



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 01:46 PM EST

PDB ID : 9BSL
EMDB ID : EMD-44869
Title : 45SRbgA particle in complex with RbgA and YphC. Class A
Authors : Arpin, D.; Ortega, J.
Deposited on : 2024-05-13
Resolution : 3.10 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.40

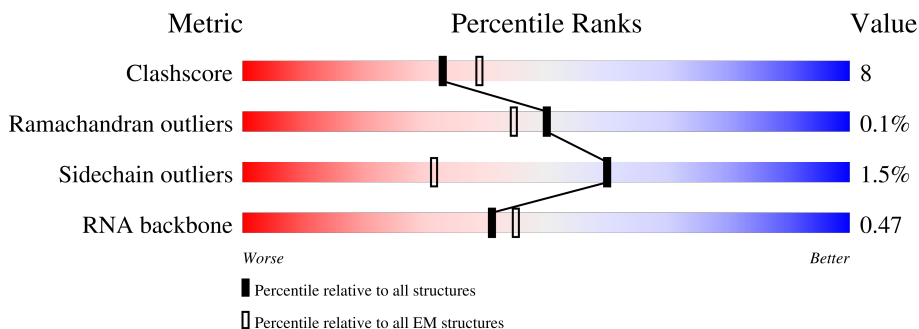
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	A	2927	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9% 45% 26% 12% 18%</p>
2	C	277	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 81% 8% 11%</p>
3	D	209	<div style="display: flex; align-items: center;"> <div style="width: 0.5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">. 90% 9% .</p>
4	E	207	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 90% 6% .</p>
5	F	179	<div style="display: flex; align-items: center;"> <div style="width: 95%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95% 67% 30% ..</p>
6	G	145	<div style="display: flex; align-items: center;"> <div style="width: 0.5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2.5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0.5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">. 97% ..</p>
7	H	122	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="text-align: center;">13% 91% 9%</p>

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Mol	Chain	Length	Quality of chain
8	I	146	
9	J	120	
10	K	115	
11	L	118	
12	M	102	
13	N	113	
14	O	95	
15	P	103	
16	R	66	
17	S	59	
18	T	59	
19	U	44	
20	V	282	
21	W	436	
22	Y	232	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 75353 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2414	51839	23125	9565	16735	2414	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 467326

- Molecule 2 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	246	1895	1177	373	340	5	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	207	1575	988	290	292	5	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	200	1511	951	278	280	2	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	175	1285	793	237	254	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	108	Total	C	N	O	S	0	0
			753	461	146	145	1		

- Molecule 9 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 10 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	113	Total	C	N	O	0	0
			925	589	180	156		

- Molecule 11 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	117	Total	C	N	O	S	0	0
			934	588	186	156	4		

- Molecule 12 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 13 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 14 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	92	Total	C	N	O	S	0	0
			741	464	136	138	3		

- Molecule 15 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	98	Total	C	N	O	S	0	0
			737	463	137	133	4		

- Molecule 16 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL32.

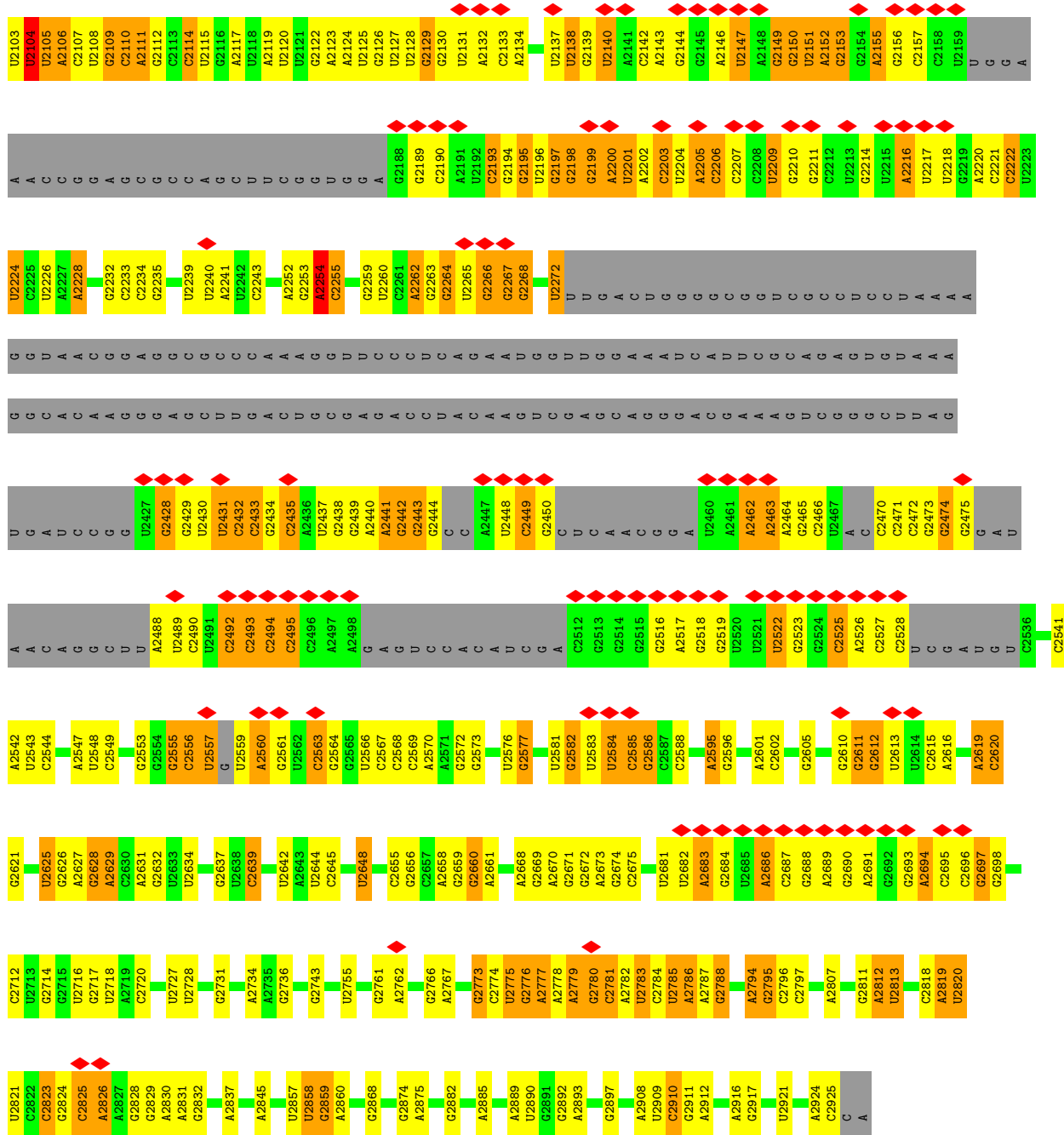
Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	54	Total	C	N	O	S	0	0
			394	241	80	68	5		

- Molecule 19 is a protein called Large ribosomal subunit protein bL34.

