



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 07:15 pm BST

PDB ID : 5NCO / pdb_00005nco
EMDB ID : EMD-3617
Title : Quaternary complex between SRP, SR, and SecYEG bound to the translating ribosome
Authors : Jomaa, A.; Hwang Fu, Y.; Boerhinger, D.; Leibundgut, M.; Shan, S.O.; Ban, N.
Deposited on : 2017-03-06
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

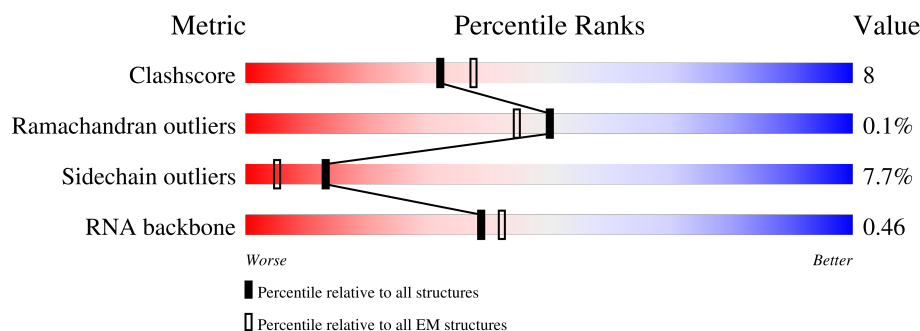
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.





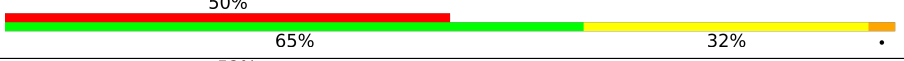
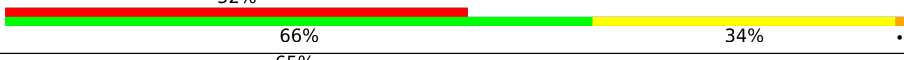
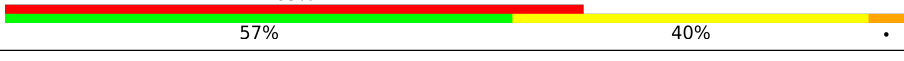
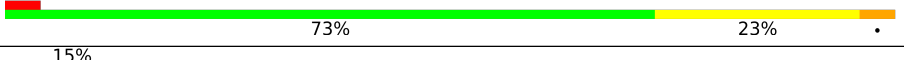

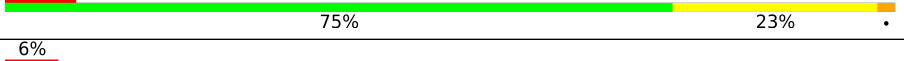

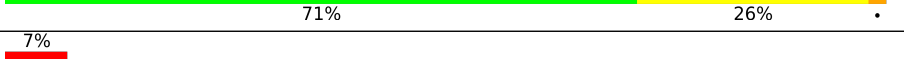
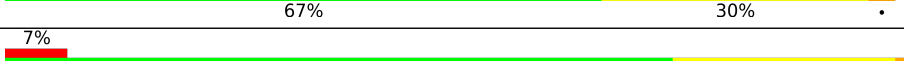
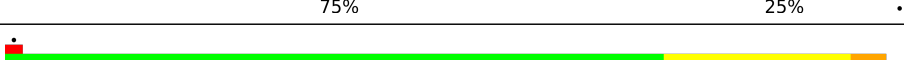
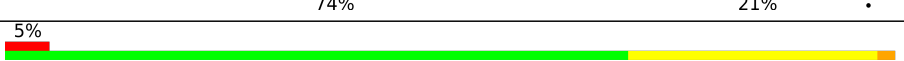
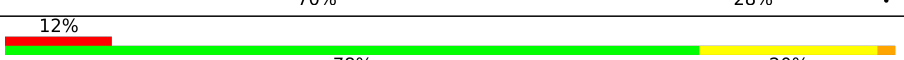
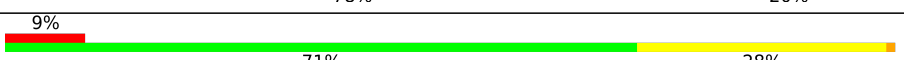
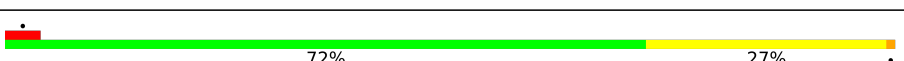
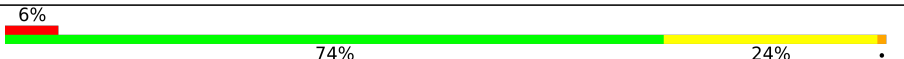
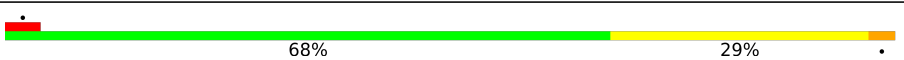


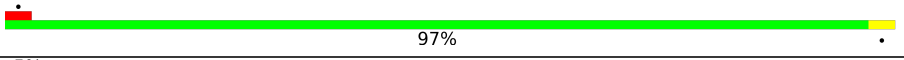
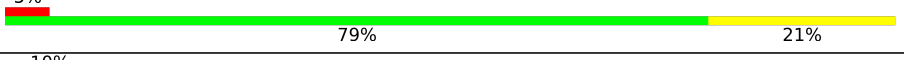
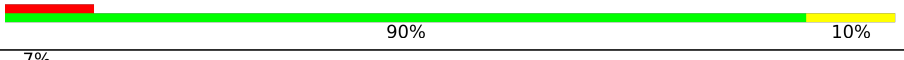
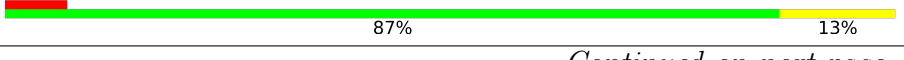

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	104	<div> <div>12%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
2	2	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	A	2903	<div> <div>55%</div> <div>36%</div> <div>8%</div> <div>..</div> </div>
4	B	120	<div> <div>72%</div> <div>24%</div> <div>.</div> </div>
5	C	271	<div> <div>8%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
6	D	209	<div> <div>6%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
7	E	201	<div> <div>8%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	F	177	
9	G	176	
10	H	149	
11	I	125	
12	J	134	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	125	
18	P	117	
19	Q	114	
20	R	117	
21	S	103	
22	T	110	
23	U	95	
24	V	102	
25	W	94	
26	X	76	
27	Y	77	
28	Z	62	
29	a	58	
30	b	56	
31	c	51	
32	d	46	

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Mol	Chain	Length	Quality of chain
33	e	64	
34	f	38	
35	g	416	
36	h	56	
37	i	450	
38	j	71	
39	k	23	
40	l	271	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 101694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 4.5S SRP RNA (Ffs).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	104	Total	C	N	O	P	0	0
			2224	991	401	728	104		

- Molecule 2 is a RNA chain called P-site tRNA-CCA end.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	416	Total	C	N	O	0	0
			1664	832	416	416		

- Molecule 36 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	56	Total	C	N	O	0	0
			224	112	56	56		

- Molecule 37 is a protein called Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	450	Total	C	N	O	S	0	0
			3384	2129	609	628	18		

- Molecule 38 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	j	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 39 is a protein called Signal sequence (1A9L).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	23	Total	C	N	O	0	0
			159	107	25	27		

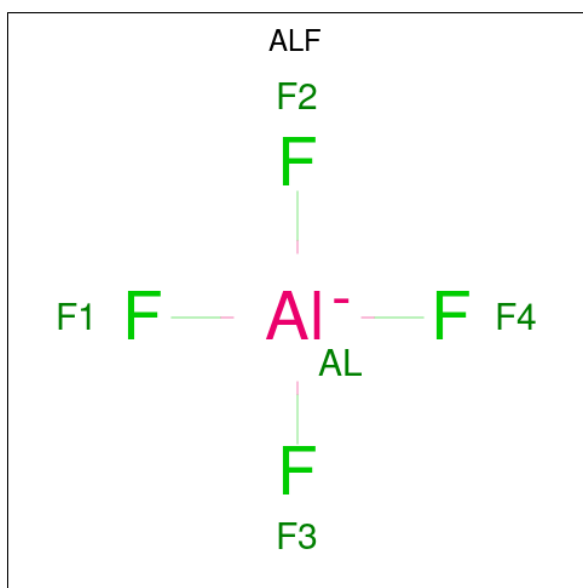
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	271	Total	C	N	O	S	0	0
			2067	1306	356	399	6		

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	f	1	Total	Zn	0
			1	1	

- Molecule 42 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

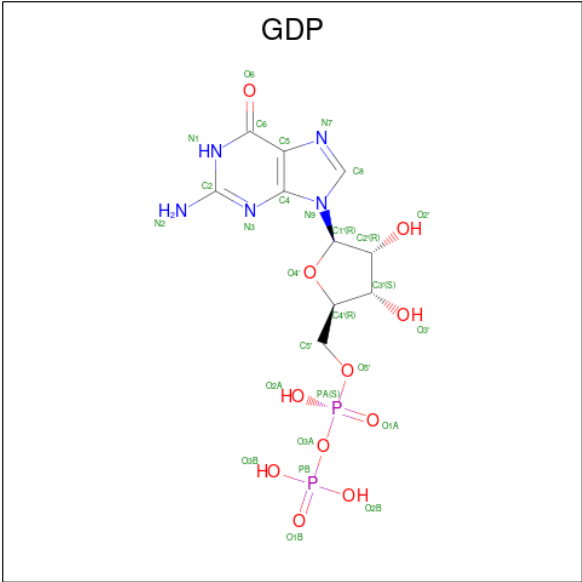


Mol	Chain	Residues	Atoms			AltConf
42	i	1	Total	Al	F	0
			5	1	4	
42	1	1	Total	Al	F	0
			5	1	4	

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	i	1	Total	Mg	0
			1	1	
43	1	1	Total	Mg	0
			1	1	

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

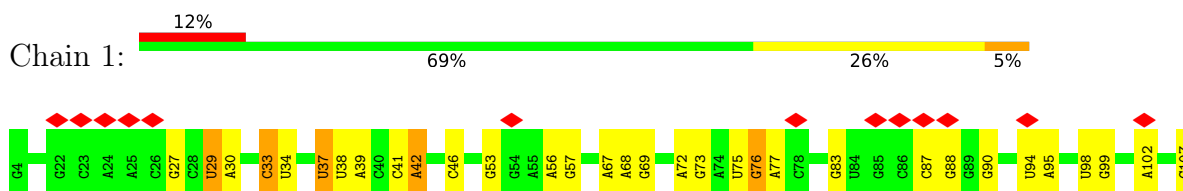


Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
44	1	1	Total	C	N	O	P	0
			28	10	5	11	2	

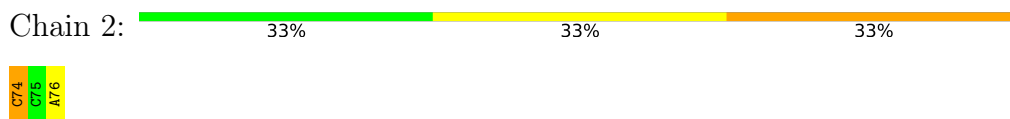
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

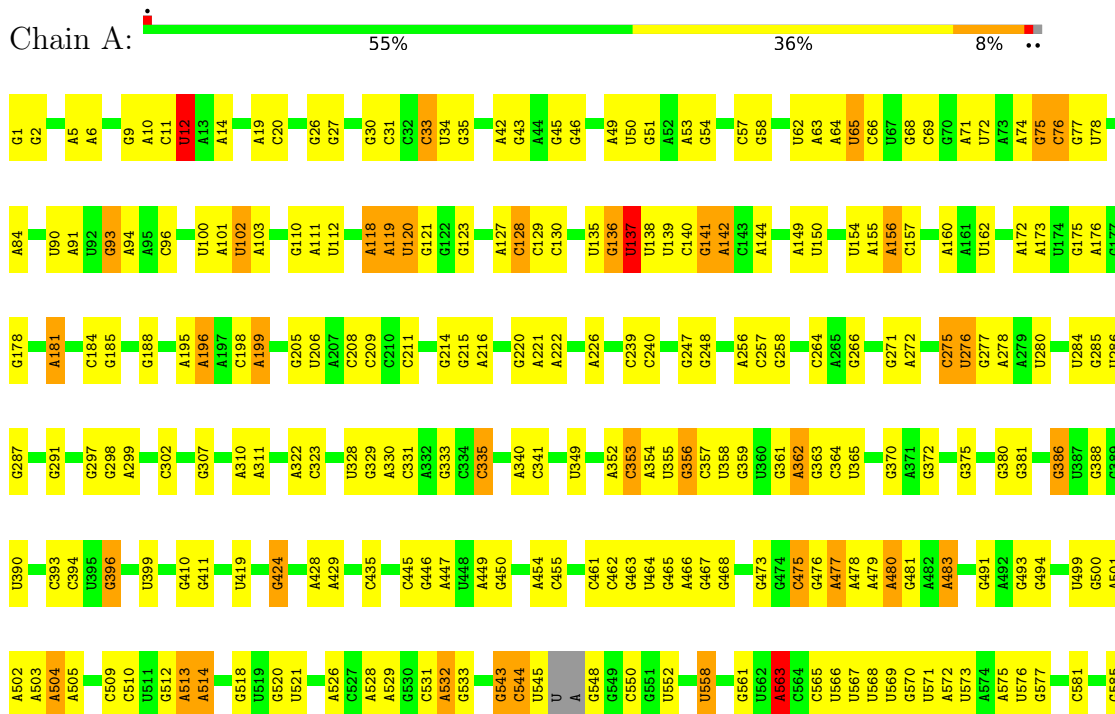
- Molecule 1: 4.5S SRP RNA (Ffs)



