



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:15 am BST

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

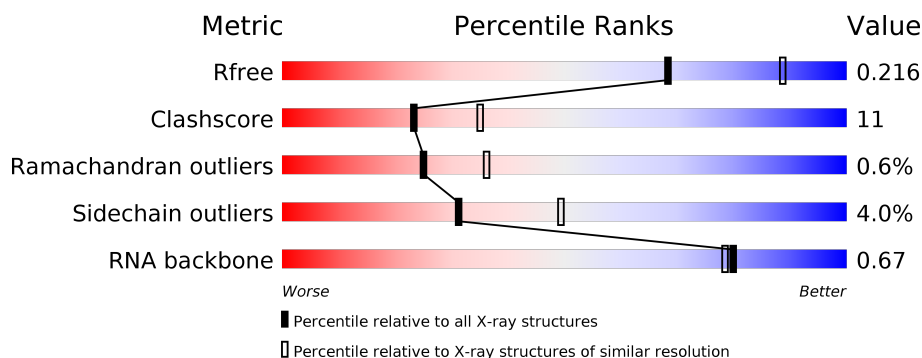
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



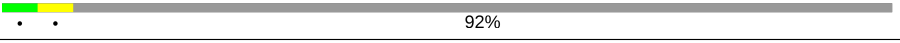















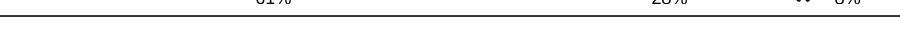
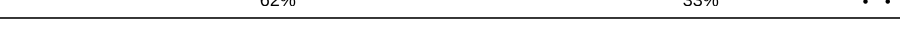
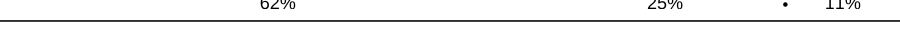
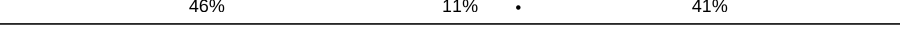
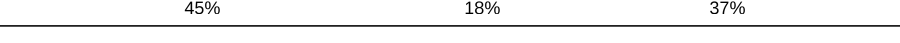
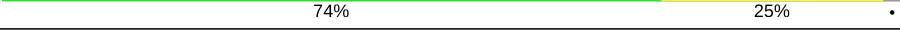



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% ..
2	B	338	71% 25% .
3	C	246	75% 21% .
4	D	177	47% 29% . 21%
5	E	178	69% 28% ..
6	F	120	73% 26% ..

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

## 2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			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 SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	73	Total Na 73 73	0	0
33	J	1	Total Na 1 1	0	0
33	Q	1	Total Na 1 1	0	0
33	H	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	A	1	Total Na 1 1	0	0
33	R	2	Total Na 2 2	0	0
33	9	3	Total Na 3 3	0	0
33	L	1	Total Na 1 1	0	0
33	S	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	10	Total Cl 10 10	0	0
34	J	3	Total Cl 3 3	0	0
34	B	1	Total Cl 1 1	0	0
34	A	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0
34	Y	1	Total Cl 1 1	0	0
34	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	3	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total 1	Cd 1	0	0
35	Z	1	Total 1	Cd 1	0	0
35	1	1	Total 1	Cd 1	0	0
35	3	1	Total 1	Cd 1	0	0
35	U	1	Total 1	Cd 1	0	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	2	Total 2	K 2	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
37	G	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
37	2	40	Total 40	O 40	0	0

