



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 01:00 pm GMT

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

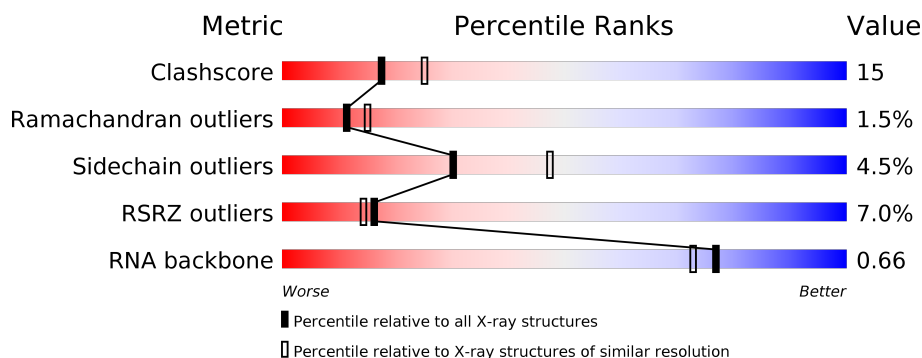
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)
RNA backbone	2636	1023 (2.80-2.00)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div>62% 27% 5% 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57% 32% 11%</div> </div>
3	4	4	<div> <div>50% 50%</div> </div>
4	5	6	<div> <div>17% 17%</div> <div>67% 17%</div> </div>
5	A	240	<div> <div>5%</div> <div>61% 33% 5%</div> </div>
6	B	338	<div> <div>3%</div> <div>57% 39%</div> </div>

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Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

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Mol	Chain	Length	Quality of chain
32	3	92	
33	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
34	MG	0	8047	-	-	-	X
36	NA	0	9152	-	-	-	X
36	NA	0	9184	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 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			

- 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'-R(*CP*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	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 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

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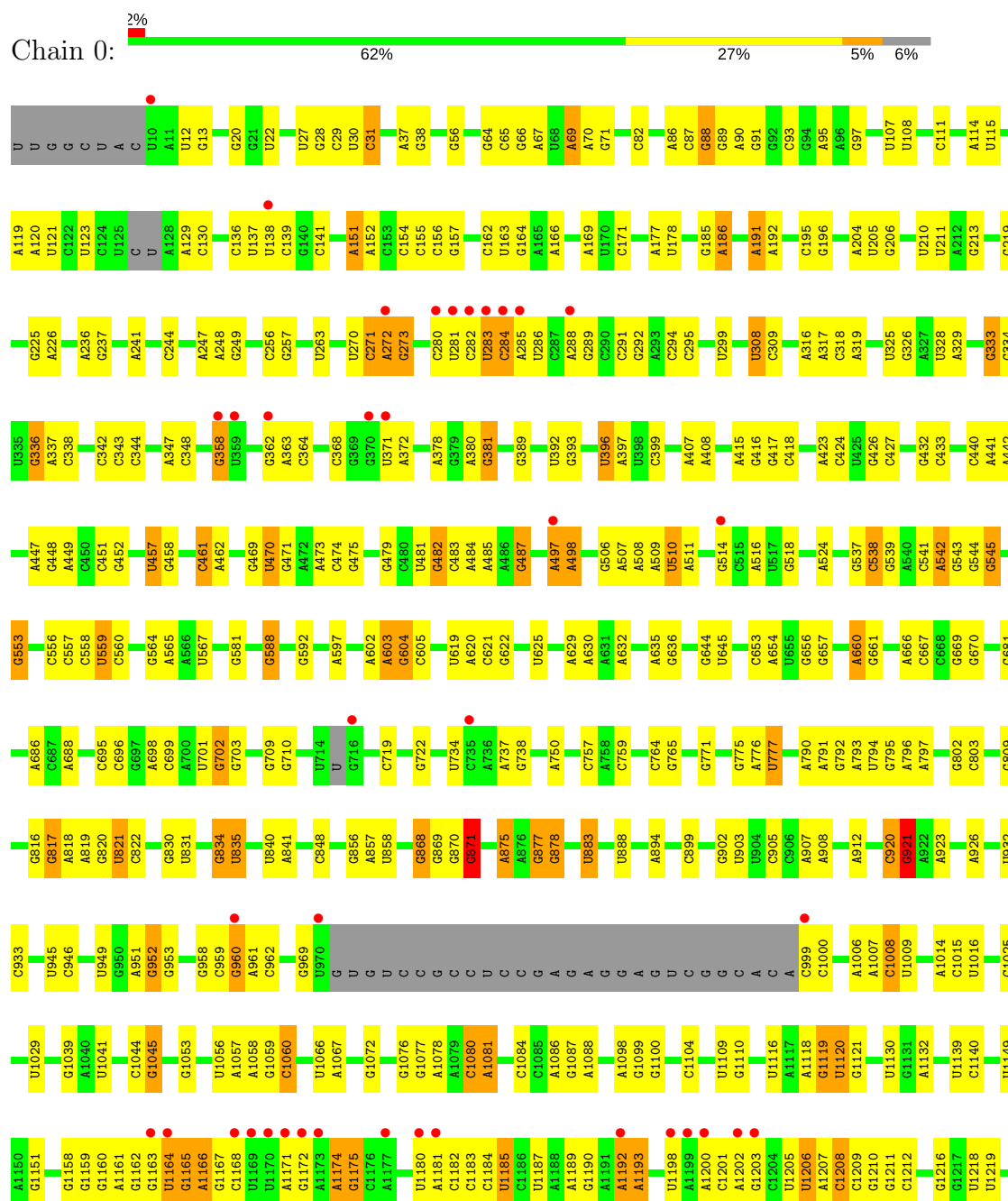
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

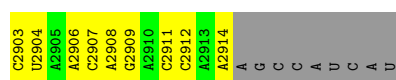
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

