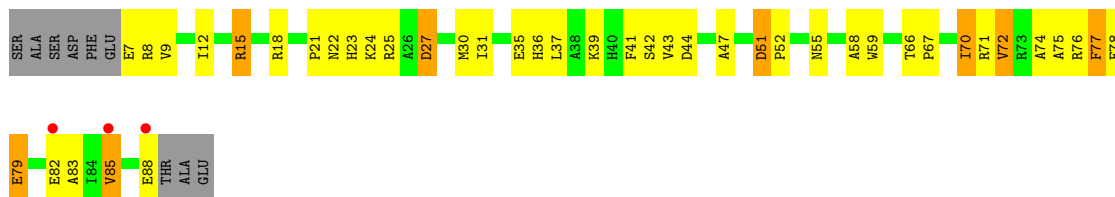
- Molecule 24: RIBOSOMAL PROTEIN L30

Chain X: 51% 42% 6%



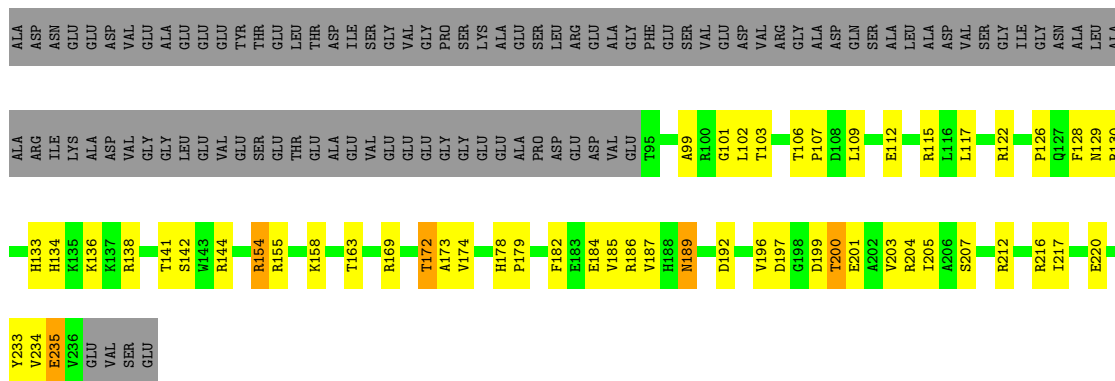
- Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y: 3% 43% 38% 9% 10%



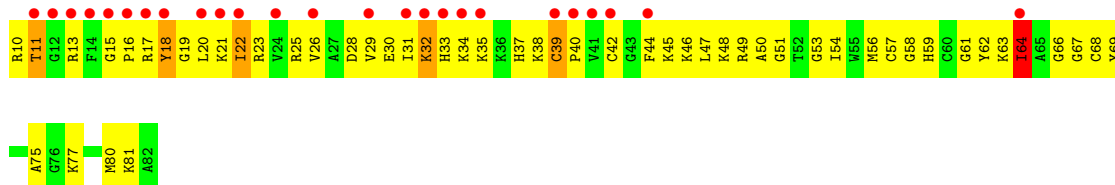
- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z: 36% 21% 41%



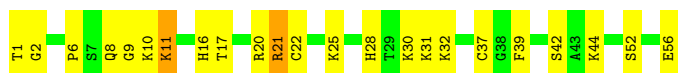
- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1: 34% 27% 64% 7%



- Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2:  59% 38%




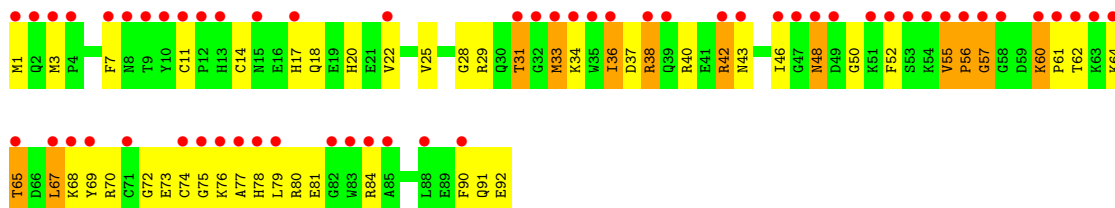
● Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 3:  54% 40%



● Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4:  45% 63% 42% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.00) 93.0 (20.00-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.96Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.265 0.215 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	98560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: K, CL, CD, MG, CAI, NA