- Molecule 2: P-site tRNA-CCA end

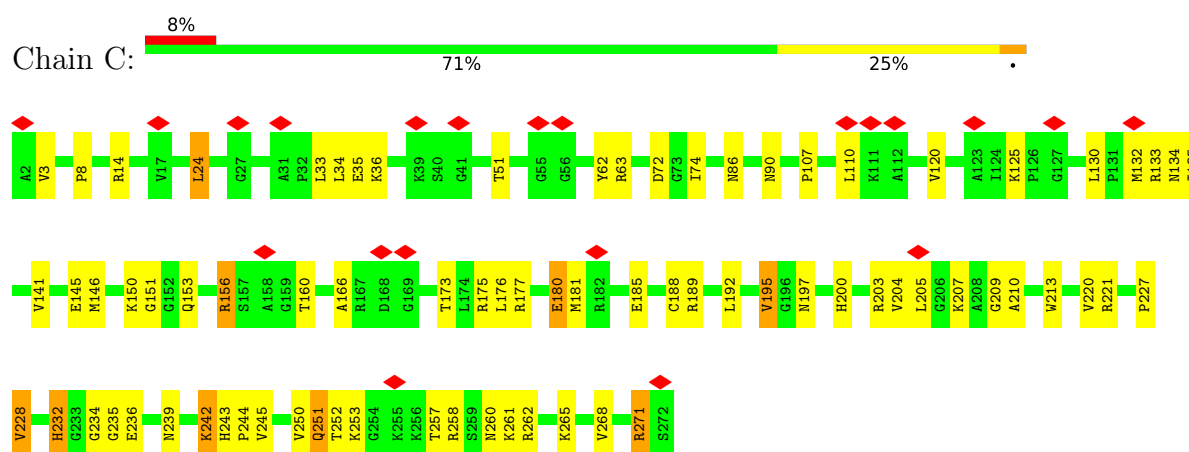


- Molecule 3: 23S rRNA

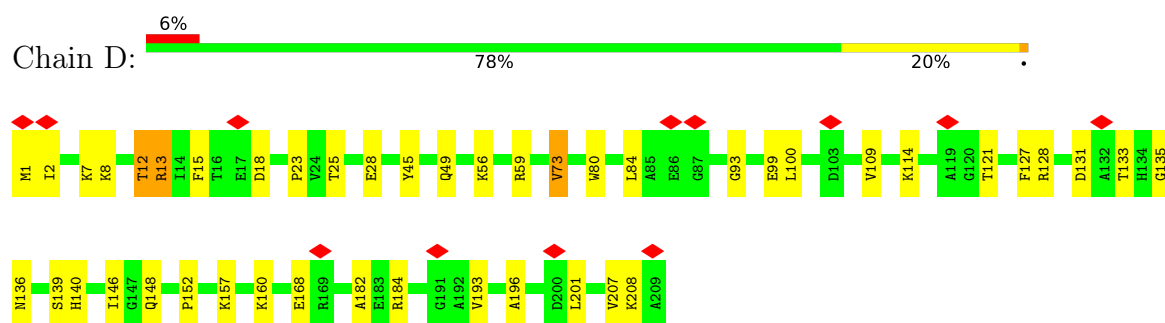


A1785	A1786	A1789	A1790	A1791	A1794	C1795	A1796	G1797	G1798	G1799	C1800	A1801	A1802	G1807	A1808	A1809	A1810	G1811	C1816	G1817	U1818	A1819	U1820	A1821	C1822	U1825	G1826	U1827	A1829	C1837	C1838	A1846	A1848	G1849	G1850	A1853	A1858	U1859	G1869	C1870	A1871	A1872	G1873	C1874	A1875	A1780	U1781	U1782	A1877			
A1677	A1678	G1681	A1689	G1695	A1697	A1698	A1699	A1700	C1706	U1709	G1710	A1711	G1715	G1721	A1722	U1725	U1729	G1730	G1731	G1732	A1735	U1736	U1737	G1738	G1743	A1744	U1751	C1752	A1757	U1758	A1759	C1760	G1761	G1762	G1763	C1764	U1769	G1770	A1773	A1774	U1775	A1780	U1781	U1782	A1877							
U1584	C1585	A1590	A1591	A1592	U1506	C1507	A1508	A1509	G1510	G1511	A1515	G1516	G1517	G1524	A1525	C1526	A1527	A1528	G1529	G1530	C1531	A1532	C1533	U1534	A1535	C1536	G1537	U1542	G1543	A1544	A1545	G1546	U1554	U1564	A1565	A1569	A1570	A1572	U1576	C1577	U1578	G1581	C1582	A1583								
A1439	A1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	G1432	A1433	A1434	G1435	G1436	C1437	U1438	A1439	U1442	U1443	C1446	C1447	G1448	G1449	A1450	C1451	G1452	A1453	U1460	C1463	G1464	G1465	U1466	U1467	U1468	A1469	A1470	G1471	C1472	G1473	U1474	G1482	G1483	U1484	U1485	C1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496
A1327	A1328	U1329	G1332	G1337	G1338	G1339	U1340	G1341	A1342	U1344	A1345	G1346	C1351	A1354	G1355	C1362	C1363	G1364	A1365	A1366	A1367	G1374	U1379	A1383	C1386	A1387	G1388	U1394	A1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	A1403	C1404	U1405	U1406	G1410	C1414	U1415	G1416	G1417	G1418						
G1212	G1218	U1230	A1231	U1234	G1235	G1236	A1237	G1243	A1247	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	C1261	A1262	U1266	U1267	A1268	A1269	C1270	G1271	A1272	A1275	A1287	G1288	C1289	U1290	U1294	G1300	A1301	A1302	G1303	A1308	U1313	C1314	A1321	G1324											
U1105	G1106	G1110	A1111	G1112	G1115	G1116	G1125	A1126	A1127	G1128	A1129	U1130	G1131	U1132	A1133	A1134	C1135	G1136	G1139	C1140	U1141	A1142	A1143	G1149	C1150	G1154	A1155	G1168	C1172	U1173	U	A	U	G1177	C1178	G1179	U1180	U1181	G1182	G1187	U1188	U1198	U1199	A1205	G1206	U1101	G1210	C1211				
A1028	U1033	G1038	A1039	A1040	C1044	C1045	A1046	G1047	A1048	G1056	A1057	U1060	U1061	G1062	C1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	C1072	A1073	G1074	C1075	C1076	U1077	U1078	C1079	U1082	U1083	A1084	A1085	A1086	C1087	A1088	A1089	A1090	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103		
C946	A947	C948	G949	G953	C957	U958	A959	A960	C961	C968	U970	G971	A972	A973	G974	A975	G976	A981	C982	A983	A984	C987	A990	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	C1005	C1006	C1007	A1008	C908	A909	A1010	G1011	U1012	C1013	A1021	G1022	U1023	G1024	G1025	G1026	A1027			
C848	A849	U850	G857	G858	G859	A861	G862	A863	G864	C865	G869	U870	U871	U872	C876	A877	G878	G879	G880	G881	C882	G	U	C	A	U	C	C	C	G	A	C	U894	U895	A896	C897	C898	A899	U906	G907	C908	G831	A910	A911	G914	C915	G916	A917	G930	U931	U932	A933
A870	C871	C872	C873	G874	A877	A878	A879	A880	A885	U886	A706	G707	G711	G712	G713	G714	A715	A716	C717	A718	C719	U720	A721	A722	G729	A730	G733	G738	U741	A742	A743	U747	A753	U754	U755	A756	G757	C758	G759	A763	A764	C765	C772	U773	G774	G775						
A536	U591	A592	U593	U594	C595	C601	A602	A603	G604	G605	A608	A609	C610	C611	G612	A613	A614	A616	G620	A621	G622	A627	G628	G629	G630	A631	A632	A633	C634	A637	G638	U639	C640	U641	U642	C645	U646	G647	G648	G649	C650	U653	A654	A655	G656	U657	U658	A668	G669			

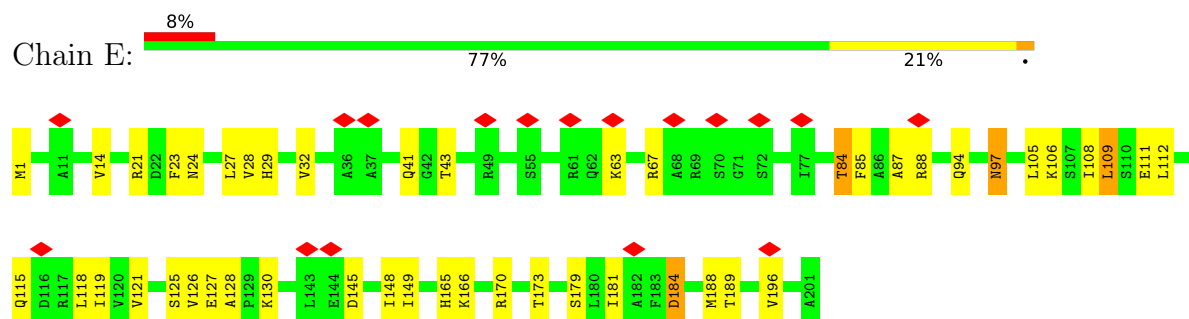




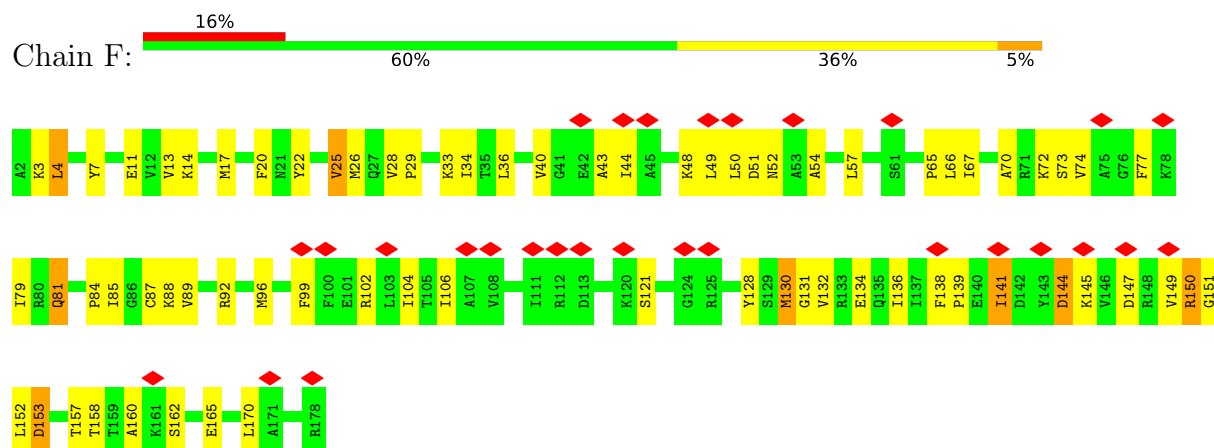
• Molecule 6: 50S ribosomal protein L3



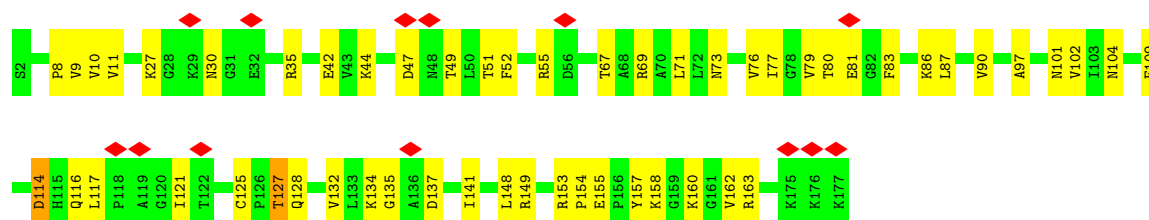
• Molecule 7: 50S ribosomal protein L4



• Molecule 8: 50S ribosomal protein L5



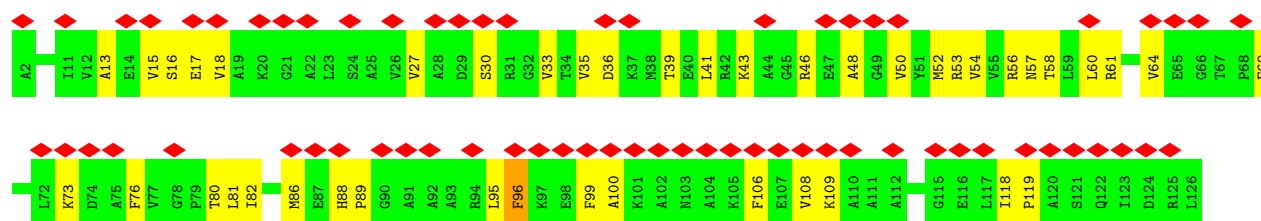
- Molecule 9: 50S ribosomal protein L6



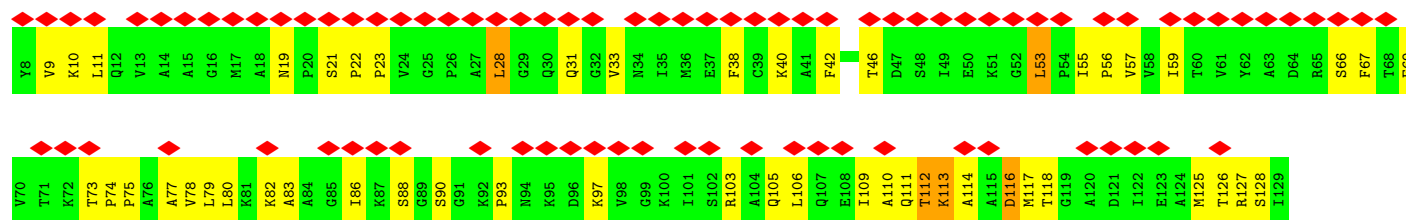
- Molecule 10: 50S ribosomal protein L9

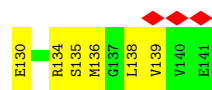


- Molecule 11: 50S ribosomal protein L10



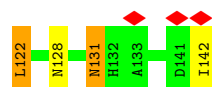
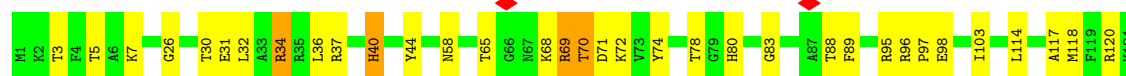
- Molecule 12: 50S ribosomal protein L11





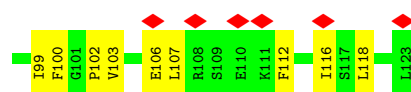
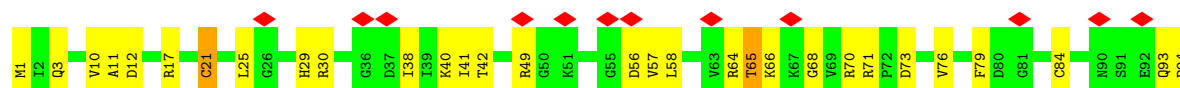
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 23%



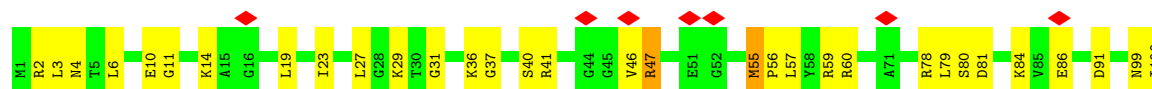
- Molecule 14: 50S ribosomal protein L14

Chain L: 15% 68% 30%



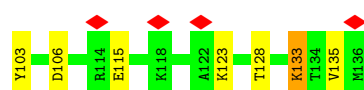
- Molecule 15: 50S ribosomal protein L15

Chain M: 8% 75% 23%

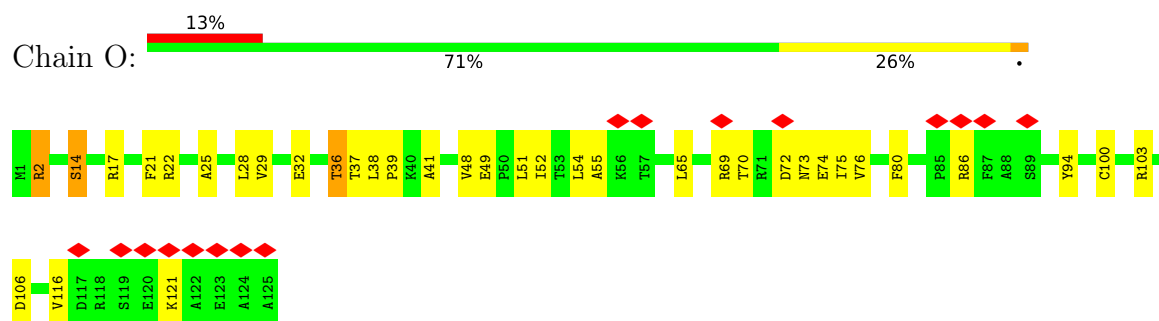


- Molecule 16: 50S ribosomal protein L16

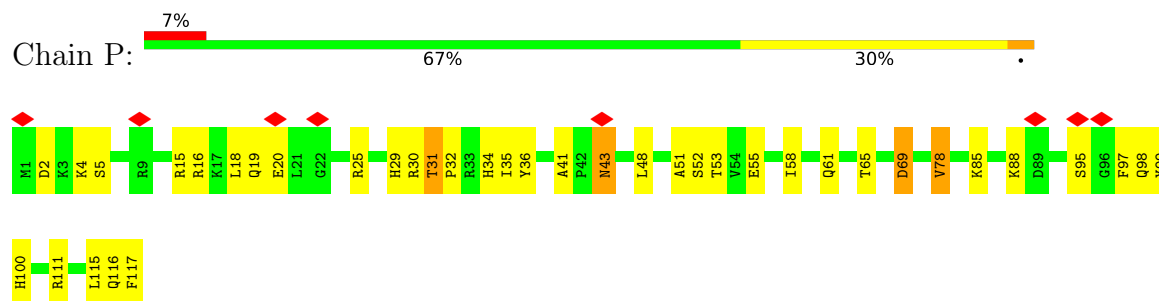
Chain N: 6% 71% 26%



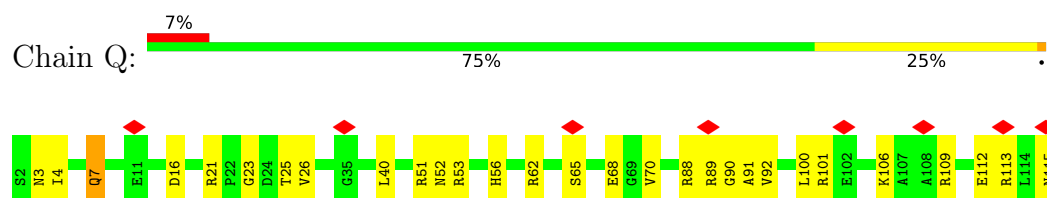
- Molecule 17: 50S ribosomal protein L17



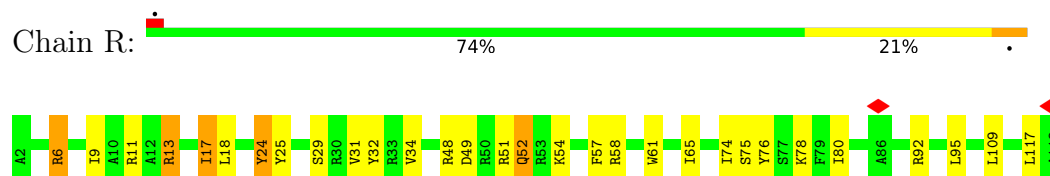
- Molecule 18: 50S ribosomal protein L18



