



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:53 pm BST

PDB ID : 1VQ5  
Title : The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.60 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 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

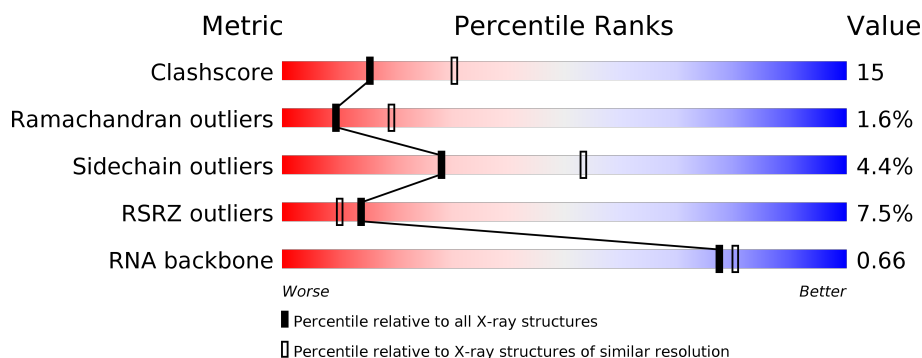
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	0	2922	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>10%</div> </div> </div>
3	4	8	<div> <div></div> <div> <div></div> <div>38%</div> <div>63%</div> </div> </div>
4	A	240	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>••</div> </div> </div>
5	B	338	<div> <div>9%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>5%</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>6%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
32	I	162	

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	MG	0	8049	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9121	-	-	-	X
35	NA	0	9155	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9182	-	-	-	X
35	NA	0	9184	-	-	-	X
35	NA	B	9158	-	-	-	X
35	NA	R	9186	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-D\*(DC)P\*(DC)P\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*C\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			126	61	23	37	5			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.



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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	106	Total	Mg	0	0
			106	106		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	3	Total K 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5820	Total 5820	O 5820	0	0
38	9	133	Total 133	O 133	0	0
38	4	8	Total 8	O 8	0	0
38	A	117	Total 117	O 117	0	0
38	B	150	Total 150	O 150	0	0
38	C	165	Total 165	O 165	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	21	Total 21	O 21	0	0
38	G	16	Total 16	O 16	0	0
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	54	Total 54	O 54	0	0
38	L	83	Total 83	O 83	0	0
38	M	118	Total 118	O 118	0	0
38	N	66	Total 66	O 66	0	0
38	O	39	Total 39	O 39	0	0
38	P	65	Total 65	O 65	0	0
38	Q	52	Total 52	O 52	0	0
38	R	85	Total 85	O 85	0	0
38	S	31	Total 31	O 31	0	0
38	T	39	Total 39	O 39	0	0
38	U	25	Total 25	O 25	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	92	Total 92	O 92	0	0

*Continued on next page...*

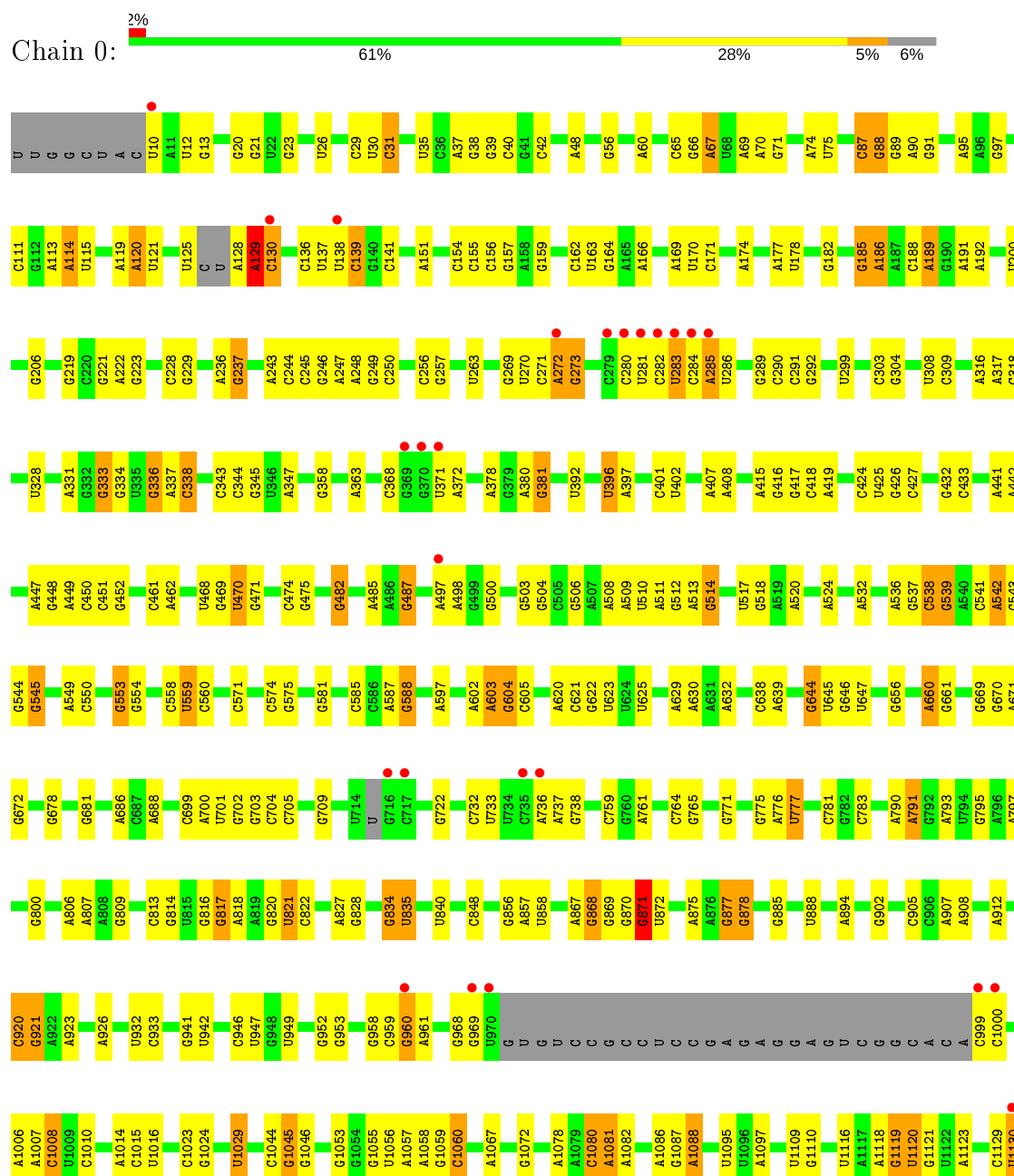
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	30	Total 30	O 30	0	0
38	1	59	Total 59	O 59	0	0
38	2	42	Total 42	O 42	0	0
38	3	74	Total 74	O 74	0	0
38	I	10	Total 10	O 10	0	0