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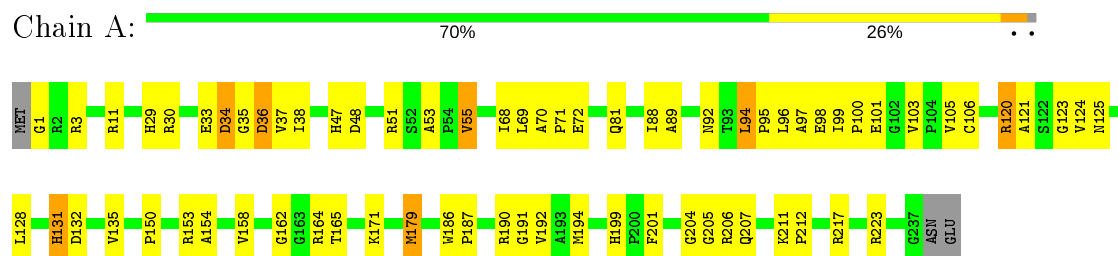
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	72	Total 72	O 72	0	0
37	0	5949	Total 5949	O 5949	0	0
37	9	139	Total 139	O 139	0	0

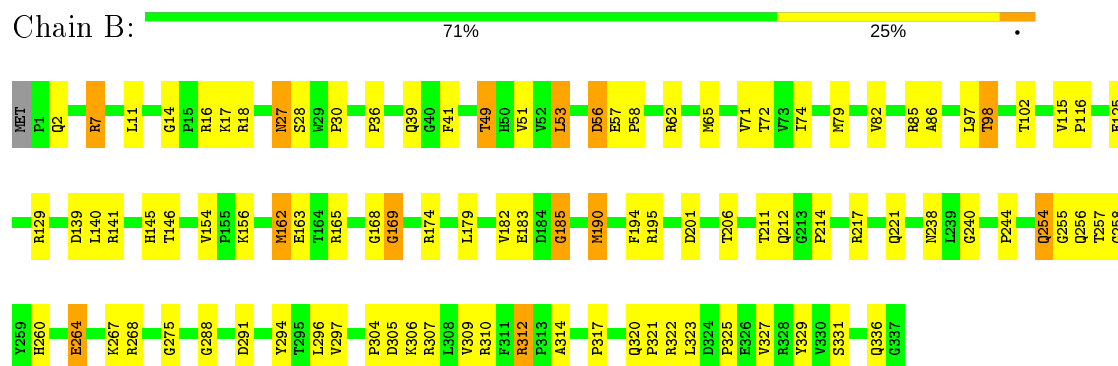
### 3 Residue-property plots [i](#)

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

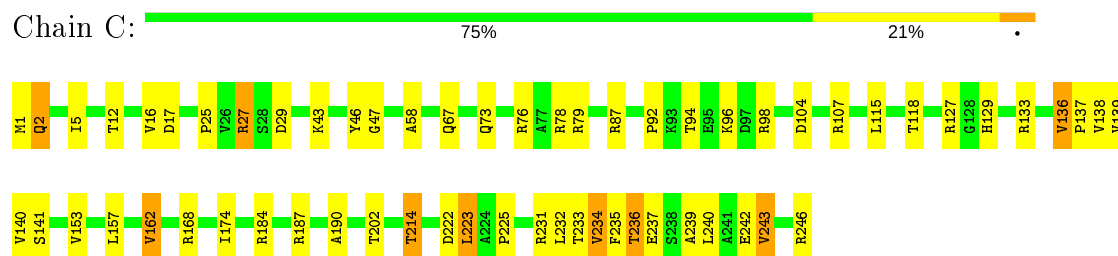
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P



- Molecule 3: 50S ribosomal protein L4P

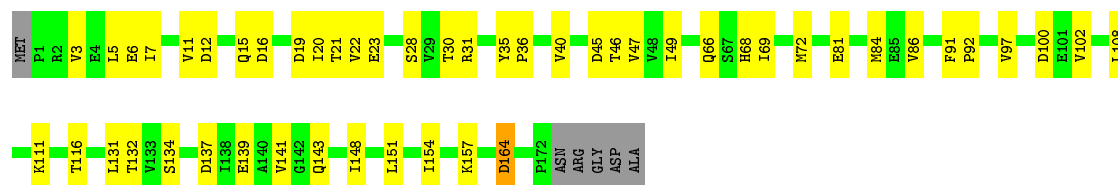


- Molecule 4: 50S ribosomal protein L5P



- Molecule 5: 50S ribosomal protein L6P

Chain E:  69% 28% ..