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	0.54	5/66076 (0.0%)	0.78	70/103052 (0.1%)
2	B	0.56	0/2905	0.85	9/4528 (0.2%)
3	C	0.65	1/1787 (0.1%)	1.18	12/2409 (0.5%)
4	D	0.66	1/2689 (0.0%)	1.15	19/3652 (0.5%)
5	E	0.70	0/1883	1.15	15/2551 (0.6%)
6	F	0.51	0/1111	1.00	5/1498 (0.3%)
7	G	0.63	0/1382	0.99	7/1880 (0.4%)
8	H	0.56	0/896	0.98	2/1219 (0.2%)
9	I	0.54	0/241	0.81	0/324
10	J	0.68	0/1246	1.36	18/1686 (1.1%)
11	K	0.68	0/1135	1.03	3/1530 (0.2%)
12	L	0.64	0/1003	1.14	10/1351 (0.7%)
13	M	0.59	0/1126	1.11	5/1504 (0.3%)
14	N	0.87	1/1633 (0.1%)	1.27	13/2180 (0.6%)
15	O	0.58	0/1473	1.19	15/1999 (0.8%)
16	P	0.68	0/873	1.07	4/1181 (0.3%)
17	Q	0.61	0/1143	1.00	3/1521 (0.2%)
18	R	0.65	0/748	1.18	6/1005 (0.6%)
19	S	0.76	1/1172 (0.1%)	1.15	10/1578 (0.6%)
20	T	0.55	0/648	1.01	5/875 (0.6%)
21	U	0.57	0/957	1.11	6/1289 (0.5%)
22	V	1.00	1/417 (0.2%)	1.17	2/562 (0.4%)
23	W	0.57	0/502	1.04	3/675 (0.4%)
24	X	0.76	0/1218	1.09	7/1655 (0.4%)
25	Y	0.68	0/664	1.07	4/895 (0.4%)
26	Z	0.69	0/1146	1.07	2/1536 (0.1%)
27	1	1.10	2/575 (0.3%)	1.25	7/763 (0.9%)
28	2	0.70	0/437	1.12	2/578 (0.3%)
29	3	0.53	0/398	0.83	0/527
30	4	1.32	5/771 (0.6%)	1.13	6/1024 (0.6%)
All	All	0.59	17/98255 (0.0%)	0.89	270/147027 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	165
2	B	0	3
All	All	1	168

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	145	MET	SD-CE	7.54	1.98	1.79
1	A	2539	U	C5'-C4'	7.30	1.62	1.51
30	4	1	MET	SD-CE	7.01	1.97	1.79
1	A	2540	G	O5'-C5'	6.89	1.52	1.42
30	4	33	MET	SD-CE	6.64	1.96	1.79

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.64	64.07	108.00
1	A	1164	U	OP2-P-O3'	-14.30	65.11	108.00
1	A	1563	G	C2'-C3'-O3'	13.46	129.69	109.50
10	J	141	ASN	N-CA-C	-12.89	97.65	113.50
15	O	135	VAL	N-CA-C	-12.34	101.00	113.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 168 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	U	Sidechain
1	A	162	C	Sidechain
1	A	170	U	Sidechain
1	A	22	U	Sidechain
1	A	48	A	Sidechain

## 5.2 Too-close contacts [i](#)

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	59017	0	29799	1357	0
2	B	2600	0	1326	83	0
3	C	1754	0	1763	132	0
4	D	2624	0	2533	200	0
5	E	1858	0	1816	155	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	90	0
8	H	885	0	854	68	0
9	I	240	0	231	21	0
10	J	1215	0	1215	170	0
11	K	1119	0	1098	76	0
12	L	993	0	1027	70	0
13	M	1114	0	1072	80	0
14	N	1605	0	1676	203	0
15	O	1444	0	1401	151	0
16	P	864	0	873	46	0
17	Q	1133	0	1127	62	0
18	R	734	0	728	29	0
19	S	1149	0	1122	66	0
20	T	641	0	605	32	0
21	U	949	0	923	58	0
22	V	410	0	366	40	0
23	W	499	0	511	31	0
24	X	1195	0	1137	101	0
25	Y	654	0	653	49	0
26	Z	1130	0	1133	66	0
27	1	563	0	600	79	0
28	2	430	0	426	26	0
29	3	393	0	406	30	0
30	4	755	0	731	52	0
31	A	59	0	63	4	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	69	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	4	1	0	0	0	0
34	A	10	0	0	3	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	3	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	41	0	0	16	0
37	2	58	0	0	5	0
37	3	41	0	0	8	0
37	4	68	0	0	11	0
37	A	5858	0	0	321	0
37	B	141	0	0	15	0
37	C	138	0	0	14	0
37	D	154	0	0	33	0
37	E	177	0	0	45	0
37	F	49	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	44	0	0	13	0
37	H	26	0	0	12	0
37	I	21	0	0	4	0
37	J	79	0	0	23	0
37	K	53	0	0	5	0
37	L	59	0	0	12	0
37	M	87	0	0	22	0
37	N	130	0	0	29	0
37	O	69	0	0	23	0
37	P	44	0	0	11	0
37	Q	68	0	0	7	0
37	R	51	0	0	5	0
37	S	81	0	0	5	0
37	T	37	0	0	8	0
37	U	37	0	0	5	0
37	V	28	0	0	7	0
37	W	14	0	0	3	0
37	X	69	0	0	7	0
37	Y	28	0	0	10	0
37	Z	100	0	0	18	0
All	All	98560	0	59566	3455	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 23.

The worst 5 of 3455 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)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.61	1.15
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.46	1.15
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.24	1.14
5:E:236:THR:HG22	5:E:239:ALA:H	1.06	1.13
1:A:1160:G:H5'	1:A:1161:A:H5'	1.30	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	
3	C	235/239 (98%)	207 (88%)	25 (11%)	3 (1%)	9	38
4	D	335/337 (99%)	303 (90%)	24 (7%)	8 (2%)	4	24
5	E	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	0	3
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	4	23
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	14 (9%)	6 (4%)	2	14
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	3	20
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	8	35
13	M	141/164 (86%)	118 (84%)	21 (15%)	2 (1%)	9	36
14	N	192/194 (99%)	170 (88%)	20 (10%)	2 (1%)	12	45
15	O	184/186 (99%)	163 (89%)	15 (8%)	6 (3%)	3	17
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	18	53
18	R	93/95 (98%)	84 (90%)	8 (9%)	1 (1%)	11	43
19	S	148/154 (96%)	138 (93%)	9 (6%)	1 (1%)	18	53
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	18
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	53
25	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	4	23
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	62 (87%)	8 (11%)	1 (1%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3295 (91%)	279 (8%)	59 (2%)	7	34