### 3 Residue-property plots [i](#)

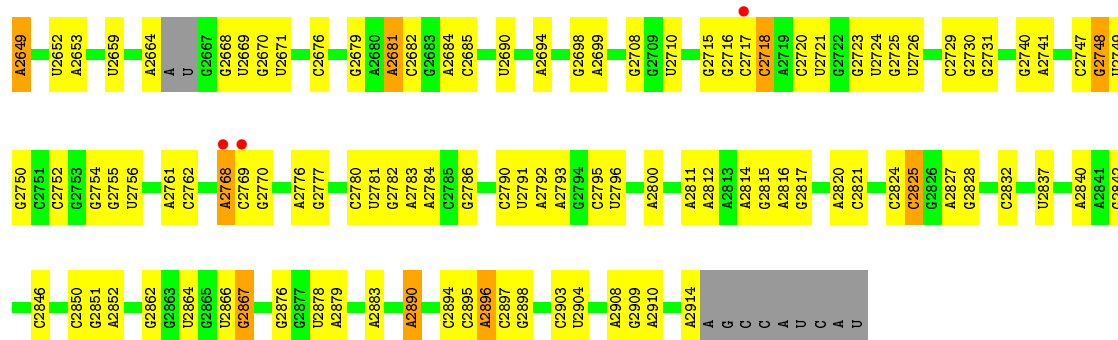
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 23S ribosomal rna

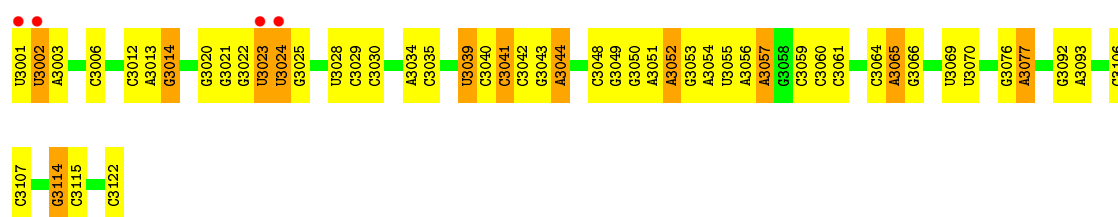


C2526	U2527	C2533	C2534	C2535	C2536	C2537	U2541	C2542	C2548	C2551	C2552	A2553	U2563	C2564	C2565	A2577	C2578	U2586	U2587	C2588	U2589	U2590	C2591	C2592	U2597	U2598	A2601	C2602	C2603	A2604	U2607	C2608	C2613	C2614	U2619	U2620	C2630	C2634	A2637	C2643	U2644	U2645											
G2421	U2422	C2423	G2426	C2427	G2428	C2438	C2439	C2443	U2444	U2445	G2446	A2455	A2456	U2457	G2462	C2467	A2468	A2469	C2472	C2476	G2480	A2483	C2487	A2490	C2491	U2492	C2493	C2502	A2503	A2504	C2505	A2506	C2507	C2508	A2509	C2510	A2511	U2512	C2515	G2516	A2521	G2524	G2525										
C2329	U2330	C2331	G2338	A	C	A	A	A	A	A	A	A2353	A2354	G2355	A2356	C2357	A2361	A2362	C2363	A2364	C2365	A2369	A2372	U2373	U2377	U2378	G2379	A2380	C2381	G2385	U2386	U2387	C2388	C2392	A2401	A2402	C2403	G2404	A2408	G2412	A2413	A2414	A2415	G2418	U2419	C2420							
A	G	A	C	A	C	U	U	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	U									
C	G	G	U	G	C	C	U	C	C	C	C	C2241	U2242	C2243	C2248	G2249	G2250	G2251	A2252	G2253	G2254	A2255	G2256	G2257	A2258	U2265	A2266	G2267	C2268	G2269	G2270	G2271	G2272	C2281	U2282	A2291	A2300	A2301	A2302	C2309	G2312	C2313	C2314	C2315	G2316	C2317	U2320	A2321	G2324				
A2067	G2068	U	A	A	C	U	U	C	C	C	C	A1839	A1840	A1845	U1846	A1847	G1848	G1849	G1855	C1856	G1863	G1867	G1868	G1877	G1878	U1879	A1881	A1904	U1905	A1919	C1920	A1921	A1922	G1926	A1927	A1930	A1931	G1932	G1933	A1934	C1940	A1941	A1942	A1943	G1948	G1949							
G1806	A1811	G1819	G1820	A1829	C1830	C1834	U1835	A1839	A1840	A1845	U1846	A1847	G1848	G1849	G1855	C1856	G1863	G1867	G1868	G1877	G1878	U1879	A1881	A1904	U1905	A1919	C1920	A1921	A1922	G1926	A1927	A1930	A1931	G1932	G1933	A1934	C1940	A1941	A1942	A1943	G1948	G1949											
A1701	U1702	A1710	A1711	A1712	G1713	C1714	C1715	A1716	A1717	G1718	U1722	G1723	U1724	C1725	G1730	C1731	A1732	A1733	C1734	U1741	A1742	G1743	G1745	A1755	G1756	U1761	U1766	U1771	C1772	G1773	G1774	A1778	A1779	G1785	C1786	C1787	U1788	G1789	C1790	U1791	C1798	G1805											
U1595	U1596	A1597	A1598	A1603	G1604	G1605	C1613	G1614	A1624	U1625	A1626	A1631	A1632	C1633	G1634	U1635	G1636	A1637	A1641	A1642	C1643	C1644	U1654	G1655	A1656	A1657	A1658	G1663	A1664	G1665	C1666	U1668	A1669	G1670	C1675	C1679	G1681	A1682	G1683	A1684	A1685	C1686	C1687	C1692	G1697	U1698							
C1450	C1451	G1452	G1453	A1458	C1462	A1463	C1474	C1477	U1478	C1483	G1484	A1485	A1494	C1495	G1496	U1500	U1503	A1504	U1505	U1506	C1513	C1514	U1524	G1525	A1526	A1527	A1528	G1529	G1535	C1536	U1544	C1545	U1559	U1561	C1562	G1563	A1564	U1567	G1568	G1592	C1593	C1594											
A1328	A1331	U1332	U1333	C1334	C1335	U1336	G1340	C1342	C1343	G1351	A1352	C1353	C1360	G1363	A1372	A1375	G1376	C1377	U1380	G1385	G1391	A1392	G1398	A1399	A1406	U1407	U1408	G1409	G1417	U1418	U1419	C1420	C1423	A1424	A1427	A1434	U1435	G1436	U1440	G1441	A1442												
G1209	G1210	C1213	G1214	A1215	G1216	G1224	C1225	C1229	U1234	G1235	A1236	U1237	C1238	G1239	A1242	C1243	U1244	G1245	A1246	U1249	C1250	C1251	A1252	C1253	C1268	G1269	U1270	C1273	A1278	U1279	C1289	G1290	A1294	G1299	G1300	U1304	C1305	A1307	A1308	U1309	U1310	G1311	U1314										
G1131	A1132	G1135	U1136	G1137	A1150	G1151	G1158	G1159	G1160	A1161	G1162	G1163	U1164	G1165	A1166	G1167	C1168	U1169	U1170	A1171	G1172	A1173	A1174	C1175	A1176	A1177	G1178	C1179	U1180	A1181	C1182	C1183	C1184	U1185	C1186	U1187	A1188	G1189	G1190	A1191	A1192	A1193	A1194	G1195	U1198	A1199	A1200	A1202	G1203	C1204	U1205	U1206	C1208