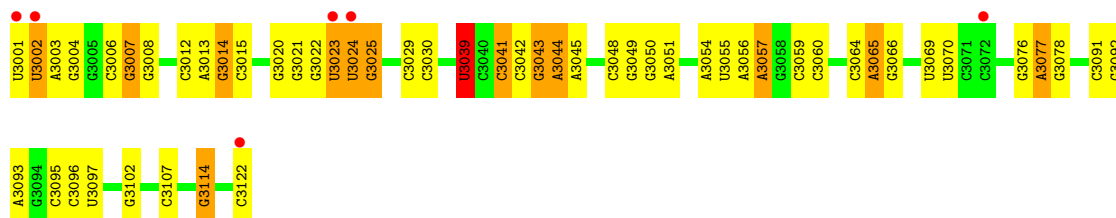
- Molecule 1: 23S ribosomal rna



U2796	U2671	G2564	A2467	C2351	C2243	U1846	U1741	C1633	A1482	C1343	A1232
A2800	C2672	C2565	A2468	A2352	C2248	A1847	G1744	G1634	G1482	U1350	A1233
U2807	U2673	A2568	A2469	A2353	G2249	G1848	G1745	U1635	G1484	U1351	U1234
U2808	C2676	A2569	C2472	A2354	G2250	G1849	U1748	G1636	G1491	A1352	A1236
G2809	A2681	G2578	C2476	A2355	G2251	C1853	U1751	A1637	G1503	C1353	U1237
G2810	C2682	U2586	C2477	A2356	G2252	G1856	G1752	A1641	U1504	C1360	C1238
A2811	A2694	U2587	A2478	G2357	G2253	G1863	G1756	A1642	A1505	G1363	G1239
A2812	G2712	G2588	G2479	A2361	G2254	G1867	U1755	U1654	U1506	A1242	A1243
G2814	G2713	U2589	G2480	A2362	A2255	G1868	G1756	G1655	U1506	A1244	A1245
G2815	U2714	G2590	G2481	A2363	G2256	G1869	U1766	A1657	U1511	C1245	C1246
A2816	U2715	C2591	A2482	A2364	G2257	G1870	U1771	A1658	G1512	A1372	A1250
G2817	G2716	G2592	A2483	G2365	A2258	G1877	U1772	A1666	U1524	C1251	A1252
G2818	G2717	U2599	C2487	A2369	U2265	G1878	U1773	A1667	G1525	U1378	C1253
G2819	C2718	A2600	A2490	A2372	A2266	U1879	G1773	A1668	A1528	A1407	A1261
A2820	A2719	G2601	G2491	U2373	G2270	A1881	U1777	U1669	C1529	U1408	U1266
C2821	G2720	G2602	U2492	A2374	G2271	C1882	A1778	A1670	G1535	G1409	C1267
C2824	U2721	C2493	C2493	G2375	G2272	U1883	A1779	C1679	C1536	C1384	C1268
G2825	U2724	U2607	C2502	C2376	A2291	G1884	U1783	C1680	G1552	A1406	A1261
G2826	G2725	C2608	A2503	U2377	U2297	A1885	U1784	G1681	C1553	A1407	U1266
G2827	U2726	G2613	A2504	U2378	U2297	A1886	G1785	A1682	U1554	U1408	C1267
G2828	U2727	G2614	A2505	U2379	U2297	G1887	U1786	G1683	U1555	G1409	C1268
G2829	U2728	U2609	A2506	A2401	A2301	G1888	U1787	A1684	G1556	A1414	A1278
U2837	U2735	U2610	A2507	A2402	A2302	G1889	U1788	A1685	A1559	G1415	U1279
A2840	U2736	U2611	C2508	G2412	A2303	G1890	U1789	A1686	U	U1418	U1279
A2841	G2737	C2509	A2509	A2413	A2304	A1919	G1795	A1687	U1561	U1418	C1289
G2842	U2738	G2627	A2511	U2414	U2309	A1921	U1796	C1692	U1562	U1422	G1290
G2851	G2743	G2630	U2512	A2415	C2313	A1922	A1797	C1700	C1574	C1423	A1294
G2852	U2749	U2631	C2515	U2416	U2317	G1926	C1798	A1701	C1575	G1426	U1298
U2853	G2750	G2632	G2516	G2417	C2317	A1927	G1799	U1702	G1589	A1427	G1299
G2856	G2761	A2633	A2521	U2418	U2320	C1928	U1801	A1716	U1597	U1435	U1306
C2857	C2762	G2634	A2522	U2419	A2321	G1929	U1802	A1717	A1598	U1440	A1307
U2858	U2767	A2637	G2524	G2420	A2324	G1940	U1803	U1722	G1451	G1441	A1308
G2862	A2768	G2642	G2525	U2421	C2324	A1941	U1804	G1723	C1452	U1442	G1311
G2863	C2769	U2643	G2526	G2422	U2325	C1942	U1805	U1724	G1453	U1454	G1312
G2864	G2770	C2644	C2527	G2423	U2326	G1943	U1806	G1725	G1604	G1314	G1315
U2866	A2776	U2645	U2531	C2424	C2329	C1944	U1807	A1606	A1458	G1325	G1325
G2867	G2777	A2648	A2532	U2425	U2330	G1947	U1808	A1607	C1462	A1328	A1328
G2876	A2778	U2649	C2533	C2426	G2333	G1948	U1809	A1615	C1463	U1333	U1333
U2877	G2779	U2650	U2534	U2427	C2334	G1949	U1810	U1736	U1473	C1334	C1334
U2878	C2780	G2651	U2535	U2428	U2335	G1950	U1811	A1737	C1474	G1340	G1340
A2879	U2781	A2653	C2537	G2429	G2336	G1951	U1812	A1738	A1630	U1478	C1342
G2883	G2782	U2654	U2538	G2430	U2337	U	U1813	U1739	U1627	C1477	A1341
G2884	A2783	U2661	U2541	G2431	G2338	A	U1814	A1739	A1628	C1478	A1341
G2885	U2784	G2662	C2542	U2432	U2339	A	U1815	A1740	G1627	U1478	C1342
G2886	G2785	U2663	C2543	A2456	C	A	U1816	A1741	A1629	U1478	C1342
A2890	U2786	A2664	C2544	U2457	U	U	U1817	A1742	A1630	U1478	C1342
C2894	C2787	A	C2545	G2462	A	U	U1818	A1743	A1631	U1478	C1342
G2895	A2793	U	A2546	A	A	A	U1819	A1744	A1632	U1478	C1342
A2896	G2794	G2667	G2344	A2465	G2345	A	U1820	A1745	A1633	U1478	C1342
G2897	C2795	G2670	C2346	C2466	C2346	C	U1821	A1746	A1634	U1478	C1342



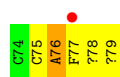
• Molecule 2: 5S ribosomal RNA



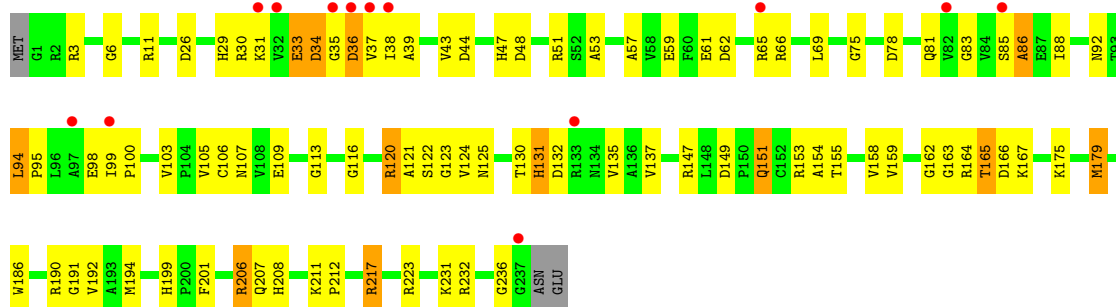
• Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