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU

### 5.3.2 Protein sidechains [i](#)

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	C	179/181 (99%)	168 (94%)	11 (6%)	17	49
4	D	282/282 (100%)	263 (93%)	19 (7%)	15	46
5	E	193/193 (100%)	178 (92%)	15 (8%)	11	39
6	F	117/147 (80%)	108 (92%)	9 (8%)	12	40
7	G	152/155 (98%)	147 (97%)	5 (3%)	33	67
8	H	92/92 (100%)	91 (99%)	1 (1%)	65	83
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	109 (89%)	13 (11%)	6	26
11	K	118/121 (98%)	110 (93%)	8 (7%)	14	45
12	L	106/106 (100%)	103 (97%)	3 (3%)	38	70
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	71
14	N	166/166 (100%)	158 (95%)	8 (5%)	23	57
15	O	149/149 (100%)	141 (95%)	8 (5%)	20	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	90 (97%)	3 (3%)	34	67
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	71
18	R	79/79 (100%)	74 (94%)	5 (6%)	16	48
19	S	117/121 (97%)	114 (97%)	3 (3%)	40	72
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
21	U	105/105 (100%)	101 (96%)	4 (4%)	29	63
22	V	44/52 (85%)	43 (98%)	1 (2%)	44	74
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
24	X	130/130 (100%)	120 (92%)	10 (8%)	12	40
25	Y	66/73 (90%)	62 (94%)	4 (6%)	17	49
26	Z	120/195 (62%)	112 (93%)	8 (7%)	15	46
27	1	56/56 (100%)	53 (95%)	3 (5%)	20	53
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
30	4	79/79 (100%)	74 (94%)	5 (6%)	16	48
All	All	3027/3441 (88%)	2872 (95%)	155 (5%)	21	55

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	39	THR
26	Z	200	THR
21	U	47	THR
24	X	122	ARG
30	4	14	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	22	GLN
23	W	60	GLN
30	4	48	ASN
19	S	98	ASN
20	T	51	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	258 (9%)	35 (1%)
2	B	121/122 (99%)	15 (12%)	6 (4%)
All	All	2868/3044 (94%)	273 (9%)	41 (1%)

5 of 273 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2313	C
2	B	3002	U
1	A	2467	A
1	A	2718	C
2	B	3023	U

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 233 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CAI	A	4000	1	61,62,62	2.84	19 (31%)	75,90,90	1.90	21 (28%)

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
31	CAI	A	4000	1	-	9/66/110/110	0/3/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	4000	CAI	C2-C3	-10.37	1.29	1.52
31	A	4000	CAI	C20-C21	8.22	1.71	1.50
31	A	4000	CAI	C6-C5	-6.34	1.40	1.52
31	A	4000	CAI	O21-C21	5.63	1.52	1.20
31	A	4000	CAI	O3-C3	5.44	1.55	1.46

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4000	CAI	O21-C21-C20	-7.74	102.86	125.38
31	A	4000	CAI	C5-C4-C3	4.50	121.25	113.16
31	A	4000	CAI	C19-O4-C4	-3.65	105.09	114.47
31	A	4000	CAI	O3-C17-O17	-3.44	116.34	122.99
31	A	4000	CAI	C4A-C3A-N3A	-3.37	103.71	111.68