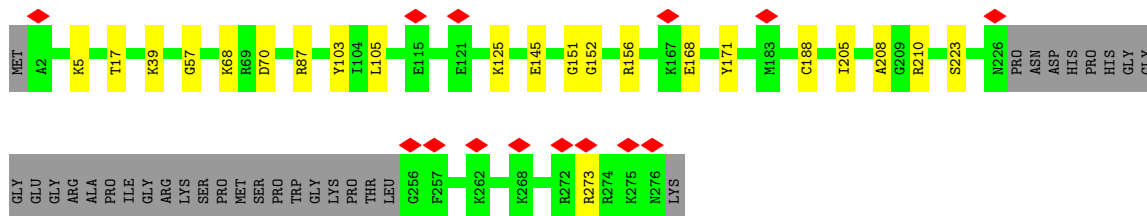
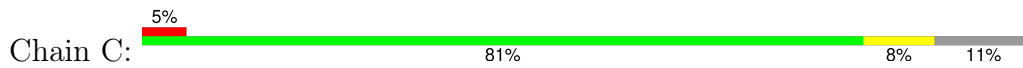
Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 20 is a protein called Ribosome biogenesis GTPase A.

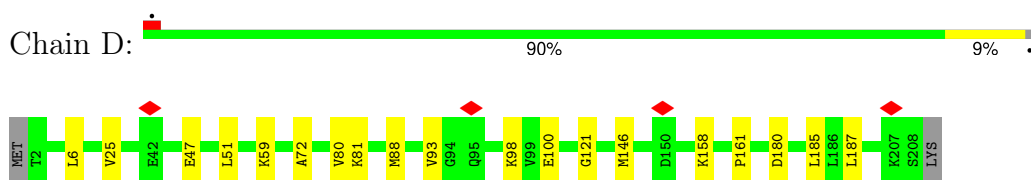
A	G1068	G1192	G1311	G1427	U1505	U1684	U1790	G	G	A	G2002
C	U1069	G1209	A1312	G1428	A1506	A1685	A1791	U	U	A	A
U	G1070	A1210	A1313	U1433	U1507	G1690	A1792	A	A	U	G
G	A1071	U1212	A1314	A1434	C1508	A1691	G1793	A	A	U	
A	A1072	U1213	G1315	U1435	G1512	U1692	A1802	C	C	A	
U	A1073	U1214	C1328	U1436	G1513	C1693	A1805	A	A	A	
U	A1074	U1215	C1334	C1437	C1514	G1696	U1808	A	A	U	
G	A1075	U1216	A1335	C1438	C1515	A1697	U1809	A	A	G	
G	A1076	U1217	A1336	U1439	A1516	A1698	G1810	A	A	G	
G	G1077	U1218	A1337	U1440	A1517	A1699	C1811	A	A	G	
A	A1078	U1219	U1339	C1441	G1518	G1712	A1812	C	C	G	
U	U1079	U1220	A1340	C1442	A1519	A1713	A1813	C	C	G	
A	U1080	A1221	C1343	U1443	A1520	A1714	A1814	U	U	C	
G	U1081	G1220	C1344	U1444	G1521	C1715	C1819	C	C	C	
G	G1082	A1242	C1345	U1445	A1522	G1719	U1820	C	C	C	
C	A1083	U1243	U1346	C1446	G1523	U1756	C1824	U	U	A	
C	A1084	U1244	A1347	U1447	G1524	G1757	U1825	A	A	G	
C	A1085	U1245	U1348	U1448	G1525	U1758	U1829	A	A	G	
C	G1086	G1246	G1349	U1449	C1526	U1759	G1830	G	G	A	
U	U1087	G1247	U1350	U1450	C1527	U1760	A1831	A	A	A	
A	A	U1249	U1351	U1451	U1528	A1761	A1832	A	A	A	
C	U1009	U1250	C1352	U1452	U1529	G	G1833	A	A	A	
C	C1010	U1251	C1353	U1453	A1533	U1626	U1834	A	A	A	
C	C1011	U1252	A1360	U1454	A1534	U1627	U1837	A	A	A	
G	G1012	A1253	A1361	U1455	U1535	U1628	A1838	A	A	A	
G	G1015	A1254	U1362	U1456	U1536	U1629	U1846	A	A	A	
U	U1016	A1260	G1363	U1457	U1537	U1630	U1847	A	A	A	
U	C1017	G1263	A1364	U1458	U1538	G1630	A1850	A	A	A	
A	G1018	U1268	U1365	U1459	U1539	A1631	G1851	A	A	A	
C	A1019	A1276	G1366	U1460	U1540	C1632	G1852	A	A	A	
C	A1020	A1277	A1368	U1461	U1541	G1633	C1855	A	A	A	
G	A1025	G1278	U1391	U1462	U1542	U1634	A1858	A	A	A	
A	A1026	U1279	G1394	U1463	U1543	A1638	C1859	A	A	A	
U	A1027	G1281	C1395	U1464	U1544	U1639	G1860	A	A	A	
U	C1028	A1287	C1396	U1465	U1545	U1640	C1862	A	A	A	
C	C1029	U1288	G1397	U1466	U1546	U1641	U1863	A	A	A	
U	C1041	G1289	A1404	U1467	U1547	G1773	G	A	A	A	
C	A1042	U1290	A1405	U1468	U1548	A1774	U	A	A	A	
A	A1046	G1291	A1406	U1469	U1549	G1775	A	A	A	A	
A	A1047	U1292	U1407	U1494	U1550	A1776	C	A	A	A	
A	G1048	G1293	G1407	U1495	U1551	G1777	C	A	A	A	
C	G1049	A1293	A1408	U1496	U1552	A1778	C	A	A	A	
U	U1050	U1294	U1409	U1497	U1553	G1779	C	A	A	A	
C	C1051	G1296	U1410	U1498	U1554	G1782	C	A	A	A	
G	C1054	U1299	G1414	U1499	U1555	C1783	C	A	A	A	
A	A1054	G1292	U1418	U1500	U1556	A1784	C	A	A	A	
A	A1055	A1295	A1423	U1501	U1557	G1785	C	A	A	A	
U	A1056	U1297	A1424	U1502	U1558	U1786	C	A	A	A	
A	G1057	A1298	A1425	U1503	U1559	G1787	C	A	A	A	
G	U1058	U1299	A1426	G1503	U1560	A1788	C	A	A	A	
C	A1059	G1170	U1306	U1504	U1561	U1789	C	A	A	A	
C	A1063	C1171	G1306	U1504	U1562	A1789	C	A	A	A	
A	U1064	U1172	C1310	U1504	U1563	U1790	C	A	A	A	
U	U1065	A1173	U1310	U1504	U1564	G1792	C	A	A	A	
U	U1065	A1174	U1310	U1504	U1565	C1783	C	A	A	A	
U	U1065	A1175	U1310	U1504	U1566	A1784	C	A	A	A	
U	U1065	U1176	U1310	U1504	U1567	G1785	C	A	A	A	
U	U1065	G1177	U1310	U1504	U1568	U1786	C	A	A	A	
U	U1065	A1092	U1310	U1504	U1569	G1787	C	A	A	A	
U	U1065	A1093	U1310	U1504	U1570	A1788	C	A	A	A	
U	U1065	A1094	U1310	U1504	U1571	U1789	C	A	A	A	
U	U1065	A1095	U1310	U1504	U1572	A1789	C	A	A	A	
U	U1065	A1096	U1310	U1504	U1573	U1790	C	A	A	A	
U	U1065	A1097	U1310	U1504	U1574	A1790	C	A	A	A	
U	U1065	C1098	U1310	U1504	U1575	G1792	C	A	A	A	
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U	U1065	A1100	U1310	U1504	U1577	A1784	C	A	A	A	
U	U1065	G1101	U1310	U1504	U1578	G1785	C	A	A	A	
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U	U1065	U	U1310	U1504	U1628	G1787	C	A	A	A	
U	U1065	U	U1310	U1504	U1629	A1788	C	A	A	A	
U	U1065	U	U1310	U1504	U1630	U1789	C	A	A	A	
U	U1065	U	U1310	U1504	U1631	G1790	C	A	A	A	
U	U1065	U	U1310	U1504	U1632	C1783	C	A	A	A	
U	U1065	U	U1310	U1504	U1633	A1784	C	A	A	A	
U	U1065	U	U1310	U1504	U1634	G1785	C	A	A	A	
U	U1065	U	U1310	U1504	U1635	U1786	C	A	A	A	
U	U1065	U	U1310	U1504	U1636	G1787	C	A	A	A	
U	U1065	U	U1310	U1504	U1637	A1788	C	A	A	A	
U	U1065	U	U1310	U1504	U1638	U1789	C	A	A	A	
U	U1065	U	U1310	U1504	U1639	G1790	C	A	A	A	
U	U1065	U	U1310	U1504	U1640	C1783	C	A	A	A	
U	U1065	U	U1310	U1504	U1641	A1784	C	A	A	A	
U	U1065	U	U1310	U1504	U1642	G1785	C	A	A	A	
U	U1065	U	U1310	U1504	U1643	U1786	C				