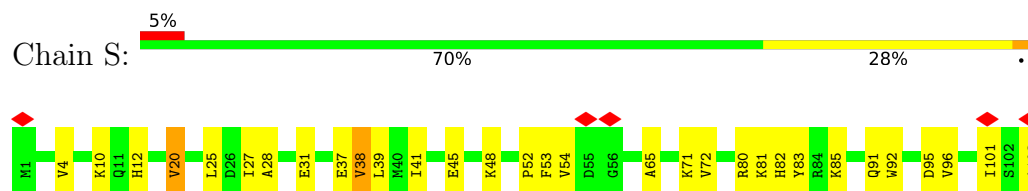
- Molecule 19: 50S ribosomal protein L19



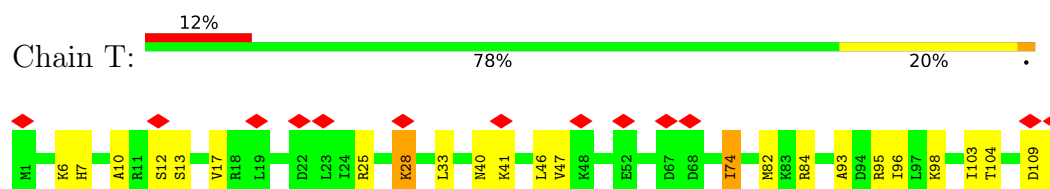
- Molecule 20: 50S ribosomal protein L20



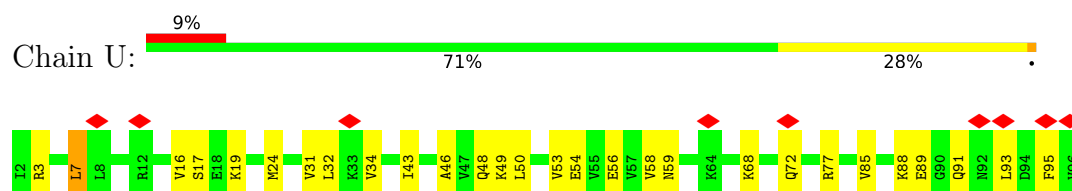
- Molecule 21: 50S ribosomal protein L21



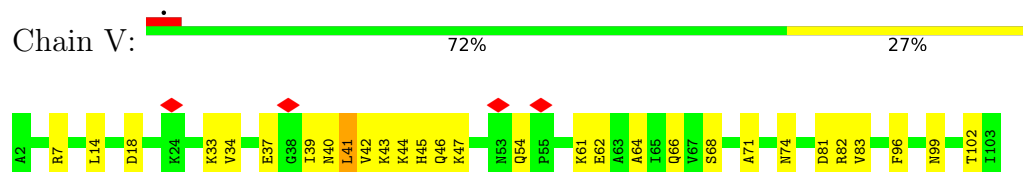
- Molecule 22: 50S ribosomal protein L22



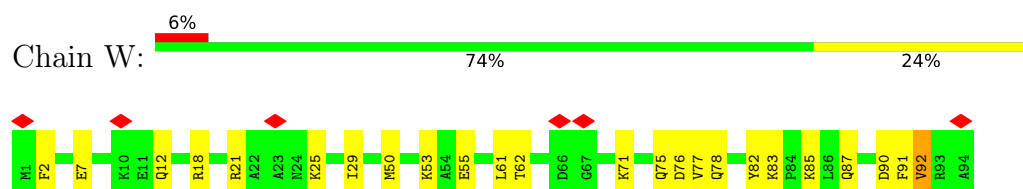
- Molecule 23: 50S ribosomal protein L23



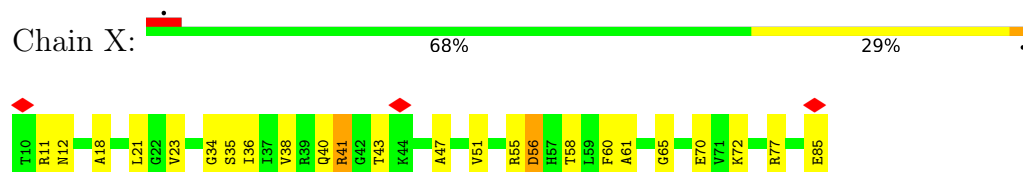
- Molecule 24: 50S ribosomal protein L24



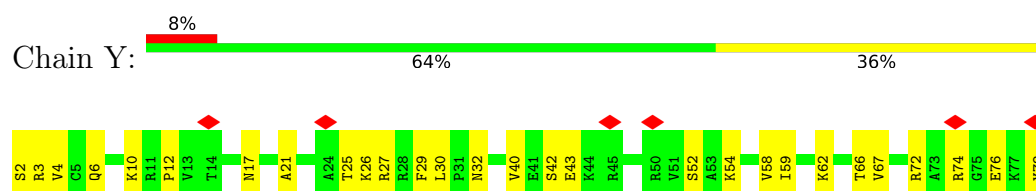
- Molecule 25: 50S ribosomal protein L25



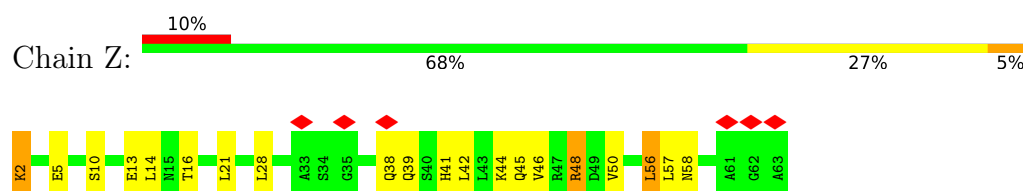
- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28



- Molecule 28: 50S ribosomal protein L29

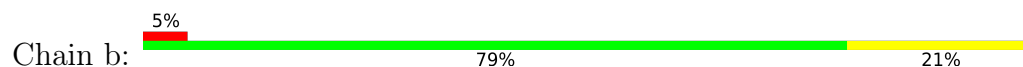


- Molecule 29: 50S ribosomal protein L30

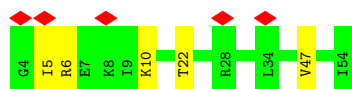




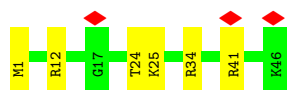
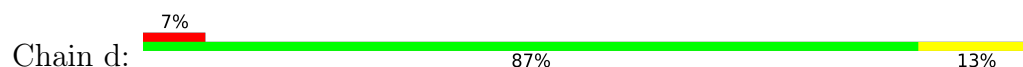
- Molecule 30: 50S ribosomal protein L32



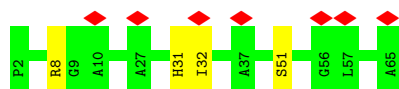
- Molecule 31: 50S ribosomal protein L33



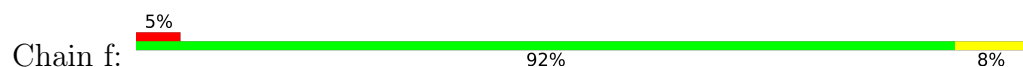
- Molecule 32: 50S ribosomal protein L34



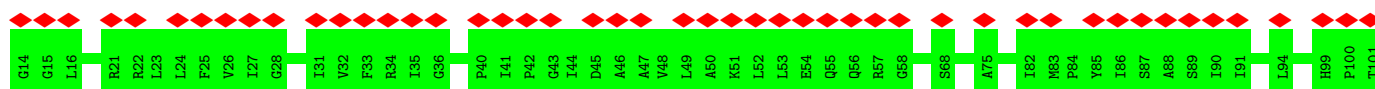
- Molecule 33: 50S ribosomal protein L35

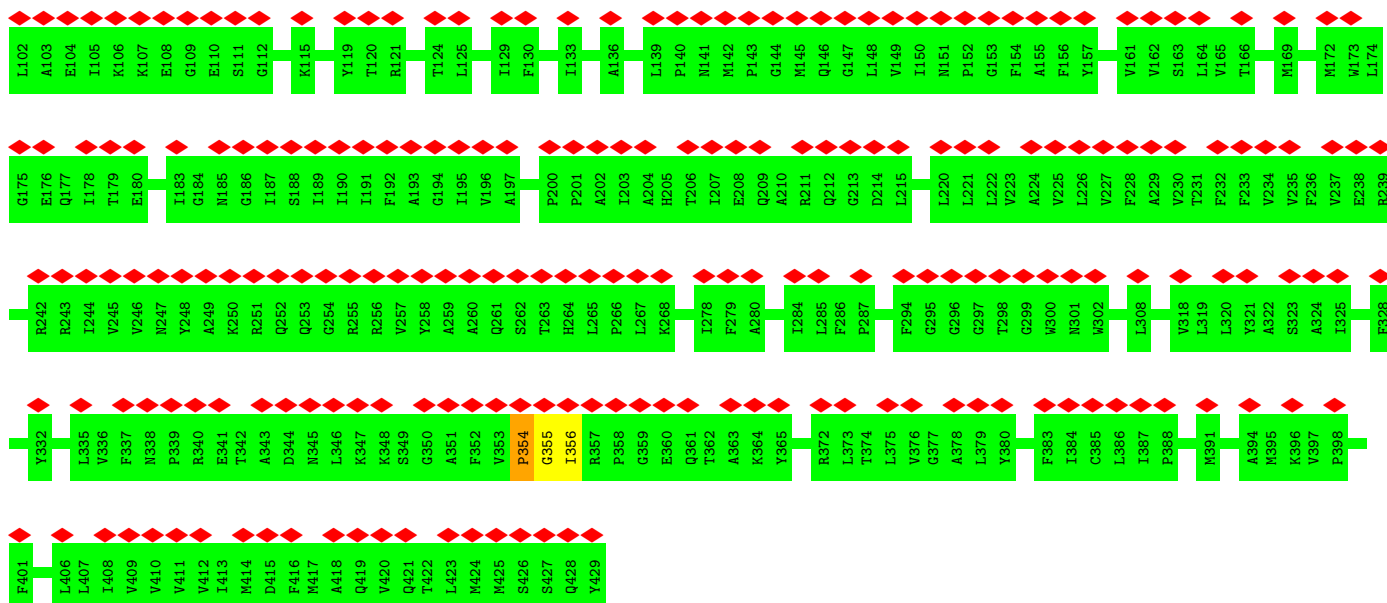


- Molecule 34: 50S ribosomal protein L36

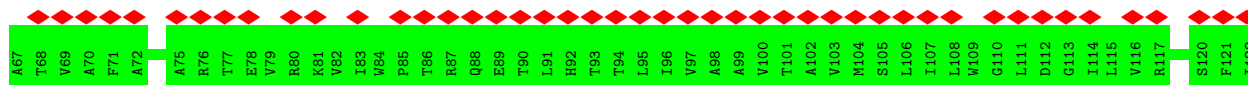
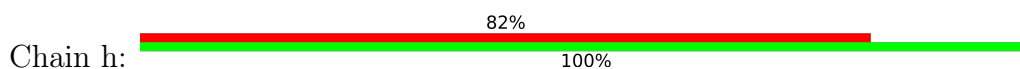


- Molecule 35: Protein translocase subunit SecY

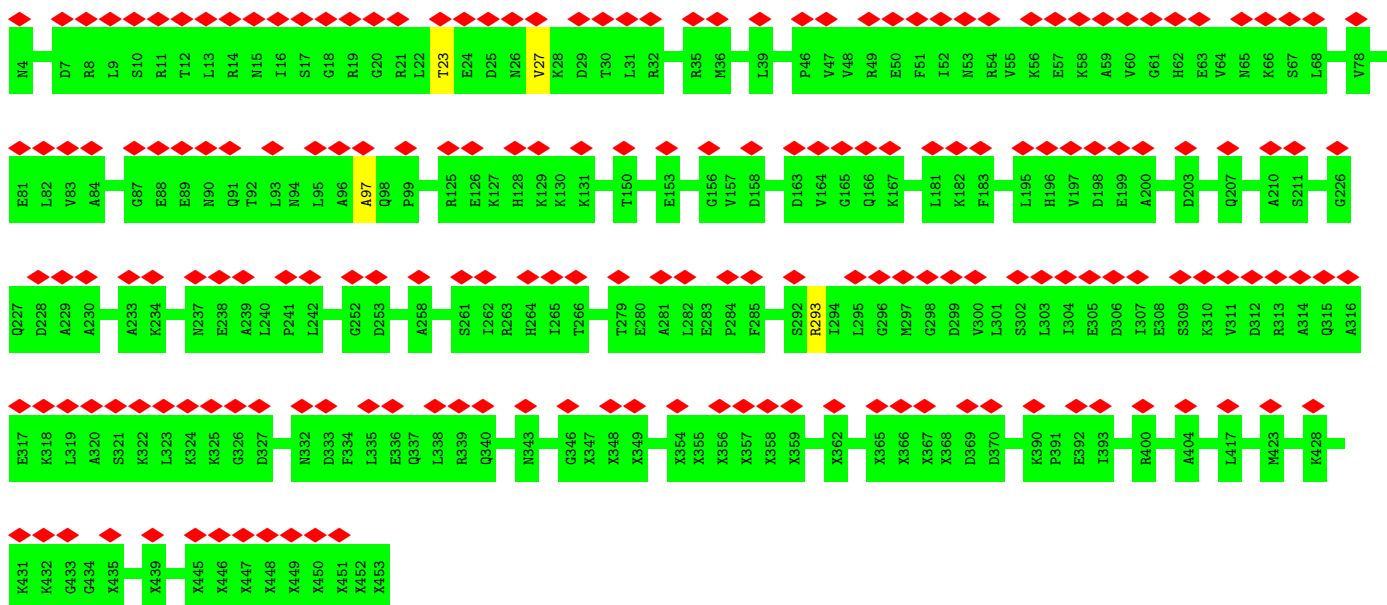
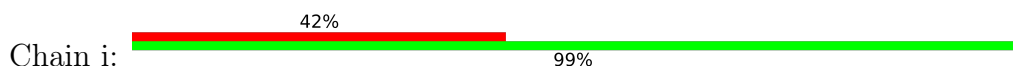




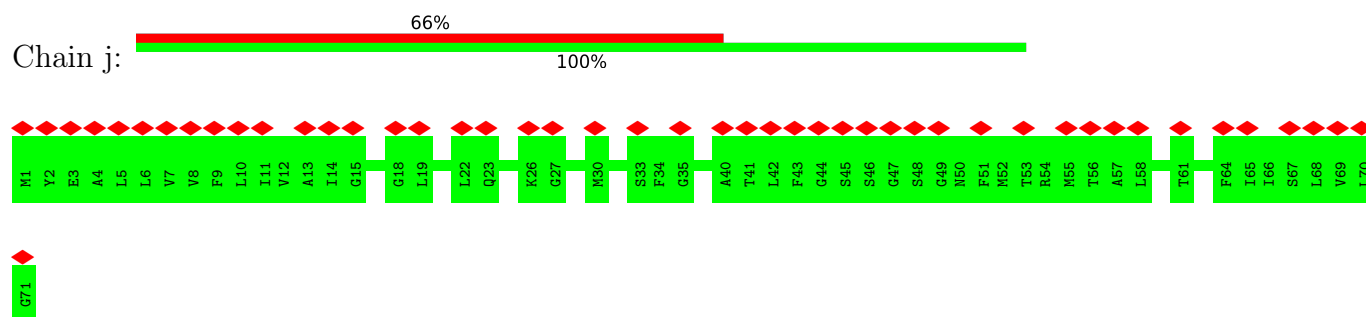
• Molecule 36: Protein translocase subunit SecE



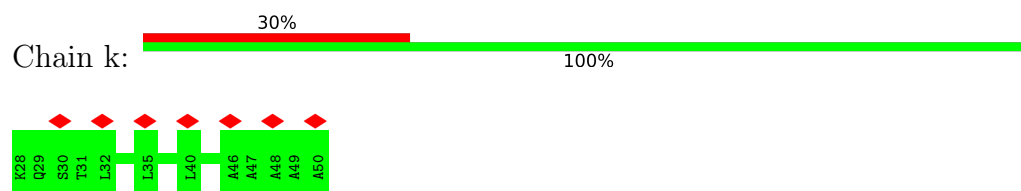
• Molecule 37: Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein



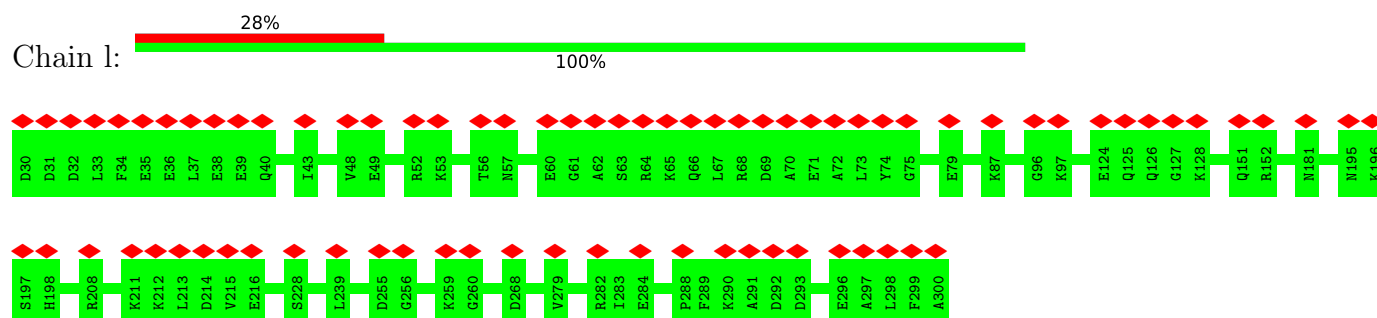
• Molecule 38: Protein-export membrane protein SecG