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

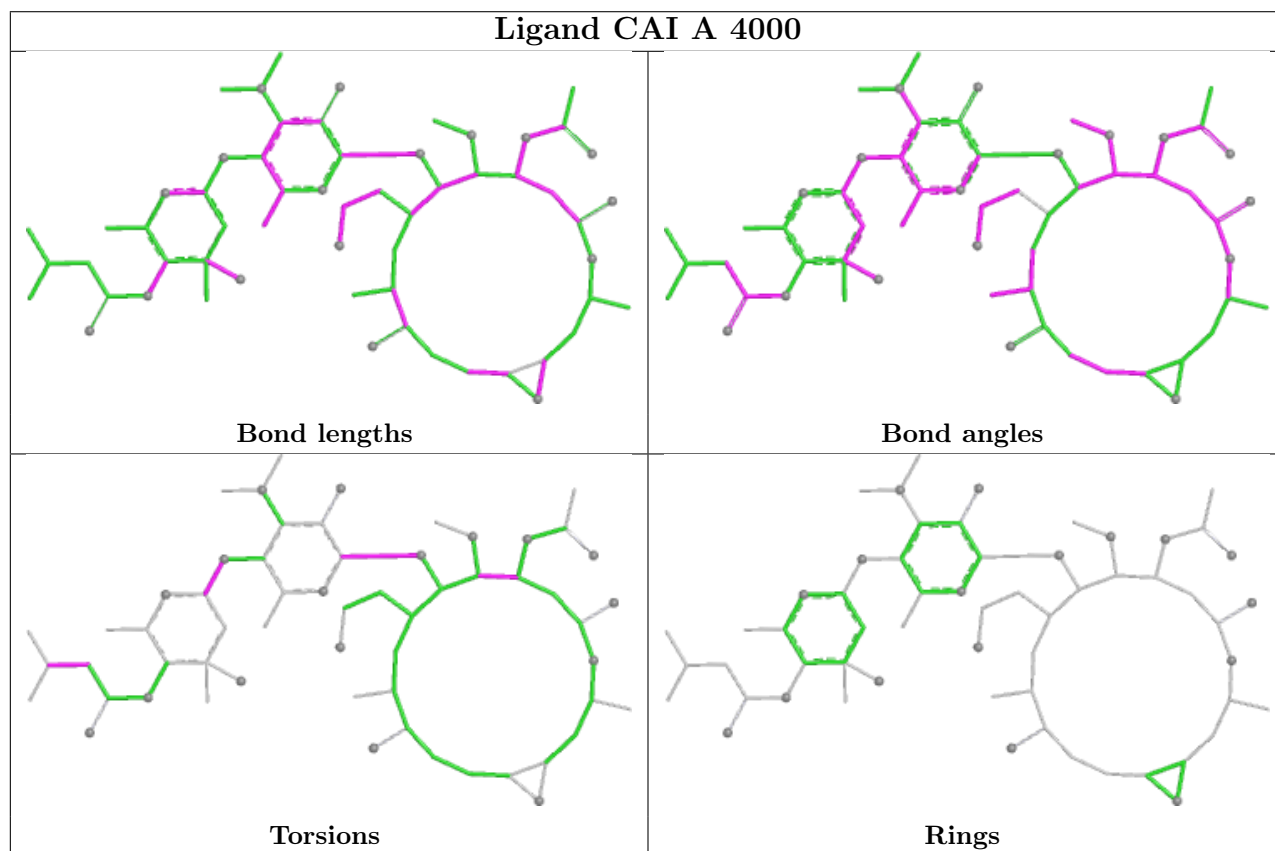
Mol	Chain	Res	Type	Atoms
31	A	4000	CAI	C2-C3-C4-C5
31	A	4000	CAI	C2B-C1B-O1B-C4A
31	A	4000	CAI	O5B-C1B-O1B-C4A
31	A	4000	CAI	C2-C3-C4-O4
31	A	4000	CAI	O3-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	4000	CAI	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.18	45 (1%) 70 47	25, 51, 97, 142	0
2	B	122/122 (100%)	0.30	5 (4%) 41 23	33, 69, 99, 152	0
3	C	237/239 (99%)	0.15	2 (0%) 82 64	30, 64, 95, 112	0
4	D	337/337 (100%)	-0.02	1 (0%) 90 79	24, 57, 84, 96	0
5	E	246/246 (100%)	-0.10	1 (0%) 88 76	23, 50, 74, 84	0
6	F	140/176 (79%)	0.93	8 (5%) 29 15	63, 104, 122, 128	0
7	G	172/177 (97%)	0.21	4 (2%) 61 38	41, 68, 90, 94	0
8	H	119/119 (100%)	0.55	1 (0%) 82 64	63, 81, 102, 108	0
9	I	29/348 (8%)	1.14	4 (13%) 6 4	77, 93, 100, 104	0
10	J	156/167 (93%)	0.17	2 (1%) 75 53	36, 57, 84, 93	0
11	K	142/145 (97%)	-0.12	0 100 100	30, 50, 75, 84	0
12	L	132/132 (100%)	-0.00	0 100 100	34, 56, 79, 85	0
13	M	145/164 (88%)	0.27	4 (2%) 55 32	30, 75, 106, 114	0
14	N	194/194 (100%)	0.37	18 (9%) 14 7	36, 56, 95, 105	0
15	O	186/186 (100%)	0.61	13 (6%) 22 12	45, 74, 112, 124	0
16	P	115/115 (100%)	0.12	0 100 100	40, 57, 75, 79	0
17	Q	143/148 (96%)	0.06	2 (1%) 73 51	40, 61, 77, 84	0
18	R	95/95 (100%)	-0.11	1 (1%) 78 57	36, 50, 65, 79	0
19	S	150/154 (97%)	-0.34	0 100 100	31, 45, 67, 75	0
20	T	81/84 (96%)	0.06	0 100 100	48, 66, 86, 89	0
21	U	119/119 (100%)	0.19	2 (1%) 69 45	44, 62, 88, 100	0
22	V	53/66 (80%)	1.42	8 (15%) 5 3	84, 96, 103, 112	0
23	W	65/70 (92%)	0.40	3 (4%) 37 20	56, 81, 110, 116	0
24	X	154/154 (100%)	-0.21	0 100 100	32, 46, 65, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.11	3 (3%) 45 25	41, 59, 84, 100	0
26	Z	142/240 (59%)	-0.18	0 100 100	27, 46, 69, 87	0
27	1	73/73 (100%)	1.79	25 (34%) 1 1	82, 97, 105, 106	0
28	2	56/56 (100%)	-0.50	0 100 100	28, 38, 45, 49	0
29	3	46/48 (95%)	0.23	0 100 100	38, 68, 89, 104	0
30	4	92/92 (100%)	2.43	58 (63%) 0 0	94, 109, 114, 119	0
All	All	6577/7279 (90%)	0.07	210 (3%) 50 29	23, 57, 104, 152	0

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	80	GLY	6.8
23	W	1	THR	6.7
14	N	89	ASN	6.4
1	A	1173	A	6.2
30	4	12	PRO	6.1

