



wwPDB X-ray Structure Validation Summary Report

May 8, 2014 – 03:42 AM EDT

PDB ID : 3CC2
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors : Gurel, G.; Blaha, G.
Deposited on : 2008-02-23
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

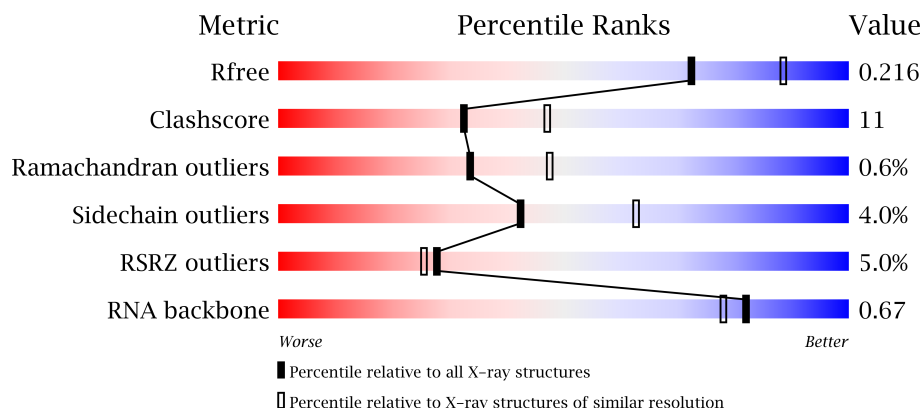
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

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.













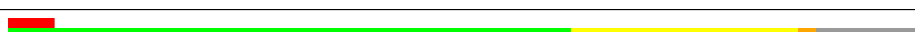
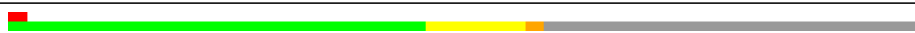





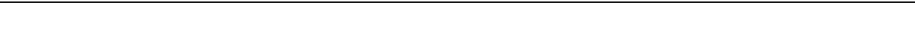
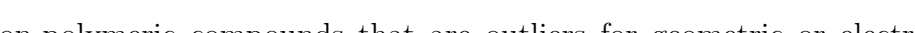

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8007	-	X
32	MG	0	8034	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8049	-	X
32	MG	0	8057	-	X
32	MG	0	8060	-	X
32	MG	0	8066	-	X
32	MG	0	8082	-	X
32	MG	0	8087	-	X
32	MG	0	8101	-	X
32	MG	0	8103	-	X
34	NA	0	8302	-	X
34	NA	0	8306	-	X
34	NA	0	8307	-	X
34	NA	0	8308	-	X
34	NA	0	8311	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8314	-	X
34	NA	0	8318	-	X
34	NA	0	8320	-	X
34	NA	0	8326	-	X
34	NA	0	8328	-	X
34	NA	0	8329	-	X
34	NA	0	8335	-	X
34	NA	0	8340	-	X
34	NA	0	8350	-	X
34	NA	0	8355	-	X
34	NA	0	8358	-	X
34	NA	0	8359	-	X
34	NA	0	8361	-	X
34	NA	0	8362	-	X
34	NA	0	8363	-	X
34	NA	0	8364	-	X
34	NA	0	8365	-	X
34	NA	0	8366	-	X
34	NA	0	8367	-	X
34	NA	0	8369	-	X
34	NA	0	8370	-	X
34	NA	0	8371	-	X
34	NA	0	8372	-	X
34	NA	0	8373	-	X
34	NA	0	8374	-	X
34	NA	0	8376	-	X
34	NA	0	8377	-	X
34	NA	0	8378	-	X
34	NA	0	8379	-	X
34	NA	0	8382	-	X
34	NA	0	8385	-	X
34	NA	9	8383	-	X
34	NA	L	8380	-	X
34	NA	R	8386	-	X
35	CL	0	8522	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	73	Total Na 73 73	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	3	Total Na 3 3	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5949	Total 5949	O 5949	0	0
37	A	117	Total 117	O 117	0	0
37	B	146	Total 146	O 146	0	0
37	C	170	Total 170	O 170	0	0
37	D	47	Total 47	O 47	0	0
37	E	42	Total 42	O 42	0	0
37	F	24	Total 24	O 24	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	19	Total 19	O 19	0	0
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0

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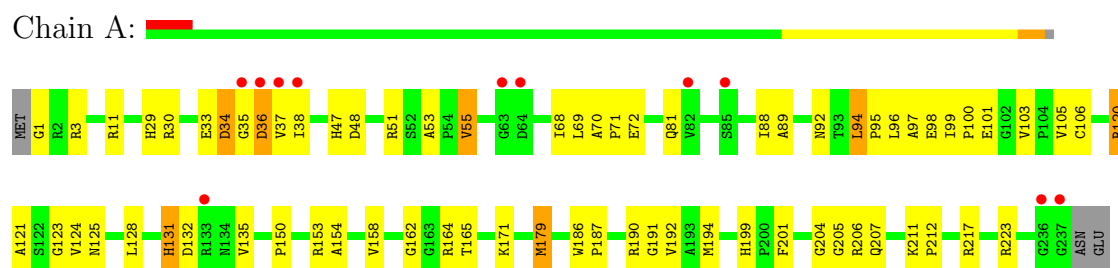
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	40	Total 40	O 40	0	0
37	3	72	Total 72	O 72	0	0
37	9	139	Total 139	O 139	0	0