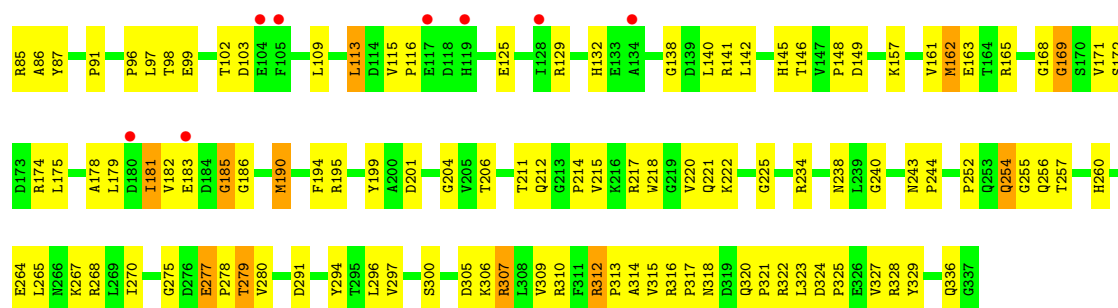


• Molecule 5: 50S ribosomal protein L2P



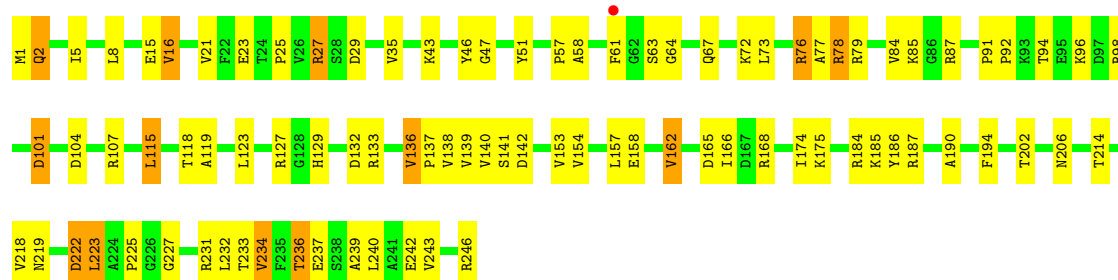
• Molecule 6: 50S ribosomal protein L3P





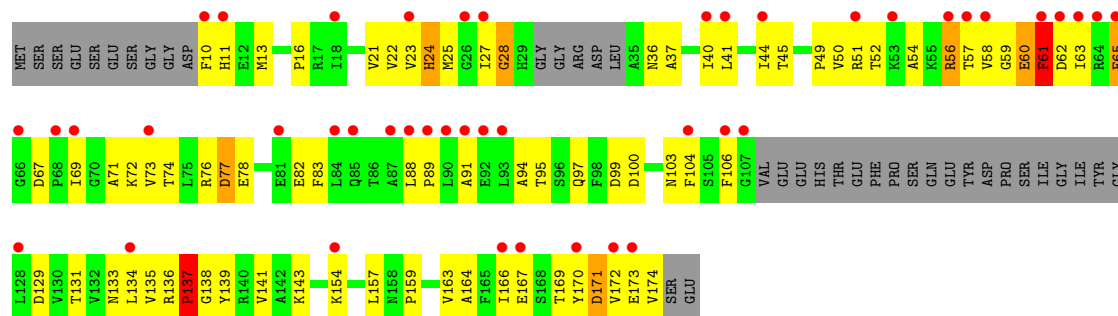
• Molecule 7: 50S ribosomal protein L4E

Chain C: 63% 31% 5%



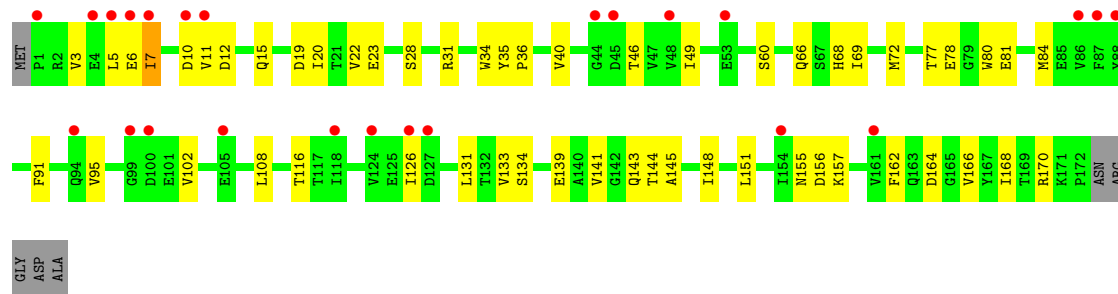
• Molecule 8: 50S ribosomal protein L5P

Chain D: 25% 36% 38% 21%



• Molecule 9: 50S ribosomal protein L6P

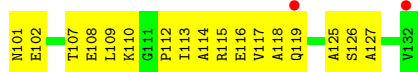
Chain E: 13% 66% 30%



• Molecule 10: 50S ribosomal protein L7AE



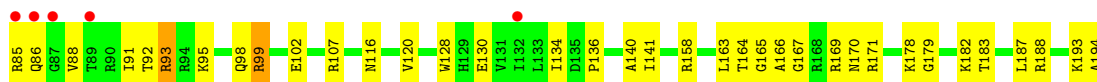
• Molecule 14: 50S ribosomal protein L14P



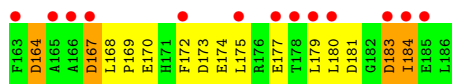
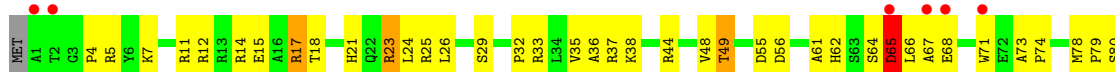
• Molecule 15: 50S ribosomal protein L15P



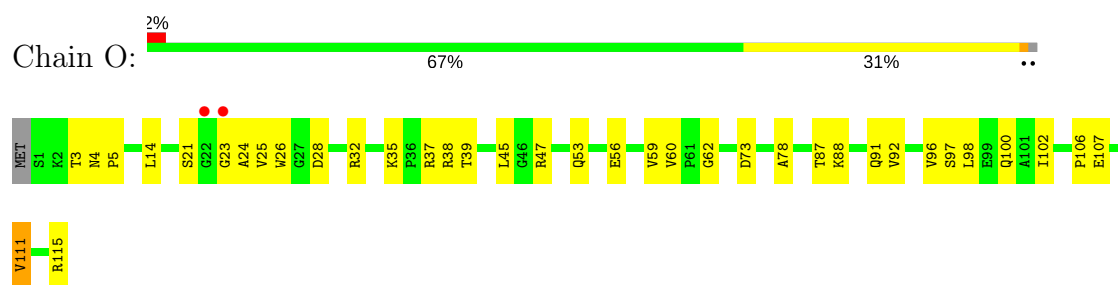
• Molecule 16: 50S Ribosomal Protein L15E



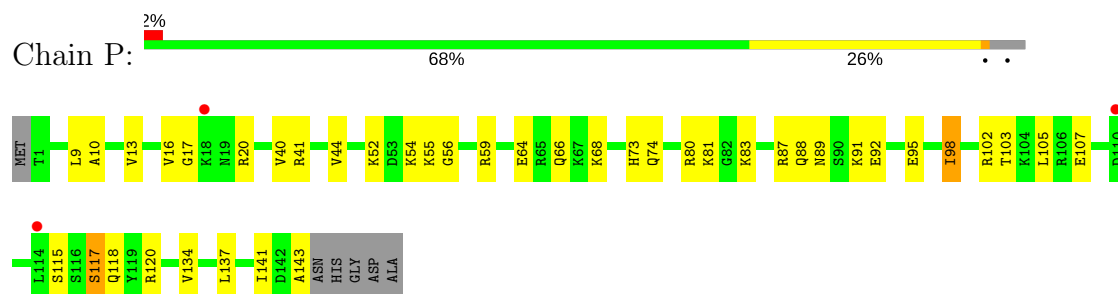
• Molecule 17: 50S ribosomal protein L18P