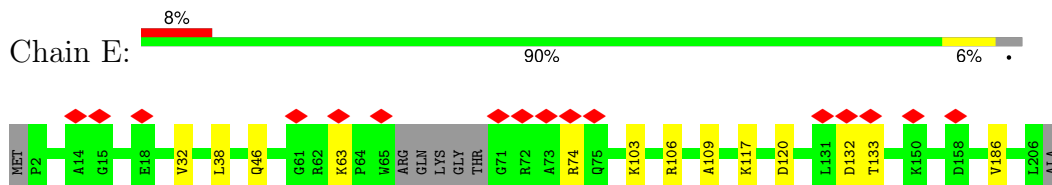
• Molecule 2: Large ribosomal subunit protein uL2



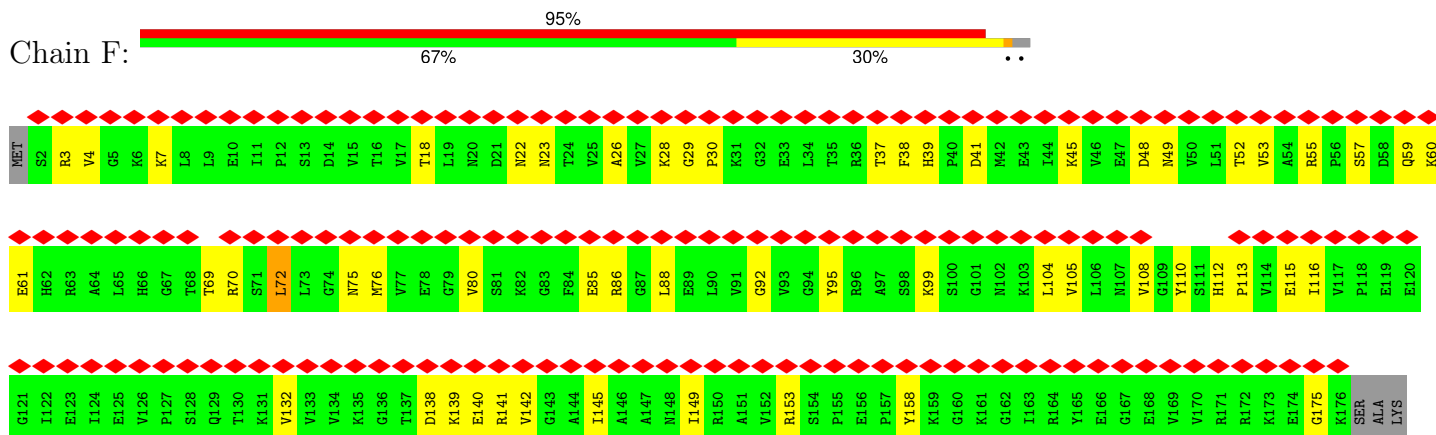
- Molecule 3: Large ribosomal subunit protein uL3



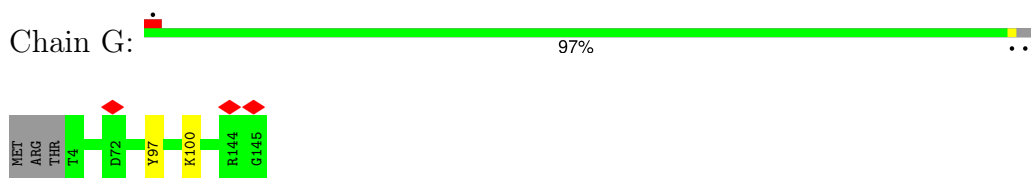
- Molecule 4: Large ribosomal subunit protein uL4



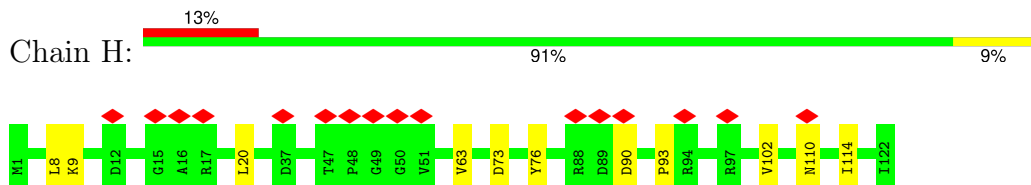
- Molecule 5: Large ribosomal subunit protein uL6