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

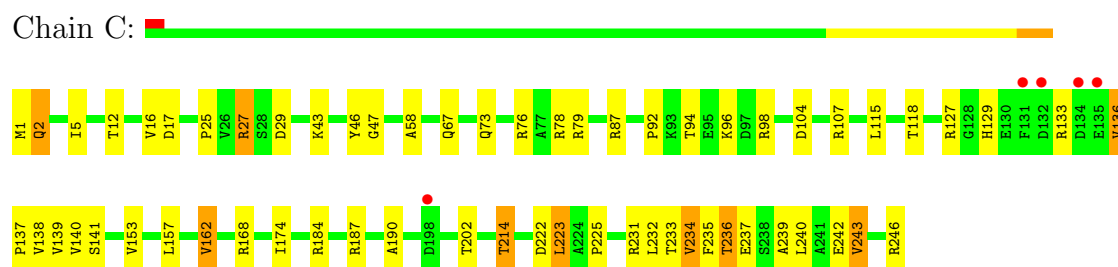
- Molecule 1: 50S ribosomal protein L2P



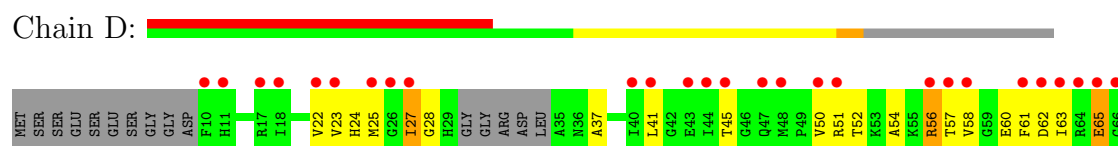
- Molecule 2: 50S ribosomal protein L3P



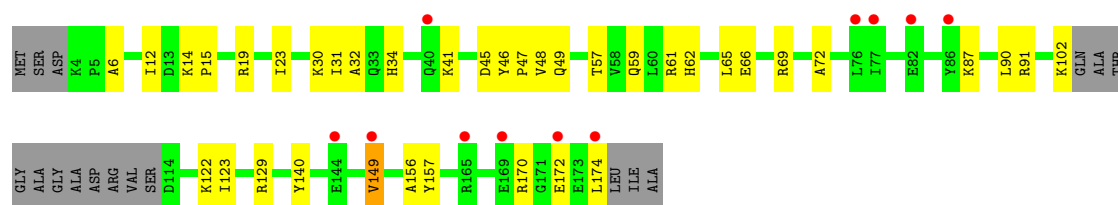
- Molecule 3: 50S ribosomal protein L4P



- Molecule 4: 50S ribosomal protein L5P

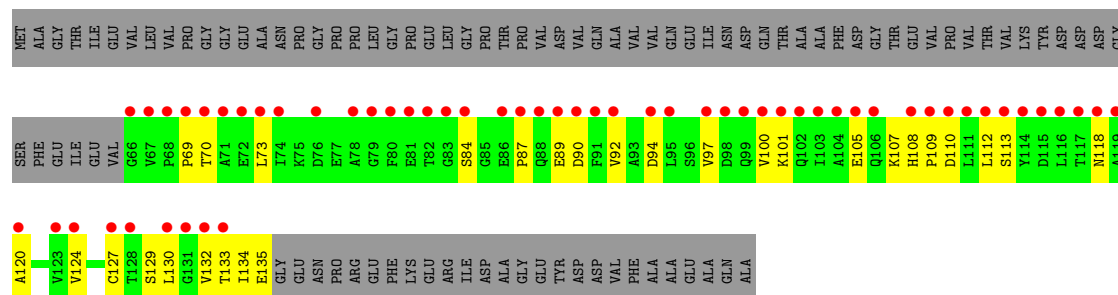






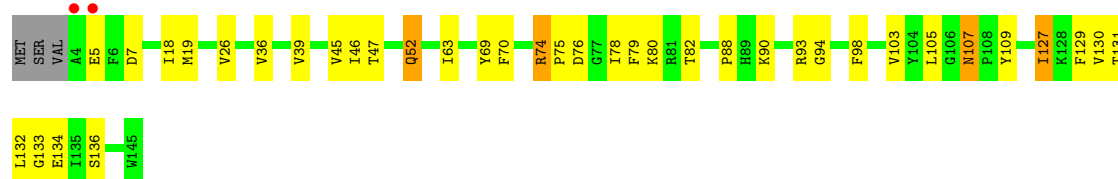
• Molecule 9: 50S ribosomal protein L11P

Chain I:



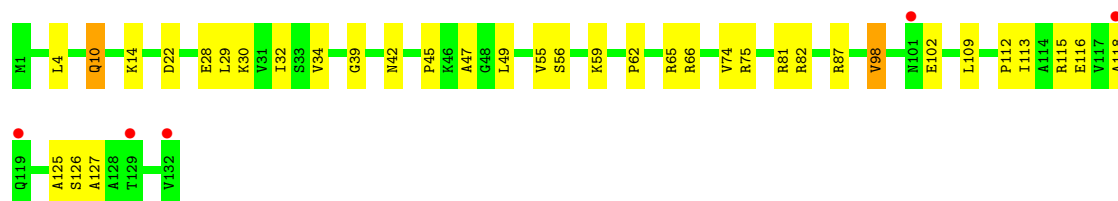
• Molecule 10: 50S ribosomal protein L13P

Chain J:



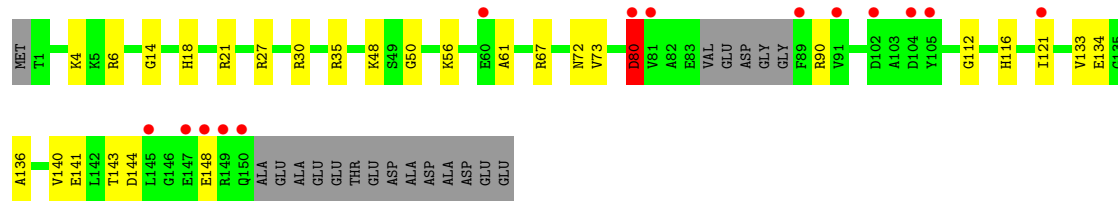
• Molecule 11: 50S ribosomal protein L14P

Chain K:



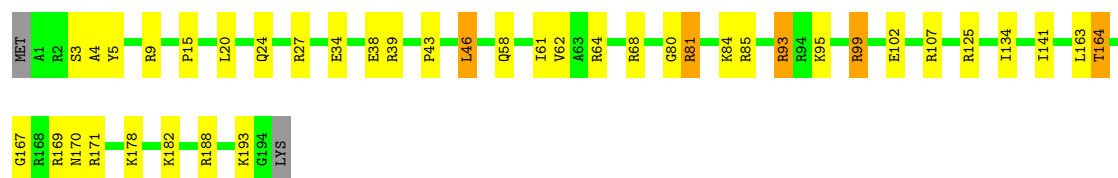
• Molecule 12: 50S ribosomal protein L15P

Chain L:



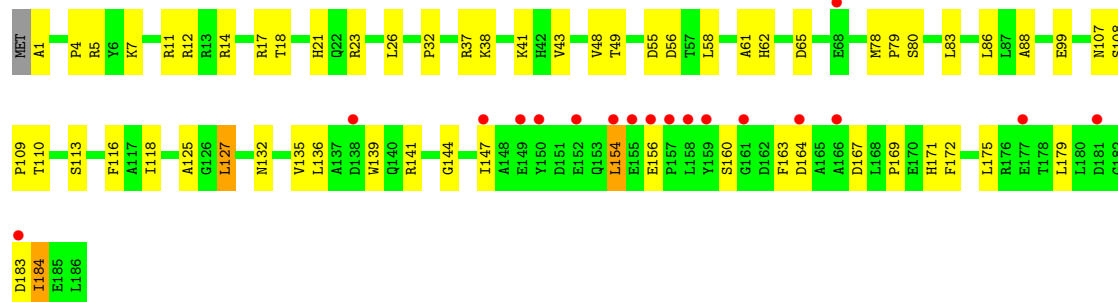
• Molecule 13: 50S ribosomal protein L15e

Chain M: 



- Molecule 14: 50S ribosomal protein L18P

Chain N: 



- Molecule 15: 50S ribosomal protein L18e

Chain O: 



- Molecule 16: 50S ribosomal protein L19e

Chain P: 



- Molecule 17: 50S ribosomal protein L21e

Chain Q: 



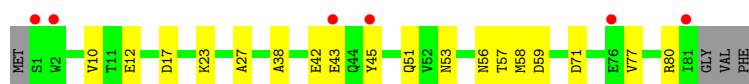
- Molecule 18: 50S ribosomal protein L22P

Chain R: 



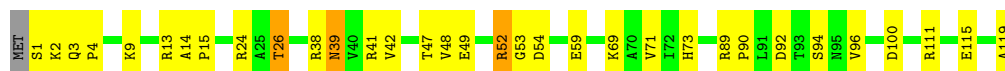
- Molecule 19: 50S ribosomal protein L23P

Chain S: 



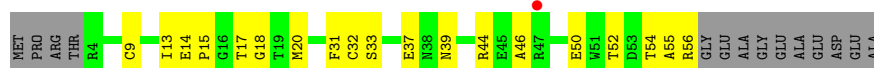
- Molecule 20: 50S ribosomal protein L24P

Chain T:



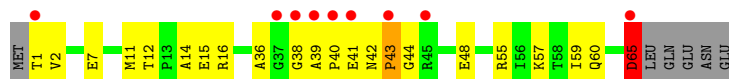
- Molecule 21: 50S ribosomal protein L24e

Chain U:



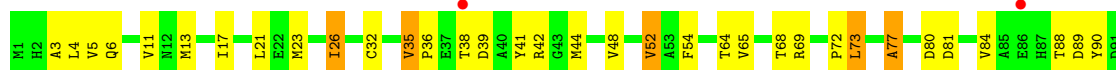
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



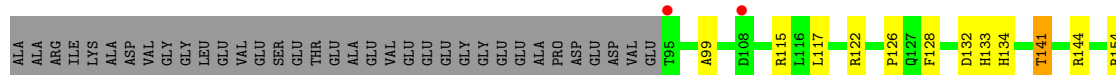
- Molecule 24: 50S ribosomal protein L31e

Chain X:



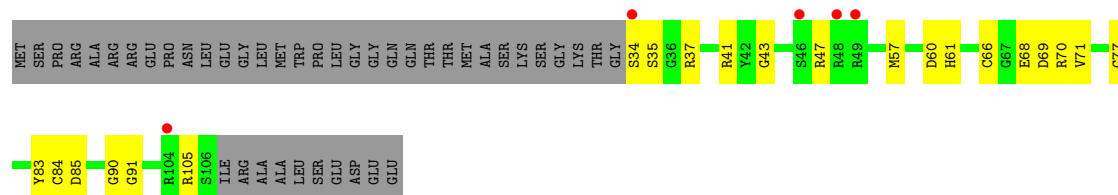
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



- Molecule 28: 50S ribosomal protein L39e

Chain 2:



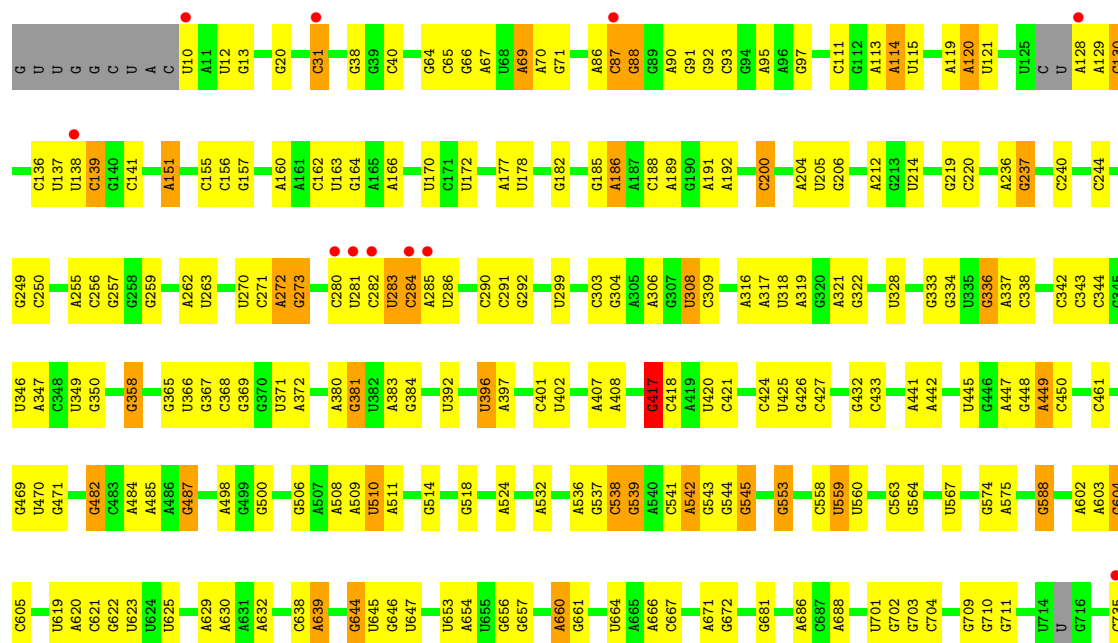
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