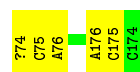




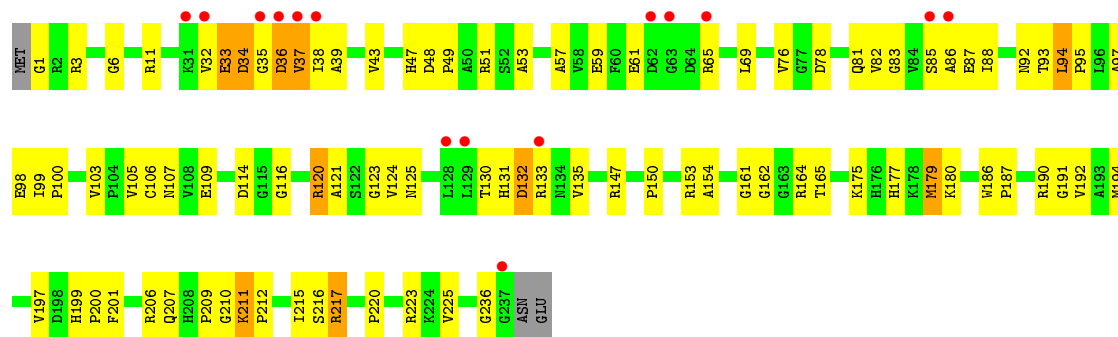
• Molecule 2: 5S ribosomal RNA



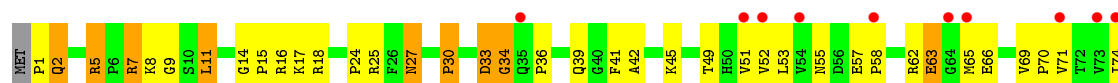
• Molecule 3: 5'-D\*(DC)P\*(DC)P\*(5AA)P\*(2OP)P\*(PO2)P\*AP\*C\*C)-3''

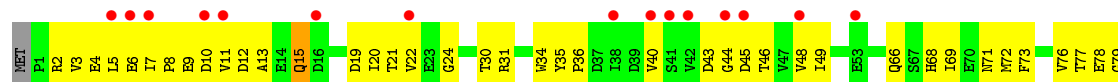


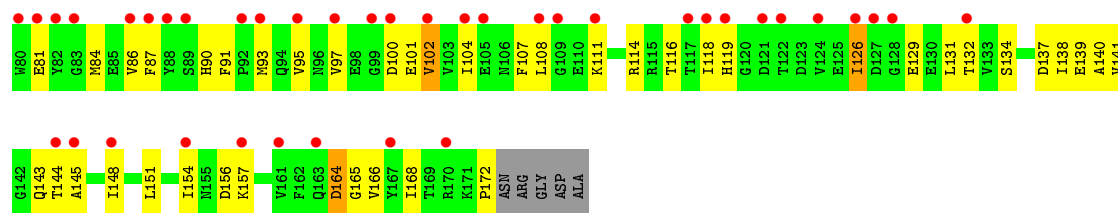
• Molecule 4: 50S ribosomal protein L2P



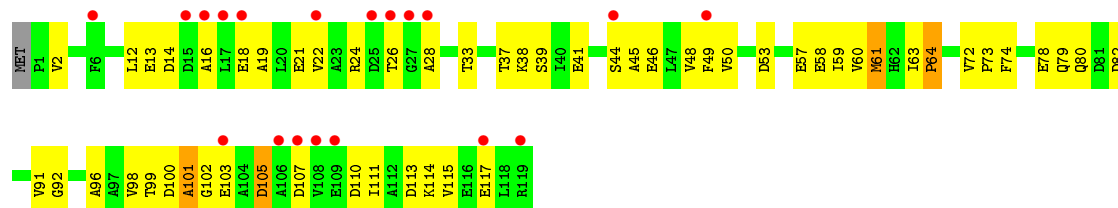
• Molecule 5: 50S ribosomal protein L3P



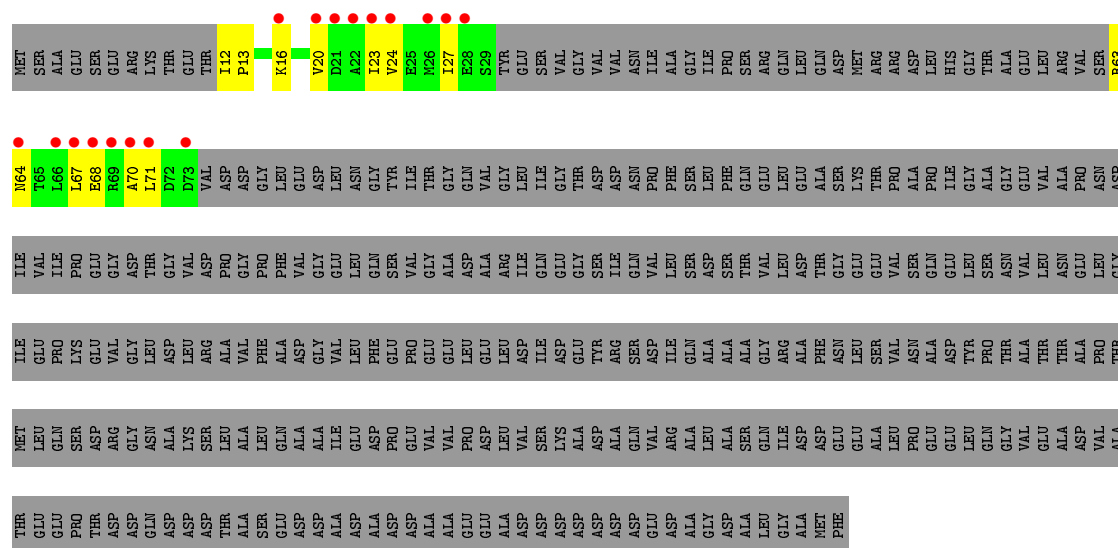




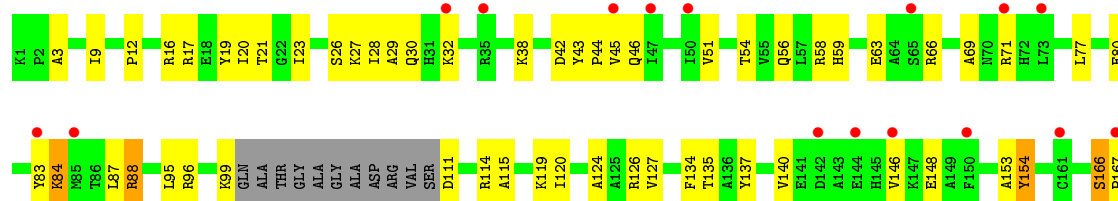
• Molecule 9: 50S ribosomal protein L7AE



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

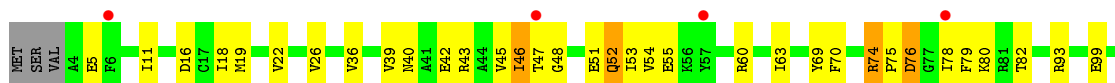


• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

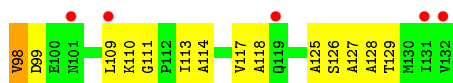




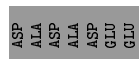
- Molecule 12: 50S ribosomal protein L13P



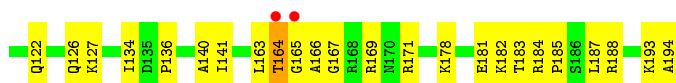
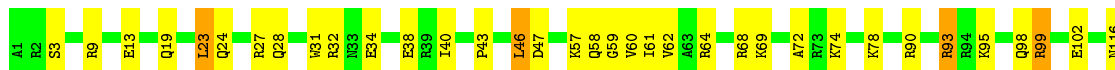
- Molecule 13: 50S ribosomal protein L14P