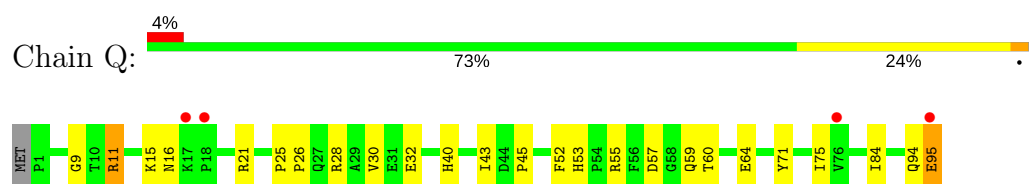
• Molecule 18: 50S ribosomal protein L18e



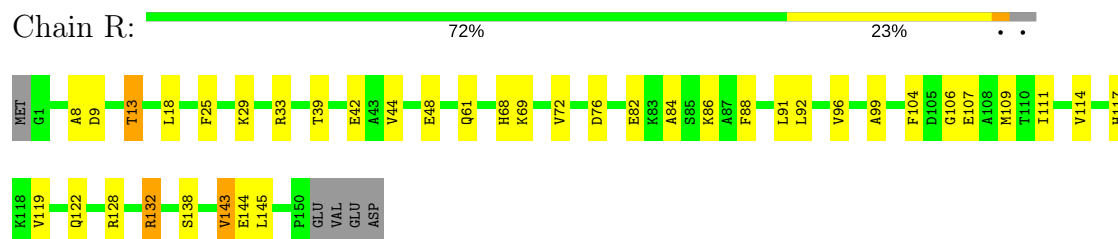
- Molecule 19: 50S ribosomal protein L19E



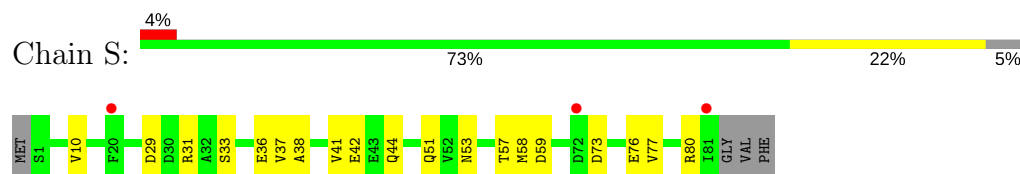
- Molecule 20: 50S ribosomal protein L21e



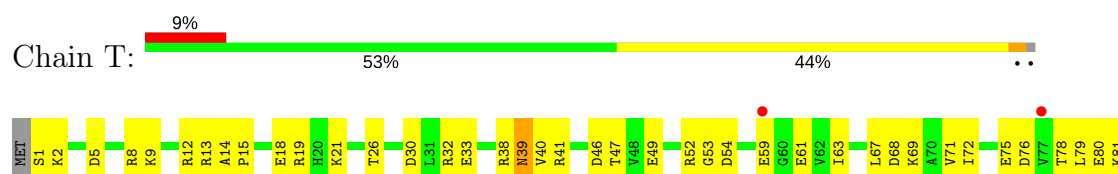
- Molecule 21: 50S ribosomal protein L22P



- Molecule 22: 50S ribosomal protein L23P



- Molecule 23: 50S ribosomal protein L24P

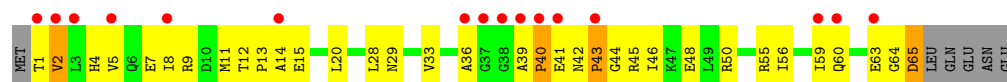




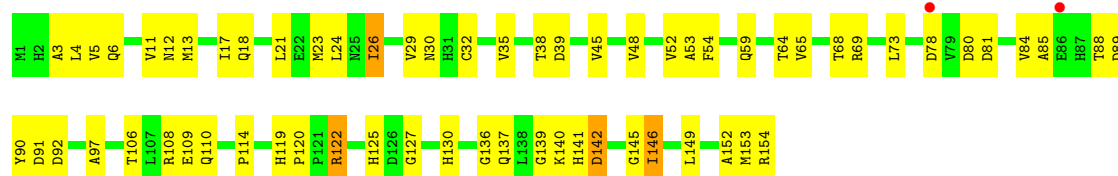
- Molecule 24: 50S ribosomal protein L24E



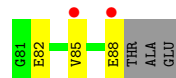
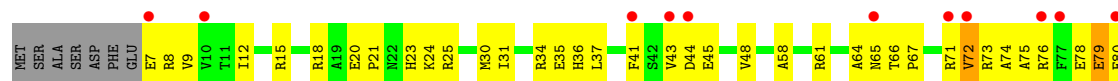
- Molecule 25: 50S ribosomal protein L29P



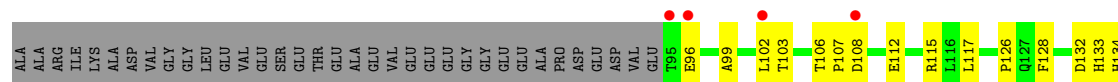
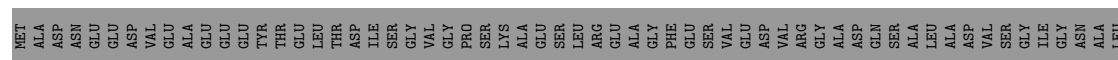
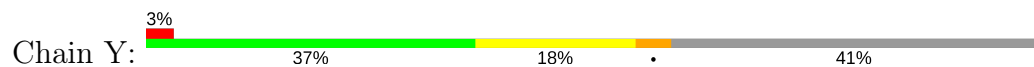
- Molecule 26: 50S ribosomal protein L30P



- Molecule 27: 50S ribosomal protein L31e



- Molecule 28: 50S ribosomal protein L32E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, 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	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (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	0	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	22	U	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 15.

The worst 5 of 2220 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04

There are no symmetry-related clashes.

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	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	13	18
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	11	15
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	21	31
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	6	6
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	6	6
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	5	4
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	21	31
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	12	17
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	31	44
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	2	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	10	13
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	6	7
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	22
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	5	4
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	11	15

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER

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	
5	A	179/182 (98%)	165 (92%)	14 (8%)	14	21
6	B	282/283 (100%)	267 (95%)	15 (5%)	25	40
7	C	193/193 (100%)	173 (90%)	20 (10%)	8	11
8	D	117/148 (79%)	112 (96%)	5 (4%)	32	49
9	E	152/156 (97%)	146 (96%)	6 (4%)	35	54
10	F	93/94 (99%)	91 (98%)	2 (2%)	55	74
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	36	55
13	J	118/121 (98%)	108 (92%)	10 (8%)	12	18
14	K	106/106 (100%)	101 (95%)	5 (5%)	29	45
15	L	113/127 (89%)	110 (97%)	3 (3%)	48	68
16	M	158/158 (100%)	153 (97%)	5 (3%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	149/150 (99%)	142 (95%)	7 (5%)	29	45
18	O	93/94 (99%)	92 (99%)	1 (1%)	76	88
19	P	113/117 (97%)	110 (97%)	3 (3%)	48	68
20	Q	79/80 (99%)	75 (95%)	4 (5%)	26	42
21	R	117/122 (96%)	114 (97%)	3 (3%)	49	70
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	36	55
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	58	77
26	W	130/130 (100%)	124 (95%)	6 (5%)	29	46
27	X	66/74 (89%)	63 (96%)	3 (4%)	30	47
28	Y	120/196 (61%)	109 (91%)	11 (9%)	10	15
29	Z	60/68 (88%)	59 (98%)	1 (2%)	63	80
30	1	46/47 (98%)	45 (98%)	1 (2%)	55	74
31	2	42/46 (91%)	41 (98%)	1 (2%)	52	72
32	3	79/79 (100%)	77 (98%)	2 (2%)	50	71
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	30	47