- Molecule 6: Large ribosomal subunit protein uL13

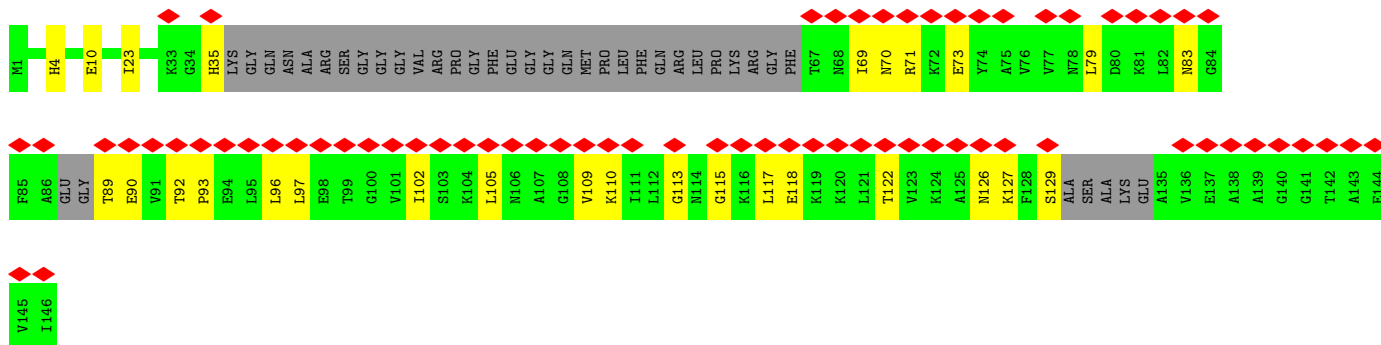


- Molecule 7: Large ribosomal subunit protein uL14



- Molecule 8: Large ribosomal subunit protein uL15





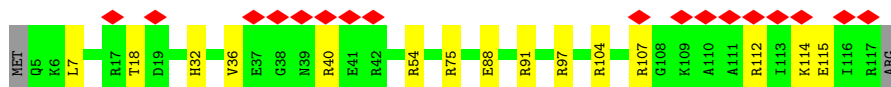
• Molecule 9: Large ribosomal subunit protein bL17

Chain J: 94% 5%



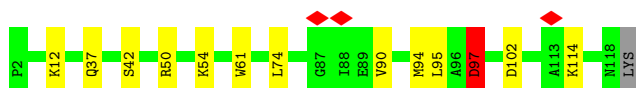
• Molecule 10: Large ribosomal subunit protein bL19

Chain K: 15% 85% 13%



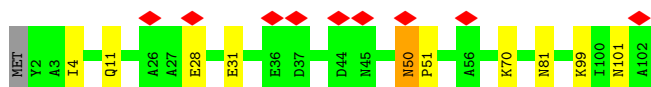
• Molecule 11: Large ribosomal subunit protein bL20

Chain L: 88% 10%



• Molecule 12: Large ribosomal subunit protein bL21

Chain M: 9% 89% 9%

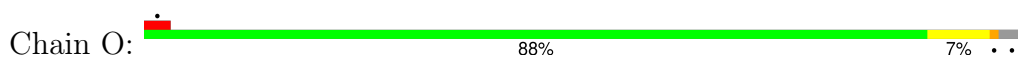


• Molecule 13: Large ribosomal subunit protein uL22

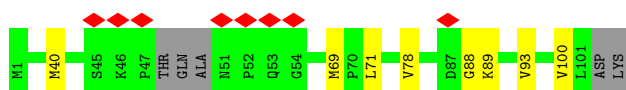
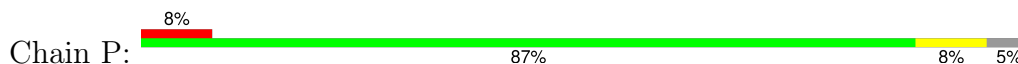
Chain N: 88% 8%



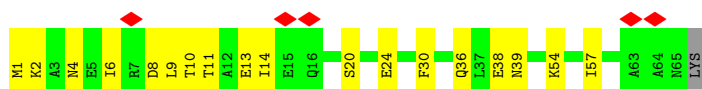
• Molecule 14: Large ribosomal subunit protein uL23



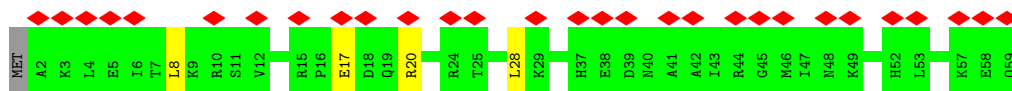
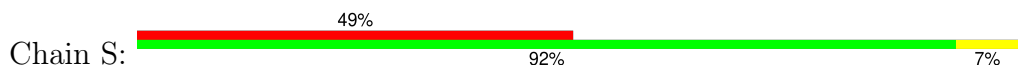
- Molecule 15: Large ribosomal subunit protein uL24



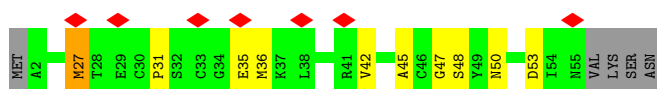
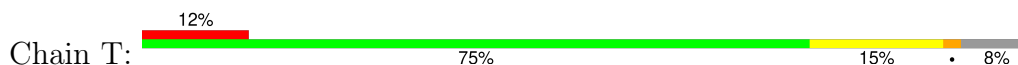
- Molecule 16: Large ribosomal subunit protein uL29



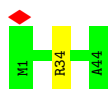
- Molecule 17: Large ribosomal subunit protein uL30



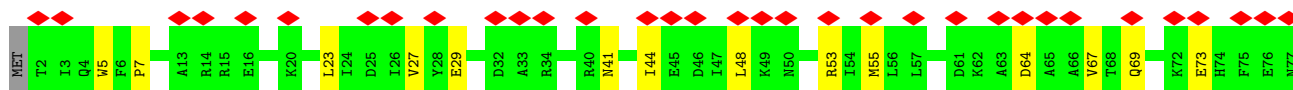
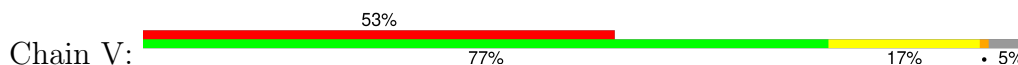
- Molecule 18: Large ribosomal subunit protein bL32