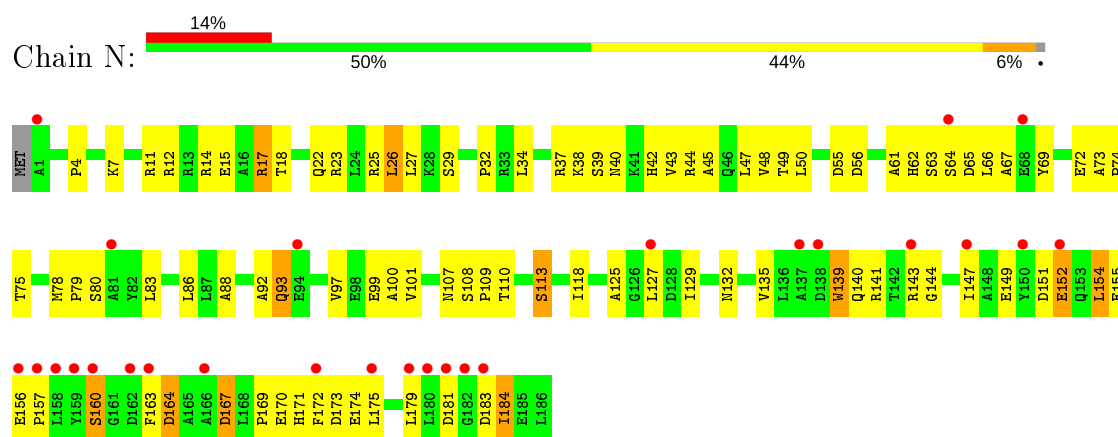
- Molecule 14: 50S ribosomal protein L15P



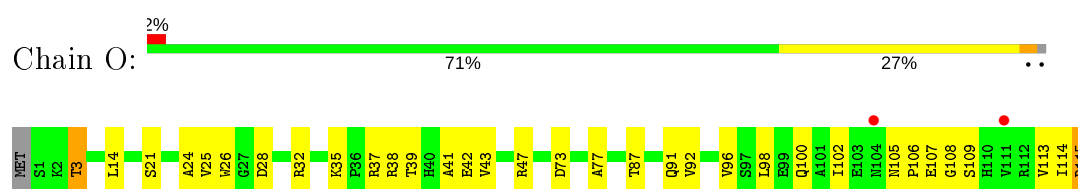
- Molecule 15: 50S Ribosomal Protein L15E



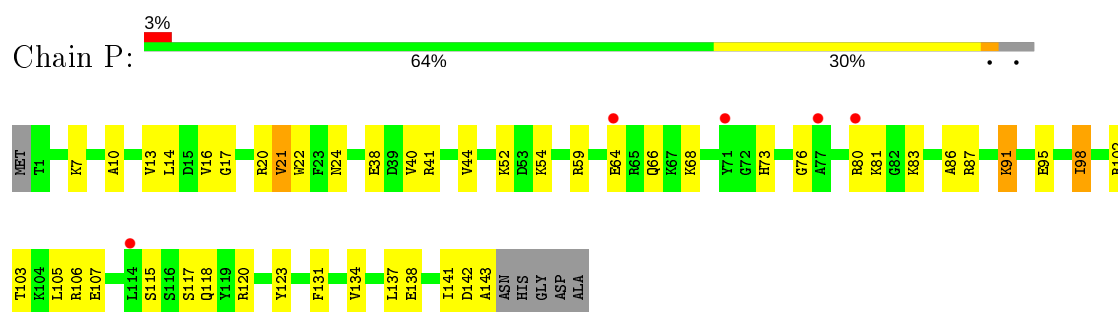
- Molecule 16: 50S ribosomal protein L18P



- Molecule 17: 50S ribosomal protein L18e

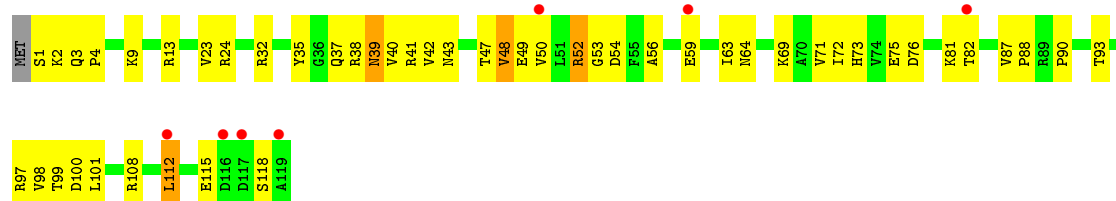


- Molecule 18: 50S ribosomal protein L19E

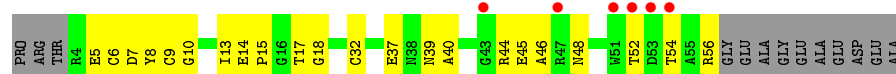




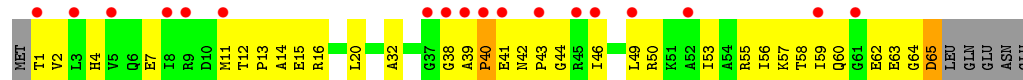
- Molecule 22: 50S ribosomal protein L24P



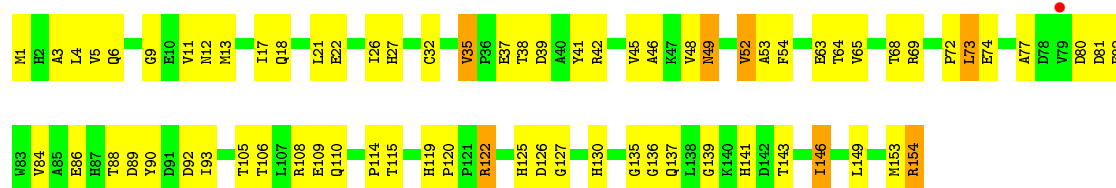
- Molecule 23: 50S ribosomal protein L24E



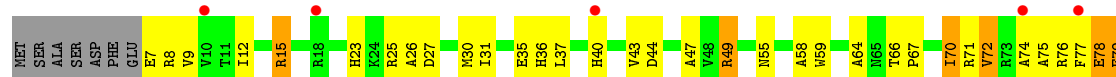
- Molecule 24: 50S ribosomal protein L29P

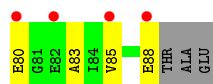


- Molecule 25: 50S ribosomal protein L30P

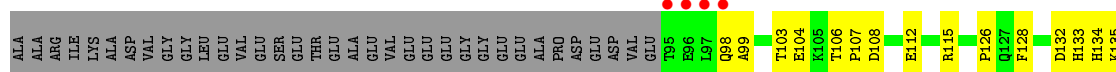


- Molecule 26: 50S ribosomal protein L31e





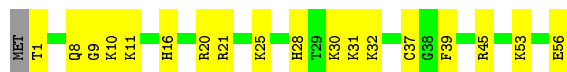
- Molecule 27: 50S ribosomal protein L32E



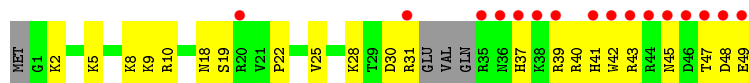
- Molecule 28: 50S ribosomal protein L37Ae