- Molecule 6: 50S ribosomal protein L7Ae

Chain F:  73% 26%



- Molecule 7: 50S ribosomal protein L10E


Chain G:  92%

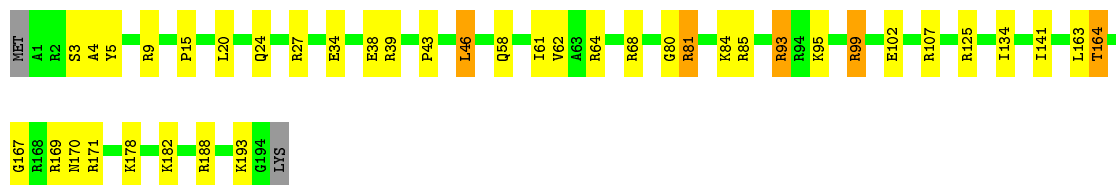


- Molecule 8: 50S ribosomal protein L10e

Chain H:  69% 21% • 10%

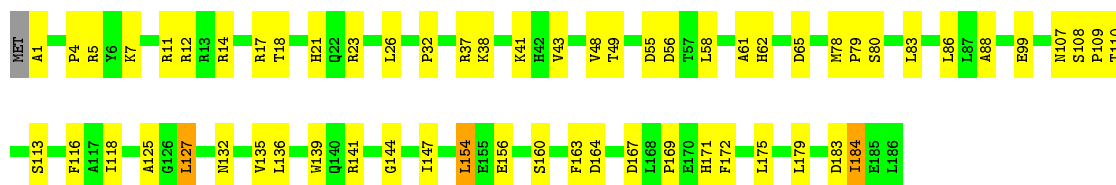


Chain M:  79% 18% ..




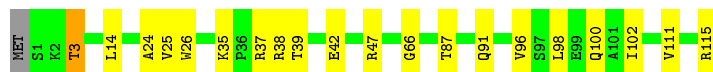
- Molecule 14: 50S ribosomal protein L18P

Chain N:  67% 31% ..




- Molecule 15: 50S ribosomal protein L18e

Chain O:  82% 16% ..




- Molecule 16: 50S ribosomal protein L19e

Chain P:  82% 14% .



- Molecule 17: 50S ribosomal protein L21e

Chain Q:  83% 14% ..



- Molecule 18: 50S ribosomal protein L22P

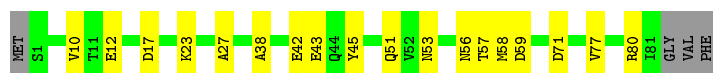
Chain R:  78% 17% ..



- Molecule 19: 50S ribosomal protein L23P

Chain S:  74% 21% 5%





- Molecule 20: 50S ribosomal protein L24P

Chain T: 72% 25% ..



- Molecule 21: 50S ribosomal protein L24e

Chain U: 51% 28% 21%



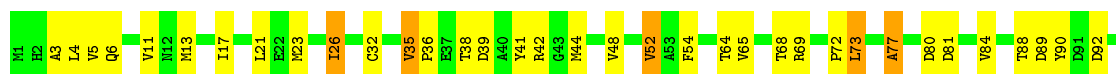
- Molecule 22: 50S ribosomal protein L29P

Chain V: 61% 28% 8%



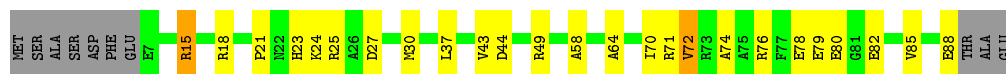
- Molecule 23: 50S ribosomal protein L30P

Chain W: 62% 33% ..