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
36	CD	4	8404	1/1	0.48	0.30	202,202,202,202	0
32	MG	A	8092	1/1	0.61	0.26	115,115,115,115	0
32	MG	A	8050	1/1	0.62	0.13	85,85,85,85	0
34	CL	4	8504	1/1	0.64	0.14	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	A	8384	1/1	0.67	0.25	109,109,109,109	0
33	NA	S	8337	1/1	0.68	0.12	40,40,40,40	0
33	NA	A	8329	1/1	0.69	0.24	64,64,64,64	0
32	MG	A	8093	1/1	0.70	0.11	37,37,37,37	0
33	NA	B	8383	1/1	0.72	0.63	103,103,103,103	0
32	MG	A	8116	1/1	0.74	0.15	85,85,85,85	0
33	NA	T	8312	1/1	0.74	0.11	61,61,61,61	0
34	CL	A	8515	1/1	0.75	0.28	92,92,92,92	0
33	NA	A	8326	1/1	0.75	0.14	61,61,61,61	0
33	NA	A	8373	1/1	0.75	0.17	71,71,71,71	0
33	NA	A	8356	1/1	0.77	0.24	52,52,52,52	0
35	K	A	8602	1/1	0.78	0.18	69,69,69,69	0
32	MG	A	8104	1/1	0.78	0.14	54,54,54,54	0
36	CD	1	8403	1/1	0.79	0.15	180,180,180,180	0
34	CL	P	8508	1/1	0.79	0.14	91,91,91,91	0
32	MG	A	8024	1/1	0.80	0.11	81,81,81,81	0
33	NA	A	8371	1/1	0.81	0.30	56,56,56,56	0
33	NA	A	8341	1/1	0.81	0.08	44,44,44,44	0
36	CD	V	8401	1/1	0.82	0.23	202,202,202,202	0
33	NA	A	8357	1/1	0.83	0.10	60,60,60,60	0
34	CL	R	8511	1/1	0.84	0.15	84,84,84,84	0
33	NA	A	8363	1/1	0.84	0.29	56,56,56,56	0
32	MG	A	8049	1/1	0.84	0.11	81,81,81,81	0
32	MG	A	8067	1/1	0.84	0.15	57,57,57,57	0
32	MG	A	8070	1/1	0.84	0.17	62,62,62,62	0
33	NA	B	8351	1/1	0.84	0.10	44,44,44,44	0
33	NA	A	8364	1/1	0.85	0.18	53,53,53,53	0
34	CL	C	8509	1/1	0.85	0.15	82,82,82,82	0
33	NA	A	8327	1/1	0.85	0.13	27,27,27,27	0
33	NA	A	8302	1/1	0.86	0.12	27,27,27,27	0
34	CL	A	8522	1/1	0.87	0.26	83,83,83,83	0
33	NA	A	8372	1/1	0.87	0.27	71,71,71,71	0
32	MG	A	8041	1/1	0.87	0.07	68,68,68,68	0
33	NA	A	8382	1/1	0.88	0.19	59,59,59,59	0
32	MG	A	8113	1/1	0.88	0.09	45,45,45,45	0
33	NA	A	8366	1/1	0.88	0.08	45,45,45,45	0
33	NA	A	8367	1/1	0.88	0.11	50,50,50,50	0
33	NA	E	8304	1/1	0.88	0.10	43,43,43,43	0
33	NA	N	8365	1/1	0.88	0.16	50,50,50,50	0
33	NA	A	8306	1/1	0.88	0.25	65,65,65,65	0
33	NA	A	8320	1/1	0.88	0.12	35,35,35,35	0
33	NA	A	8331	1/1	0.88	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8101	1/1	0.89	0.14	59,59,59,59	0
34	CL	A	8505	1/1	0.89	0.17	95,95,95,95	0
33	NA	A	8303	1/1	0.89	0.14	43,43,43,43	0
32	MG	A	8053	1/1	0.89	0.06	45,45,45,45	0
32	MG	A	8119	1/1	0.89	0.08	19,19,19,19	0
33	NA	A	8301	1/1	0.89	0.10	19,19,19,19	0
32	MG	A	8102	1/1	0.90	0.50	109,109,109,109	0
34	CL	D	8519	1/1	0.90	0.14	71,71,71,71	0
34	CL	M	8510	1/1	0.90	0.18	108,108,108,108	0
33	NA	A	8355	1/1	0.90	0.19	54,54,54,54	0
33	NA	A	8328	1/1	0.90	0.07	47,47,47,47	0
33	NA	A	8324	1/1	0.90	0.39	61,61,61,61	0
33	NA	A	8374	1/1	0.90	0.27	75,75,75,75	0
32	MG	4	8078	1/1	0.90	0.15	74,74,74,74	0
33	NA	A	8332	1/1	0.90	0.13	57,57,57,57	0
33	NA	A	8340	1/1	0.90	0.07	42,42,42,42	0
32	MG	D	8055	1/1	0.91	0.06	77,77,77,77	0
34	CL	A	8523	1/1	0.91	0.15	56,56,56,56	0
33	NA	A	8319	1/1	0.91	0.12	49,49,49,49	0
32	MG	A	8082	1/1	0.91	0.08	63,63,63,63	0
33	NA	A	8336	1/1	0.91	0.07	49,49,49,49	0
33	NA	A	8339	1/1	0.91	0.10	33,33,33,33	0
33	NA	A	8369	1/1	0.91	0.21	60,60,60,60	0
32	MG	A	8114	1/1	0.91	0.12	97,97,97,97	0
32	MG	A	8046	1/1	0.91	0.07	48,48,48,48	0
32	MG	A	8066	1/1	0.91	0.13	66,66,66,66	0
34	CL	A	8512	1/1	0.91	0.09	39,39,39,39	0
33	NA	A	8305	1/1	0.91	0.07	20,20,20,20	0
32	MG	A	8089	1/1	0.92	0.12	64,64,64,64	0
33	NA	A	8378	1/1	0.92	0.16	37,37,37,37	0
33	NA	A	8362	1/1	0.92	0.13	56,56,56,56	0
31	CAI	A	4000	59/59	0.92	0.11	40,47,60,62	0
33	NA	A	8368	1/1	0.92	0.08	41,41,41,41	0
33	NA	A	8316	1/1	0.93	0.12	53,53,53,53	0
33	NA	A	8318	1/1	0.93	0.18	42,42,42,42	0
32	MG	A	8022	1/1	0.93	0.32	56,56,56,56	0
33	NA	A	8352	1/1	0.93	0.12	46,46,46,46	0
36	CD	P	8405	1/1	0.93	0.09	136,136,136,136	0
32	MG	C	8105	1/1	0.93	0.09	40,40,40,40	0