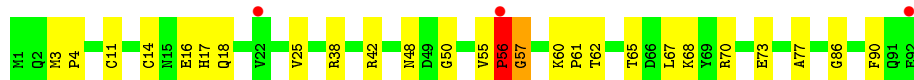
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



•	A125	•	SER	•	MET
•	K126	•	PHE	•	ALA
•	E127	•	GLU	•	GLY
•	V128	•	ILE	•	THR
•	V129	•	GLU	•	ILE
•	G130	•	VAL	•	GLU
•	T131	•	G71	•	VAL
•	C132	•	V72	•	LEU
•	T133	•	P73	•	VAL
•	S134	•	P74	•	PRO
•	L135	•	T75	•	GLY
•	G136	•	A76	•	GLY
•	V137	•	E77	•	GLU
•	T138	•	L78	•	ALA
•	I139	•	I79	•	ASN
•	E140	•	K30	•	PRO
		•	D81	•	GLY
		•	E82	•	PRO
		•	A83	•	PRO
		•	G84	•	LEU
		•	F85	•	GLY
		•	E86	•	PRO
		•	T87	•	GLU
		•	G88	•	LEU
		•	S89	•	GLY
		•	G90	•	PRO
		•	E91	•	THR
		•	P92	•	PRO
		•	Q93	•	VAL
		•	E94	•	ASP
		•	D95	•	VAL
		•	F96	•	GLN
		•	V97	•	ALA
		•	A98	•	VAL
			D99		VAL
			L100		GLN
			S101		GLU
			V102		ILE
		•	D103	•	ASN
		•	Q104	•	ASP
		•	V105	•	GLN
		•	K106	•	THR
		•	Q107	•	ALA
		•	I108	•	ALA
		•	A109	•	PHE
		•	E110	•	ASP
		•	Q111	•	GLY
		•	K112	•	THR
		•	H113	•	GLU
		•	P114	•	VAL
		•	D115	•	PRO
		•	L116	•	VAL
		•	L117	•	THR
		•	S118	•	VAL
		•	Y119	•	LYS
		•	D120	•	TYR
		•	L121	•	ASP
		•	T122	•	ASP
		•	N123	•	ASP
		•	A124	•	GLY



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 90.1 (49.67-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.197 , 0.237 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, PO2, CD, 5AA, DCZ, OMU, UR3, 2OP, 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	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.53	0/83	0.82	0/119
4	A	0.33	0/1786	0.64	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.29	0/241	0.45	0/324
11	H	0.34	0/1287	0.63	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.35	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.62	0/1999
17	O	0.34	0/874	0.59	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.37	0/749	0.68	0/1005
20	R	0.35	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	0/875
22	T	0.32	0/958	0.65	1/1289 (0.1%)
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.51	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.37	0/589	0.65	0/787
29	1	0.41	0/438	0.64	0/578
30	2	0.32	0/401	0.55	0/529
31	3	0.38	0/771	0.59	0/1024
32	I	0.29	0/526	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.37	0/98775	0.67	22/147696 (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
1	0	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.50	130.40	109.50
1	0	1942	A	C5'-C4'-C3'	7.87	128.58	116.00
2	9	3039	U	N1-C1'-C2'	6.80	122.84	114.00
1	0	871	G	C5'-C4'-O4'	-6.76	100.98	109.10
1	0	1819	G	C5'-C4'-C3'	6.21	125.94	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	189	A	Sidechain
1	0	26	U	Sidechain
1	0	333	G	Sidechain
1	0	48	A	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	0	59021	0	29813	777	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	158	1
6	C	1859	0	1816	111	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	78	0
9	F	890	0	843	51	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	51	1
14	L	1118	0	1076	53	0
15	M	1560	0	1568	62	0
16	N	1445	0	1401	109	0
17	O	865	0	873	29	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	50	0
23	U	410	0	364	21	0
24	V	499	0	511	34	0
25	W	1196	0	1137	95	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	53	0
28	Z	578	0	539	24	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	58	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	3	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	9	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	4	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0
38	Z	30	0	0	2	0
All	All	99060	0	59975	2235	3

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 15.

The worst 5 of 2235 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1160:G:H5'	1:O:1161:A:H5'	1.26	1.12
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:O:156:C:H5''	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:O:1171:A:N3	1:O:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	7	13
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	8	16
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	34	57
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	1	0
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	25	47
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	3	5
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	8	15
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	11	22
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	6	11
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	11	22
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	4	6
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	17	35
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	11	22
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	7	14
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	4	6
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	22	43
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	5	9
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2	2

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	6	12
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100	100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	9	19

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	21	42
5	B	282/283 (100%)	265 (94%)	17 (6%)	19	39
6	C	193/193 (100%)	176 (91%)	17 (9%)	10	19
7	D	117/148 (79%)	112 (96%)	5 (4%)	29	54
8	E	152/156 (97%)	148 (97%)	4 (3%)	46	72
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	88
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	27	52
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	26
13	K	106/106 (100%)	101 (95%)	5 (5%)	26	50
14	L	113/127 (89%)	107 (95%)	6 (5%)	22	45
15	M	158/158 (100%)	151 (96%)	7 (4%)	28	53

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	63
17	O	93/94 (99%)	90 (97%)	3 (3%)	39	65
18	P	113/117 (97%)	109 (96%)	4 (4%)	36	62
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	59
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	72
21	S	71/74 (96%)	69 (97%)	2 (3%)	43	69
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	59
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	78
25	W	130/130 (100%)	124 (95%)	6 (5%)	27	51
26	X	66/74 (89%)	61 (92%)	5 (8%)	13	26
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	27
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	74
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	59
32	I	58/130 (45%)	57 (98%)	1 (2%)	60	81
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	28	53

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	46	ILE
14	L	35	ARG
27	Y	174	VAL
12	J	74	ARG
13	K	7	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	170	ASN
19	Q	16	ASN
30	2	41	HIS
16	N	40	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	P	66	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	250 (8%)	33 (1%)

5 of 250 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1692	C
1	0	2726	U
1	0	1450	C
1	0	1563	G

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	0	2621	1	17,21,22	1.64	3 (17%)	20,30,33	5.44	4 (20%)
1	1MA	0	628	1	15,25,26	0.78	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1,35	14,22,23	1.02	1 (7%)	14,31,34	1.15	1 (7%)
1	OMG	0	2588	1,3	18,26,27	1.10	2 (11%)	20,38,41	2.57	4 (20%)
1	UR3	0	2619	1	14,22,23	0.86	1 (7%)	15,32,35	0.56	0
3	5AA	4	76	1,3	18,26,27	0.74	0	15,38,41	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1,35	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.95	1.48	1.52
1	0	2588	OMG	C6-N1	3.45	1.39	1.33
1	0	2621	PSU	C4-N3	3.03	1.38	1.33
1	0	2587	OMU	C4-N3	2.78	1.37	1.33
1	0	2621	PSU	C2-N1	2.66	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.18	114.77	128.43
1	0	2621	PSU	C4-N3-C2	14.43	127.32	115.14
1	0	2588	OMG	C5-C6-N1	-8.58	111.70	123.43
1	0	2621	PSU	C5-C4-N3	-8.36	114.59	125.36
1	0	2588	OMG	C6-N1-C2	5.77	125.09	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
3	4	76	5AA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:A	O3'	175:C	P	8.45