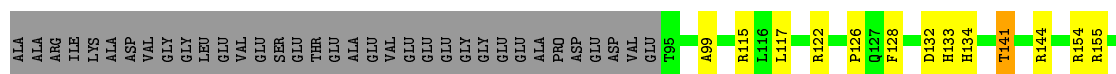
- Molecule 24: 50S ribosomal protein L31e

Chain X: 62% 25% 11%



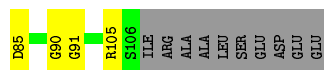
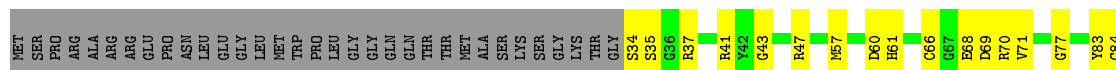
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 46% 11% 41%





- Molecule 26: 50S ribosomal protein L37Ae



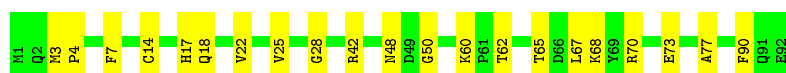
- Molecule 27: 50S ribosomal protein L37e



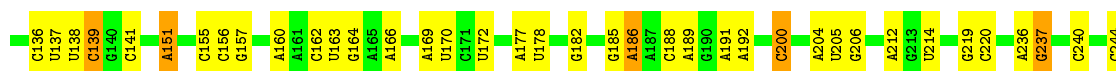
- Molecule 28: 50S ribosomal protein L39e



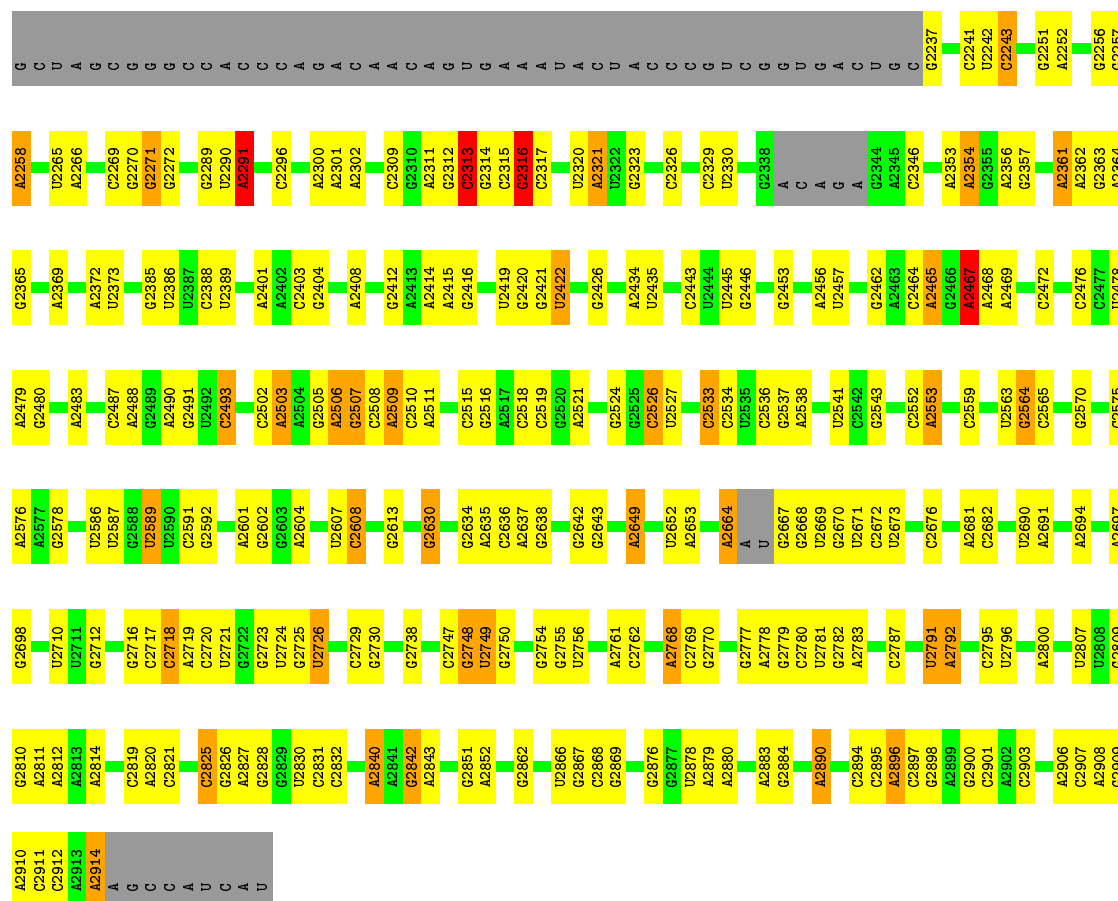
- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA

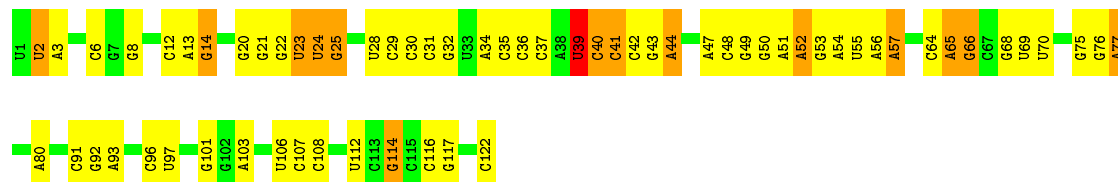


C2114	U1996	G1878	A1733	A1615	A1482	C1360	U1244	G1187	G1059	U	A867	G716	G604	G469
U2115	A1997	U1879	G1734	A1624	C1483	A1367	G1245	C1188	C1060	G	G868	G735	C605	U470
U2116	G2001	C1380	C1735	A1694	A1484	U1368	A1246	A1171	G1072	U	G869	A736	U619	G471
G2128	G2002	A1881	A1736	U1625	A1485	A1369	U1249	A1172	G1076	C	A620	A737	A620	G482
G2134	U2003	C1882	U1741	A1626	A1493	G1370	C1250	A1173	G1077	G	G871	G738	C621	C483
A2135	U2004	U1893	A1742	G1627	G1497	U1371	C1251	A1174	A1078	C	G872	G739	G622	A484
G2136	G2005	G1894	G1752	A1632	U1500	A1372	C1252	G1175	A1079	U	U872	C757	U623	A485
A	U2008	A1909	G1753	C1633	U1501	C1377	U1253	U1180	A1079	C	A875	A758	U624	A486
C	G2009	A1919	U1766	G1634	U1502	C1384	C1257	A1181	A1081	C	A876	C759	U625	G487
G	A2010	C1920	U1771	A1635	U1503	G1384	G1258	A1182	A1082	G	A877	G764	A629	A498
U	A2011	A1921	U1772	G1636	U1504	C1384	U1259	C1183	A1083	A	A878	G765	A630	A499
G	U2012	A1922	C1772	A1637	U1505	A1389	U1266	C1184	C1084	G	U883	G775	A631	G499
G2013	G2013	G1925	G1773	U1506	U1506	C1394	C1267	U1185	C1085	A	G885	A776	A632	G500
U	A2015	A1926	A1778	U1524	U1524	A1406	G1268	A1186	A1086	G	A884	G777	G638	G506
C	G2016	A1927	U1779	U1525	U1525	A1407	G1269	A1187	A1087	G	A885	U777	A639	A507
C	A2019	C1940	A1783	U1654	U1526	U1408	A1278	A1188	A1088	A	G888	A790	G644	A508
G	G2020	A1941	U1784	G1655	A1527	G1409	U1279	G1189	A1097	U	C899	A791	U645	A509
A	C2031	A1942	G1785	A1656	A1528	G1409	C1289	A1191	A1098	C	U899	G792	U646	U510
U	U2032	C1943	C1787	A1658	G1529	A1414	G1290	A1192	G1099	G	G902	U794	U647	A511
G	G2033	G1944	U1788	A1666	G1535	A1414	A1291	A1193	C1103	C	G905	G795	G514	G514
U	U2034	C1946	G1789	C1666	U1536	G1417	A1291	A1200	G1103	A	C906	A796	U653	G518
G	G2044	G1947	U1790	A1667	C1536	U1418	A1294	C1201	U1109	C	A907	A797	A654	G518
C	A2044	G1948	C1798	U1668	C1545	U1418	G1295	A1202	G1110	A	U907	G809	U655	A524
C	G2050	G1949	G1799	C1675	G1546	U1419	G1295	G1203	U1116	C	G956	G809	G656	A524