• Molecule 39: Signal sequence (1A9L)



• Molecule 40: Signal recognition particle receptor FtsY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; After 3D reconstruction 3D maps were sharpened	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GDP, ALF

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	1	0.15	0/2486	0.70	0/3874
2	2	0.57	0/68	1.27	1/103 (1.0%)
3	A	0.69	13/69329 (0.0%)	1.17	188/108152 (0.2%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2122	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1435	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
10	H	0.43	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1290 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.60	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.46	0/763	0.65	0/1021
24	V	0.38	0/788	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.42	0/502	0.54	0/667
29	a	0.38	0/453	0.56	0/605
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.47	0/513	0.63	0/676
34	f	0.49	0/303	0.58	0/397
35	g	0.27	0/1663	0.51	5/2077 (0.2%)
36	h	0.16	0/223	0.29	0/277
37	i	0.21	0/3170	0.39	0/4255
38	j	0.16	0/283	0.27	0/352
39	k	0.21	0/159	0.40	0/218
40	l	0.20	0/2091	0.36	0/2822
All	All	0.60	13/109794 (0.0%)	1.02	198/163369 (0.1%)

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
5	C	0	1
9	G	0	1
12	J	0	1
35	g	0	1
37	i	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.93	1.33	1.37
3	A	1254	A	N9-C4	-6.48	1.33	1.37
3	A	1321	A	N9-C4	6.30	1.41	1.37
3	A	776	G	N9-C4	6.01	1.42	1.38
3	A	1490	A	N9-C4	5.92	1.41	1.37
3	A	2114	A	N9-C4	5.90	1.41	1.37
3	A	563	A	N9-C4	-5.71	1.34	1.37
3	A	1254	A	N3-C4	-5.48	1.31	1.34
3	A	1010	A	N9-C4	-5.33	1.34	1.37
3	A	960	A	N9-C4	-5.27	1.34	1.37
3	A	586	A	N3-C4	-5.24	1.31	1.34
3	A	1678	A	N9-C4	-5.21	1.34	1.37
3	A	514	A	N9-C4	-5.11	1.34	1.37

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.21	113.67	121.00
3	A	2422	C	O4'-C1'-N1	9.37	115.69	108.20
3	A	1838	C	C6-N1-C2	9.15	123.96	120.30
35	g	354	PRO	C-N-CA	-8.94	103.53	122.30
3	A	2423	U	C5-C6-N1	8.77	127.08	122.70
3	A	1584	U	C2-N1-C1'	8.55	127.95	117.70
3	A	776	G	C8-N9-C4	-7.97	103.21	106.40
3	A	2431	U	N3-C2-O2	-7.91	116.67	122.20
3	A	275	C	C6-N1-C2	-7.67	117.23	120.30
3	A	1760	C	C6-N1-C2	7.58	123.33	120.30
3	A	2422	C	N3-C2-O2	-7.30	116.79	121.90
3	A	1584	U	N1-C2-O2	7.26	127.88	122.80
3	A	2177	C	C6-N1-C2	-7.10	117.46	120.30
3	A	1992	G	C4-C5-N7	7.02	113.61	110.80
3	A	2614	A	C6-N1-C2	-6.92	114.45	118.60
3	A	2431	U	C5-C4-O4	6.90	130.04	125.90
3	A	214	G	N3-C4-C5	-6.89	125.16	128.60
3	A	137	U	C5-C4-O4	-6.85	121.79	125.90
3	A	2422	C	C6-N1-C2	-6.83	117.57	120.30
3	A	2636	C	C2-N1-C1'	6.80	126.28	118.80
3	A	2424	C	O4'-C1'-N1	6.78	113.62	108.20
3	A	2207	C	C6-N1-C2	-6.76	117.60	120.30
35	g	355	GLY	CA-C-O	-6.75	108.44	120.60
3	A	1607	C	C6-N1-C2	-6.71	117.62	120.30
3	A	1027	A	C8-N9-C4	6.62	108.45	105.80
3	A	102	U	C2-N1-C1'	6.62	125.64	117.70
3	A	776	G	C4-N9-C1'	6.54	135.01	126.50
3	A	1064	C	C6-N1-C2	-6.49	117.70	120.30
3	A	2542	A	C2-N3-C4	-6.48	107.36	110.60
3	A	1531	C	C5-C6-N1	6.47	124.24	121.00
3	A	784	G	P-O3'-C3'	6.47	127.47	119.70
3	A	906	U	C5-C4-O4	6.47	129.78	125.90
3	A	1849	G	C8-N9-C4	-6.46	103.81	106.40
3	A	2000	C	C6-N1-C2	6.46	122.88	120.30
3	A	1313	U	N3-C2-O2	-6.45	117.68	122.20
3	A	1128	G	C8-N9-C4	6.43	108.97	106.40
3	A	1849	G	N7-C8-N9	6.38	116.29	113.10
3	A	2456	C	C6-N1-C2	-6.32	117.77	120.30
3	A	1652	A	C8-N9-C4	6.28	108.31	105.80
3	A	12	U	N3-C2-O2	-6.28	117.81	122.20
3	A	733	G	C4-C5-N7	6.28	113.31	110.80
3	A	2104	C	C6-N1-C2	-6.27	117.79	120.30
3	A	483	A	C8-N9-C4	6.24	108.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1606	C	N3-C2-O2	-6.24	117.53	121.90
3	A	1848	A	C8-N9-C4	-6.23	103.31	105.80
3	A	1695	G	N9-C4-C5	-6.21	102.92	105.40
3	A	832	U	C5-C6-N1	-6.18	119.61	122.70
3	A	611	C	C6-N1-C2	-6.17	117.83	120.30
3	A	805	G	C8-N9-C4	6.15	108.86	106.40
3	A	774	G	C8-N9-C4	6.13	108.85	106.40
3	A	1470	A	C8-N9-C4	-6.11	103.36	105.80
3	A	804	A	C8-N9-C4	6.11	108.24	105.80
3	A	758	C	C6-N1-C2	-6.10	117.86	120.30
3	A	1362	C	C6-N1-C2	-6.10	117.86	120.30
3	A	776	G	N3-C4-C5	-6.07	125.56	128.60
3	A	2691	C	C6-N1-C2	6.07	122.73	120.30
3	A	2499	C	N1-C2-O2	6.07	122.54	118.90
3	A	1261	C	C6-N1-C2	6.06	122.72	120.30
3	A	2704	C	C6-N1-C2	-6.04	117.89	120.30
3	A	1272	A	C8-N9-C4	6.03	108.21	105.80
3	A	2052	A	N1-C6-N6	6.02	122.21	118.60
3	A	102	U	N1-C2-O2	6.00	127.00	122.80
3	A	2542	A	N3-C4-C5	6.00	131.00	126.80
3	A	2171	A	O4'-C1'-N9	6.00	113.00	108.20
3	A	2109	U	C6-N1-C2	-5.98	117.41	121.00
3	A	130	C	N3-C4-C5	5.97	124.29	121.90
3	A	1992	G	N9-C4-C5	-5.97	103.01	105.40
3	A	1584	U	C5-C6-N1	5.96	125.68	122.70
3	A	2433	A	N1-C2-N3	5.96	132.28	129.30
3	A	832	U	C2-N3-C4	-5.93	123.44	127.00
3	A	2440	C	C6-N1-C2	5.89	122.66	120.30
3	A	2423	U	N3-C4-C5	-5.88	111.07	114.60
3	A	776	G	O4'-C1'-N9	5.87	112.90	108.20
3	A	2820	A	C8-N9-C4	5.87	108.15	105.80
3	A	1531	C	C6-N1-C2	-5.86	117.96	120.30
3	A	205	G	O4'-C1'-N9	5.84	112.87	108.20
12	J	53	LEU	CA-CB-CG	5.82	128.69	115.30
3	A	790	U	N1-C2-O2	5.82	126.88	122.80
3	A	2077	A	C6-N1-C2	-5.81	115.11	118.60
3	A	1072	C	C6-N1-C2	-5.80	117.98	120.30
3	A	141	G	N7-C8-N9	5.79	116.00	113.10
3	A	1584	U	N3-C2-O2	-5.78	118.15	122.20
3	A	793	A	C2-N3-C4	5.77	113.49	110.60
3	A	2580	U	C6-N1-C2	-5.74	117.56	121.00
3	A	2153	C	C5-C6-N1	5.71	123.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	741	U	C5-C6-N1	-5.71	119.84	122.70
3	A	1871	A	C8-N9-C4	-5.70	103.52	105.80
3	A	1643	G	C8-N9-C4	-5.70	104.12	106.40
3	A	1045	C	C6-N1-C2	5.69	122.58	120.30
7	E	109	LEU	CA-CB-CG	-5.68	102.23	115.30
3	A	2588	G	N3-C4-C5	5.68	131.44	128.60
3	A	1659	G	N3-C4-C5	5.67	131.44	128.60
3	A	2582	G	N3-C4-C5	-5.67	125.76	128.60
3	A	816	C	C6-N1-C2	-5.67	118.03	120.30
3	A	1993	U	C5-C6-N1	-5.67	119.87	122.70
3	A	76	C	C5-C6-N1	5.66	123.83	121.00
3	A	2243	U	C5-C6-N1	-5.66	119.87	122.70
3	A	2845	U	C2-N3-C4	-5.65	123.61	127.00
3	A	793	A	C5-C6-N6	-5.63	119.20	123.70
11	I	95	LEU	CA-CB-CG	5.62	128.24	115.30
3	A	987	C	N3-C4-C5	5.62	124.15	121.90
35	g	355	GLY	N-CA-C	-5.61	99.08	113.10
3	A	130	C	C6-N1-C2	5.60	122.54	120.30
3	A	783	A	C8-N9-C4	-5.58	103.57	105.80
3	A	410	G	N3-C4-C5	-5.57	125.82	128.60
3	A	2636	C	C6-N1-C1'	-5.56	114.13	120.80
3	A	1303	G	C8-N9-C4	5.56	108.62	106.40
3	A	2145	C	C6-N1-C2	-5.55	118.08	120.30
3	A	1526	C	C6-N1-C2	-5.54	118.08	120.30
3	A	972	A	N1-C6-N6	-5.54	115.28	118.60
3	A	1078	U	C5-C6-N1	5.51	125.45	122.70
3	A	2498	C	C6-N1-C2	-5.51	118.10	120.30
3	A	825	A	C6-N1-C2	-5.51	115.30	118.60
3	A	1125	G	C8-N9-C4	-5.50	104.20	106.40
3	A	2022	U	C6-N1-C2	5.50	124.30	121.00
3	A	2614	A	C5-C6-N1	5.49	120.45	117.70
3	A	1314	C	C6-N1-C2	-5.49	118.11	120.30
3	A	1604	C	C5-C6-N1	-5.48	118.26	121.00
3	A	1351	C	C6-N1-C2	5.48	122.49	120.30
3	A	1584	U	C6-N1-C1'	-5.48	113.53	121.20
3	A	776	G	N7-C8-N9	5.45	115.82	113.10
3	A	206	U	C2-N1-C1'	5.44	124.23	117.70
3	A	135	U	C5-C6-N1	5.44	125.42	122.70
3	A	2153	C	C6-N1-C2	-5.42	118.13	120.30
3	A	280	U	P-O3'-C3'	5.41	126.19	119.70
3	A	2595	G	C4-N9-C1'	-5.41	119.47	126.50
3	A	613	A	P-O3'-C3'	5.40	126.18	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	356	ILE	N-CA-C	5.39	125.54	111.00
3	A	2423	U	N1-C2-N3	5.38	118.13	114.90
3	A	755	U	C5-C6-N1	-5.38	120.01	122.70
3	A	1642	G	N3-C4-C5	5.37	131.29	128.60
3	A	12	U	N1-C2-O2	5.37	126.56	122.80
3	A	793	A	C5-C6-N1	5.37	120.38	117.70
3	A	1172	C	C6-N1-C2	-5.36	118.16	120.30
3	A	2090	A	C8-N9-C4	5.35	107.94	105.80
3	A	1848	A	N7-C8-N9	5.34	116.47	113.80
3	A	2380	C	C6-N1-C2	-5.34	118.17	120.30
3	A	790	U	C2-N1-C1'	5.33	124.10	117.70
3	A	1606	C	N1-C2-O2	5.33	122.10	118.90
3	A	1494	A	P-O3'-C3'	5.33	126.09	119.70
3	A	672	C	N3-C2-O2	-5.32	118.17	121.90
3	A	642	U	O4'-C1'-N1	5.31	112.45	108.20
3	A	2645	G	C4-N9-C1'	5.31	133.41	126.50
4	B	42	C	C6-N1-C2	-5.31	118.18	120.30
3	A	569	U	C5-C6-N1	-5.30	120.05	122.70
3	A	946	C	N3-C2-O2	-5.30	118.19	121.90
3	A	906	U	O4'-C1'-N1	5.30	112.44	108.20
3	A	2645	G	N3-C4-C5	-5.29	125.96	128.60
3	A	1664	A	C8-N9-C4	-5.29	103.69	105.80
35	g	356	ILE	C-N-CA	5.27	134.87	121.70
3	A	1848	A	O4'-C1'-N9	5.26	112.41	108.20
3	A	2000	C	C5-C6-N1	-5.24	118.38	121.00
3	A	264	C	N3-C2-O2	-5.24	118.23	121.90
3	A	375	G	N3-C4-N9	5.22	129.13	126.00
3	A	128	C	C6-N1-C2	5.22	122.39	120.30
3	A	809	G	N3-C4-C5	-5.22	125.99	128.60
3	A	906	U	C2-N1-C1'	-5.21	111.45	117.70
3	A	1072	C	C5-C6-N1	5.21	123.60	121.00
3	A	375	G	N3-C4-C5	-5.20	126.00	128.60
3	A	1769	U	C5-C6-N1	-5.20	120.10	122.70
3	A	1970	A	N1-C2-N3	5.20	131.90	129.30
3	A	2516	A	C8-N9-C4	5.20	107.88	105.80
3	A	2074	U	N3-C2-O2	-5.19	118.57	122.20
2	2	74	C	C5-C6-N1	5.19	123.59	121.00
3	A	2022	U	C5-C6-N1	-5.18	120.11	122.70
3	A	2074	U	C2-N1-C1'	5.18	123.91	117.70
3	A	972	A	N9-C4-C5	5.15	107.86	105.80
3	A	828	U	C5-C6-N1	-5.15	120.12	122.70
3	A	981	A	C8-N9-C4	5.13	107.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1617	C	C5-C6-N1	-5.13	118.43	121.00
3	A	2847	U	C5-C6-N1	-5.12	120.14	122.70
3	A	66	C	N3-C2-O2	-5.11	118.32	121.90
3	A	1617	C	C2-N3-C4	-5.11	117.34	119.90
3	A	2421	G	C4-C5-N7	5.11	112.84	110.80
3	A	807	U	C5-C6-N1	-5.09	120.15	122.70
3	A	2115	G	N3-C4-C5	-5.09	126.05	128.60
3	A	646	U	C6-N1-C2	-5.07	117.96	121.00
3	A	1958	C	C6-N1-C2	-5.07	118.27	120.30
3	A	2614	A	C8-N9-C4	-5.07	103.77	105.80
3	A	906	U	C6-N1-C1'	5.06	128.28	121.20
3	A	809	G	C8-N9-C4	-5.05	104.38	106.40
3	A	30	G	C8-N9-C4	5.05	108.42	106.40
3	A	878	A	C8-N9-C4	-5.05	103.78	105.80
3	A	2365	G	C8-N9-C4	5.05	108.42	106.40
3	A	76	C	C6-N1-C2	-5.04	118.28	120.30
3	A	1903	G	C8-N9-C4	5.04	108.42	106.40
3	A	1470	A	N9-C4-C5	5.04	107.82	105.80
3	A	2114	A	C8-N9-C4	-5.04	103.79	105.80
3	A	2421	G	C6-C5-N7	-5.04	127.38	130.40
3	A	211	C	C6-N1-C2	5.03	122.31	120.30
3	A	1314	C	C2-N1-C1'	5.03	124.33	118.80
3	A	733	G	C5-N7-C8	-5.02	101.79	104.30
3	A	2064	C	C6-N1-C2	-5.02	118.29	120.30
3	A	102	U	C6-N1-C1'	-5.02	114.17	121.20
3	A	2542	A	C8-N9-C4	5.02	107.81	105.80
3	A	271	G	C8-N9-C4	5.01	108.41	106.40
3	A	804	A	C2-N3-C4	-5.00	108.10	110.60
3	A	1102	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	g	354	PRO	Peptide
37	i	293	ARG	Peptide

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	1	2224	0	1124	11	0
2	2	62	0	34	1	0
3	A	61902	0	31134	679	0
4	B	2569	0	1301	19	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	33	0
7	E	1552	0	1619	27	0
8	F	1411	0	1444	44	0
9	G	1323	0	1371	33	0
10	H	1110	0	1148	24	0
11	I	946	0	976	30	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	23	0
14	L	946	0	1023	21	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	24	0
17	O	993	0	1034	24	0
18	P	900	0	935	22	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	20	0
24	V	780	0	831	16	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0
28	Z	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	g	1664	0	476	0	0
36	h	224	0	58	0	0
37	i	3384	0	3512	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	284	0	95	0	0
39	k	159	0	189	0	0
40	l	2067	0	2114	0	0
41	f	1	0	0	0	0
42	i	5	0	0	0	0
42	l	5	0	0	0	0
43	i	1	0	0	0	0
43	l	1	0	0	0	0
44	i	28	0	12	0	0
44	l	28	0	12	0	0
All	All	101694	0	68522	1166	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 8.