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	0.03	65 (2%) 59 53	24, 51, 98, 161	0
2	9	122/122 (100%)	0.19	4 (3%) 46 39	46, 68, 96, 153	0
3	4	4/8 (50%)	-0.08	0 100 100	42, 42, 46, 46	0
4	A	237/240 (98%)	0.51	15 (6%) 20 15	31, 55, 94, 120	0
5	B	337/338 (99%)	0.97	32 (9%) 8 5	33, 65, 94, 103	0
6	C	246/246 (100%)	-0.01	5 (2%) 65 60	26, 51, 75, 86	0
7	D	140/177 (79%)	2.30	65 (46%) 0 0	64, 110, 134, 141	0
8	E	172/178 (96%)	1.66	54 (31%) 0 0	50, 81, 105, 115	0
9	F	119/120 (99%)	0.81	19 (15%) 1 1	57, 81, 107, 122	0
10	G	29/348 (8%)	2.93	17 (58%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	0.91	17 (10%) 6 4	42, 63, 94, 101	0
12	J	142/145 (97%)	0.68	4 (2%) 53 46	42, 59, 82, 97	0
13	K	132/132 (100%)	0.83	11 (8%) 11 8	37, 62, 86, 90	0
14	L	145/165 (87%)	0.74	19 (13%) 3 2	28, 74, 118, 131	0
15	M	194/194 (100%)	0.12	2 (1%) 82 80	33, 48, 64, 72	0
16	N	186/187 (99%)	0.83	27 (14%) 2 1	43, 69, 118, 124	0
17	O	115/116 (99%)	0.19	2 (1%) 70 66	43, 61, 79, 89	0
18	P	143/149 (95%)	0.52	5 (3%) 44 36	46, 62, 75, 81	0
19	Q	95/96 (98%)	0.35	2 (2%) 63 58	40, 50, 66, 77	0
20	R	150/155 (96%)	0.19	2 (1%) 77 73	36, 51, 72, 82	0
21	S	81/85 (95%)	0.34	4 (4%) 29 23	48, 65, 85, 94	0
22	T	119/120 (99%)	0.42	7 (5%) 22 17	44, 61, 90, 111	0
23	U	53/66 (80%)	0.97	6 (11%) 5 3	48, 63, 80, 88	0
24	V	65/71 (91%)	1.40	18 (27%) 0 0	59, 83, 117, 124	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.39	1 (0%) 89 88	41, 57, 78, 88	0
26	X	82/92 (89%)	0.79	9 (10%) 5 3	49, 66, 89, 106	0
27	Y	142/241 (58%)	0.50	8 (5%) 24 19	32, 51, 74, 95	0
28	Z	73/83 (87%)	0.25	3 (4%) 37 30	45, 64, 78, 96	0
29	1	56/57 (98%)	-0.10	0 100 100	31, 38, 46, 61	0
30	2	46/50 (92%)	1.64	16 (34%) 0 0	40, 70, 123, 128	0
31	3	92/92 (100%)	0.37	3 (3%) 46 39	37, 60, 74, 89	0
32	I	70/162 (43%)	3.96	58 (82%) 0 0	108, 129, 152, 155	0
All	All	6650/7482 (88%)	0.44	500 (7%) 14 10	24, 58, 109, 161	0