32	MG	A	8094	1/1	0.93	0.17	63,63,63,63	0
33	NA	A	8310	1/1	0.93	0.09	42,42,42,42	0
32	MG	A	8045	1/1	0.94	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	8040	1/1	0.94	0.20	124,124,124,124	0
33	NA	A	8323	1/1	0.94	0.15	53,53,53,53	0
32	MG	A	8062	1/1	0.94	0.06	80,80,80,80	0
33	NA	A	8350	1/1	0.94	0.11	38,38,38,38	0
34	CL	A	8514	1/1	0.94	0.07	57,57,57,57	0
32	MG	A	8088	1/1	0.94	0.06	24,24,24,24	0
34	CL	A	8516	1/1	0.94	0.13	43,43,43,43	0
32	MG	A	8001	1/1	0.94	0.07	30,30,30,30	0
33	NA	A	8377	1/1	0.94	0.18	71,71,71,71	0
32	MG	A	8103	1/1	0.94	0.14	57,57,57,57	0
33	NA	A	8379	1/1	0.94	0.09	44,44,44,44	0
33	NA	A	8314	1/1	0.94	0.14	35,35,35,35	0
34	CL	N	8518	1/1	0.94	0.12	51,51,51,51	0
33	NA	A	8330	1/1	0.94	0.07	39,39,39,39	0
32	MG	U	8073	1/1	0.94	0.04	40,40,40,40	0
32	MG	A	8090	1/1	0.94	0.22	67,67,67,67	0
33	NA	C	8345	1/1	0.94	0.06	43,43,43,43	0
35	K	A	8603	1/1	0.94	0.09	67,67,67,67	0
33	NA	A	8334	1/1	0.94	0.08	30,30,30,30	0
33	NA	K	8346	1/1	0.94	0.06	27,27,27,27	0
33	NA	M	8380	1/1	0.94	0.07	52,52,52,52	0
33	NA	N	8347	1/1	0.94	0.06	25,25,25,25	0
32	MG	A	8117	1/1	0.95	0.04	17,17,17,17	0
33	NA	A	8325	1/1	0.95	0.10	60,60,60,60	0
32	MG	A	8086	1/1	0.95	0.05	44,44,44,44	0
33	NA	A	8308	1/1	0.95	0.09	53,53,53,53	0
34	CL	A	8513	1/1	0.95	0.10	60,60,60,60	0
33	NA	A	8375	1/1	0.95	0.13	54,54,54,54	0
33	NA	A	8353	1/1	0.95	0.05	32,32,32,32	0
32	MG	A	8087	1/1	0.95	0.06	41,41,41,41	0
32	MG	A	8076	1/1	0.95	0.06	76,76,76,76	0
33	NA	A	8381	1/1	0.95	0.05	42,42,42,42	0
33	NA	A	8315	1/1	0.95	0.06	40,40,40,40	0
33	NA	A	8359	1/1	0.95	0.11	64,64,64,64	0
33	NA	A	8385	1/1	0.95	0.13	34,34,34,34	0
33	NA	A	8360	1/1	0.95	0.16	36,36,36,36	0
34	CL	O	8507	1/1	0.95	0.08	58,58,58,58	0
32	MG	A	8079	1/1	0.95	0.05	56,56,56,56	0
32	MG	A	8081	1/1	0.95	0.06	44,44,44,44	0
34	CL	Z	8520	1/1	0.95	0.07	39,39,39,39	0
33	NA	A	8333	1/1	0.95	0.10	37,37,37,37	0
35	K	A	8601	1/1	0.95	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	J	8309	1/1	0.95	0.07	21,21,21,21	0
33	NA	J	8322	1/1	0.95	0.11	59,59,59,59	0
32	MG	A	8091	1/1	0.95	0.07	53,53,53,53	0
32	MG	A	8075	1/1	0.95	0.09	33,33,33,33	0
33	NA	A	8338	1/1	0.95	0.09	79,79,79,79	0
32	MG	A	8085	1/1	0.95	0.06	77,77,77,77	0
32	MG	A	8043	1/1	0.96	0.06	52,52,52,52	0
32	MG	A	8012	1/1	0.96	0.08	25,25,25,25	0
32	MG	A	8118	1/1	0.96	0.14	22,22,22,22	0
33	NA	A	8321	1/1	0.96	0.12	50,50,50,50	0
34	CL	K	8501	1/1	0.96	0.05	50,50,50,50	0
32	MG	A	8071	1/1	0.96	0.05	66,66,66,66	0
32	MG	A	8106	1/1	0.96	0.06	59,59,59,59	0
33	NA	R	8348	1/1	0.96	0.03	23,23,23,23	0
32	MG	A	8112	1/1	0.96	0.06	52,52,52,52	0
33	NA	A	8313	1/1	0.96	0.06	75,75,75,75	0
34	CL	S	8506	1/1	0.96	0.10	48,48,48,48	0
33	NA	U	8343	1/1	0.96	0.03	18,18,18,18	0
34	CL	A	8503	1/1	0.96	0.09	63,63,63,63	0
32	MG	A	8099	1/1	0.96	0.07	51,51,51,51	0
33	NA	A	8344	1/1	0.96	0.04	24,24,24,24	0
32	MG	A	8072	1/1	0.96	0.07	83,83,83,83	0
32	MG	A	8115	1/1	0.96	0.05	47,47,47,47	0
33	NA	A	8317	1/1	0.96	0.05	27,27,27,27	0
33	NA	A	8354	1/1	0.96	0.08	44,44,44,44	0
34	CL	A	8517	1/1	0.96	0.04	52,52,52,52	0
33	NA	A	8307	1/1	0.97	0.05	34,34,34,34	0
32	MG	A	8098	1/1	0.97	0.17	23,23,23,23	0
33	NA	A	8370	1/1	0.97	0.15	39,39,39,39	0
32	MG	A	8051	1/1	0.97	0.05	57,57,57,57	0
33	NA	A	8311	1/1	0.97	0.05	34,34,34,34	0
32	MG	A	8100	1/1	0.97	0.08	65,65,65,65	0
32	MG	A	8027	1/1	0.97	0.07	69,69,69,69	0
32	MG	A	8060	1/1	0.97	0.06	62,62,62,62	0
33	NA	A	8361	1/1	0.97	0.09	63,63,63,63	0
32	MG	A	8047	1/1	0.97	0.07	41,41,41,41	0
32	MG	A	8064	1/1	0.97	0.17	23,23,23,23	0
33	NA	A	8349	1/1	0.97	0.06	56,56,56,56	0
32	MG	A	8096	1/1	0.97	0.06	48,48,48,48	0
32	MG	B	8095	1/1	0.97	0.05	67,67,67,67	0
34	CL	K	8521	1/1	0.97	0.05	43,43,43,43	0
32	MG	A	8083	1/1	0.98	0.07	44,44,44,44	0