G	C2050	G1950	C1787	G1676	U1556	C1420	G1299	C1204	A1117	C	G957	G812	G657	A532
U	A2054	G1951	U1788	A1677	G1556	A1424	G1300	U1205	A1118	A	U658	A812	A660	A532
A	U2054	U	C1816	A1678	G1557	A1424	G1301	U1206	G1119	C	A661	G813	A661	A536
U	C2061	A	G1819	C1679	G1558	A1427	U1304	A1207	G1119	A	G921	G814	G661	A536
A	A2062	C	G1820	G1680	A1559	C1428	C1305	C1208	U1120	C	A922	U815	G537	G537
G	U2063	U	U1821	A1682	U	U1429	U1306	G1209	G1121	G	U923	G816	U664	C538
U	U2064	A	U1825	G1683	C1562	G1430	A1313	C1211	G1127	C	U932	G817	U665	G539
U	G2070	G	C1826	A1684	C1565	G1433	U1314	G1212	U1128	A	A933	A818	A666	A540
G	C2071	A	A1829	A1685	G1571	A1434	G1315	G1213	C1129	C	G940	A819	C667	C541
G	G2072	C	C1834	C1692	G1571	U1435	G1316	G1214	U1130	C	G941	G820	A542	A542
G	A2074	C	U1835	G1697	G1588	C1436	G1325	G1216	A1132	C	U942	U821	A543	G543
C	A2081	U1964	A1840	U1698	G1589	C1439	G1328	U1218	G1135	C	G946	G828	G681	G545
U	G2089	G1971	C1841	A1701	G1592	U1440	G1329	U1219	U1136	A	U947	G834	A686	G553
U	G2090	A1972	A1842	U1702	C1593	G1441	A1330	C1229	G1137	C	U948	U835	A687	C558
A	G2091	A1973	A1845	C1714	C1594	A1442	U1333	A1230	G1138	C	U949	U840	A688	C558
C	C2091	C	A1845	C1715	G1595	C1450	C1334	A1231	G1139	C	U950	A841	U560	U560
A	A2096	G1976	G1848	A1716	U1596	G1453	G1339	A1232	C1140	C	G952	A844	G699	A563
G	G2097	U1977	C1856	A1717	A1598	G1453	G1340	U1233	G1151	C	G953	U701	A700	G563
A	A2101	A1978	C1856	U1722	A1603	C1462	A1341	U1234	C1043	C	G958	G702	G701	G564
G	G2102	U1980	C1862	U1723	A1604	U1463	G1342	G1235	C1044	C	C959	G703	G703	U567
U	G2103	C	G1863	U1724	G1605	A1470	C1343	U1237	G1045	C	G960	C704	G704	G574
C	C2104	U1985	C1863	C1725	G1605	A1470	U1350	G1239	G1046	C	A961	G709	G709	A575
A	G2110	U1992	G1867	U1730	G1611	C1474	U1351	G1240	G1053	C	G962	G710	G710	A575
C	G2111	C1993	G1868	C1731	A1612	C1477	G1352	G1241	G1163	C	U969	U858	G711	G888
G	A2112	A1994	C1613	C1732	A1613	C1477	C1353	G1242	U1164	C	U970	U860	U714	A602
C	G2113	G1995	G1877	A1732	G1614	C1477	C1353	C1243	G1165	C	A603	A861	U	A603