The worst 5 of 500 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	93	GLN	11.8
32	I	133	THR	9.5
24	V	1	THR	8.2
7	D	88	LEU	8.1
32	I	137	VAL	8.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMG	0	2588	24/25	0.90	0.20	30,33,38,40	0
1	UR3	0	2619	21/22	0.92	0.22	33,38,39,42	0
1	1MA	0	628	23/24	0.93	0.21	28,34,37,38	0
1	OMU	0	2587	21/22	0.93	0.17	31,35,40,41	0
3	5AA	4	76	24/25	0.93	0.23	40,44,46,47	0
1	PSU	0	2621	20/21	0.94	0.17	31,34,40,41	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
33	MG	0	8063	1/1	0.30	0.19	71,71,71,71	0
35	NA	0	9184	1/1	0.32	0.89	83,83,83,83	0
33	MG	0	8116	1/1	0.46	0.18	62,62,62,62	0
33	MG	0	8091	1/1	0.50	0.07	79,79,79,79	0
33	MG	0	8068	1/1	0.53	0.07	60,60,60,60	0
35	NA	0	9110	1/1	0.53	0.34	43,43,43,43	0
35	NA	R	9186	1/1	0.56	0.43	78,78,78,78	0
35	NA	0	9177	1/1	0.59	0.45	68,68,68,68	0
35	NA	0	9124	1/1	0.59	0.22	66,66,66,66	0
33	MG	0	8090	1/1	0.60	0.31	65,65,65,65	0
35	NA	0	9102	1/1	0.61	0.25	45,45,45,45	0
36	CL	J	9302	1/1	0.63	0.21	79,79,79,79	0
35	NA	0	9170	1/1	0.64	0.29	49,49,49,49	0
33	MG	0	8103	1/1	0.64	0.26	65,65,65,65	0
35	NA	0	9155	1/1	0.64	0.49	79,79,79,79	0
35	NA	0	9182	1/1	0.64	0.49	81,81,81,81	0
35	NA	0	9129	1/1	0.66	0.25	57,57,57,57	0
33	MG	0	8025	1/1	0.66	0.14	46,46,46,46	0
35	NA	0	9157	1/1	0.67	0.11	73,73,73,73	0
33	MG	0	8058	1/1	0.68	0.16	56,56,56,56	0
33	MG	9	8052	1/1	0.68	0.12	54,54,54,54	0
33	MG	0	8101	1/1	0.69	0.40	72,72,72,72	0
35	NA	0	9105	1/1	0.69	0.26	44,44,44,44	0
36	CL	J	9301	1/1	0.69	0.20	78,78,78,78	0
35	NA	0	9176	1/1	0.69	0.33	49,49,49,49	0
33	MG	0	8059	1/1	0.70	0.15	51,51,51,51	0
33	MG	0	8053	1/1	0.70	0.16	57,57,57,57	0
33	MG	0	8113	1/1	0.70	0.20	52,52,52,52	0
33	MG	0	8034	1/1	0.71	0.13	38,38,38,38	0
33	MG	0	8117	1/1	0.72	0.15	37,37,37,37	0
33	MG	0	8084	1/1	0.72	0.13	38,38,38,38	0
35	NA	0	9111	1/1	0.73	0.21	61,61,61,61	0
36	CL	N	9307	1/1	0.73	0.33	72,72,72,72	0
35	NA	S	9112	1/1	0.73	0.28	73,73,73,73	0
35	NA	0	9121	1/1	0.73	0.82	55,55,55,55	0
35	NA	0	9162	1/1	0.75	0.56	64,64,64,64	0
35	NA	0	9133	1/1	0.76	0.15	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	8056	1/1	0.76	0.10	47,47,47,47	0
36	CL	J	9321	1/1	0.77	0.18	55,55,55,55	0
33	MG	0	8092	1/1	0.77	0.45	90,90,90,90	0
33	MG	0	8021	1/1	0.78	0.17	32,32,32,32	0
33	MG	B	8055	1/1	0.78	0.20	62,62,62,62	0
33	MG	0	8093	1/1	0.78	0.20	66,66,66,66	0
35	NA	0	9181	1/1	0.79	0.35	56,56,56,56	0
35	NA	B	9158	1/1	0.79	0.85	70,70,70,70	0
36	CL	0	9315	1/1	0.79	0.26	80,80,80,80	0
33	MG	0	8049	1/1	0.79	0.43	81,81,81,81	0
33	MG	0	8050	1/1	0.79	0.14	69,69,69,69	0
33	MG	0	8079	1/1	0.79	0.10	29,29,29,29	0
33	MG	0	8088	1/1	0.80	0.15	38,38,38,38	0
33	MG	0	8047	1/1	0.80	0.18	86,86,86,86	0
33	MG	0	8038	1/1	0.80	0.17	32,32,32,32	0
36	CL	3	9304	1/1	0.80	0.12	61,61,61,61	0
33	MG	0	8033	1/1	0.80	0.11	38,38,38,38	0
35	NA	0	9144	1/1	0.80	0.14	33,33,33,33	0
35	NA	0	9142	1/1	0.81	0.26	47,47,47,47	0
35	NA	0	9126	1/1	0.81	0.17	41,41,41,41	0
33	MG	9	8095	1/1	0.81	0.10	77,77,77,77	0
33	MG	0	8111	1/1	0.82	0.09	52,52,52,52	0
35	NA	0	9101	1/1	0.82	0.25	40,40,40,40	0
35	NA	0	9113	1/1	0.82	0.36	67,67,67,67	0
33	MG	0	8018	1/1	0.82	0.16	42,42,42,42	0
35	NA	0	9161	1/1	0.82	0.22	56,56,56,56	0
35	NA	0	9125	1/1	0.82	0.22	59,59,59,59	0
33	MG	0	8006	1/1	0.82	0.09	37,37,37,37	0
33	MG	0	8023	1/1	0.82	0.24	52,52,52,52	0
33	MG	0	8099	1/1	0.82	0.17	53,53,53,53	0
33	MG	0	8044	1/1	0.83	0.13	55,55,55,55	0
33	MG	0	8104	1/1	0.83	0.17	55,55,55,55	0
33	MG	0	8008	1/1	0.83	0.08	37,37,37,37	0
35	NA	0	9117	1/1	0.84	0.26	61,61,61,61	0
35	NA	0	9171	1/1	0.84	0.21	52,52,52,52	0
35	NA	0	9169	1/1	0.84	0.33	60,60,60,60	0
35	NA	C	9104	1/1	0.84	0.14	40,40,40,40	0
33	MG	K	8069	1/1	0.84	0.09	52,52,52,52	0
33	MG	0	8003	1/1	0.84	0.15	31,31,31,31	0
33	MG	Y	8109	1/1	0.84	0.34	44,44,44,44	0
35	NA	0	9139	1/1	0.84	0.16	31,31,31,31	0
35	NA	0	9173	1/1	0.84	0.22	62,62,62,62	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8071	1/1	0.85	0.18	66,66,66,66	0
33	MG	0	8032	1/1	0.85	0.20	41,41,41,41	0
33	MG	0	8045	1/1	0.85	0.19	73,73,73,73	0
33	MG	0	8007	1/1	0.85	0.11	27,27,27,27	0
35	NA	0	9164	1/1	0.85	0.28	53,53,53,53	0
35	NA	9	9151	1/1	0.86	0.14	64,64,64,64	0
36	CL	L	9310	1/1	0.86	0.16	63,63,63,63	0
33	MG	0	8082	1/1	0.86	0.16	76,76,76,76	0
35	NA	H	9122	1/1	0.86	0.17	72,72,72,72	0
33	MG	3	8078	1/1	0.86	0.10	43,43,43,43	0
33	MG	0	8072	1/1	0.86	0.26	60,60,60,60	0
35	NA	0	9131	1/1	0.86	0.20	41,41,41,41	0
35	NA	0	9156	1/1	0.86	0.32	49,49,49,49	0
33	MG	0	8026	1/1	0.87	0.10	24,24,24,24	0
33	MG	0	8057	1/1	0.87	0.15	42,42,42,42	0
37	CD	U	9201	1/1	0.87	0.11	74,74,74,74	0
33	MG	0	8064	1/1	0.87	0.15	30,30,30,30	0
35	NA	0	9135	1/1	0.87	0.40	52,52,52,52	0
35	NA	R	9138	1/1	0.88	0.14	63,63,63,63	0
36	CL	0	9311	1/1	0.88	0.16	53,53,53,53	0
35	NA	0	9119	1/1	0.88	0.10	44,44,44,44	0
36	CL	0	9316	1/1	0.88	0.31	66,66,66,66	0
35	NA	0	9174	1/1	0.88	0.35	62,62,62,62	0
34	K	0	9003	1/1	0.88	0.20	64,64,64,64	0
35	NA	0	9166	1/1	0.88	0.12	69,69,69,69	0
33	MG	0	8009	1/1	0.88	0.13	30,30,30,30	0
35	NA	0	9141	1/1	0.89	0.10	45,45,45,45	0
35	NA	0	9123	1/1	0.89	0.30	44,44,44,44	0
33	MG	0	8080	1/1	0.89	0.18	41,41,41,41	0
35	NA	0	9179	1/1	0.89	0.29	70,70,70,70	0
35	NA	9	9183	1/1	0.89	0.14	60,60,60,60	0
35	NA	H	9109	1/1	0.89	0.13	34,34,34,34	0
35	NA	0	9149	1/1	0.89	0.18	38,38,38,38	0