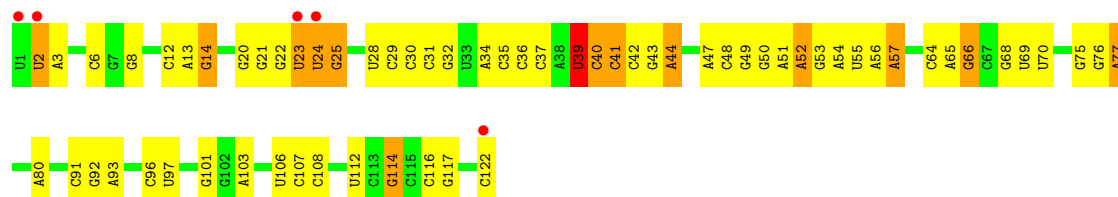


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



A252	G2111	C1993	G1868	G1730	A1612	C1477	A1352	G1241	U1170	G1072	C	A736
G2256	A2112	A1994	G1877	C1731	C1613	C1477	C1383	A1242	A1171	G1072	C	A737
G2257	G2113	G1995	G1878	A1732	G1614	A1482	C1360	C1243	A1172	G1076	C	G738
A2258	C2114	U1996	G1879	A1733	A1615	A1483	C1360	U1244	A1173	G1077	G	C757
U2265	U2115	A1997	G1880	C1734	A1624	G1484	A1367	A1245	A1174	A1078	C	A758
U2265	U2116	A1981	U1825	A1735	U1626	A1485	U1368	C1246	G1175	C1080	U	C759
A2266	G2128	C2001	C1882	A1736	A1626	A1485	A1369	U1249	C1176	A1081	C	C764
C2269	G2134	C2002	G1884	U1741	G1627	A1493	U1370	C1250	A1177	A1082	G	G765
G2270	A2135	U2003	G1884	A1742	A1632	G1497	A1372	C1251	U1180	C1083	A	G775
G2271	G2136	G2005	G1884	A1742	A1633	G1497	A1372	A1252	C1181	C1084	G	U883
G2272	A	A1909	A1909	G1752	G1633	U1500	C1377	C1253	C1182	C1085	A	A776
G2289	C	A1919	U1666	U1766	U1635	U1500	C1377	C1257	C1184	G1087	G	U777
U2290	G	C1920	U1771	U1771	G1636	U1503	C1384	G1258	U1185	A1088	A	A790
A2291	U	A1921	U1771	U1771	A1637	A1504	A1393	U1266	A1187	A1097	G	A791
G2296	C	A1922	C1772	C1772	A1641	U1505	A1394	C1267	A1188	A1098	C	G792
A2300	U	G1925	G1773	G1773	A1642	U1506	C1394	C1268	A1189	G1099	G	A793
A2301	G	G1926	A1778	A1778	U1654	U1524	A1406	G1289	G1190	C1103	C	U794
A2302	C	A1927	A1779	A1779	G1655	A1527	A1407	U1278	A1191	U1109	A	G795
C2309	C	C1940	A1783	A1783	A1656	A1527	U1408	U1279	A1192	C	A	A796
G2310	A	A1941	U1784	U1784	A1657	A1528	G1409	C1289	A1193	G1110	A	A797
A2311	U	C1943	C1787	C1787	C1666	G1535	A1413	G1290	G1194	U1116	C	G809
G2312	G	C1946	U1788	U1788	A1667	C1536	A1414	A1291	G1195	A1117	C	A812
C2313	G	G1947	G1789	G1789	U1668	U1536	G1417	A1291	C1196	A1118	C	C813
G2314	C	G1948	C1798	C1798	U1668	U1536	U1418	A1294	U1197	G1119	C	G814
C2315	A	G1949	G1799	G1799	C1675	C1545	U1419	G1295	A1199	U1120	C	U815
G2316	C	G1950	U1800	U1800	U1676	G1546	C1420	G1299	C1201	G1121	C	G816
C2317	C	U1951	U1800	U1800	U1677	G1556	A1423	G1300	A1202	C1127	C	C817
U2320	A	A	U1800	U1800	U1678	C1557	A1424	U1304	C1204	U1128	C	A818
A2321	U	A	A	A	A1679	C1558	A1424	U1305	U1206	G1130	C	A819
U2322	C	C	C	C	C1680	A1559	A1427	U1306	U1207	A1131	C	G820
G2323	C	U	U	U	A1681	U1561	C1428	U1306	C1208	G1131	C	U821
C2326	C	U	U	U	A1682	C1562	U1429	A1306	C1209	U132	C	A827
C2329	C	U	U	U	G1683	C1565	G1430	A1313	G1210	G1135	C	G828
U2330	C	G	A	A	A1684	C1565	U1434	U1314	C1211	U1136	C	G834
G2338	C	C	C	C	A1685	C1571	U1435	G1316	C1212	G1137	C	U835
A2344	C	C	C	C	C1692	G1571	C1436	G1325	G1214	U1139	C	U840
A2345	C	U1964	G1697	U1935	G1697	G1588	C1439	A1328	A1215	C1140	C	A841
C2346	C	G1971	U1998	U1998	U1698	G1589	U1440	G1328	G1216	G1151	C	A844
A2363	C	U1972	A1701	C1841	A1701	C1592	G1441	A1330	U1218	C1043	C	G848
A2364	C	A1973	U1702	A1842	U1702	C1594	A1442	U1333	U1219	G1045	C	G856
G2355	C	G1976	C1714	A1845	C1714	G1595	C1460	C1334	C1229	G1046	C	U857
A2356	C	U1977	C1715	G1848	C1715	U1596	G1453	G1339	G1159	G1160	C	U858
G2357	C	A1978	A1717	U1717	A1717	A1597	G1453	G1340	G1161	C1162	C	C859
	C	U1979	U1722	C1856	U1722	A1598	C1462	G1340	U1234	G1163	C	U860
	C	U1980	G1723	C1862	G1723	A1603	U1463	C1342	G1235	U1066	C	A861
	C	U1985	C1725	G1863	C1725	G1604	U1463	C1343	U1237	A1057	C	A867
	C	U1992	C1725	G1867	C1725	G1605	A1470	U1350	G1238	G1167	C	G868
	C	U1992	C1725	G1867	C1725	G1611	C1474	G1351	G1239	C1168	C	G869
	C	U1992	C1725	G1867	C1725	G1611	C1474	G1351	G1240	U1169	C	