All (1166) 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)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
23:U:24:MET:SD	23:U:93:LEU:CD1	2.60	0.90
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:276:U:O2	3:A:278:A:N6	2.07	0.86
1:1:42:A:H61	1:1:67:A:H62	1.23	0.86
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
3:A:287:G:O6	3:A:352:A:N6	2.10	0.85
3:A:2135:A:HO2'	3:A:2159:G:HO2'	1.24	0.85
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.84
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.83
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.83
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.79
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.78
11:I:18:VAL:HG13	11:I:86:MET:SD	2.23	0.78
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.76
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.75
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.73
23:U:24:MET:SD	23:U:93:LEU:HD12	2.27	0.73
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.72
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.71
13:K:131:ASN:OD1	13:K:131:ASN:N	2.22	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.88	0.71
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.71
3:A:1069:A:H4'	3:A:1070:A:H5''	1.71	0.70
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.70
3:A:545:U:O2	3:A:548:G:N1	2.19	0.69
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.69
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.69
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.69
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.69
3:A:1536:C:H4'	3:A:1537:G:H5''	1.75	0.69
3:A:2830:C:H5''	6:D:56:LYS:HE3	1.75	0.68
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.73	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.68
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.67
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:196:A:OP2	15:M:47:ARG:NH1	2.28	0.67
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.67
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.67
3:A:2713:U:H3'	3:A:2714:G:H5''	1.77	0.67
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.65
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.65
3:A:1597:A:H5''	3:A:1598:A:H5'	1.78	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.61	0.65
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.65
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.65
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.65
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.65
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.64
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.64
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.64
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.64
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.64
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.64
3:A:284:U:H3	3:A:356:G:H1	1.44	0.64
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.64
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.64
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.63
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.29	0.63
8:F:144:ASP:N	8:F:144:ASP:OD1	2.30	0.63
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.63
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.63
3:A:2424:C:H5''	3:A:2425:A:H5'	1.79	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.62	0.63
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.63
1:1:29:U:O4	1:1:77:A:N6	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.63
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.63
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.62
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.48	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
19:Q:4:ILE:HD12	19:Q:4:ILE:H	1.65	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.79	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.62
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.61
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
26:X:56:ASP:OD1	26:X:56:ASP:N	2.28	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.46	0.61
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.65	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.61
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
1:1:37:U:O4	1:1:68:A:N6	2.34	0.60
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.60
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.60
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
7:E:97:ASN:N	7:E:97:ASN:OD1	2.34	0.60
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.60
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.60
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.60
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.59
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.59
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.59
3:A:2584:U:H3'	3:A:2585:U:H5''	1.84	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.59
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.59
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.58
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.58
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.39	0.58
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.58
3:A:1645:G:H5''	3:A:1646:C:H5'	1.86	0.57
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.57
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
3:A:1403:A:HO2'	3:A:1471:G:HO2'	1.38	0.57
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.56
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.56
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.56
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.05	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
3:A:480:A:OP2	24:V:44:LYS:NZ	2.23	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.56
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.56
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.56
3:A:2162:G:H5''	3:A:2171:A:H2'	1.86	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.56
3:A:1800:C:H5'	5:C:146:MET:HE1	1.88	0.56
3:A:2491:U:H5''	3:A:2570:G:H5''	1.88	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
3:A:849:A:H2'	3:A:850:U:H6	1.70	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
17:O:2:ARG:NH1	17:O:2:ARG:HB3	2.21	0.56
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
17:O:48:VAL:O	17:O:51:LEU:HB2	2.05	0.55
3:A:591:U:H2'	3:A:592:A:H8	1.72	0.55
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.55
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.55
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.41	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.55
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.54
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.54
3:A:833:A:H2'	3:A:834:G:H8	1.73	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:609:A:H2'	3:A:610:C:O4'	2.08	0.54
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.54
3:A:2619:C:H5''	6:D:157:LYS:HG3	1.89	0.54
7:E:88:ARG:HA	7:E:88:ARG:HH21	1.72	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.54
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.54
3:A:2267:A:H5''	3:A:2268:A:H5''	1.89	0.54
3:A:2424:C:H5''	3:A:2425:A:C5'	2.37	0.54
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.54
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.54
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.54
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.53
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
3:A:2845:U:H5''	19:Q:52:ASN:O	2.08	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
3:A:1056:G:H5''	3:A:1057:A:H5'	1.90	0.53
3:A:1056:G:O2'	3:A:1103:A:N6	2.40	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.53
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53
23:U:24:MET:CG	23:U:93:LEU:HD12	2.39	0.53
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.52
3:A:1069:A:C2	3:A:1096:A:H5''	2.44	0.52
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.52
4:B:93:C:OP2	25:W:18:ARG:NH1	2.41	0.52
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.52
3:A:1428:C:C5	3:A:1569:A:H5''	2.45	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.44	0.52
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
3:A:120:U:H4'	3:A:121:G:H5''	1.89	0.52
3:A:284:U:O2	3:A:356:G:N2	2.37	0.52
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.52
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.52
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
23:U:53:VAL:HB	23:U:91:GLN:CD	2.30	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
25:W:55:GLU:H	25:W:55:GLU:CD	2.13	0.52
3:A:653:U:H1'	3:A:654:A:H5''	1.91	0.52
3:A:845:A:H61	3:A:932:U:H3	1.58	0.52
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.52
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.52
3:A:1115:G:O2'	3:A:1116:G:H5''	2.10	0.52
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.52
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.52
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.51
23:U:93:LEU:HD13	23:U:95:PHE:CZ	2.45	0.51
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.51
3:A:1798:U:H5''	5:C:258:ARG:HB2	1.92	0.51
19:Q:16:ASP:OD1	19:Q:16:ASP:N	2.33	0.51
23:U:56:GLU:HA	23:U:88:LYS:HE3	1.92	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
3:A:2502:G:H5''	3:A:2503:A:H5''	1.92	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.51
24:V:18:ASP:OD2	24:V:40:ASN:N	2.38	0.51
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:2439:A:H4'	3:A:2440:C:H5''	1.91	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
3:A:2271:G:H5''	26:X:18:ALA:HB1	1.93	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.51
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.93	0.51
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.51
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.51
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.51
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.93	0.50
3:A:2564:A:OP1	3:A:2648:G:O2'	2.19	0.50
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.50
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.50
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.50
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.50
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.46	0.50
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
23:U:54:GLU:H	23:U:91:GLN:NE2	2.08	0.50
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.50
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.50
3:A:2850:A:N7	3:A:2868:A:O2'	2.39	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.50
23:U:24:MET:SD	23:U:93:LEU:HD13	2.50	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.49
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.49
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.49
28:Z:39:GLN:HB3	28:Z:41:HIS:CE1	2.47	0.49
3:A:1021:A:H3'	3:A:1021:A:N3	2.27	0.49
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.49
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.49
3:A:184:C:H2'	3:A:185:G:H8	1.76	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.49
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:671:C:H2'	3:A:672:C:C6	2.48	0.49
3:A:1187:G:HO2'	3:A:1188:U:H6	1.60	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.49
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.49
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.49
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.45	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
3:A:160:A:N3	3:A:2208:C:O2'	2.43	0.48
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.48
22:T:96:ILE:HD13	22:T:96:ILE:HA	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
1:1:98:U:H2'	1:1:99:G:H8	1.79	0.48
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.48
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
5:C:175:ARG:HG3	5:C:181:MET:HE1	1.95	0.48
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.48
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.48
1:1:53:G:N2	1:1:56:A:OP2	2.45	0.48
7:E:184:ASP:OD1	7:E:184:ASP:N	2.43	0.48
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.78	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.48
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.48
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.48	0.48
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.48
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:1819:A:H5''	5:C:160:THR:HG21	1.94	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.48
3:A:136:G:H2'	3:A:137:U:O4'	2.13	0.48
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.48
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.53	0.48
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.48
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.48
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.48
3:A:914:G:H5'	3:A:915:C:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.48
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.48
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.43	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
3:A:957:C:C5	3:A:959:A:C5	3.01	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.94	0.48
1:1:76:G:H2'	1:1:77:A:C8	2.48	0.48
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.48
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.48
3:A:2209:G:H1	3:A:2215:C:N4	2.12	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.47
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.47
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.47
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.47
3:A:1007:C:H5''	13:K:37:ARG:NH2	2.29	0.47
3:A:1846:G:H5''	3:A:1847:A:OP2	2.14	0.47
3:A:2305:U:H5''	8:F:131:GLY:HA3	1.96	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.96	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
3:A:175:G:N2	3:A:176:A:N3	2.62	0.47
3:A:1132:U:H3'	3:A:1133:A:H5''	1.95	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.47
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.47
3:A:910:A:H2'	3:A:911:A:C8	2.49	0.47
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.47
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.47
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.47
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.47
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.47
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.47
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.95	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.47
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
3:A:127:A:H5''	3:A:128:C:O4'	2.14	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.47
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.47
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:2557:G:H2'	3:A:2558:C:C6	2.50	0.47
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.47
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.47
9:G:155:GLU:OE1	9:G:157:TYR:N	2.44	0.47
10:H:40:THR:HG22	10:H:41:LYS:H	1.79	0.47
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
25:W:2:PHE:HB3	25:W:50:MET:CE	2.44	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.47
3:A:2431:U:H5	3:A:2433:A:H5''	1.79	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
3:A:1062:G:N2	12:J:93:PRO:HG2	2.29	0.47
3:A:2339:C:H2'	3:A:2340:A:H8	1.80	0.47
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.47
19:Q:100:LEU:HA	19:Q:100:LEU:HD23	1.67	0.47
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.47
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.47
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.47
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.47
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.46
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.46
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.46
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.46
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.50	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.78	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.46
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.46
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.46
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.46
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.46
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
3:A:861:A:C6	3:A:917:A:C8	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.46
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.46
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.46
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.46
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
5:C:125:LYS:HE2	5:C:125:LYS:HB2	1.77	0.46
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.46
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.46
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.46
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.46
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.30	0.46
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.46
3:A:532:A:N3	3:A:532:A:H2'	2.31	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.46
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.46
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.79	0.46
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.19	0.46
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.45
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.45
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.45
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.45
3:A:483:A:H5''	24:V:47:LYS:HG2	1.97	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.45
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.16	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.45
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.17	0.45
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.45
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:831:G:H5''	15:M:37:GLY:HA2	1.97	0.45
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.45
3:A:1466:U:H5''	3:A:1467:U:H5'	1.98	0.45
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.16	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
3:A:499:U:H5''	24:V:43:LYS:HE3	1.99	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.45
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.45
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.45
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
18:P:85:LYS:HE2	18:P:85:LYS:HB3	1.79	0.45
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.45
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.45
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.45
3:A:629:G:H5''	3:A:650:C:O2'	2.16	0.45
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.60	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.84	0.45
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.45
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.45
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.45
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.45
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:2313:C:H5''	8:F:88:LYS:HD3	1.98	0.45
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.45
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.45
11:I:52:MET:HE3	11:I:81:LEU:HD11	1.99	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
17:O:2:ARG:HB3	17:O:2:ARG:CZ	2.46	0.45
3:A:141:G:C8	3:A:141:G:H3'	2.51	0.44
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.44
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.44
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.44
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.44
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.44
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.53	0.44
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:1972:G:H2'	3:A:1973:G:H8	1.82	0.44
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.44
13:K:65:THR:O	13:K:68:LYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
3:A:239:C:HO2'	3:A:622:G:HO2'	1.60	0.44
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.44
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.44
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.33	0.44
21:S:27:ILE:HG22	21:S:28:ALA:O	2.18	0.44
22:T:46:LEU:HD23	22:T:46:LEU:HA	1.82	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.17	0.44
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.44
22:T:28:LYS:HB2	22:T:28:LYS:HE2	1.41	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.98	0.44
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.44
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.53	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.44
3:A:997:G:H5''	20:R:92:ARG:NH1	2.33	0.44
3:A:1230:A:H2'	3:A:1231:U:O4'	2.17	0.44
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.44
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
28:Z:56:LEU:HD22	28:Z:56:LEU:HA	1.82	0.44
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.44
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.99	0.44
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	2.00	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.44
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44
23:U:24:MET:CG	23:U:93:LEU:CD1	2.96	0.44
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.44
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.44
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.44
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.44
9:G:44:LYS:HE3	9:G:44:LYS:HB2	1.80	0.44
16:N:95:LEU:HA	16:N:95:LEU:HD23	1.77	0.44
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.44
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.43
3:A:1266:G:O2'	3:A:2012:G:O6	2.34	0.43
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.43
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.43
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.43
3:A:463:G:N1	3:A:467:G:C6	2.86	0.43
3:A:566:U:H5''	15:M:29:LYS:HE3	1.99	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.01	0.43
8:F:138:PHE:HA	8:F:139:PRO:HD3	1.90	0.43
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.43
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.99	0.43
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.43
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.43
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.43
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.43
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.43
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.43
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.53	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
18:P:18:LEU:HA	18:P:18:LEU:HD23	1.71	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
3:A:475:C:N4	3:A:476:G:C6	2.86	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.01	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.43
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.43
5:C:33:LEU:HA	5:C:33:LEU:HD23	1.58	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
20:R:9:ILE:H	20:R:9:ILE:HD12	1.84	0.43
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.43
1:1:72:A:H2'	1:1:73:G:H8	1.82	0.43
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.43
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.43
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.43
3:A:2512:C:H5''	3:A:2513:A:OP2	2.17	0.43
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.43
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.43
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
15:M:41:ARG:H	15:M:41:ARG:HG2	1.62	0.43
3:A:195:A:H5''	15:M:47:ARG:HH22	1.84	0.43
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.43
3:A:1494:A:H2'	3:A:1495:A:H8	1.84	0.43
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.43
6:D:148:GLN:OE1	6:D:148:GLN:N	2.51	0.43
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.43
7:E:181:ILE:H	7:E:181:ILE:HG13	1.69	0.43
14:L:3:GLN:HE21	14:L:3:GLN:HB3	1.66	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.43
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.43
1:1:33:C:H6	1:1:33:C:O5'	2.02	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:1088:A:H61	12:J:135:SER:HB3	1.83	0.43
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.43
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.43
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.43
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.62	0.43
3:A:464:U:C2	3:A:788:A:C6	3.06	0.42
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.42
3:A:2518:A:H2'	3:A:2518:A:N3	2.34	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
5:C:200:HIS:CD2	5:C:200:HIS:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.42
10:H:104:THR:HA	10:H:108:VAL:O	2.19	0.42
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.42
19:Q:40:LEU:HD23	19:Q:40:LEU:HA	1.75	0.42
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
3:A:307:G:N1	3:A:310:A:OP2	2.52	0.42
3:A:653:U:C1'	3:A:654:A:H5''	2.49	0.42
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.42
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.42
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
8:F:4:LEU:HD23	8:F:4:LEU:HA	1.73	0.42
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.42
14:L:11:ALA:O	14:L:100:PHE:N	2.46	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:819:A:N3	3:A:819:A:H2'	2.34	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.42
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.42
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.42
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.20	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.42
15:M:6:LEU:HD23	15:M:6:LEU:HA	1.82	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.42
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.42
3:A:1064:C:H5''	12:J:88:SER:HB2	2.01	0.42
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.84	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.42
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
20:R:24:TYR:N	20:R:24:TYR:HD1	2.17	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.19	0.42
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.42
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.42
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.42
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
1:I:72:A:H2'	1:I:73:G:C8	2.55	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
7:E:109:LEU:HA	7:E:109:LEU:HD23	1.79	0.42
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.42
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.42
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.42
5:C:24:LEU:HA	5:C:24:LEU:HD12	1.66	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.01	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.42
13:K:96:ARG:HA	13:K:97:PRO:HD2	1.92	0.42
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.34	0.42
3:A:1482:G:H2'	3:A:1483:G:H8	1.84	0.42
3:A:1877:A:H2'	3:A:1878:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.42
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.42
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.42
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.42
8:F:79:ILE:HD12	8:F:79:ILE:O	2.20	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
3:A:335:C:H5''	24:V:82:ARG:HD2	2.02	0.41
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.41
3:A:2339:C:O3'	4:B:41:G:N2	2.52	0.41
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.41
22:T:33:LEU:HD23	22:T:33:LEU:HA	1.66	0.41
27:Y:26:LYS:HD3	27:Y:26:LYS:HA	1.88	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.20	0.41
3:A:877:A:C6	3:A:899:A:C6	3.08	0.41
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:2796:U:HO2'	3:A:2797:U:H6	1.63	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.41
25:W:2:PHE:HB3	25:W:50:MET:HE3	2.02	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.41
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.41
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.41
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.41
3:A:2267:A:H5''	3:A:2268:A:C5'	2.50	0.41
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
8:F:130:MET:HE3	8:F:130:MET:HB2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:43:LYS:HE2	12:J:118:THR:HA	2.01	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.41
3:A:799:G:C6	3:A:800:A:C6	3.08	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.21	0.41
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.21	0.41
3:A:1110:G:HO2'	3:A:1111:A:P	2.44	0.41
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.73	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:2860:A:H5''	3:A:2861:U:OP2	2.21	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.41
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
7:E:170:ARG:HD3	7:E:170:ARG:HA	1.91	0.41
14:L:71:ARG:HA	14:L:71:ARG:HD3	1.81	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.85	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.55	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
15:M:3:LEU:HD23	15:M:3:LEU:HA	1.77	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
1:1:98:U:H2'	1:1:99:G:C8	2.55	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.41
3:A:601:C:O2'	3:A:605:G:H5''	2.21	0.41
3:A:776:G:HO2'	3:A:777:G:P	2.41	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.41
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.20	0.41
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.41
9:G:9:VAL:HG23	9:G:52:PHE:HE1	1.86	0.41
16:N:6:ARG:CZ	16:N:6:ARG:HB2	2.50	0.41
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.41
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.41
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.41
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.41
4:B:7:G:H5''	18:P:29:HIS:CE1	2.56	0.41
14:L:17:ARG:HA	14:L:17:ARG:HD3	1.77	0.41
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.41
28:Z:21:LEU:HD23	28:Z:21:LEU:HA	1.82	0.41
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:74:C:O5'	2:2:74:C:H6	2.04	0.40
3:A:141:G:C8	3:A:141:G:C3'	3.04	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.56	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:778:G:H5''	3:A:779:U:OP2	2.21	0.40
3:A:997:G:OP1	20:R:92:ARG:HD2	2.21	0.40
3:A:1332:G:N7	3:A:1609:A:O2'	2.46	0.40
3:A:1365:A:N3	3:A:1365:A:H2'	2.36	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.03	0.40
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.40
7:E:67:ARG:HE	7:E:67:ARG:HB3	1.61	0.40
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.02	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.03	0.40
18:P:115:LEU:HD23	18:P:117:PHE:CE2	2.56	0.40
18:P:115:LEU:HD23	18:P:117:PHE:HE2	1.86	0.40
21:S:85:LYS:HE2	21:S:85:LYS:HB3	1.80	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.86	0.40
28:Z:42:LEU:HA	28:Z:42:LEU:HD23	1.81	0.40
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.40
3:A:863:A:H2'	3:A:864:G:H8	1.86	0.40
3:A:2423:U:H2'	3:A:2424:C:C1'	2.51	0.40
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.40
3:A:2600:A:H2'	3:A:2601:C:C6	2.56	0.40
8:F:28:VAL:HA	8:F:29:PRO:HD3	1.91	0.40
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.40
1:1:68:A:H2'	1:1:69:G:C8	2.56	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.89	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:719:C:H2'	3:A:720:U:C6	2.57	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.56	0.40
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.40
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2421:G:H4'	3:A:2421:G:OP1	2.21	0.40
4:B:68:C:H2'	4:B:69:G:O4'	2.22	0.40
11:I:13:ALA:O	11:I:17:GLU:HB2	2.22	0.40
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.03	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40
14:L:103:VAL:HB	14:L:107:LEU:HD12	2.02	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
17:O:65:LEU:HA	17:O:65:LEU:HD12	1.85	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
3:A:1:G:H2'	3:A:2:G:C8	2.56	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.40
3:A:1127:A:N7	3:A:2488:G:O2'	2.54	0.40
3:A:1275:A:OP2	3:A:1646:C:N4	2.52	0.40
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.40
3:A:2365:G:P	26:X:55:ARG:HG2	2.61	0.40
3:A:2388:A:H5'	3:A:2389:G:OP2	2.21	0.40
5:C:251:GLN:HE21	5:C:251:GLN:HB2	1.58	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
11:I:100:ALA:HB2	11:I:106:PHE:CE1	2.56	0.40
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.40
17:O:22:ARG:HG3	17:O:70:THR:HA	2.03	0.40
3:A:362:A:H3'	3:A:363:G:C8	2.48	0.40
3:A:447:A:C5	3:A:473:G:C5	3.10	0.40
3:A:863:A:H2'	3:A:864:G:C8	2.57	0.40
3:A:1139:G:H8	3:A:1139:G:OP2	2.05	0.40
3:A:1234:U:H2'	3:A:1235:G:O4'	2.21	0.40
3:A:1945:G:C5	3:A:1946:U:C4	3.09	0.40
3:A:2283:C:C2	3:A:2389:G:C2	3.09	0.40
3:A:2563:U:O2	3:A:2566:A:C5	2.75	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
6:D:13:ARG:HD2	6:D:15:PHE:CE2	2.56	0.40
10:H:60:GLU:HA	10:H:63:ALA:HB3	2.04	0.40
12:J:97:LYS:HE2	12:J:139:VAL:HG12	2.03	0.40
18:P:25:ARG:O	18:P:25:ARG:HG3	2.22	0.40
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.40