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	H	18	GLU
14	K	4	LEU
28	Y	174	VAL
12	H	88	ARG
13	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
19	P	50	GLN
21	R	61	GLN
31	2	16	ASN
19	P	66	GLN

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Mol	Chain	Res	Type
19	P	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1730	G
1	0	2761	A
1	0	1684	A
1	0	1685	A

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

8 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	OMU	0	2587	1	14,22,23	1.00	2 (14%)	18,31,34	3.61	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.08	2 (10%)	22,38,41	2.47	4 (18%)
1	UR3	0	2619	1,38	13,22,23	0.96	0	15,32,35	0.67	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	5.42	4 (20%)
1	1MA	0	628	1,36	16,25,26	1.03	1 (6%)	12,37,40	1.25	1 (8%)
3	PPU	4	76	1,3	17,26,41	0.71	0	16,38,60	1.03	1 (6%)
3	HFA	4	77	3	11,11,12	0.88	1 (9%)	13,13,15	0.73	1 (7%)
4	ACA	5	78	4	7,7,8	2.14	1 (14%)	5,6,8	1.04	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	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1,38	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1
4	ACA	5	78	4	-	0/4/5/6	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	78	ACA	C3-C2	-5.05	1.32	1.52
1	0	2621	PSU	C5-C1'	-4.71	1.48	1.52
1	0	2588	OMG	C8-N7	-2.16	1.30	1.34
1	0	2587	OMU	C6-C5	-2.09	1.33	1.38
3	4	77	HFA	OA-CA	2.13	1.48	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.23	114.56	128.41
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	2588	OMG	C5-C6-N1	-8.29	111.69	123.47
1	0	628	1MA	C2-N3-C4	-3.72	110.83	116.51
1	0	2587	OMU	C5-C4-N3	-3.60	114.82	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	3	0
1	0	2619	UR3	1	0
3	4	76	PPU	1	0
4	5	78	ACA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.63	62 (2%) 60 57	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.24	6 (4%) 29 28	41, 69, 93, 152	0
3	4	2/4 (50%)	-1.10	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	-0.08	1 (25%) 0 0	55, 57, 58, 66	0
5	A	237/240 (98%)	0.33	13 (5%) 25 24	31, 54, 86, 106	0
6	B	337/338 (99%)	0.14	11 (3%) 46 44	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.06	1 (0%) 92 91	27, 49, 70, 87	0
8	D	140/177 (79%)	1.71	44 (31%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.74	24 (13%) 2 2	44, 66, 86, 92	0
10	F	119/120 (99%)	1.00	27 (22%) 0 0	49, 74, 100, 112	0
11	G	29/348 (8%)	2.39	18 (62%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	16 (10%) 7 6	47, 65, 96, 103	0
13	J	142/145 (97%)	-0.01	3 (2%) 63 60	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.15	2 (1%) 73 71	37, 48, 71, 84	0
15	L	145/165 (87%)	0.60	15 (10%) 6 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.52	19 (9%) 7 7	37, 48, 85, 93	0
17	N	186/187 (99%)	0.90	33 (17%) 1 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.16	2 (1%) 70 67	40, 59, 73, 81	0
19	P	143/149 (95%)	0.24	3 (2%) 63 60	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.05	4 (4%) 36 34	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.14	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	3 (3%) 41 40	43, 61, 84, 97	0
23	T	119/120 (99%)	0.67	11 (9%) 9 8	41, 59, 85, 110	0
24	U	53/66 (80%)	0.26	2 (3%) 40 39	42, 56, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.61	16 (24%) 0 0	56, 78, 115, 120	0
26	W	154/154 (100%)	0.02	2 (1%) 77 75	40, 53, 74, 82	0
27	X	82/92 (89%)	0.67	13 (15%) 2 1	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.10	8 (5%) 24 23	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	29 (39%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.44	15 (32%) 0 0	41, 68, 96, 102	0
32	3	92/92 (100%)	0.33	6 (6%) 19 17	41, 61, 73, 86	0
33	I	70/162 (43%)	5.01	57 (81%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.03	466 (7%) 16 14	24, 54, 100, 153	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.4
25	V	1	THR	14.2
33	I	79	ILE	12.3
33	I	76	ALA	12.1
33	I	133	THR	11.9