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.231 0.183 , 0.216	Depositor DCC
R_{free} test set	6200 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 666819 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	270	U	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	F	24	0	0	2	0
37	G	19	0	0	1	0
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 1694 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5''	1.61	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08

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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	25	35
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	25	35
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	7	5
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	14	17
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	30	43
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	27	39
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	30	43
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	14	18
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	11	13
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	14	18
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	30	43
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	18	24
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	8	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	33	47

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	38	57
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	51
3	C	193/193 (100%)	179 (93%)	14 (7%)	20	30
4	D	117/148 (79%)	112 (96%)	5 (4%)	40	59
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	79
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	94
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	66
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	66
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	89
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	34
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	77
12	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
13	M	158/160 (99%)	152 (96%)	6 (4%)	44	65
14	N	149/150 (99%)	146 (98%)	3 (2%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	93/94 (99%)	90 (97%)	3 (3%)	51	72
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	88
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	50
18	R	117/122 (96%)	115 (98%)	2 (2%)	73	89
19	S	71/74 (96%)	69 (97%)	2 (3%)	56	77
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	35
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	64
23	W	130/130 (100%)	123 (95%)	7 (5%)	31	47
24	X	66/74 (89%)	60 (91%)	6 (9%)	14	20
25	Y	120/196 (61%)	112 (93%)	8 (7%)	23	35
26	Z	60/94 (64%)	58 (97%)	2 (3%)	50	71
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	81
29	3	79/79 (100%)	78 (99%)	1 (1%)	80	93
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	42	63

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ILE
13	M	68	ARG
25	Y	172	THR
10	J	74	ARG
11	K	49	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	88	GLN
28	2	18	ASN
13	M	137	ASN
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	240 (8%)	0

5 of 240 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	OMU	0	2587	30	20,22,23	1.36	1 (5%)	24,31,34	0.73	0
30	OMG	0	2588	30	24,26,27	0.84	0	33,38,41	5.30	4 (12%)
30	UR3	0	2619	30	20,22,23	1.41	1 (5%)	23,32,35	0.76	0
30	PSU	0	2621	30	19,21,22	1.39	1 (5%)	23,30,33	0.94	0
30	1MA	0	628	30,34	23,25,26	0.95	1 (4%)	32,37,40	0.96	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,34	-	1/8/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2619	UR3	C5-C4	5.48	1.43	1.37
30	0	2587	OMU	C5-C4	5.10	1.43	1.37
30	0	2621	PSU	C5-C1'	-4.69	1.48	1.52
30	0	628	1MA	C6-N6	2.30	1.33	1.29

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.58	130.29	134.14
30	0	2588	OMG	C6-N1-C2	8.95	125.25	120.20
30	0	628	1MA	C2-N3-C4	-3.43	110.65	116.23
30	0	2588	OMG	C2-N3-C4	-2.91	111.81	115.30
30	0	2588	OMG	C5-C4-N3	2.12	128.50	126.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 231 ligands modelled in this entry, 231 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	237/240 (98%)	0.18	11 (4%) 31 29	19, 38, 77, 98	0
2	B	337/338 (99%)	0.20	10 (2%) 48 45	21, 46, 74, 84	0
3	C	246/246 (100%)	0.07	5 (2%) 62 59	15, 36, 60, 71	0
4	D	140/177 (79%)	2.21	68 (48%) 1 0	47, 90, 115, 123	0
5	E	172/178 (96%)	0.64	14 (8%) 12 10	39, 61, 81, 85	0
6	F	119/120 (99%)	0.65	12 (10%) 7 7	34, 61, 90, 104	0
7	G	29/348 (8%)	1.98	12 (41%) 1 0	69, 86, 95, 98	0
8	H	160/177 (90%)	0.54	11 (6%) 17 15	30, 48, 83, 90	0
9	I	70/162 (43%)	3.98	57 (81%) 0 0	122, 136, 154, 155	0
10	J	142/145 (97%)	0.20	2 (1%) 72 71	29, 43, 66, 89	0
11	K	132/132 (100%)	0.02	5 (3%) 38 36	27, 42, 65, 77	0
12	L	145/165 (87%)	0.51	14 (9%) 8 7	18, 55, 101, 117	0
13	M	194/196 (98%)	-0.33	0 100 100	20, 31, 47, 55	0
14	N	186/187 (99%)	0.52	18 (9%) 8 7	32, 53, 102, 112	0
15	O	115/116 (99%)	0.04	3 (2%) 53 51	29, 45, 62, 70	0
16	P	143/149 (95%)	0.10	1 (0%) 84 84	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.04	1 (1%) 77 77	26, 35, 54, 66	0
18	R	150/155 (96%)	-0.13	1 (0%) 84 84	22, 37, 58, 71	0
19	S	81/85 (95%)	0.43	6 (7%) 14 13	31, 48, 72, 82	0
20	T	119/120 (99%)	0.27	0 100 100	29, 46, 78, 98	0
21	U	53/67 (79%)	0.09	1 (1%) 64 61	34, 48, 66, 76	0
22	V	65/71 (91%)	1.50	9 (13%) 4 3	40, 62, 106, 113	0
23	W	154/154 (100%)	0.26	4 (2%) 53 51	28, 42, 59, 71	0
24	X	82/92 (89%)	0.41	5 (6%) 21 18	36, 50, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.09	5 (3%) 42 40	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.19	5 (6%) 17 15	34, 48, 68, 87	0
27	1	56/57 (98%)	-0.26	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	0.41	3 (6%) 18 17	26, 50, 75, 89	0
29	3	92/92 (100%)	0.05	1 (1%) 77 77	22, 45, 62, 76	0
30	0	2754/2923 (94%)	-0.19	55 (1%) 62 59	16, 36, 81, 155	0
31	9	122/122 (100%)	-0.09	5 (4%) 35 33	31, 54, 77, 138	0
All	All	6651/7517 (88%)	0.13	344 (5%) 28 24	15, 42, 89, 155	0