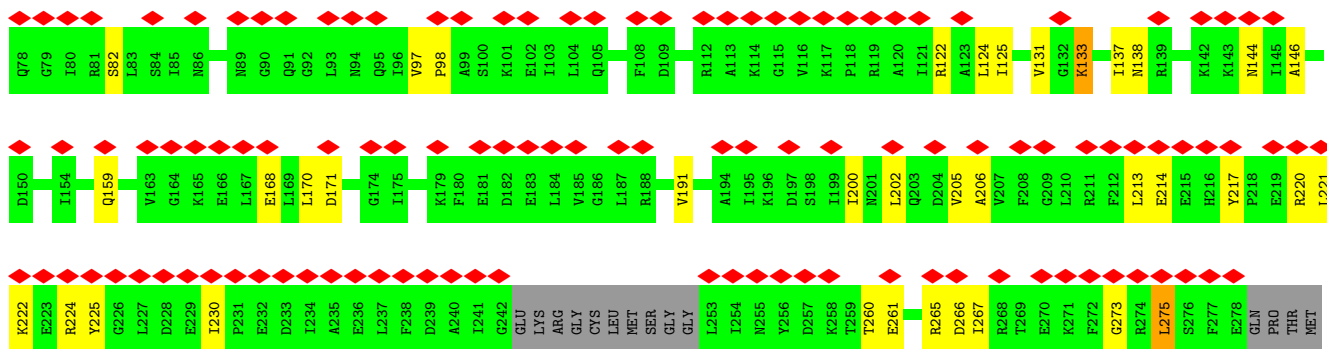


- Molecule 19: Large ribosomal subunit protein bL34

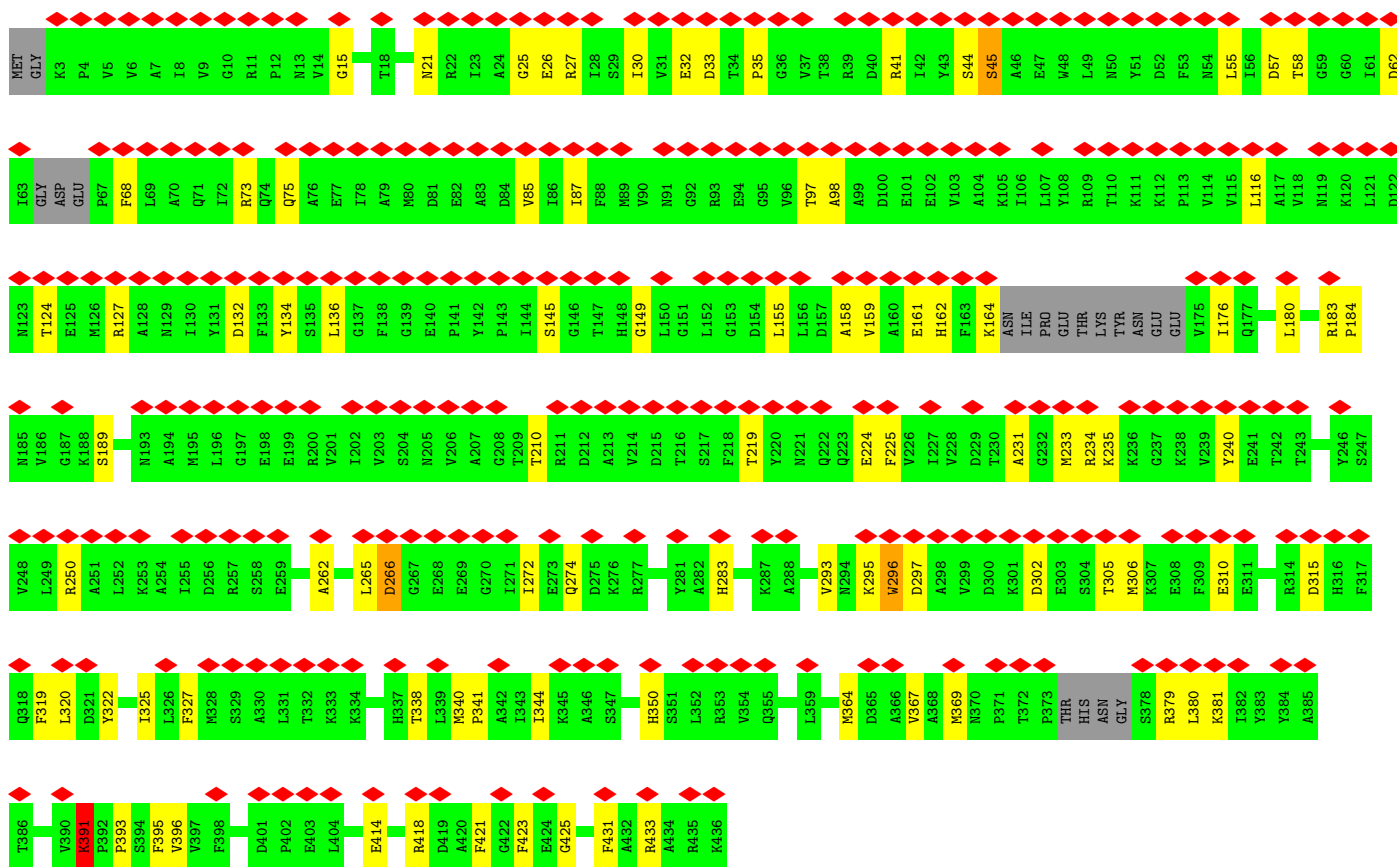
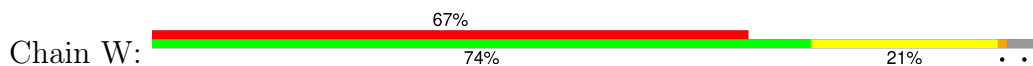