33	MG	0	8096	1/1	0.89	0.15	53,53,53,53	0
35	NA	0	9185	1/1	0.89	0.37	51,51,51,51	0
35	NA	0	9165	1/1	0.89	0.23	47,47,47,47	0
33	MG	0	8100	1/1	0.89	0.44	70,70,70,70	0
35	NA	R	9137	1/1	0.89	0.15	44,44,44,44	0
33	MG	0	8037	1/1	0.89	0.11	45,45,45,45	0
35	NA	Q	9148	1/1	0.89	0.21	38,38,38,38	0
33	MG	0	8108	1/1	0.90	0.11	58,58,58,58	0
33	MG	0	8070	1/1	0.90	0.10	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8077	1/1	0.90	0.09	28,28,28,28	0
35	NA	0	9178	1/1	0.90	0.48	57,57,57,57	0
33	MG	0	8036	1/1	0.90	0.13	35,35,35,35	0
33	MG	0	8027	1/1	0.90	0.09	37,37,37,37	0
33	MG	0	8106	1/1	0.90	0.07	54,54,54,54	0
35	NA	A	9145	1/1	0.90	0.20	48,48,48,48	0
35	NA	0	9106	1/1	0.90	0.37	38,38,38,38	0
33	MG	0	8015	1/1	0.90	0.12	33,33,33,33	0
33	MG	0	8081	1/1	0.90	0.16	52,52,52,52	0
33	MG	0	8013	1/1	0.91	0.19	33,33,33,33	0
33	MG	0	8016	1/1	0.91	0.29	50,50,50,50	0
33	MG	0	8107	1/1	0.91	0.10	53,53,53,53	0
36	CL	0	9317	1/1	0.91	0.09	61,61,61,61	0
33	MG	0	8014	1/1	0.91	0.07	43,43,43,43	0
37	CD	1	9202	1/1	0.91	0.07	62,62,62,62	0
33	MG	0	8115	1/1	0.91	0.09	57,57,57,57	0
33	MG	0	8085	1/1	0.91	0.19	72,72,72,72	0
33	MG	0	8030	1/1	0.91	0.17	35,35,35,35	0
35	NA	0	9127	1/1	0.91	0.12	42,42,42,42	0
36	CL	Y	9320	1/1	0.91	0.12	52,52,52,52	0
33	MG	0	8086	1/1	0.91	0.12	50,50,50,50	0
33	MG	0	8002	1/1	0.91	0.14	39,39,39,39	0
33	MG	4	8118	1/1	0.91	0.13	41,41,41,41	0
33	MG	T	8073	1/1	0.92	0.13	59,59,59,59	0
33	MG	0	8022	1/1	0.92	0.09	35,35,35,35	0
33	MG	0	8061	1/1	0.92	0.08	37,37,37,37	0
35	NA	0	9172	1/1	0.92	0.26	62,62,62,62	0
33	MG	0	8001	1/1	0.92	0.11	35,35,35,35	0
33	MG	0	8094	1/1	0.92	0.11	73,73,73,73	0
35	NA	J	9146	1/1	0.92	0.08	42,42,42,42	0
33	MG	0	8010	1/1	0.92	0.11	28,28,28,28	0
33	MG	0	8060	1/1	0.92	0.23	46,46,46,46	0
36	CL	B	9319	1/1	0.92	0.22	55,55,55,55	0
33	MG	0	8041	1/1	0.92	0.25	79,79,79,79	0
34	K	0	9002	1/1	0.92	0.12	48,48,48,48	0
35	NA	0	9136	1/1	0.92	0.09	55,55,55,55	0
33	MG	0	8119	1/1	0.92	0.20	62,62,62,62	0
33	MG	0	8046	1/1	0.92	0.09	59,59,59,59	0
33	MG	0	8035	1/1	0.92	0.12	49,49,49,49	0
35	NA	0	9163	1/1	0.92	0.20	65,65,65,65	0
35	NA	0	9140	1/1	0.93	0.26	47,47,47,47	0
35	NA	0	9134	1/1	0.93	0.15	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CD	O	9205	1/1	0.93	0.05	143,143,143,143	0
35	NA	0	9130	1/1	0.93	0.12	45,45,45,45	0
35	NA	0	9115	1/1	0.93	0.14	37,37,37,37	0
35	NA	0	9128	1/1	0.93	0.09	43,43,43,43	0
33	MG	0	8011	1/1	0.93	0.19	20,20,20,20	0
35	NA	0	9114	1/1	0.93	0.21	64,64,64,64	0
36	CL	A	9309	1/1	0.93	0.25	61,61,61,61	0
33	MG	0	8114	1/1	0.93	0.07	56,56,56,56	0
35	NA	0	9108	1/1	0.93	0.10	49,49,49,49	0
33	MG	0	8075	1/1	0.93	0.16	57,57,57,57	0
33	MG	0	8012	1/1	0.93	0.13	32,32,32,32	0
36	CL	0	9313	1/1	0.94	0.13	60,60,60,60	0
33	MG	0	8089	1/1	0.94	0.10	56,56,56,56	0
33	MG	0	8005	1/1	0.94	0.19	36,36,36,36	0
36	CL	0	9303	1/1	0.94	0.12	53,53,53,53	0
33	MG	0	8031	1/1	0.94	0.13	30,30,30,30	0
33	MG	0	8051	1/1	0.94	0.08	72,72,72,72	0
35	NA	0	9152	1/1	0.94	0.50	61,61,61,61	0
33	MG	0	8083	1/1	0.94	0.09	42,42,42,42	0
36	CL	0	9314	1/1	0.94	0.11	49,49,49,49	0
36	CL	0	9312	1/1	0.94	0.28	59,59,59,59	0
33	MG	A	8066	1/1	0.94	0.06	66,66,66,66	0
35	NA	0	9168	1/1	0.94	0.08	49,49,49,49	0
33	MG	0	8102	1/1	0.94	0.10	58,58,58,58	0
33	MG	0	8098	1/1	0.94	0.10	47,47,47,47	0
35	NA	0	9116	1/1	0.94	0.17	42,42,42,42	0
35	NA	0	9175	1/1	0.94	0.34	52,52,52,52	0
35	NA	0	9120	1/1	0.95	0.26	52,52,52,52	0
35	NA	0	9103	1/1	0.95	0.26	43,43,43,43	0
35	NA	0	9107	1/1	0.95	0.17	46,46,46,46	0
35	NA	0	9150	1/1	0.95	0.23	42,42,42,42	0
33	MG	0	8028	1/1	0.95	0.18	41,41,41,41	0
33	MG	0	8040	1/1	0.95	0.14	56,56,56,56	0
33	MG	0	8020	1/1	0.95	0.13	31,31,31,31	0
33	MG	0	8097	1/1	0.95	0.09	40,40,40,40	0
33	MG	0	8048	1/1	0.95	0.07	56,56,56,56	0
35	NA	0	9160	1/1	0.95	0.35	46,46,46,46	0
33	MG	0	8087	1/1	0.95	0.27	59,59,59,59	0
35	NA	0	9167	1/1	0.95	0.07	52,52,52,52	0
33	MG	0	8039	1/1	0.96	0.05	52,52,52,52	0
33	MG	0	8067	1/1	0.96	0.16	49,49,49,49	0
33	MG	0	8042	1/1	0.96	0.06	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	A	8065	1/1	0.96	0.17	45,45,45,45	0
35	NA	0	9159	1/1	0.96	0.24	50,50,50,50	0
36	CL	R	9306	1/1	0.96	0.13	57,57,57,57	0
35	NA	M	9147	1/1	0.96	0.14	25,25,25,25	0
33	MG	0	8110	1/1	0.96	0.15	32,32,32,32	0
36	CL	0	9322	1/1	0.96	0.18	77,77,77,77	0
35	NA	L	9180	1/1	0.96	0.46	51,51,51,51	0
33	MG	0	8043	1/1	0.96	0.11	47,47,47,47	0
33	MG	0	8062	1/1	0.96	0.07	51,51,51,51	0
33	MG	0	8112	1/1	0.97	0.07	39,39,39,39	0
37	CD	Z	9203	1/1	0.97	0.09	67,67,67,67	0
33	MG	0	8004	1/1	0.97	0.09	34,34,34,34	0
35	NA	0	9154	1/1	0.97	0.14	33,33,33,33	0
33	MG	0	8029	1/1	0.97	0.07	36,36,36,36	0
33	MG	0	8024	1/1	0.97	0.17	39,39,39,39	0
35	NA	0	9153	1/1	0.97	0.19	21,21,21,21	0
33	MG	0	8017	1/1	0.97	0.14	29,29,29,29	0
35	NA	0	9118	1/1	0.97	0.22	62,62,62,62	0
33	MG	2	8076	1/1	0.97	0.14	55,55,55,55	0
35	NA	0	9143	1/1	0.98	0.17	33,33,33,33	0
37	CD	3	9204	1/1	0.98	0.06	64,64,64,64	0
34	K	0	9001	1/1	0.98	0.14	71,71,71,71	0
35	NA	0	9132	1/1	0.98	0.06	34,34,34,34	0
33	MG	0	8054	1/1	0.98	0.10	29,29,29,29	0
33	MG	0	8019	1/1	0.98	0.14	35,35,35,35	0
36	CL	M	9318	1/1	0.98	0.17	47,47,47,47	0
36	CL	O	9308	1/1	0.98	0.27	79,79,79,79	0
36	CL	0	9305	1/1	0.98	0.11	55,55,55,55	0
33	MG	0	8074	1/1	0.99	0.08	37,37,37,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.