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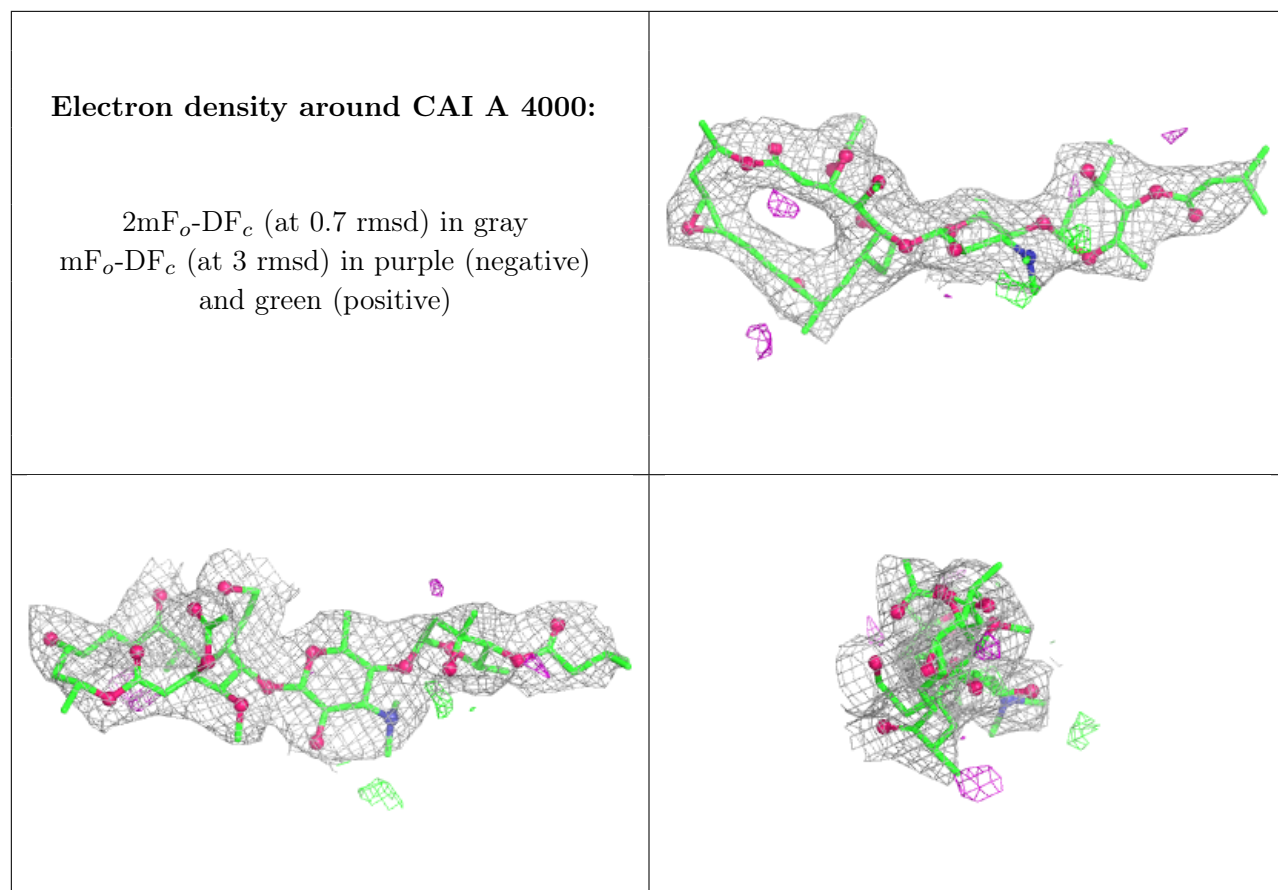
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8084	1/1	0.98	0.09	40,40,40,40	0
34	CL	K	8502	1/1	0.98	0.03	48,48,48,48	0
32	MG	A	8033	1/1	0.98	0.06	19,19,19,19	0
32	MG	A	8039	1/1	0.98	0.09	76,76,76,76	0
32	MG	A	8068	1/1	0.98	0.04	52,52,52,52	0
32	MG	A	8052	1/1	0.98	0.05	43,43,43,43	0
32	MG	L	8069	1/1	0.98	0.05	78,78,78,78	0
32	MG	A	8006	1/1	0.98	0.03	61,61,61,61	0
33	NA	A	8335	1/1	0.98	0.09	61,61,61,61	0
32	MG	Z	8109	1/1	0.98	0.08	42,42,42,42	0
32	MG	A	8056	1/1	0.98	0.06	40,40,40,40	0
32	MG	A	8111	1/1	0.98	0.03	47,47,47,47	0
32	MG	A	8057	1/1	0.98	0.05	48,48,48,48	0
32	MG	A	8059	1/1	0.98	0.03	35,35,35,35	0
33	NA	A	8342	1/1	0.98	0.09	60,60,60,60	0
32	MG	A	8008	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8048	1/1	0.98	0.03	54,54,54,54	0
32	MG	A	8042	1/1	0.98	0.08	46,46,46,46	0
32	MG	C	8065	1/1	0.99	0.03	48,48,48,48	0
32	MG	A	8030	1/1	0.99	0.03	19,19,19,19	0
32	MG	A	8097	1/1	0.99	0.10	29,29,29,29	0
32	MG	A	8007	1/1	0.99	0.03	25,25,25,25	0
32	MG	A	8035	1/1	0.99	0.04	49,49,49,49	0
32	MG	A	8037	1/1	0.99	0.04	30,30,30,30	0
32	MG	A	8080	1/1	0.99	0.06	31,31,31,31	0
32	MG	A	8054	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8013	1/1	0.99	0.03	56,56,56,56	0
32	MG	A	8014	1/1	0.99	0.05	14,14,14,14	0
32	MG	A	8058	1/1	0.99	0.03	57,57,57,57	0
32	MG	A	8107	1/1	0.99	0.02	40,40,40,40	0