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACA	5	78	8/9	0.88	0.30	66,72,83,86	0
3	HFA	4	77	11/12	0.95	0.20	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	39,42,45,48	0
1	OMG	0	2588	24/25	0.98	0.13	31,34,39,41	0
1	OMU	0	2587	21/22	0.98	0.13	32,37,40,40	0
3	PPU	4	76	24/38	0.98	0.13	41,44,45,49	0
1	1MA	0	628	23/24	0.98	0.12	32,35,37,38	0
1	PSU	0	2621	20/21	0.98	0.14	36,38,43,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
38	SR	0	9529	1/1	-0.08	0.27	131,131,131,131	0
38	SR	0	9484	1/1	0.32	0.14	149,149,149,149	0
36	NA	0	9184	1/1	0.40	0.41	87,87,87,87	0
38	SR	0	9537	1/1	0.50	0.23	157,157,157,157	0
38	SR	0	9547	1/1	0.52	0.39	194,194,194,194	0
34	MG	0	8047	1/1	0.56	0.54	107,107,107,107	0
36	NA	0	9122	1/1	0.57	0.40	90,90,90,90	0
38	SR	9	9588	1/1	0.59	0.14	143,143,143,143	0
38	SR	B	9521	1/1	0.59	0.63	200,200,200,200	0
34	MG	0	8101	1/1	0.61	0.29	80,80,80,80	0
36	NA	0	9182	1/1	0.63	0.39	90,90,90,90	0
38	SR	0	9501	1/1	0.65	0.20	159,159,159,159	0
34	MG	0	8108	1/1	0.68	0.14	103,103,103,103	0
36	NA	D	9151	1/1	0.70	0.23	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	54,54,54,54	0
36	NA	0	9135	1/1	0.72	0.30	55,55,55,55	0
36	NA	0	9141	1/1	0.74	0.13	73,73,73,73	0
36	NA	9	9183	1/1	0.75	0.38	75,75,75,75	0
35	K	0	9002	1/1	0.75	0.18	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	84,84,84,84	0
36	NA	0	9114	1/1	0.76	0.20	65,65,65,65	0
36	NA	0	9116	1/1	0.77	0.35	52,52,52,52	0
36	NA	0	9152	1/1	0.77	1.03	83,83,83,83	0
36	NA	0	9126	1/1	0.78	0.11	63,63,63,63	0
34	MG	0	8093	1/1	0.79	0.13	49,49,49,49	0
36	NA	J	9146	1/1	0.79	0.11	55,55,55,55	0
36	NA	0	9129	1/1	0.80	0.13	72,72,72,72	0
34	MG	0	8090	1/1	0.80	0.35	68,68,68,68	0
34	MG	0	8092	1/1	0.82	0.34	77,77,77,77	0
34	MG	0	8065	1/1	0.82	0.34	107,107,107,107	0
34	MG	0	8059	1/1	0.83	0.42	84,84,84,84	0
34	MG	0	8052	1/1	0.83	0.25	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9172	1/1	0.83	0.35	76,76,76,76	0
34	MG	0	8037	1/1	0.84	0.10	46,46,46,46	0
34	MG	0	8104	1/1	0.84	0.13	57,57,57,57	0
36	NA	R	9186	1/1	0.84	0.38	80,80,80,80	0
34	MG	0	8107	1/1	0.84	0.17	65,65,65,65	0
34	MG	0	8013	1/1	0.84	0.34	25,25,25,25	0
34	MG	0	8102	1/1	0.85	0.12	68,68,68,68	0
36	NA	0	9158	1/1	0.85	0.44	66,66,66,66	0
36	NA	0	9185	1/1	0.85	0.61	54,54,54,54	0
34	MG	0	8022	1/1	0.85	0.94	112,112,112,112	0
36	NA	0	9132	1/1	0.86	0.22	68,68,68,68	0
36	NA	0	9161	1/1	0.86	0.72	68,68,68,68	0
34	MG	0	8061	1/1	0.86	0.19	87,87,87,87	0
36	NA	0	9169	1/1	0.86	0.39	116,116,116,116	0
36	NA	0	9164	1/1	0.87	0.57	61,61,61,61	0
34	MG	0	8113	1/1	0.87	0.12	52,52,52,52	0
36	NA	0	9102	1/1	0.87	0.22	63,63,63,63	0
36	NA	S	9112	1/1	0.87	0.23	80,80,80,80	0
35	K	0	9001	1/1	0.87	0.31	74,74,74,74	0
34	MG	0	8030	1/1	0.87	0.08	37,37,37,37	0
38	SR	0	9581	1/1	0.87	0.08	130,130,130,130	0
38	SR	0	9500	1/1	0.88	1.54	200,200,200,200	0
34	MG	0	8089	1/1	0.88	0.17	61,61,61,61	0
34	MG	0	8024	1/1	0.88	0.41	86,86,86,86	0
34	MG	5	8118	1/1	0.88	0.34	45,45,45,45	0
34	MG	0	8050	1/1	0.88	0.22	89,89,89,89	0
34	MG	0	8106	1/1	0.88	0.09	51,51,51,51	0
38	SR	0	9539	1/1	0.88	0.38	157,157,157,157	0
34	MG	0	8091	1/1	0.89	0.15	64,64,64,64	0
38	SR	0	9532	1/1	0.89	0.05	120,120,120,120	0
34	MG	0	8072	1/1	0.89	0.65	89,89,89,89	0
36	NA	0	9143	1/1	0.89	0.14	40,40,40,40	0
36	NA	0	9165	1/1	0.89	0.30	45,45,45,45	0
36	NA	0	9140	1/1	0.89	0.15	57,57,57,57	0
34	MG	0	8103	1/1	0.89	0.17	67,67,67,67	0
36	NA	0	9170	1/1	0.89	0.28	77,77,77,77	0
36	NA	0	9166	1/1	0.89	0.09	74,74,74,74	0
38	SR	0	9590	1/1	0.89	0.12	131,131,131,131	0
34	MG	0	8040	1/1	0.90	0.21	92,92,92,92	0
34	MG	0	8058	1/1	0.90	0.21	41,41,41,41	0
34	MG	0	8025	1/1	0.90	0.42	27,27,27,27	0
36	NA	0	9131	1/1	0.90	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9482	1/1	0.90	0.35	135,135,135,135	0
36	NA	0	9128	1/1	0.90	0.15	49,49,49,49	0
34	MG	0	8014	1/1	0.90	0.38	73,73,73,73	0
34	MG	0	8051	1/1	0.90	0.21	36,36,36,36	0
38	SR	9	9503	1/1	0.90	0.05	122,122,122,122	0
36	NA	0	9168	1/1	0.90	0.17	69,69,69,69	0
38	SR	0	9626	1/1	0.91	0.25	154,154,154,154	0
34	MG	0	8055	1/1	0.91	0.31	97,97,97,97	0
36	NA	0	9111	1/1	0.91	0.31	63,63,63,63	0
36	NA	0	9167	1/1	0.91	0.10	65,65,65,65	0
38	SR	0	9504	1/1	0.91	0.11	108,108,108,108	0
36	NA	0	9177	1/1	0.91	0.35	77,77,77,77	0
34	MG	0	8099	1/1	0.91	0.14	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	103,103,103,103	0
38	SR	0	9468	1/1	0.91	0.05	128,128,128,128	0
34	MG	0	8043	1/1	0.91	0.06	52,52,52,52	0
36	NA	0	9174	1/1	0.91	0.38	65,65,65,65	0
36	NA	0	9179	1/1	0.91	0.60	121,121,121,121	0
37	CL	L	9310	1/1	0.92	0.12	58,58,58,58	0
34	MG	0	8094	1/1	0.92	0.50	72,72,72,72	0
36	NA	0	9101	1/1	0.92	0.13	46,46,46,46	0
34	MG	0	8019	1/1	0.92	0.06	51,51,51,51	0