- Molecule 20: Ribosome biogenesis GTPase A

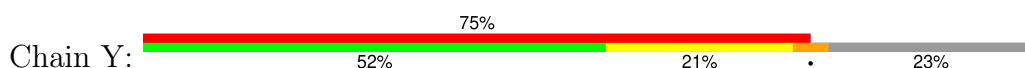




• Molecule 21: GTPase Der



• Molecule 22: Large ribosomal subunit protein uL1



M121	G122	E123	V124	G125	K126	I127	G128	R129	V130	L131	G132	P133	K134	G135	L136	M137	P138	N139	P140	K141	T142	G143	T144	V145	T146	F147	E148	V149	E150	K151	A152	I153	G154	E155	I156	K157	ALA	GLY	LYS	VAL	GLU	TYR	ARG	VAL	ASP	LYS	A168	G169	N170	I171	H172	V173	P174	I175	G176	K177	V178	S179	F180
E181	D182	E183	K184	L185	V186	E187	M188	F189	T190	T191	M192	Y193	D194	T195	I196	L197	K198	A199	K200	P201	A202	A203	A204	K205	G206	V207	Y208	V209	K210	N211	V212	A213	V214	THR	SER	THR	MET	GLY	PRO	GLY	VAL	VAL	LYS	VAL	ASP	SER	SER	THR	THR	PHE	ASN	VAL	VAL	LYS					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.576	Depositor
Minimum map value	-0.191	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.142	Depositor
Map size (Å)	383.04, 383.04, 383.04	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GNP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/58047	0.86	49/90517 (0.1%)
2	C	0.27	0/1921	0.57	2/2570 (0.1%)
3	D	0.27	0/1597	0.52	0/2140
4	E	0.28	0/1529	0.52	0/2064
5	F	0.25	0/1303	0.58	1/1760 (0.1%)
6	G	0.26	0/1146	0.50	0/1542
7	H	0.28	0/927	0.61	0/1245
8	I	0.27	0/754	0.58	0/1007
9	J	0.26	0/960	0.58	0/1284
10	K	0.28	0/938	0.59	0/1255
11	L	0.30	0/946	0.55	1/1259 (0.1%)
12	M	0.30	0/797	0.54	0/1070
13	N	0.29	0/851	0.55	0/1146
14	O	0.30	0/748	0.64	1/997 (0.1%)
15	P	0.27	0/746	0.53	0/996
16	R	0.29	0/531	0.59	0/707
17	S	0.27	0/457	0.58	0/613
18	T	0.26	0/400	0.65	0/536
19	U	0.27	0/370	0.64	0/483
20	V	0.25	0/2152	0.52	0/2902
21	W	0.25	0/3295	0.54	2/4463 (0.0%)
22	Y	0.35	0/1352	0.71	1/1822 (0.1%)
All	All	0.33	0/81767	0.79	57/122378 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	W	0	1