32	MG	A	8108	1/1	0.99	0.07	67,67,67,67	0
32	MG	A	8110	1/1	0.99	0.05	41,41,41,41	0
32	MG	A	8015	1/1	0.99	0.03	43,43,43,43	0
32	MG	A	8016	1/1	0.99	0.03	59,59,59,59	0
32	MG	A	8018	1/1	0.99	0.03	43,43,43,43	0
32	MG	A	8063	1/1	0.99	0.04	67,67,67,67	0
32	MG	A	8044	1/1	0.99	0.08	70,70,70,70	0
32	MG	A	8004	1/1	0.99	0.03	52,52,52,52	0
32	MG	A	8023	1/1	0.99	0.02	29,29,29,29	0
32	MG	A	8009	1/1	0.99	0.05	24,24,24,24	0
32	MG	A	8010	1/1	0.99	0.03	48,48,48,48	0
36	CD	2	8402	1/1	0.99	0.04	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8028	1/1	0.99	0.06	34,34,34,34	0
32	MG	A	8019	1/1	1.00	0.04	34,34,34,34	0
32	MG	A	8031	1/1	1.00	0.04	32,32,32,32	0
32	MG	A	8032	1/1	1.00	0.08	23,23,23,23	0
32	MG	A	8020	1/1	1.00	0.03	33,33,33,33	0
32	MG	A	8034	1/1	1.00	0.03	15,15,15,15	0
32	MG	A	8021	1/1	1.00	0.02	19,19,19,19	0
32	MG	A	8036	1/1	1.00	0.02	28,28,28,28	0
32	MG	A	8074	1/1	1.00	0.09	12,12,12,12	0
32	MG	A	8002	1/1	1.00	0.03	25,25,25,25	0
32	MG	A	8038	1/1	1.00	0.01	33,33,33,33	0
32	MG	A	8077	1/1	1.00	0.04	21,21,21,21	0
32	MG	A	8011	1/1	1.00	0.04	24,24,24,24	0
32	MG	A	8005	1/1	1.00	0.03	41,41,41,41	0
32	MG	A	8025	1/1	1.00	0.02	41,41,41,41	0
32	MG	A	8026	1/1	1.00	0.04	12,12,12,12	0
32	MG	A	8017	1/1	1.00	0.03	24,24,24,24	0
32	MG	A	8061	1/1	1.00	0.04	33,33,33,33	0
32	MG	A	8003	1/1	1.00	0.04	14,14,14,14	0
32	MG	A	8029	1/1	1.00	0.01	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.