The worst 5 of 344 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	13.0
22	V	39	ALA	10.8
14	N	166	ALA	9.9
4	D	63	ILE	9.8
22	V	40	PRO	9.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.14	0.95	24,27,31,36	0
30	1MA	0	628	23/24	0.14	0.19	20,22,23,25	0
30	PSU	0	2621	20/21	0.13	-0.89	20,23,27,27	0
30	OMU	0	2587	21/22	0.10	-1.25	22,25,27,28	0
30	OMG	0	2588	24/25	0.12	-1.84	22,25,27,28	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8370	1/1	0.60	40.06	70,70,70,70	0
32	MG	0	8082	1/1	0.20	33.50	62,62,62,62	0
34	NA	0	8358	1/1	0.36	31.78	73,73,73,73	0
34	NA	0	8367	1/1	0.28	18.26	46,46,46,46	0
34	NA	0	8366	1/1	0.18	15.53	63,63,63,63	0
34	NA	0	8372	1/1	0.35	15.29	60,60,60,60	0
34	NA	0	8320	1/1	0.20	15.26	37,37,37,37	0
34	NA	0	8371	1/1	0.22	14.17	48,48,48,48	0
34	NA	0	8350	1/1	0.28	13.36	41,41,41,41	0
32	MG	0	8101	1/1	0.18	12.63	44,44,44,44	0
32	MG	0	8087	1/1	0.14	12.57	57,57,57,57	0
34	NA	0	8376	1/1	0.27	10.41	42,42,42,42	0
34	NA	R	8386	1/1	0.38	10.15	80,80,80,80	0
34	NA	0	8340	1/1	0.18	10.03	49,49,49,49	0
35	CL	0	8522	1/1	0.19	9.67	44,44,44,44	0
34	NA	0	8364	1/1	0.20	8.39	40,40,40,40	0
34	NA	L	8380	1/1	0.30	7.79	44,44,44,44	0
34	NA	0	8379	1/1	0.22	7.09	46,46,46,46	0
34	NA	0	8308	1/1	0.19	7.04	45,45,45,45	0
34	NA	0	8363	1/1	0.21	7.02	50,50,50,50	0
34	NA	0	8318	1/1	0.20	6.72	47,47,47,47	0
34	NA	0	8374	1/1	0.15	6.53	47,47,47,47	0
32	MG	0	8066	1/1	0.39	6.22	88,88,88,88	0
32	MG	0	8103	1/1	0.17	5.91	55,55,55,55	0
34	NA	0	8329	1/1	0.13	5.40	55,55,55,55	0
34	NA	0	8382	1/1	0.18	5.25	67,67,67,67	0
32	MG	0	8047	1/1	0.15	5.23	59,59,59,59	0
34	NA	0	8361	1/1	0.19	5.16	41,41,41,41	0
34	NA	0	8307	1/1	0.17	5.16	42,42,42,42	0
34	NA	0	8306	1/1	0.21	4.97	29,29,29,29	0
32	MG	0	8049	1/1	0.18	4.79	54,54,54,54	0
34	NA	0	8385	1/1	0.21	4.67	44,44,44,44	0
34	NA	0	8326	1/1	0.15	4.64	37,37,37,37	0
34	NA	0	8373	1/1	0.16	3.90	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8365	1/1	0.25	3.59	31,31,31,31	0
32	MG	0	8060	1/1	0.19	3.57	33,33,33,33	0
34	NA	0	8311	1/1	0.14	3.48	52,52,52,52	0
34	NA	0	8302	1/1	0.15	3.48	44,44,44,44	0
34	NA	0	8335	1/1	0.18	3.31	31,31,31,31	0
34	NA	0	8362	1/1	0.19	3.29	46,46,46,46	0
34	NA	0	8355	1/1	0.33	3.23	53,53,53,53	0
34	NA	0	8377	1/1	0.16	3.10	50,50,50,50	0
34	NA	0	8314	1/1	0.18	3.05	38,38,38,38	0
34	NA	0	8378	1/1	0.23	3.02	40,40,40,40	0
34	NA	0	8359	1/1	0.18	3.01	39,39,39,39	0
32	MG	0	8057	1/1	0.14	2.80	34,34,34,34	0
32	MG	0	8007	1/1	0.17	2.78	21,21,21,21	0
34	NA	0	8328	1/1	0.14	2.75	31,31,31,31	0
34	NA	9	8383	1/1	0.20	2.69	46,46,46,46	0
32	MG	0	8034	1/1	0.13	2.68	30,30,30,30	0
34	NA	0	8369	1/1	0.18	2.53	42,42,42,42	0
32	MG	0	8041	1/1	0.14	2.11	34,34,34,34	0
34	NA	0	8384	1/1	0.12	1.96	53,53,53,53	0
32	MG	0	8090	1/1	0.28	1.50	56,56,56,56	0
34	NA	0	8360	1/1	0.15	1.48	41,41,41,41	0
34	NA	0	8325	1/1	0.16	1.47	50,50,50,50	0
32	MG	0	8013	1/1	0.15	1.29	22,22,22,22	0
34	NA	0	8324	1/1	0.14	1.17	48,48,48,48	0
34	NA	0	8368	1/1	0.12	1.15	48,48,48,48	0
34	NA	0	8331	1/1	0.17	1.09	35,35,35,35	0
34	NA	0	8342	1/1	0.16	0.99	35,35,35,35	0
32	MG	0	8023	1/1	0.16	0.94	28,28,28,28	0
34	NA	H	8322	1/1	0.21	0.83	54,54,54,54	0
32	MG	0	8015	1/1	0.16	0.71	25,25,25,25	0
34	NA	0	8321	1/1	0.17	0.65	42,42,42,42	0
32	MG	0	8070	1/1	0.15	0.49	44,44,44,44	0
32	MG	0	8080	1/1	0.15	0.47	40,40,40,40	0
32	MG	0	8079	1/1	0.16	0.46	20,20,20,20	0
32	MG	0	8012	1/1	0.12	0.44	30,30,30,30	0
32	MG	0	8104	1/1	0.21	0.42	50,50,50,50	0
34	NA	0	8341	1/1	0.11	0.32	41,41,41,41	0
32	MG	0	8099	1/1	0.16	0.26	40,40,40,40	0