34	MG	0	8063	1/1	0.92	0.10	65,65,65,65	0
38	SR	0	9465	1/1	0.92	0.10	107,107,107,107	0
38	SR	0	9509	1/1	0.92	0.15	95,95,95,95	0
37	CL	A	9309	1/1	0.92	0.19	66,66,66,66	0
34	MG	0	8032	1/1	0.92	0.10	48,48,48,48	0
34	MG	9	8095	1/1	0.92	0.35	55,55,55,55	0
37	CL	J	9301	1/1	0.93	0.18	60,60,60,60	0
36	NA	0	9113	1/1	0.93	0.11	60,60,60,60	0
36	NA	M	9147	1/1	0.93	0.18	42,42,42,42	0
36	NA	0	9159	1/1	0.93	0.35	58,58,58,58	0
36	NA	0	9173	1/1	0.93	0.34	69,69,69,69	0
36	NA	0	9117	1/1	0.93	0.07	51,51,51,51	0
34	MG	0	8085	1/1	0.93	0.21	63,63,63,63	0
36	NA	0	9106	1/1	0.93	0.44	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	59,59,59,59	0
36	NA	0	9171	1/1	0.93	0.31	61,61,61,61	0
36	NA	0	9124	1/1	0.93	0.19	50,50,50,50	0
34	MG	0	8054	1/1	0.93	0.16	63,63,63,63	0
36	NA	0	9175	1/1	0.93	0.33	55,55,55,55	0
36	NA	0	9120	1/1	0.93	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8036	1/1	0.94	0.11	65,65,65,65	0
34	MG	0	8097	1/1	0.94	0.13	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	106,106,106,106	0
38	SR	0	9508	1/1	0.94	0.08	97,97,97,97	0
34	MG	T	8073	1/1	0.94	0.11	43,43,43,43	0
36	NA	0	9157	1/1	0.94	0.18	47,47,47,47	0
36	NA	0	9150	1/1	0.94	0.21	47,47,47,47	0
36	NA	0	9163	1/1	0.94	0.17	73,73,73,73	0
34	MG	2	8076	1/1	0.94	0.17	64,64,64,64	0
36	NA	0	9110	1/1	0.94	0.33	46,46,46,46	0
39	CD	O	9205	1/1	0.94	0.05	132,132,132,132	0
38	SR	0	9570	1/1	0.94	0.07	111,111,111,111	0
36	NA	0	9149	1/1	0.94	0.29	49,49,49,49	0
34	MG	0	8057	1/1	0.94	0.20	77,77,77,77	0
38	SR	0	9522	1/1	0.95	0.04	114,114,114,114	0
36	NA	0	9155	1/1	0.95	0.18	60,60,60,60	0
34	MG	0	8003	1/1	0.95	0.13	35,35,35,35	0
37	CL	0	9317	1/1	0.95	0.06	52,52,52,52	0
34	MG	0	8068	1/1	0.95	0.14	48,48,48,48	0
34	MG	0	8004	1/1	0.95	0.10	35,35,35,35	0
37	CL	0	9322	1/1	0.95	0.38	61,61,61,61	0
36	NA	0	9125	1/1	0.95	0.81	92,92,92,92	0
38	SR	H	9486	1/1	0.95	0.15	125,125,125,125	0
38	SR	0	9517	1/1	0.95	0.06	110,110,110,110	0
34	MG	0	8082	1/1	0.95	0.20	82,82,82,82	0
38	SR	0	9505	1/1	0.95	0.07	106,106,106,106	0
38	SR	0	9483	1/1	0.95	0.06	77,77,77,77	0
37	CL	J	9321	1/1	0.95	0.11	66,66,66,66	0
34	MG	0	8045	1/1	0.95	0.26	72,72,72,72	0
38	SR	0	9560	1/1	0.95	0.08	101,101,101,101	0
34	MG	0	8116	1/1	0.95	0.10	64,64,64,64	0
34	MG	0	8083	1/1	0.95	0.11	53,53,53,53	0
36	NA	C	9104	1/1	0.95	0.16	33,33,33,33	0
38	SR	0	9495	1/1	0.95	0.14	111,111,111,111	0
37	CL	M	9318	1/1	0.95	0.17	41,41,41,41	0
34	MG	0	8098	1/1	0.95	0.07	45,45,45,45	0
34	MG	0	8079	1/1	0.95	0.13	33,33,33,33	0
36	NA	0	9139	1/1	0.95	0.10	43,43,43,43	0
34	MG	0	8029	1/1	0.95	0.22	35,35,35,35	0
34	MG	0	8067	1/1	0.95	0.11	40,40,40,40	0
34	MG	0	8021	1/1	0.95	0.16	56,56,56,56	0
34	MG	0	8070	1/1	0.96	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9162	1/1	0.96	0.15	52,52,52,52	0
37	CL	J	9302	1/1	0.96	0.07	53,53,53,53	0
36	NA	R	9137	1/1	0.96	0.08	36,36,36,36	0
38	SR	F	9595	1/1	0.96	0.16	109,109,109,109	0
36	NA	0	9156	1/1	0.96	0.16	57,57,57,57	0
38	SR	0	9490	1/1	0.96	0.13	116,116,116,116	0
38	SR	0	9530	1/1	0.96	0.11	72,72,72,72	0
34	MG	0	8060	1/1	0.96	0.07	82,82,82,82	0
38	SR	0	9440	1/1	0.96	0.05	72,72,72,72	0
37	CL	Y	9320	1/1	0.96	0.08	47,47,47,47	0
36	NA	0	9178	1/1	0.96	0.45	54,54,54,54	0
38	SR	0	9585	1/1	0.96	0.08	94,94,94,94	0
37	CL	3	9304	1/1	0.96	0.07	61,61,61,61	0
36	NA	0	9107	1/1	0.96	0.40	71,71,71,71	0
38	SR	0	9433	1/1	0.96	0.12	75,75,75,75	0
36	NA	0	9115	1/1	0.96	0.18	41,41,41,41	0
34	MG	0	8042	1/1	0.96	0.11	48,48,48,48	0
34	MG	Y	8109	1/1	0.96	0.12	45,45,45,45	0
34	MG	0	8112	1/1	0.96	0.06	46,46,46,46	0
36	NA	0	9105	1/1	0.96	0.09	44,44,44,44	0
37	CL	N	9307	1/1	0.96	0.16	65,65,65,65	0
38	SR	0	9447	1/1	0.97	0.07	73,73,73,73	0
34	MG	0	8027	1/1	0.97	0.24	36,36,36,36	0
37	CL	0	9316	1/1	0.97	0.26	78,78,78,78	0
34	MG	0	8002	1/1	0.97	0.09	34,34,34,34	0
34	MG	A	8066	1/1	0.97	0.10	57,57,57,57	0
37	CL	0	9311	1/1	0.97	0.15	71,71,71,71	0
38	SR	0	9426	1/1	0.97	0.08	71,71,71,71	0
34	MG	0	8009	1/1	0.97	0.10	21,21,21,21	0
34	MG	0	8114	1/1	0.97	0.47	83,83,83,83	0
38	SR	0	9466	1/1	0.97	0.06	96,96,96,96	0
38	SR	0	9545	1/1	0.97	0.06	85,85,85,85	0
38	SR	A	9437	1/1	0.97	0.10	70,70,70,70	0
37	CL	0	9315	1/1	0.97	0.09	52,52,52,52	0
34	MG	0	8012	1/1	0.97	0.22	39,39,39,39	0
38	SR	0	9601	1/1	0.97	0.06	119,119,119,119	0
38	SR	0	9438	1/1	0.97	0.09	70,70,70,70	0
34	MG	0	8117	1/1	0.97	0.12	46,46,46,46	0
38	SR	0	9446	1/1	0.97	0.07	88,88,88,88	0
34	MG	0	8044	1/1	0.97	0.06	35,35,35,35	0
38	SR	0	9534	1/1	0.97	0.14	111,111,111,111	0
36	NA	0	9127	1/1	0.97	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9442	1/1	0.97	0.10	66,66,66,66	0
38	SR	A	9436	1/1	0.97	0.06	60,60,60,60	0
34	MG	0	8088	1/1	0.97	0.11	28,28,28,28	0
34	MG	0	8046	1/1	0.97	0.05	39,39,39,39	0