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1433	U	C2-N1-C1'	8.40	127.78	117.70
1	A	698	C	N1-C2-O2	8.23	123.84	118.90
1	A	698	C	C2-N1-C1'	7.65	127.21	118.80
1	A	100	U	C2-N1-C1'	7.52	126.73	117.70
1	A	100	U	N1-C2-O2	7.23	127.86	122.80
1	A	1433	U	N1-C2-O2	6.85	127.59	122.80
1	A	698	C	N3-C2-O2	-6.81	117.13	121.90
22	Y	54	LYS	N-CA-CB	-6.77	98.42	110.60
1	A	100	U	N3-C2-O2	-6.72	117.50	122.20
1	A	1352	U	C2-N1-C1'	6.59	125.61	117.70
2	C	152	GLY	N-CA-C	6.51	129.39	113.10
1	A	2104	U	C2-N1-C1'	6.50	125.50	117.70
1	A	401	C	C2-N1-C1'	6.39	125.83	118.80
1	A	1433	U	N3-C2-O2	-6.39	117.73	122.20
1	A	824	G	C4-N9-C1'	6.38	134.79	126.50
1	A	1353	C	C2-N1-C1'	6.35	125.79	118.80
1	A	271	C	N1-C2-O2	6.19	122.62	118.90
1	A	759	G	N3-C4-N9	5.81	129.48	126.00
1	A	824	G	C8-N9-C1'	-5.72	119.56	127.00
1	A	2104	U	N1-C2-O2	5.71	126.79	122.80
1	A	1433	U	C6-N1-C1'	-5.64	113.31	121.20
2	C	151	GLY	N-CA-C	5.60	127.09	113.10
11	L	97	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	686	C	C2-N1-C1'	5.53	124.88	118.80
1	A	271	C	N3-C2-O2	-5.52	118.03	121.90
1	A	824	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1086	U	C2-N1-C1'	5.50	124.30	117.70
1	A	303	G	N3-C4-C5	-5.42	125.89	128.60
1	A	460	C	C2-N1-C1'	5.41	124.75	118.80
1	A	872	C	N1-C2-O2	5.36	122.12	118.90
1	A	578	A	OP2-P-O3'	5.34	116.95	105.20
1	A	471	G	N1-C6-O6	-5.32	116.71	119.90
1	A	415	C	C2-N1-C1'	-5.30	112.97	118.80
1	A	698	C	C6-N1-C1'	-5.28	114.46	120.80
1	A	698	C	C6-N1-C2	-5.25	118.20	120.30
21	W	266	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	1362	G	P-O3'-C3'	5.22	125.96	119.70
1	A	824	G	N3-C4-N9	5.21	129.13	126.00
1	A	2254	A	P-O3'-C3'	5.19	125.93	119.70
1	A	158	C	C2-N1-C1'	5.18	124.50	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	A	P-O3'-C3'	5.17	125.91	119.70
1	A	2104	U	N3-C2-O2	-5.17	118.58	122.20
1	A	2470	C	N1-C2-O2	5.17	122.00	118.90
21	W	315	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	759	G	C8-N9-C1'	-5.14	120.31	127.00
1	A	276	C	N1-C2-O2	5.14	121.98	118.90
1	A	2648	U	C2-N1-C1'	5.12	123.85	117.70
1	A	401	C	C6-N1-C1'	-5.10	114.68	120.80
1	A	1353	C	C6-N1-C1'	-5.09	114.70	120.80
14	O	91	GLU	CA-CB-CG	5.09	124.59	113.40
5	F	72	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	1729	C	C2-N1-C1'	5.05	124.36	118.80
1	A	1515	C	C2-N1-C1'	5.03	124.33	118.80
1	A	1281	C	C2-N1-C1'	5.02	124.33	118.80
1	A	2470	C	C2-N1-C1'	5.02	124.32	118.80
1	A	2222	C	C2-N1-C1'	5.02	124.32	118.80
1	A	1281	C	N3-C2-O2	-5.01	118.39	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	W	391	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	51839	0	26098	657	0
2	C	1895	0	1985	11	0
3	D	1575	0	1642	12	0
4	E	1511	0	1585	9	0
5	F	1285	0	1246	43	0
6	G	1123	0	1162	1	0
7	H	920	0	977	4	0
8	I	753	0	754	23	0
9	J	953	0	983	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	925	0	995	10	0
11	L	934	0	994	10	0
12	M	786	0	826	8	0
13	N	842	0	899	5	0
14	O	741	0	781	6	0
15	P	737	0	789	5	0
16	R	530	0	568	11	0
17	S	455	0	491	2	0
18	T	394	0	373	6	0
19	U	367	0	410	1	0
20	V	2119	0	2190	31	0
21	W	3239	0	3203	104	0
22	Y	1334	0	1351	123	0
23	V	32	0	13	1	0
23	W	64	0	26	4	0
All	All	75353	0	50341	998	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 (998) 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)
21:W:132:ASP:HA	22:Y:137:MET:CE	1.21	1.59
21:W:98:ALA:N	22:Y:52:PRO:HD3	1.48	1.26
21:W:98:ALA:H	22:Y:52:PRO:CD	1.46	1.26
21:W:132:ASP:CA	22:Y:137:MET:CE	2.16	1.24
21:W:132:ASP:CA	22:Y:137:MET:HE1	1.70	1.22
22:Y:116:ALA:HB1	22:Y:121:MET:CE	1.74	1.15
1:A:2152:A:H4'	22:Y:172:HIS:CD2	1.76	1.15
21:W:98:ALA:CB	22:Y:52:PRO:HD3	1.76	1.15
21:W:180:LEU:HD23	21:W:262:ALA:HB3	1.14	1.13
22:Y:59:ILE:CD1	22:Y:201:PRO:HG2	1.79	1.12
22:Y:116:ALA:HB1	22:Y:121:MET:HE1	1.13	1.12
22:Y:59:ILE:HD12	22:Y:201:PRO:HG2	1.34	1.09
1:A:2206:C:OP1	22:Y:213:ALA:C	1.72	1.09
21:W:98:ALA:H	22:Y:52:PRO:HD3	1.00	1.09
21:W:132:ASP:HA	22:Y:137:MET:HE3	1.13	1.07
21:W:180:LEU:CD2	21:W:262:ALA:HB3	1.82	1.07
21:W:98:ALA:CA	22:Y:52:PRO:HD3	1.84	1.05
21:W:97:THR:HG23	22:Y:55:ASN:ND2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:A:N6	1:A:1512:G:H1	1.54	1.03
22:Y:59:ILE:CD1	22:Y:201:PRO:CG	2.41	0.98
21:W:98:ALA:HB3	22:Y:52:PRO:CD	1.94	0.97
22:Y:116:ALA:CB	22:Y:121:MET:SD	2.52	0.97
22:Y:59:ILE:HD12	22:Y:201:PRO:CG	1.93	0.97
1:A:2152:A:C4'	22:Y:172:HIS:CD2	2.47	0.96
21:W:132:ASP:CA	22:Y:137:MET:HE3	1.87	0.96
21:W:98:ALA:CB	22:Y:52:PRO:CD	2.44	0.95
5:F:3:ARG:HH12	5:F:55:ARG:HD3	1.31	0.95
21:W:98:ALA:CB	22:Y:52:PRO:HG3	1.98	0.94
1:A:1479:G:H1	1:A:1608:A:H61	1.14	0.93
21:W:97:THR:HG23	22:Y:55:ASN:CG	1.89	0.92
1:A:2152:A:H4'	22:Y:172:HIS:CG	2.02	0.92
21:W:132:ASP:HA	22:Y:137:MET:HE1	0.93	0.92
22:Y:117:THR:O	22:Y:121:MET:SD	2.29	0.90
21:W:98:ALA:H	22:Y:52:PRO:HD2	1.36	0.89
21:W:98:ALA:HB3	22:Y:52:PRO:HD3	1.48	0.88
1:A:2130:G:H1	1:A:2217:U:H3	1.21	0.87
5:F:99:LYS:HB3	5:F:104:LEU:HA	1.56	0.87
22:Y:116:ALA:HB3	22:Y:121:MET:SD	2.12	0.87
21:W:98:ALA:CB	22:Y:52:PRO:CG	2.53	0.87
22:Y:67:ASN:HD21	22:Y:187:GLU:HB2	1.39	0.87
22:Y:117:THR:O	22:Y:121:MET:HG2	1.75	0.86
1:A:1479:G:H1	1:A:1608:A:N6	1.73	0.86
1:A:2207:C:H4'	22:Y:47:ARG:CB	2.06	0.85
1:A:1756:U:H3	1:A:1776:A:H61	1.25	0.84
22:Y:116:ALA:HB1	22:Y:121:MET:SD	2.13	0.84