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 PDB entries followed by that with respect to all EM entries.

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	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	19	56
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	53
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	12	46
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	g	414/416 (100%)	402 (97%)	12 (3%)	0	100	100
36	h	54/56 (96%)	54 (100%)	0	0	100	100
37	i	408/450 (91%)	397 (97%)	10 (2%)	1 (0%)	44	78
38	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
39	k	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
40	l	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
All	All	4667/4779 (98%)	4520 (97%)	143 (3%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	i	97	ALA
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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 PDB entries followed by that with respect to all EM entries.

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	C	216/216 (100%)	192 (89%)	24 (11%)	5	18
6	D	164/164 (100%)	154 (94%)	10 (6%)	15	37
7	E	165/165 (100%)	152 (92%)	13 (8%)	10	29
8	F	148/148 (100%)	130 (88%)	18 (12%)	4	16
9	G	137/137 (100%)	129 (94%)	8 (6%)	17	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	114/114 (100%)	100 (88%)	14 (12%)	4	16
11	I	95/95 (100%)	90 (95%)	5 (5%)	19	41
12	J	104/104 (100%)	93 (89%)	11 (11%)	5	20
13	K	116/116 (100%)	105 (90%)	11 (10%)	7	22
14	L	104/104 (100%)	94 (90%)	10 (10%)	7	22
15	M	103/103 (100%)	94 (91%)	9 (9%)	8	26
16	N	109/109 (100%)	100 (92%)	9 (8%)	9	28
17	O	102/102 (100%)	95 (93%)	7 (7%)	13	33
18	P	87/87 (100%)	75 (86%)	12 (14%)	3	14
19	Q	99/99 (100%)	90 (91%)	9 (9%)	7	24
20	R	89/89 (100%)	82 (92%)	7 (8%)	10	29
21	S	84/84 (100%)	76 (90%)	8 (10%)	7	22
22	T	93/93 (100%)	88 (95%)	5 (5%)	18	40
23	U	82/82 (100%)	77 (94%)	5 (6%)	15	37
24	V	83/83 (100%)	76 (92%)	7 (8%)	9	28
25	W	78/78 (100%)	72 (92%)	6 (8%)	10	30
26	X	57/58 (98%)	51 (90%)	6 (10%)	5	20
27	Y	67/67 (100%)	63 (94%)	4 (6%)	16	38
28	Z	54/54 (100%)	47 (87%)	7 (13%)	3	15
29	a	48/48 (100%)	46 (96%)	2 (4%)	25	47
30	b	47/47 (100%)	35 (74%)	12 (26%)	0	3
31	c	45/46 (98%)	40 (89%)	5 (11%)	5	18
32	d	38/38 (100%)	32 (84%)	6 (16%)	2	11
33	e	51/51 (100%)	47 (92%)	4 (8%)	10	29
34	f	34/34 (100%)	31 (91%)	3 (9%)	8	25
37	i	336/338 (99%)	334 (99%)	2 (1%)	84	88
39	k	16/16 (100%)	16 (100%)	0	100	100
40	l	217/217 (100%)	217 (100%)	0	100	100
All	All	3382/3386 (100%)	3123 (92%)	259 (8%)	13	30

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	156	ARG
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	265	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	28	GLU
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	139	SER
6	D	160	LYS
6	D	168	GLU
7	E	84	THR
7	E	85	PHE
7	E	94	GLN
7	E	97	ASN
7	E	105	LEU
7	E	115	GLN
7	E	119	ILE
7	E	127	GLU
7	E	148	ILE

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Mol	Chain	Res	Type
7	E	173	THR
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	72	LYS
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	162	SER
9	G	10	VAL
9	G	11	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	125	CYS
9	G	127	THR
9	G	153	ARG
10	H	15	LEU
10	H	17	ASP
10	H	25	TYR
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	110	VAL

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Mol	Chain	Res	Type
10	H	112	LYS
10	H	116	ARG
11	I	16	SER
11	I	36	ASP
11	I	58	THR
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	55	ILE
12	J	66	SER
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
13	K	5	THR
13	K	7	LYS
13	K	34	ARG
13	K	40	HIS
13	K	44	TYR
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
14	L	1	MET
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	106	GLU
14	L	116	ILE
15	M	2	ARG
15	M	14	LYS
15	M	46	VAL

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Mol	Chain	Res	Type
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	126	ARG
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	2	ARG
17	O	14	SER
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	55	GLU
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL

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Mol	Chain	Res	Type
19	Q	115	ASN
20	R	6	ARG
20	R	13	ARG
20	R	17	ILE
20	R	24	TYR
20	R	51	ARG
20	R	52	GLN
20	R	109	LEU
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	71	LYS
21	S	72	VAL
21	S	83	TYR
21	S	101	ILE
22	T	12	SER
22	T	28	LYS
22	T	74	ILE
22	T	95	ARG
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
24	V	7	ARG
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	78	GLN
25	W	90	ASP
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU

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Mol	Chain	Res	Type
26	X	35	SER
26	X	41	ARG
26	X	56	ASP
27	Y	2	SER
27	Y	4	VAL
27	Y	42	SER
27	Y	74	ARG
28	Z	2	LYS
28	Z	16	THR
28	Z	28	LEU
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	10	LYS
31	c	22	THR
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
33	e	8	ARG
33	e	31	HIS
33	e	32	ILE

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Mol	Chain	Res	Type
33	e	51	SER
34	f	2	LYS
34	f	12	ARG
34	f	36	ARG
37	i	23	THR
37	i	27	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	200	HIS
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	165	HIS
8	F	63	GLN
8	F	81	GLN
8	F	127	ASN
10	H	11	ASN
10	H	33	GLN
10	H	43	ASN
10	H	66	ASN
12	J	31	GLN
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
17	O	18	GLN
18	P	100	HIS
19	Q	52	ASN
19	Q	66	ASN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
23	U	48	GLN
23	U	59	ASN
23	U	91	GLN
26	X	46	HIS

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Mol	Chain	Res	Type
28	Z	39	GLN
28	Z	58	ASN
32	d	26	ASN
32	d	29	GLN
37	i	91	GLN
40	l	161	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	103/104 (99%)	22 (21%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3102/3130 (99%)	554 (17%)	19 (0%)

All (554) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	G
1	1	29	U
1	1	30	A
1	1	33	C
1	1	34	U
1	1	37	U
1	1	38	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	46	C
1	1	57	G
1	1	75	U
1	1	76	G
1	1	83	G
1	1	87	C
1	1	88	G
1	1	90	G
1	1	94	U
1	1	95	A
1	1	102	A
1	1	107	C

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Mol	Chain	Res	Type
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G

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Mol	Chain	Res	Type
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A

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Mol	Chain	Res	Type
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C

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Mol	Chain	Res	Type
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A

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Mol	Chain	Res	Type
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G

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Mol	Chain	Res	Type
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A

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Mol	Chain	Res	Type
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A

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Mol	Chain	Res	Type
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A

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Mol	Chain	Res	Type
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A

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Mol	Chain	Res	Type
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G

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Mol	Chain	Res	Type
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G

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Mol	Chain	Res	Type
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A

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Mol	Chain	Res	Type
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A

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Mol	Chain	Res	Type
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	ALF	i	1001	-	0,4,4	-	-	-		
44	GDP	l	1003	43	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
44	GDP	i	1003	43	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
42	ALF	l	1001	-	0,4,4	-	-	-		

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
44	GDP	i	1003	43	-	4/12/32/32	0/3/3/3
44	GDP	l	1003	43	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	l	1003	GDP	C6-N1	-2.44	1.34	1.37
44	i	1003	GDP	C6-N1	-2.35	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	i	1003	GDP	PA-O3A-PB	-3.78	119.86	132.83
44	l	1003	GDP	PA-O3A-PB	-3.67	120.23	132.83
44	i	1003	GDP	C3'-C2'-C1'	3.00	105.49	100.98
44	l	1003	GDP	C3'-C2'-C1'	2.94	105.40	100.98
44	l	1003	GDP	C8-N7-C5	2.37	107.50	102.99
44	i	1003	GDP	C8-N7-C5	2.36	107.50	102.99
44	l	1003	GDP	C5-C6-N1	2.35	118.11	113.95
44	i	1003	GDP	C5-C6-N1	2.33	118.07	113.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

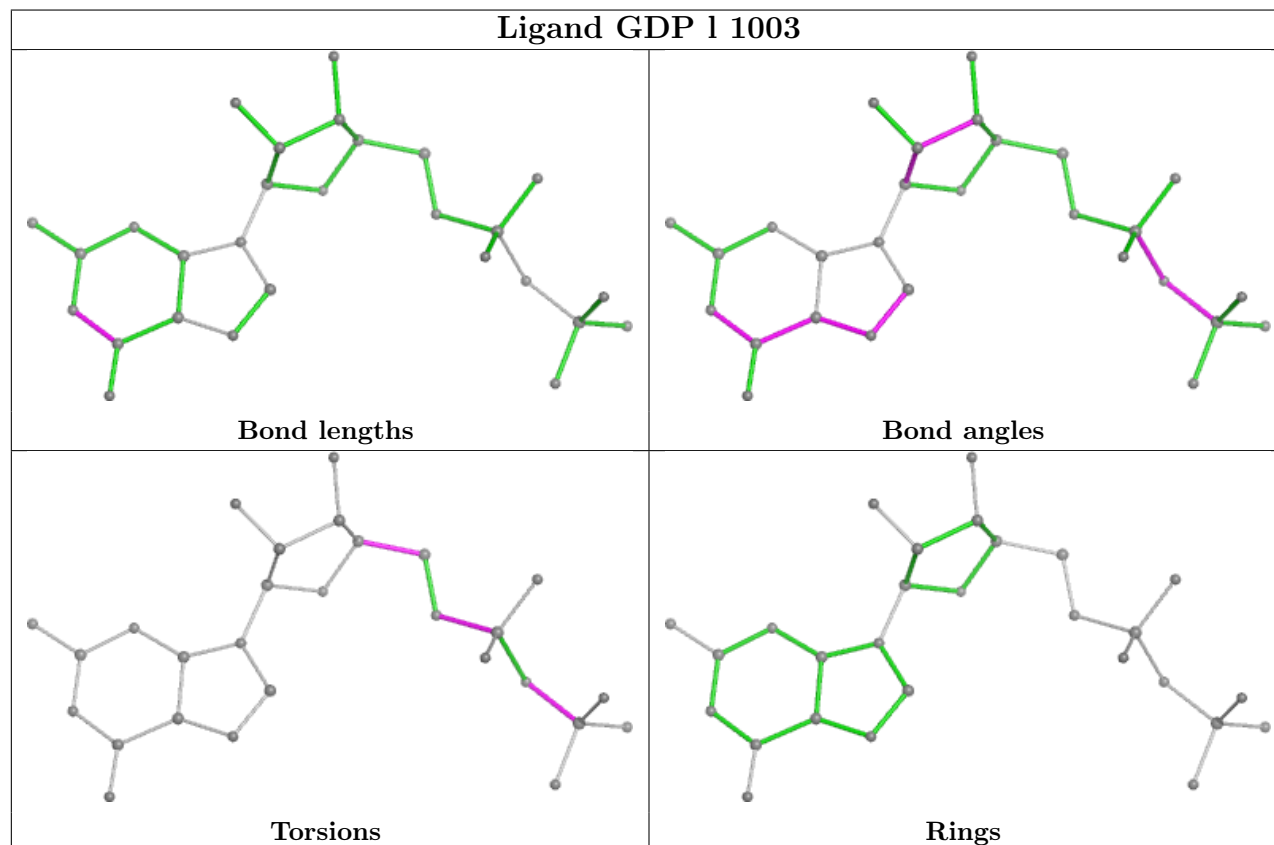
Mol	Chain	Res	Type	Atoms
44	i	1003	GDP	C5'-O5'-PA-O3A
44	i	1003	GDP	O4'-C4'-C5'-O5'
44	i	1003	GDP	C3'-C4'-C5'-O5'
44	l	1003	GDP	PA-O3A-PB-O2B
44	l	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	C5'-O5'-PA-O2A
44	l	1003	GDP	O4'-C4'-C5'-O5'
44	l	1003	GDP	C3'-C4'-C5'-O5'
44	i	1003	GDP	C5'-O5'-PA-O1A
44	l	1003	GDP	PA-O3A-PB-O1B
44	l	1003	GDP	C5'-O5'-PA-O3A