36	NA	0	9108	1/1	0.97	0.10	34,34,34,34	0
36	NA	0	9160	1/1	0.97	0.17	46,46,46,46	0
36	NA	0	9138	1/1	0.97	0.07	62,62,62,62	0
38	SR	0	9568	1/1	0.97	0.07	80,80,80,80	0
34	MG	K	8069	1/1	0.97	0.17	25,25,25,25	0
38	SR	0	9405	1/1	0.97	0.16	59,59,59,59	0
38	SR	0	9432	1/1	0.97	0.14	68,68,68,68	0
34	MG	0	8041	1/1	0.97	0.09	55,55,55,55	0
36	NA	0	9134	1/1	0.97	0.10	47,47,47,47	0
34	MG	0	8084	1/1	0.97	0.40	89,89,89,89	0
37	CL	R	9306	1/1	0.97	0.10	45,45,45,45	0
34	MG	0	8110	1/1	0.97	0.11	45,45,45,45	0
38	SR	0	9489	1/1	0.98	0.11	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	47,47,47,47	0
38	SR	0	9464	1/1	0.98	0.05	81,81,81,81	0
38	SR	0	9477	1/1	0.98	0.10	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	78,78,78,78	0
34	MG	0	8001	1/1	0.98	0.19	22,22,22,22	0
38	SR	0	9629	1/1	0.98	0.08	75,75,75,75	0
38	SR	0	9566	1/1	0.98	0.04	80,80,80,80	0
38	SR	9	9481	1/1	0.98	0.08	89,89,89,89	0
34	MG	0	8020	1/1	0.98	0.16	36,36,36,36	0
34	MG	0	8056	1/1	0.98	0.23	44,44,44,44	0
38	SR	0	9454	1/1	0.98	0.10	82,82,82,82	0
38	SR	0	9435	1/1	0.98	0.08	76,76,76,76	0
37	CL	0	9305	1/1	0.98	0.07	61,61,61,61	0
38	SR	0	9427	1/1	0.98	0.12	56,56,56,56	0
38	SR	0	9443	1/1	0.98	0.10	63,63,63,63	0
34	MG	0	8031	1/1	0.98	0.12	49,49,49,49	0
38	SR	0	9475	1/1	0.98	0.13	83,83,83,83	0
38	SR	0	9445	1/1	0.98	0.09	57,57,57,57	0
36	NA	0	9118	1/1	0.98	0.21	66,66,66,66	0
38	SR	0	9506	1/1	0.98	0.04	68,68,68,68	0
36	NA	0	9154	1/1	0.98	0.15	54,54,54,54	0
36	NA	0	9130	1/1	0.98	0.15	50,50,50,50	0
38	SR	0	9461	1/1	0.98	0.06	82,82,82,82	0
34	MG	0	8039	1/1	0.98	0.17	49,49,49,49	0
34	MG	0	8096	1/1	0.98	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9456	1/1	0.98	0.10	67,67,67,67	0
38	SR	0	9469	1/1	0.98	0.05	85,85,85,85	0
38	SR	0	9455	1/1	0.98	0.10	88,88,88,88	0
36	NA	0	9136	1/1	0.98	0.12	34,34,34,34	0
34	MG	0	8005	1/1	0.98	0.06	29,29,29,29	0
38	SR	0	9457	1/1	0.98	0.08	51,51,51,51	0
38	SR	0	9414	1/1	0.98	0.12	57,57,57,57	0
38	SR	0	9441	1/1	0.98	0.07	68,68,68,68	0
34	MG	0	8017	1/1	0.98	0.14	31,31,31,31	0
36	NA	Q	9148	1/1	0.98	0.09	49,49,49,49	0
38	SR	0	9462	1/1	0.98	0.10	74,74,74,74	0
34	MG	0	8080	1/1	0.98	0.17	57,57,57,57	0
38	SR	A	9497	1/1	0.98	0.09	96,96,96,96	0
37	CL	0	9312	1/1	0.99	0.10	57,57,57,57	0
38	SR	0	9478	1/1	0.99	0.06	77,77,77,77	0
34	MG	0	8026	1/1	0.99	0.15	30,30,30,30	0
34	MG	0	8028	1/1	0.99	0.13	37,37,37,37	0
38	SR	0	9428	1/1	0.99	0.07	55,55,55,55	0
37	CL	0	9314	1/1	0.99	0.06	51,51,51,51	0
38	SR	0	9449	1/1	0.99	0.09	67,67,67,67	0
38	SR	0	9473	1/1	0.99	0.03	82,82,82,82	0
38	SR	0	9467	1/1	0.99	0.10	86,86,86,86	0
34	MG	0	8008	1/1	0.99	0.19	16,16,16,16	0
38	SR	0	9410	1/1	0.99	0.14	41,41,41,41	0
38	SR	0	9431	1/1	0.99	0.13	65,65,65,65	0
38	SR	0	9430	1/1	0.99	0.10	49,49,49,49	0
38	SR	0	9515	1/1	0.99	0.14	100,100,100,100	0
37	CL	B	9319	1/1	0.99	0.17	54,54,54,54	0
38	SR	0	9488	1/1	0.99	0.11	86,86,86,86	0
39	CD	1	9202	1/1	0.99	0.05	54,54,54,54	0
38	SR	0	9451	1/1	0.99	0.12	60,60,60,60	0
38	SR	0	9413	1/1	0.99	0.12	49,49,49,49	0
38	SR	0	9408	1/1	0.99	0.12	36,36,36,36	0
36	NA	0	9123	1/1	0.99	0.09	52,52,52,52	0
38	SR	L	9409	1/1	0.99	0.07	37,37,37,37	0
38	SR	0	9425	1/1	0.99	0.15	56,56,56,56	0
38	SR	0	9434	1/1	0.99	0.14	64,64,64,64	0
39	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0
38	SR	1	9419	1/1	0.99	0.09	40,40,40,40	0
38	SR	0	9480	1/1	0.99	0.05	93,93,93,93	0
38	SR	3	9439	1/1	0.99	0.05	72,72,72,72	0
34	MG	0	8015	1/1	0.99	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	SR	0	9417	1/1	0.99	0.08	63,63,63,63	0
38	SR	0	9474	1/1	0.99	0.08	73,73,73,73	0
37	CL	0	9313	1/1	0.99	0.10	59,59,59,59	0
38	SR	1	9460	1/1	0.99	0.10	52,52,52,52	0
37	CL	O	9308	1/1	0.99	0.09	67,67,67,67	0
34	MG	0	8074	1/1	0.99	0.18	27,27,27,27	0
34	MG	0	8038	1/1	0.99	0.25	25,25,25,25	0
37	CL	0	9303	1/1	0.99	0.13	53,53,53,53	0
38	SR	S	9470	1/1	0.99	0.16	101,101,101,101	0
38	SR	0	9411	1/1	0.99	0.14	43,43,43,43	0
38	SR	0	9450	1/1	0.99	0.07	72,72,72,72	0
38	SR	0	9429	1/1	0.99	0.10	72,72,72,72	0
38	SR	0	9453	1/1	0.99	0.06	72,72,72,72	0
38	SR	R	9418	1/1	0.99	0.15	57,57,57,57	0
38	SR	0	9444	1/1	0.99	0.05	55,55,55,55	0
38	SR	0	9422	1/1	0.99	0.10	58,58,58,58	0
38	SR	0	9412	1/1	0.99	0.13	45,45,45,45	0
38	SR	0	9498	1/1	0.99	0.05	63,63,63,63	0
38	SR	B	9458	1/1	0.99	0.05	82,82,82,82	0
38	SR	0	9407	1/1	1.00	0.13	47,47,47,47	0
38	SR	0	9424	1/1	1.00	0.16	49,49,49,49	0
38	SR	0	9448	1/1	1.00	0.07	63,63,63,63	0
38	SR	0	9423	1/1	1.00	0.05	64,64,64,64	0
38	SR	0	9406	1/1	1.00	0.13	35,35,35,35	0
38	SR	0	9415	1/1	1.00	0.10	56,56,56,56	0
38	SR	0	9416	1/1	1.00	0.08	43,43,43,43	0
39	CD	U	9201	1/1	1.00	0.09	53,53,53,53	0
38	SR	0	9420	1/1	1.00	0.17	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.