34	NA	0	8316	1/1	0.17	0.23	38,38,38,38	0
32	MG	0	8042	1/1	0.10	0.20	31,31,31,31	0
32	MG	0	8102	1/1	0.11	0.08	48,48,48,48	0
32	MG	0	8026	1/1	0.14	-0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8010	1/1	0.14	-0.17	24,24,24,24	0
32	MG	0	8009	1/1	0.14	-0.17	25,25,25,25	0
32	MG	0	8061	1/1	0.15	-0.28	30,30,30,30	0
32	MG	0	8067	1/1	0.12	-0.42	28,28,28,28	0
35	CL	M	8518	1/1	0.12	-0.49	32,32,32,32	0
32	MG	9	8095	1/1	0.13	-0.52	64,64,64,64	0
35	CL	0	8503	1/1	0.12	-0.74	38,38,38,38	0
34	NA	C	8304	1/1	0.12	-0.75	29,29,29,29	0
34	NA	0	8327	1/1	0.12	-0.85	36,36,36,36	0
32	MG	0	8011	1/1	0.12	-0.89	21,21,21,21	0
32	MG	0	8086	1/1	0.07	-0.98	37,37,37,37	0
35	CL	A	8509	1/1	0.12	-1.03	49,49,49,49	0
34	NA	0	8354	1/1	0.15	-1.04	23,23,23,23	0
32	MG	B	8055	1/1	0.10	-1.09	42,42,42,42	0
32	MG	0	8038	1/1	0.11	-1.15	21,21,21,21	0
35	CL	J	8502	1/1	0.10	-1.22	55,55,55,55	0
32	MG	0	8116	1/1	0.13	-1.25	35,35,35,35	0
32	MG	0	8064	1/1	0.12	-1.30	26,26,26,26	0
34	NA	0	8305	1/1	0.12	-1.31	33,33,33,33	0
32	MG	0	8094	1/1	0.09	-1.33	59,59,59,59	0
35	CL	J	8501	1/1	0.09	-1.41	46,46,46,46	0
36	CD	U	8401	1/1	0.07	-1.42	48,48,48,48	0
34	NA	0	8344	1/1	0.08	-1.49	24,24,24,24	0
34	NA	0	8356	1/1	0.12	-1.54	35,35,35,35	0
32	MG	0	8016	1/1	0.10	-1.55	30,30,30,30	0
35	CL	J	8521	1/1	0.10	-1.60	47,47,47,47	0
32	MG	0	8074	1/1	0.06	-1.72	35,35,35,35	0
35	CL	Y	8520	1/1	0.08	-1.74	35,35,35,35	0
32	MG	0	8077	1/1	0.14	-1.74	22,22,22,22	0
35	CL	0	8511	1/1	0.08	-1.76	37,37,37,37	0
36	CD	1	8402	1/1	0.08	-1.80	45,45,45,45	0
32	MG	0	8100	1/1	0.10	-1.84	63,63,63,63	0
34	NA	M	8347	1/1	0.10	-1.86	19,19,19,19	0
34	NA	0	8375	1/1	0.14	-1.89	38,38,38,38	0
34	NA	0	8315	1/1	0.14	-1.89	30,30,30,30	0
35	CL	0	8516	1/1	0.10	-1.92	41,41,41,41	0
34	NA	0	8381	1/1	0.09	-1.94	43,43,43,43	0
34	NA	0	8319	1/1	0.10	-1.97	31,31,31,31	0
32	MG	0	8022	1/1	0.13	-1.99	31,31,31,31	0
34	NA	0	8332	1/1	0.10	-2.06	31,31,31,31	0
36	CD	Z	8403	1/1	0.08	-2.15	43,43,43,43	0
32	MG	0	8098	1/1	0.10	-2.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	J	8346	1/1	0.06	-2.16	37,37,37,37	0
32	MG	0	8024	1/1	0.10	-2.21	22,22,22,22	0
34	NA	A	8345	1/1	0.09	-2.21	43,43,43,43	0
35	CL	O	8508	1/1	0.06	-2.24	51,51,51,51	0
32	MG	0	8045	1/1	0.08	-2.25	55,55,55,55	0
36	CD	O	8405	1/1	0.06	-2.28	71,71,71,71	0
32	MG	0	8096	1/1	0.09	-2.32	34,34,34,34	0
36	CD	3	8404	1/1	0.06	-2.34	45,45,45,45	0
32	MG	0	8106	1/1	0.06	-2.34	31,31,31,31	0
34	NA	S	8312	1/1	0.08	-2.37	28,28,28,28	0
32	MG	0	8031	1/1	0.12	-2.39	24,24,24,24	0
34	NA	0	8339	1/1	0.11	-2.40	19,19,19,19	0
32	MG	0	8020	1/1	0.10	-2.41	22,22,22,22	0
34	NA	9	8351	1/1	0.10	-2.41	45,45,45,45	0
35	CL	N	8507	1/1	0.07	-2.45	44,44,44,44	0
32	MG	0	8053	1/1	0.11	-2.48	33,33,33,33	0
35	CL	0	8505	1/1	0.09	-2.49	41,41,41,41	0
32	MG	0	8001	1/1	0.10	-2.49	24,24,24,24	0
32	MG	0	8083	1/1	0.12	-2.53	33,33,33,33	0
35	CL	0	8512	1/1	0.08	-2.54	35,35,35,35	0
32	MG	0	8085	1/1	0.12	-2.58	37,37,37,37	0
33	K	0	8201	1/1	0.11	-2.76	60,60,60,60	0
35	CL	L	8510	1/1	0.08	-2.82	40,40,40,40	0
34	NA	0	8317	1/1	0.07	-2.82	28,28,28,28	0
32	MG	T	8073	1/1	0.06	-2.84	40,40,40,40	0
34	NA	0	8303	1/1	0.11	-2.89	32,32,32,32	0
32	MG	0	8062	1/1	0.08	-2.96	42,42,42,42	0
34	NA	0	8309	1/1	0.07	-2.97	25,25,25,25	0
35	CL	0	8514	1/1	0.11	-3.02	39,39,39,39	0
32	MG	0	8056	1/1	0.07	-3.09	34,34,34,34	0
34	NA	0	8330	1/1	0.06	-3.12	37,37,37,37	0
34	NA	Q	8348	1/1	0.06	-3.18	30,30,30,30	0
35	CL	3	8504	1/1	0.04	-3.20	43,43,43,43	0
32	MG	0	8054	1/1	0.12	-3.25	16,16,16,16	0