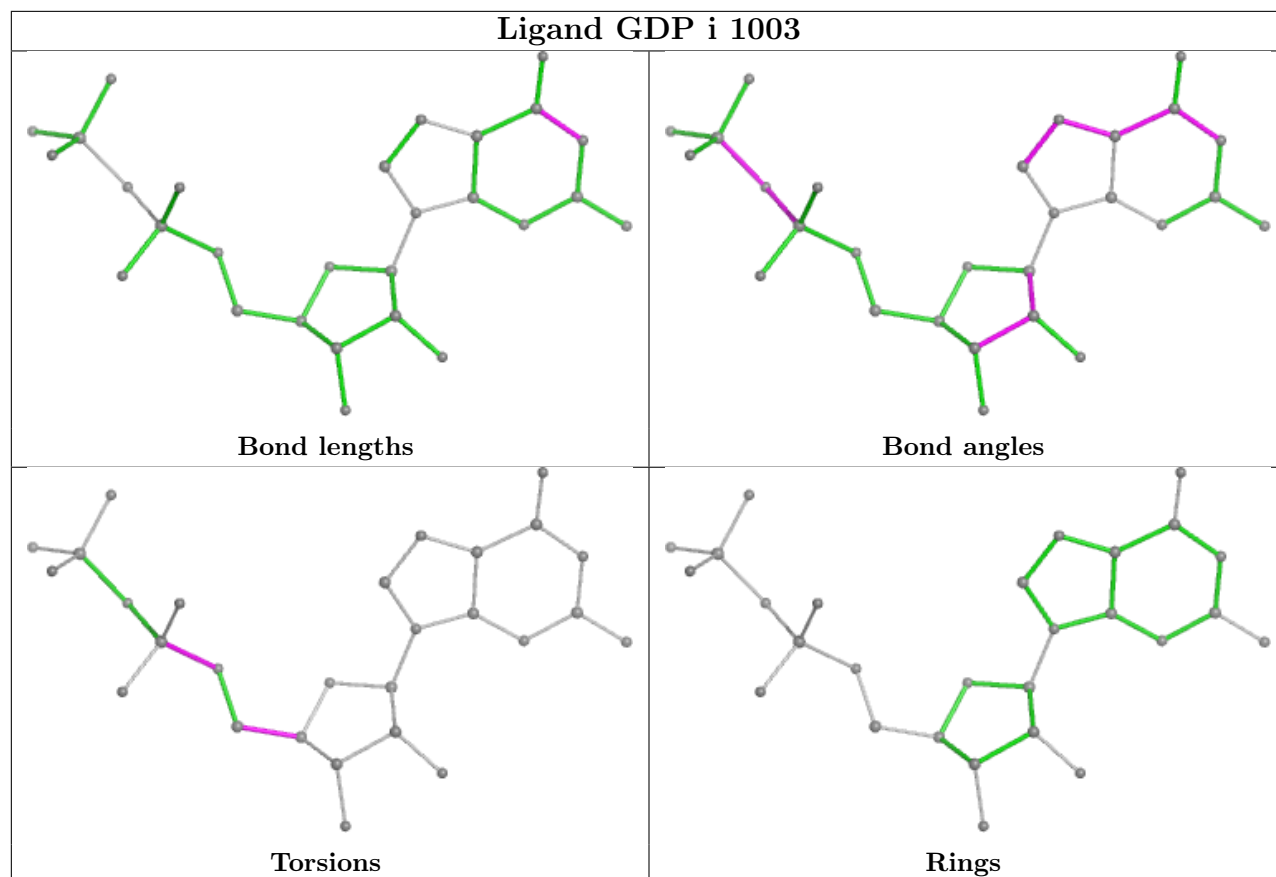
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

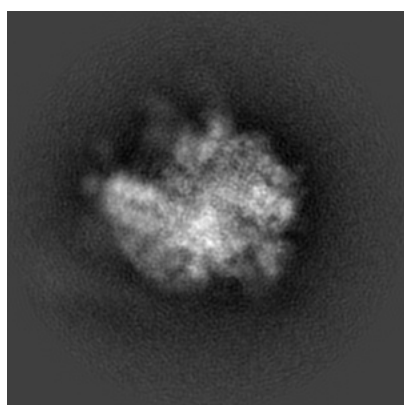
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3617. These allow visual inspection of the internal detail of the map and identification of artifacts.

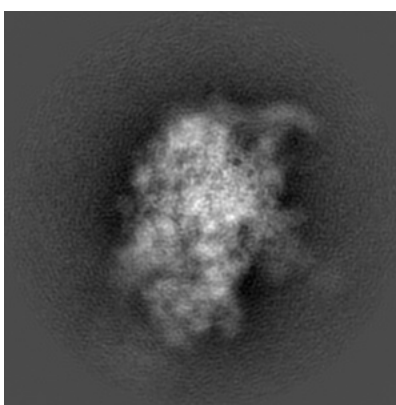
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

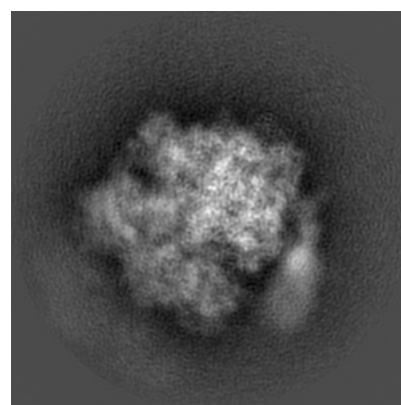
6.1.1 Primary map



X



Y

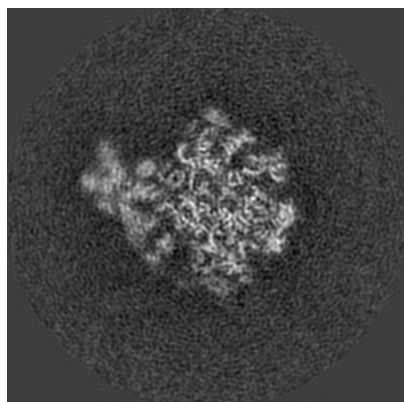


Z

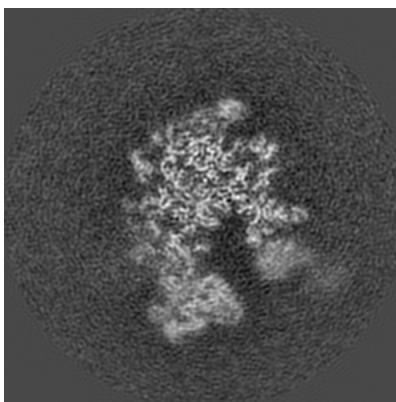
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

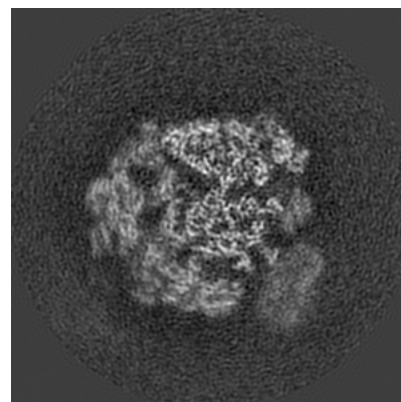
6.2.1 Primary map



X Index: 160



Y Index: 160

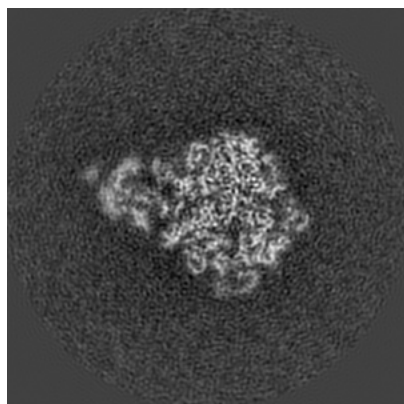


Z Index: 160

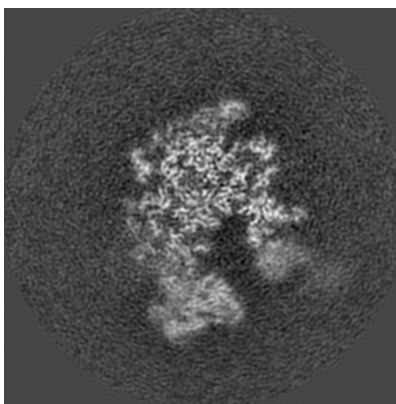
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

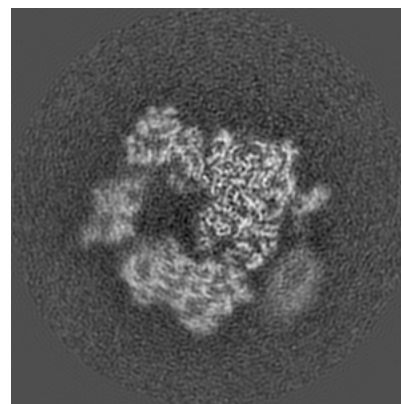
6.3.1 Primary map



X Index: 170



Y Index: 159

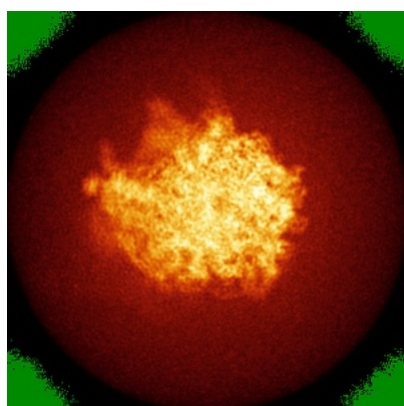


Z Index: 175

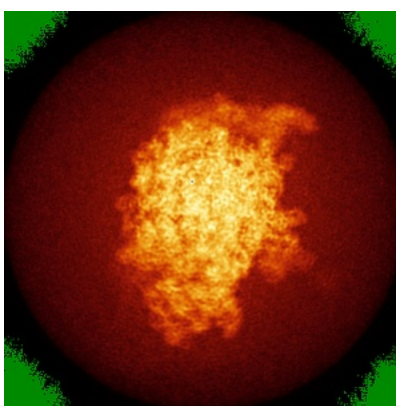
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

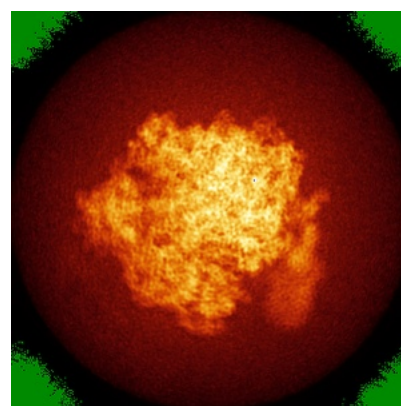
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

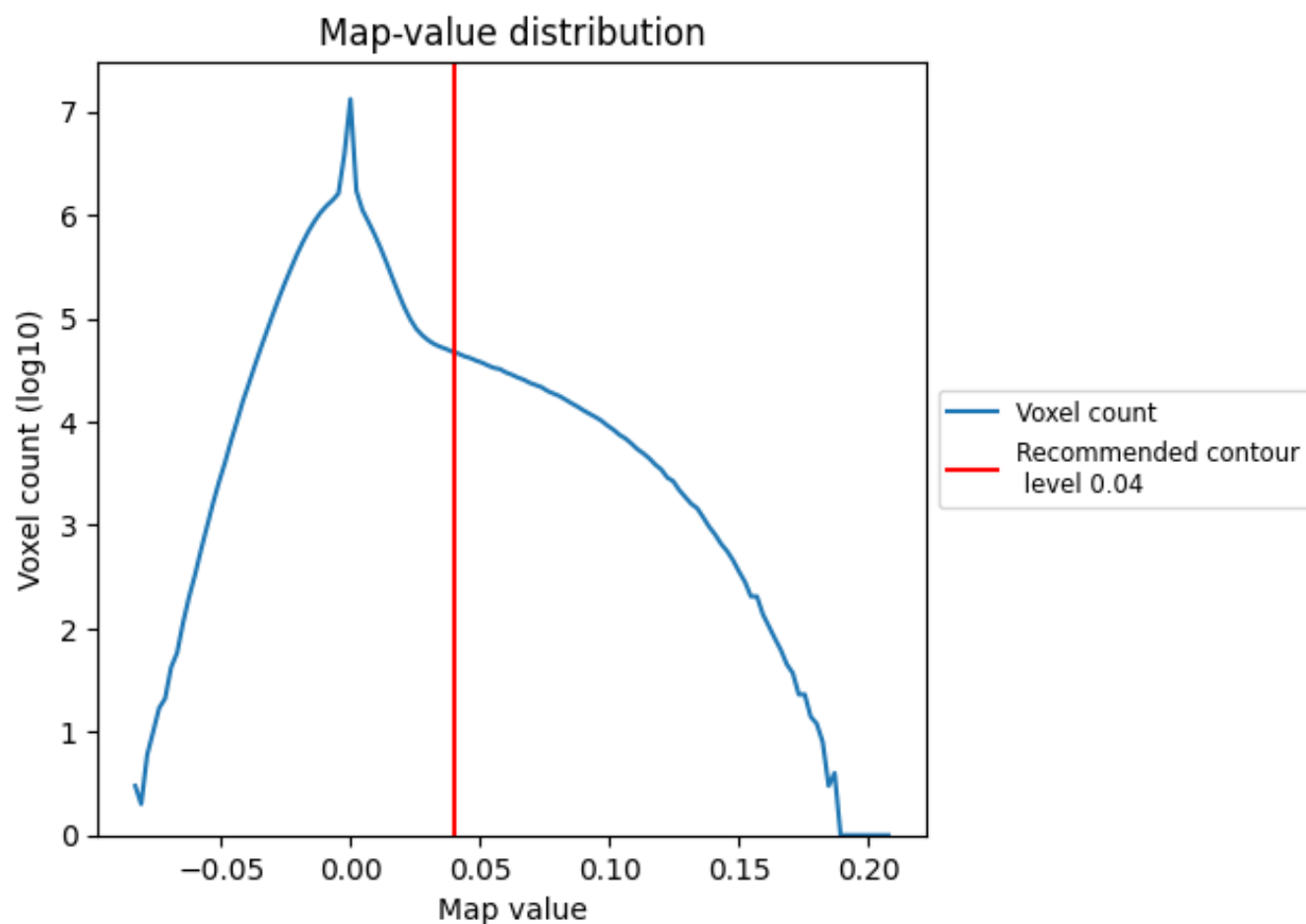
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