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9: 48% 40% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.231 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, 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 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	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
32	B	1	0	0	0	0
32	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	73	0	0	0	0
33	9	3	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	2	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	3	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	J	3	0	0	1	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	O	1	0	0	0	0
34	R	1	0	0	0	0
34	Y	1	0	0	0	0
35	1	1	0	0	0	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	2	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
37	F	24	0	0	2	0
37	G	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 11.

The worst 5 of 1694 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)
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%)	17	25
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	17	25
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	4	3
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	9	11
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%)	22	32
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	29
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	22	32
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	9	13
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%)	7	9
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9	13
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22	32
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	12	17
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	5	4
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%)	25	36

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%)	27	44
2	B	282/283 (100%)	268 (95%)	14 (5%)	24	40
3	C	193/193 (100%)	179 (93%)	14 (7%)	14	22
4	D	117/148 (79%)	112 (96%)	5 (4%)	29	46
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	66
6	F	93/94 (99%)	92 (99%)	1 (1%)	73	87
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	53
8	H	134/145 (92%)	129 (96%)	5 (4%)	34	53
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	78
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	25
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	63
12	L	113/127 (89%)	110 (97%)	3 (3%)	44	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	152 (96%)	6 (4%)	33	51
14	N	149/150 (99%)	146 (98%)	3 (2%)	55	74
15	O	93/94 (99%)	90 (97%)	3 (3%)	39	59
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	76
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
18	R	117/122 (96%)	115 (98%)	2 (2%)	60	78
19	S	71/74 (96%)	69 (97%)	2 (3%)	43	63
20	T	105/106 (99%)	98 (93%)	7 (7%)	16	26
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	50
23	W	130/130 (100%)	123 (95%)	7 (5%)	22	36
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	14
25	Y	120/196 (61%)	112 (93%)	8 (7%)	16	26
26	Z	60/94 (64%)	58 (97%)	2 (3%)	38	57
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	84
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	31	49

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

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Mol	Chain	Res	Type
14	N	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	240 (8%)	33 (1%)

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

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1856	C
30	0	2761	A
30	0	1377	C
30	0	1506	U

## 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	14,22,23	1.01	1 (7%)	14,31,34	1.15	1 (7%)
30	UR3	0	2619	30	14,22,23	0.74	0	15,32,35	0.64	0
30	1MA	0	628	33,30	15,25,26	0.73	0	15,37,40	1.37	1 (6%)
30	PSU	0	2621	30	17,21,22	1.56	3 (17%)	20,30,33	5.46	4 (20%)
30	OMG	0	2588	30	18,26,27	1.08	2 (11%)	20,38,41	2.61	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	1MA	0	628	33,30	-	0/3/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.87	1.48	1.52
30	0	2588	OMG	C6-N1	3.50	1.39	1.33
30	0	2621	PSU	C4-N3	2.84	1.38	1.33
30	0	2587	OMU	C4-N3	2.78	1.37	1.33
30	0	2621	PSU	C2-N1	2.52	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.53	114.50	128.43
30	0	2621	PSU	C4-N3-C2	14.26	127.18	115.14
30	0	2588	OMG	C5-C6-N1	-8.67	111.57	123.43
30	0	2621	PSU	C5-C4-N3	-8.15	114.85	125.36
30	0	2588	OMG	C6-N1-C2	5.87	125.25	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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