32	MG	0	8115	1/1	0.09	-3.33	41,41,41,41	0
32	MG	0	8058	1/1	0.08	-3.36	29,29,29,29	0
32	MG	0	8046	1/1	0.05	-3.38	39,39,39,39	0
34	NA	0	8334	1/1	0.06	-3.41	36,36,36,36	0
32	MG	0	8037	1/1	0.07	-3.44	35,35,35,35	0
34	NA	R	8337	1/1	0.08	-3.45	33,33,33,33	0
32	MG	0	8003	1/1	0.09	-3.48	21,21,21,21	0
35	CL	0	8513	1/1	0.07	-3.50	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8075	1/1	0.08	-3.50	27,27,27,27	0
34	NA	9	8352	1/1	0.10	-3.52	41,41,41,41	0
35	CL	0	8517	1/1	0.08	-3.54	47,47,47,47	0
32	MG	0	8008	1/1	0.10	-3.65	26,26,26,26	0
34	NA	0	8310	1/1	0.06	-3.66	30,30,30,30	0
35	CL	R	8506	1/1	0.09	-3.69	40,40,40,40	0
32	MG	0	8017	1/1	0.12	-3.80	11,11,11,11	0
32	MG	0	8072	1/1	0.09	-3.84	47,47,47,47	0
35	CL	0	8515	1/1	0.09	-3.85	53,53,53,53	0
34	NA	0	8343	1/1	0.06	-3.91	28,28,28,28	0
32	MG	0	8005	1/1	0.13	-3.91	25,25,25,25	0
34	NA	0	8333	1/1	0.06	-3.97	23,23,23,23	0
32	MG	0	8105	1/1	0.08	-4.02	45,45,45,45	0
32	MG	Y	8108	1/1	0.09	-4.07	25,25,25,25	0
32	MG	0	8035	1/1	0.08	-4.14	34,34,34,34	0
32	MG	A	8065	1/1	0.07	-4.28	23,23,23,23	0
35	CL	B	8519	1/1	0.08	-4.28	34,34,34,34	0
32	MG	0	8081	1/1	0.07	-4.39	39,39,39,39	0
32	MG	3	8078	1/1	0.07	-4.40	37,37,37,37	0
32	MG	0	8088	1/1	0.08	-4.44	24,24,24,24	0
32	MG	0	8051	1/1	0.07	-4.63	54,54,54,54	0
32	MG	0	8109	1/1	0.09	-4.63	25,25,25,25	0
32	MG	0	8107	1/1	0.07	-4.69	68,68,68,68	0
32	MG	0	8068	1/1	0.04	-4.95	46,46,46,46	0
34	NA	0	8353	1/1	0.07	-4.97	17,17,17,17	0
34	NA	0	8338	1/1	0.05	-4.97	41,41,41,41	0
32	MG	0	8084	1/1	0.07	-5.02	38,38,38,38	0
32	MG	0	8030	1/1	0.07	-5.19	21,21,21,21	0
32	MG	0	8014	1/1	0.09	-5.21	25,25,25,25	0
32	MG	0	8113	1/1	0.05	-5.49	31,31,31,31	0
32	MG	0	8029	1/1	0.07	-5.52	34,34,34,34	0
34	NA	0	8349	1/1	0.09	-5.53	32,32,32,32	0
32	MG	0	8004	1/1	0.10	-5.66	19,19,19,19	0
32	MG	0	8071	1/1	0.06	-5.83	61,61,61,61	0
32	MG	0	8032	1/1	0.06	-6.17	26,26,26,26	0
32	MG	0	8033	1/1	0.06	-6.32	19,19,19,19	0
32	MG	0	8040	1/1	0.10	-6.37	38,38,38,38	0
32	MG	0	8036	1/1	0.06	-6.44	31,31,31,31	0
32	MG	0	8025	1/1	0.06	-6.53	32,32,32,32	0
32	MG	0	8091	1/1	0.05	-6.69	41,41,41,41	0
32	MG	0	8027	1/1	0.05	-6.76	36,36,36,36	0
32	MG	0	8048	1/1	0.07	-6.80	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	K	8069	1/1	0.05	-6.91	47,47,47,47	0
32	MG	0	8044	1/1	0.07	-7.06	33,33,33,33	0
32	MG	0	8006	1/1	0.07	-7.13	29,29,29,29	0
32	MG	0	8021	1/1	0.10	-7.14	25,25,25,25	0
32	MG	0	8018	1/1	0.07	-7.26	30,30,30,30	0
34	NA	0	8323	1/1	0.10	-7.29	31,31,31,31	0
32	MG	0	8092	1/1	0.08	-7.50	66,66,66,66	0
32	MG	0	8019	1/1	0.05	-7.54	23,23,23,23	0
32	MG	0	8050	1/1	0.12	-7.80	66,66,66,66	0
32	MG	0	8111	1/1	0.05	-7.94	23,23,23,23	0
32	MG	0	8059	1/1	0.06	-7.96	22,22,22,22	0
34	NA	0	8313	1/1	0.08	-7.97	55,55,55,55	0
34	NA	0	8357	1/1	0.05	-8.36	39,39,39,39	0
33	K	0	8202	1/1	0.06	-8.76	37,37,37,37	0
32	MG	0	8110	1/1	0.05	-8.99	29,29,29,29	0
32	MG	0	8093	1/1	0.07	-9.38	37,37,37,37	0
32	MG	0	8063	1/1	0.10	-9.43	60,60,60,60	0
32	MG	0	8043	1/1	0.05	-9.72	32,32,32,32	0
32	MG	0	8076	1/1	0.04	-10.31	44,44,44,44	0
32	MG	0	8002	1/1	0.05	-10.67	25,25,25,25	0
34	NA	0	8336	1/1	0.03	-11.25	37,37,37,37	0
32	MG	0	8052	1/1	0.04	-13.26	48,48,48,48	0
32	MG	0	8039	1/1	0.05	-13.51	33,33,33,33	0
32	MG	0	8028	1/1	0.07	-16.84	27,27,27,27	0
32	MG	0	8112	1/1	0.11	-17.00	39,39,39,39	0
32	MG	0	8089	1/1	0.07	-18.91	43,43,43,43	0
32	MG	0	8114	1/1	0.05	-21.33	38,38,38,38	0
34	NA	0	8301	1/1	0.10	-21.50	34,34,34,34	0
32	MG	0	8097	1/1	0.06	-21.91	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.