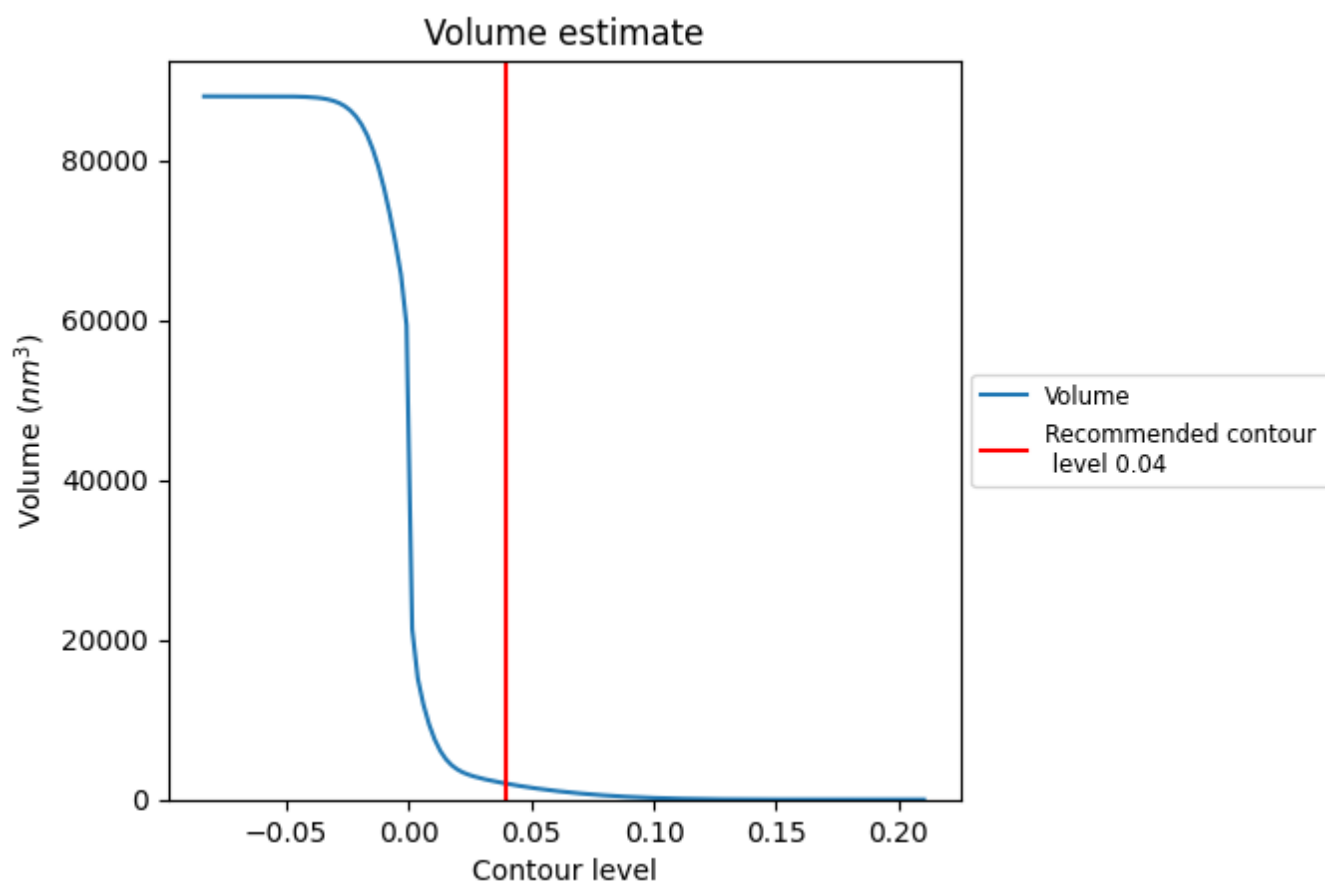
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

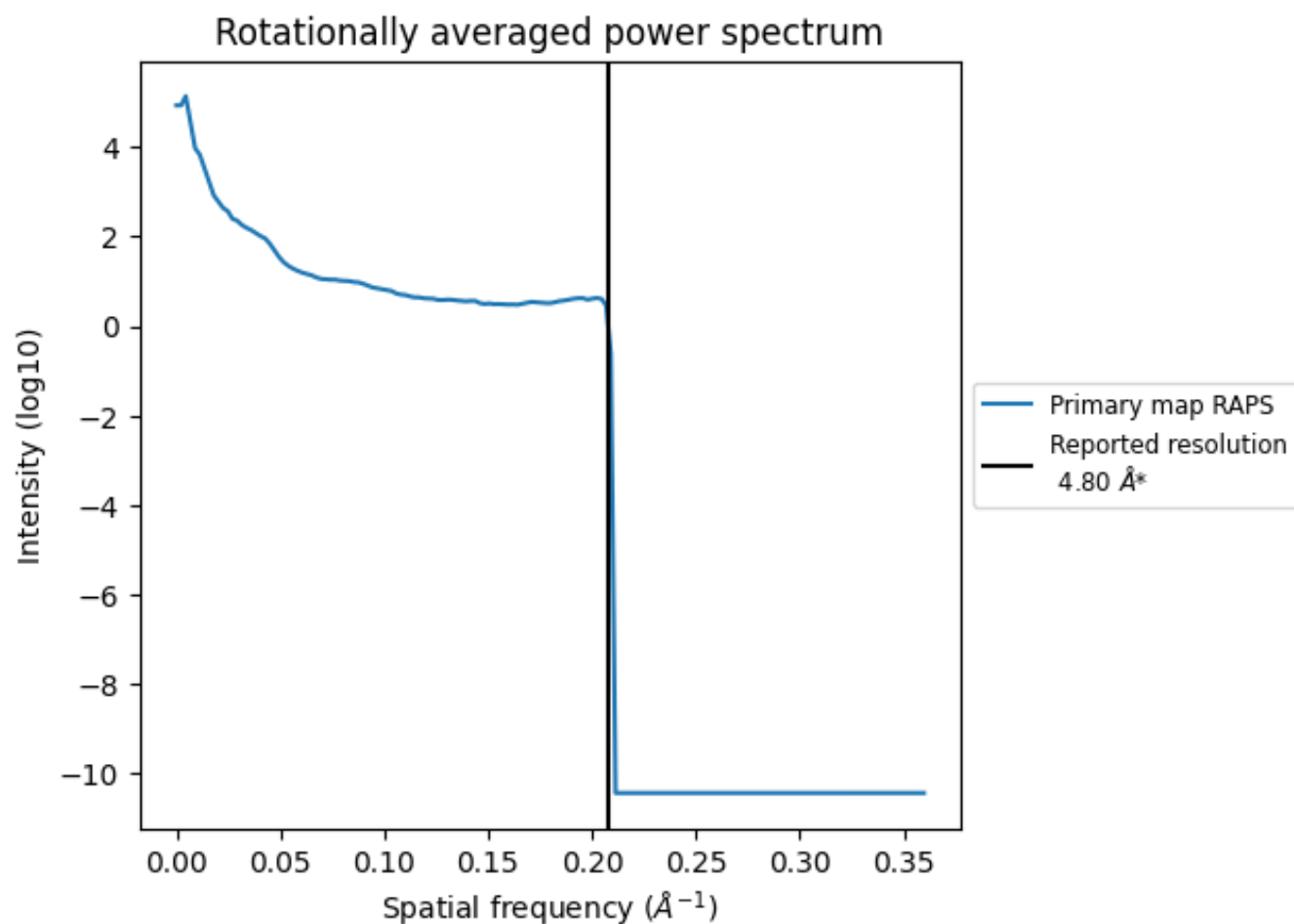
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1992 nm^3 ; this corresponds to an approximate mass of 1799 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

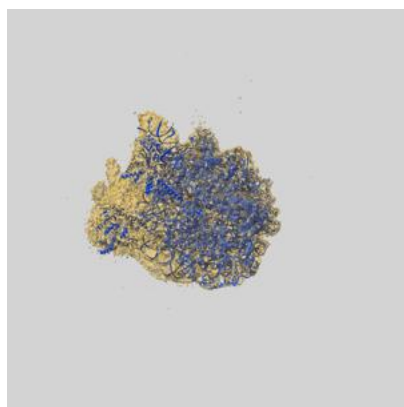
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

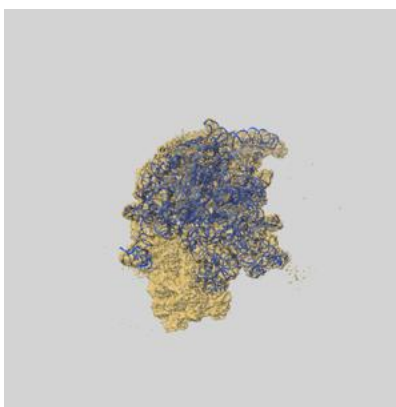
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3617 and PDB model 5NCO. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

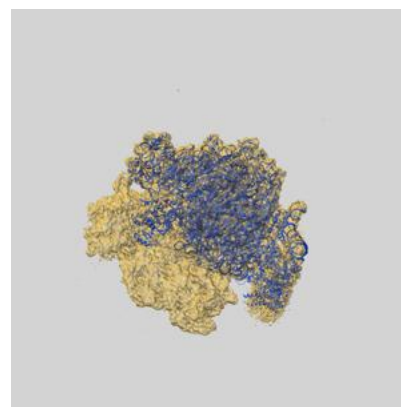
9.1 Map-model overlay [i](#)



X



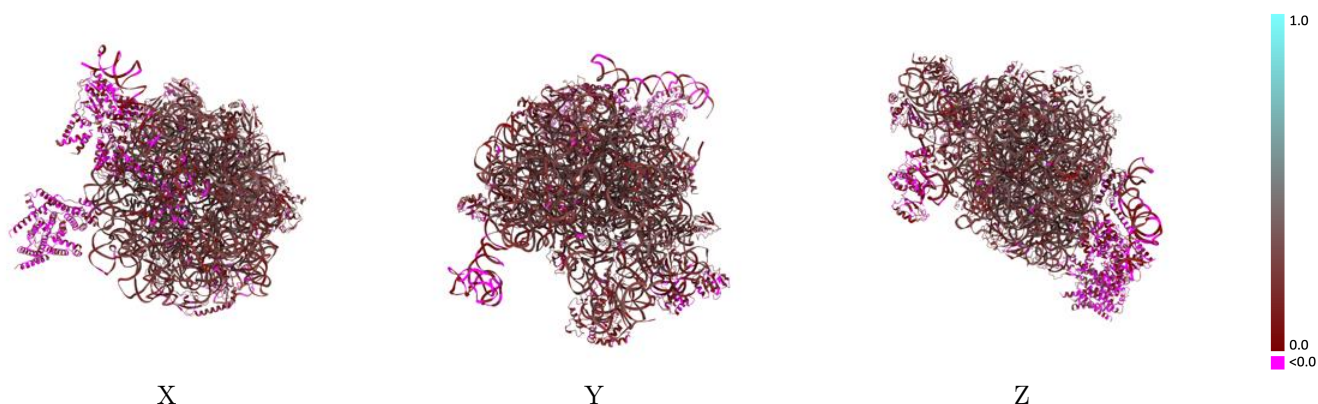
Y



Z

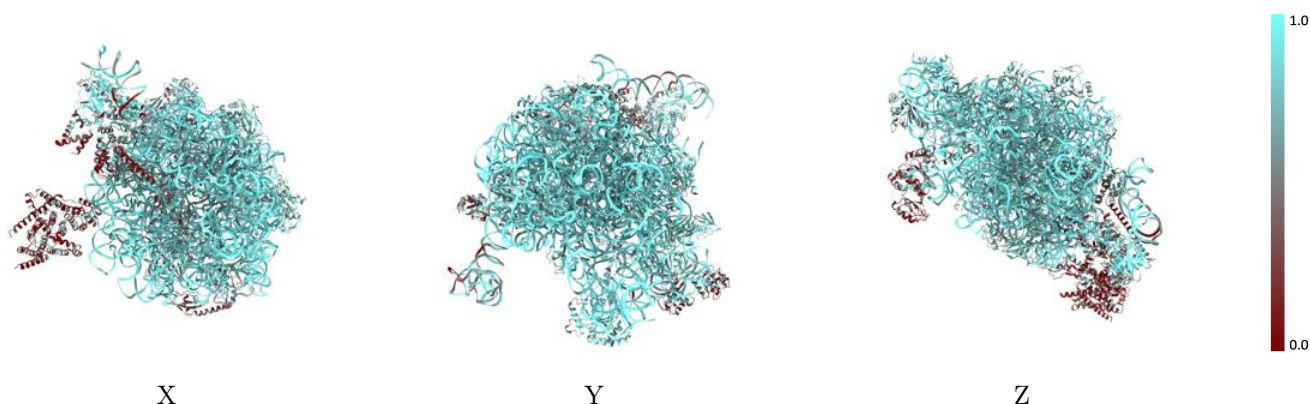
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



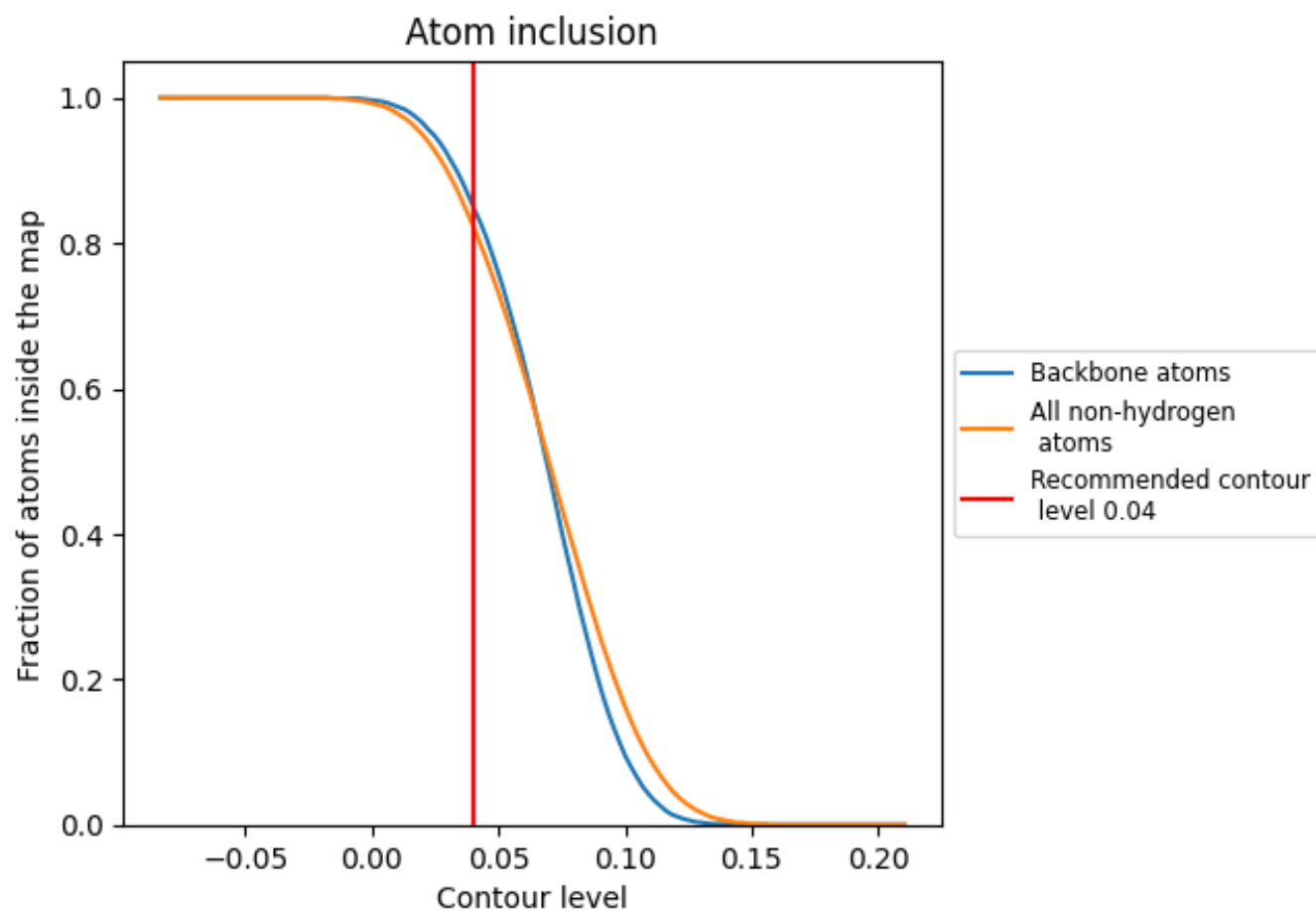
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ













The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.2180
1	 0.7470	 0.0820
2	 0.9030	 0.2780
A	 0.9270	 0.2540
B	 0.9510	 0.2450
C	 0.7000	 0.2090
D	 0.7160	 0.2310
E	 0.7210	 0.2080
F	 0.6910	 0.1350
G	 0.7310	 0.2130
H	 0.4340	 0.1410
I	 0.4080	 0.0570
J	 0.3230	 0.0500
K	 0.7270	 0.2280
L	 0.6250	 0.2120
M	 0.7440	 0.2090
N	 0.7420	 0.2390
O	 0.6560	 0.2170
P	 0.7800	 0.1880
Q	 0.6840	 0.2320
R	 0.7880	 0.2280
S	 0.7340	 0.2260
T	 0.6670	 0.2230
U	 0.6860	 0.2060
V	 0.7080	 0.2070
W	 0.7130	 0.2120
X	 0.7500	 0.1850
Y	 0.7010	 0.2080
Z	 0.6910	 0.1640
a	 0.7730	 0.2340
b	 0.7240	 0.2260
c	 0.6670	 0.1380
d	 0.7160	 0.2070
e	 0.6930	 0.2100
f	 0.7750	 0.1990



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Chain	Atom inclusion	Q-score
g	 0.2910	 0.0050
h	 0.1560	 -0.0410
i	 0.5010	 0.0590
j	 0.2820	 0.0170
k	 0.6670	 0.1140
l	 0.6440	 0.0390