1:A:1491:A:N7	1:A:1512:G:N2	2.25	0.84
21:W:134:TYR:HD2	22:Y:137:MET:SD	2.01	0.84
21:W:97:THR:HG22	22:Y:52:PRO:CD	2.08	0.83
22:Y:117:THR:O	22:Y:121:MET:CG	2.27	0.83
22:Y:116:ALA:CB	22:Y:121:MET:CE	2.57	0.82
1:A:1087:U:O2	1:A:1160:G:N2	2.11	0.81
21:W:98:ALA:HB3	22:Y:52:PRO:CG	2.10	0.81
1:A:1094:A:H61	1:A:2780:G:H1	1.23	0.81
21:W:98:ALA:HB3	22:Y:52:PRO:HG3	1.62	0.81
1:A:283:G:N2	1:A:288:C:O2	2.13	0.81
1:A:2207:C:O5'	22:Y:211:ASN:CB	2.29	0.81
21:W:97:THR:HG22	22:Y:52:PRO:N	1.95	0.80
1:A:1096:A:H2'	1:A:1097:A:H4'	1.64	0.80
22:Y:116:ALA:CB	22:Y:121:MET:HE1	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:121:MET:HE2	22:Y:121:MET:HA	1.63	0.79
22:Y:67:ASN:HB2	22:Y:188:ASN:HD21	1.47	0.79
1:A:1520:A:H61	1:A:1564:C:H42	1.30	0.78
1:A:303:G:H2'	1:A:304:G:C8	2.19	0.78
1:A:2207:C:C4'	22:Y:47:ARG:CB	2.63	0.77
1:A:202:A:N6	1:A:2463:A:OP2	2.18	0.77
1:A:2207:C:P	22:Y:211:ASN:CB	2.72	0.77
21:W:98:ALA:HB2	22:Y:52:PRO:CG	2.15	0.77
1:A:302:A:O2'	1:A:303:G:N7	2.18	0.77
1:A:2610:G:H4'	1:A:2611:G:H5'	1.66	0.76
21:W:134:TYR:CD2	22:Y:137:MET:SD	2.80	0.75
1:A:226:A:H8	1:A:454:G:H21	1.32	0.74
1:A:272:C:N4	1:A:416:U:O4	2.20	0.74
1:A:630:A:H62	1:A:1291:A:H2	1.36	0.74
21:W:180:LEU:CD2	21:W:262:ALA:CB	2.65	0.74
1:A:1444:C:H2'	1:A:1445:A:H8	1.52	0.74
1:A:1491:A:H62	1:A:1512:G:H1	0.79	0.74
21:W:98:ALA:N	22:Y:52:PRO:CD	2.23	0.74
18:T:42:VAL:HB	18:T:47:GLY:HA2	1.69	0.74
21:W:98:ALA:HB2	22:Y:52:PRO:HG3	1.67	0.73
1:A:1555:A:H1'	1:A:1556:A:N7	2.03	0.73
1:A:1340:A:H2	1:A:1671:G:H21	1.34	0.72
1:A:283:G:N2	1:A:289:C:O2	2.22	0.72
1:A:2104:U:N3	1:A:2106:A:N7	2.36	0.72
1:A:2777:A:N7	1:A:2783:U:O2	2.23	0.72
1:A:847:A:H4'	1:A:848:G:H5'	1.71	0.72
1:A:2138:U:H2'	1:A:2139:G:C8	2.26	0.71
1:A:303:G:H2'	1:A:304:G:H8	1.53	0.70
1:A:309:U:H4'	1:A:407:A:H62	1.55	0.70
22:Y:200:LYS:HE3	22:Y:201:PRO:HD2	1.73	0.70
1:A:1246:G:H1'	1:A:1247:G:H5'	1.73	0.70
1:A:1556:A:H2'	1:A:1557:G:O4'	1.92	0.70
18:T:48:SER:HA	18:T:53:ASP:HA	1.72	0.70
1:A:2125:U:H2'	1:A:2126:G:H8	1.57	0.69
21:W:97:THR:CG2	22:Y:55:ASN:ND2	2.53	0.69
22:Y:201:PRO:HG2	22:Y:208:TYR:HE1	1.57	0.69
1:A:1497:G:N1	1:A:1505:U:N3	2.38	0.69
1:A:327:G:H1	1:A:400:U:H3	1.40	0.69
1:A:2205:A:H5'	22:Y:214:VAL:C	2.12	0.69
1:A:2776:G:H21	1:A:2786:A:H62	1.38	0.69
1:A:732:A:H8	1:A:735:U:H3	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2206:C:OP1	22:Y:214:VAL:N	2.25	0.69
10:K:112:ARG:HH12	10:K:114:LYS:HA	1.58	0.69
22:Y:67:ASN:HB2	22:Y:188:ASN:ND2	2.08	0.69
5:F:61:GLU:N	5:F:61:GLU:OE1	2.26	0.68
1:A:430:C:N4	1:A:433:G:OP1	2.26	0.68
1:A:1482:G:H21	1:A:1562:A:H8	1.41	0.68
5:F:72:LEU:O	5:F:75:ASN:HB2	1.92	0.68
1:A:1094:A:N6	1:A:2780:G:H1	1.91	0.68
1:A:2824:G:N2	1:A:2826:A:OP2	2.26	0.68
21:W:234:ARG:HG2	21:W:235:LYS:H	1.58	0.68
1:A:1479:G:N2	1:A:1608:A:N1	2.42	0.68
21:W:132:ASP:C	22:Y:137:MET:HE1	2.15	0.67
1:A:1859:C:HO2'	1:A:1860:G:H8	1.38	0.67
1:A:300:G:H4'	1:A:301:U:H5'	1.76	0.67
1:A:1347:A:H62	1:A:1651:G:H8	1.43	0.67
8:I:23:ILE:HD11	12:M:81:ASN:HB3	1.76	0.67
1:A:2688:G:N2	1:A:2691:A:OP2	2.27	0.67
22:Y:59:ILE:HG21	22:Y:208:TYR:OH	1.95	0.67
1:A:1479:G:H2'	1:A:1480:A:N3	2.10	0.66
22:Y:59:ILE:CD1	22:Y:201:PRO:HG3	2.24	0.66
21:W:234:ARG:HG2	21:W:235:LYS:N	2.10	0.66
1:A:698:C:H3'	1:A:699:A:C8	2.31	0.66
22:Y:199:ALA:O	22:Y:201:PRO:HD3	1.95	0.66
1:A:2557:U:H3	1:A:2564:G:H1	1.41	0.66
1:A:1087:U:N3	1:A:1160:G:N1	2.41	0.66
1:A:1526:G:O2'	1:A:1527:C:H5'	1.96	0.65
22:Y:101:ILE:HD11	22:Y:124:VAL:HG23	1.79	0.65
1:A:1496:G:H1	1:A:1507:U:H3	1.42	0.65
1:A:2823:C:H3'	1:A:2824:G:H8	1.61	0.65
1:A:683:A:C5	1:A:698:C:H1'	2.31	0.65
1:A:1444:C:H2'	1:A:1445:A:C8	2.31	0.64
1:A:282:G:N2	1:A:283:G:O6	2.30	0.64
1:A:1268:G:OP2	11:L:12:LYS:NZ	2.28	0.64
1:A:1242:U:H2'	1:A:1243:A:H8	1.63	0.64
1:A:267:C:O2'	1:A:268:A:O5'	2.14	0.63
1:A:761:U:H2'	1:A:762:A:H3'	1.78	0.63
22:Y:194:ASP:HA	22:Y:197:LEU:HG	1.80	0.63
1:A:296:G:O2'	1:A:297:G:OP1	2.17	0.63
1:A:316:G:H2'	1:A:317:G:C8	2.32	0.63
1:A:617:G:N1	1:A:2060:A:OP1	2.27	0.63
1:A:414:C:O2'	1:A:415:C:OP1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:G:O6	1:A:444:U:O2	2.15	0.63
1:A:2152:A:C4'	22:Y:172:HIS:CG	2.78	0.63
1:A:2440:A:N6	1:A:2441:A:N3	2.47	0.63
1:A:2695:C:H4'	5:F:110:TYR:CZ	2.34	0.63
22:Y:80:LYS:NZ	22:Y:120:MET:HB2	2.14	0.63
22:Y:195:THR:HA	22:Y:198:LYS:HE2	1.80	0.62
12:M:50:ASN:HB2	12:M:51:PRO:HD3	1.80	0.62
1:A:1220:G:H2'	1:A:1221:A:H8	1.63	0.62
1:A:1759:U:OP1	1:A:1773:G:N1	2.32	0.62
5:F:3:ARG:NH1	5:F:55:ARG:HD3	2.09	0.62
1:A:2488:A:N6	1:A:2525:C:O2	2.30	0.62
1:A:437:A:H2'	1:A:438:A:H8	1.64	0.61
1:A:445:C:O2'	1:A:446:G:O5'	2.18	0.61
1:A:1025:A:H5'	1:A:1026:A:H5''	1.82	0.61
1:A:1093:G:N2	1:A:1157:A:OP2	2.29	0.61
1:A:1069:U:OP2	1:A:1071:G:N2	2.33	0.61
1:A:2091:A:N6	1:A:2639:C:N3	2.49	0.61
22:Y:201:PRO:HD2	22:Y:208:TYR:CE1	2.35	0.61
1:A:305:A:H62	1:A:411:G:H21	1.49	0.61
21:W:183:ARG:NE	21:W:272:ILE:HD12	2.16	0.61
1:A:722:A:OP1	4:E:63:LYS:NZ	2.32	0.61
1:A:2265:U:H3'	1:A:2266:G:C8	2.36	0.61
1:A:1374:C:OP1	14:O:65:ARG:NH1	2.34	0.61
1:A:1491:A:N6	1:A:1512:G:N1	2.28	0.61
1:A:510:G:N2	1:A:513:A:OP2	2.27	0.60
1:A:2435:C:N4	1:A:2438:G:N7	2.48	0.60
21:W:183:ARG:CZ	21:W:272:ILE:HD12	2.31	0.60
1:A:326:A:H3'	1:A:327:G:H5''	1.83	0.60
21:W:393:PRO:HG3	21:W:423:PHE:CE1	2.36	0.60
1:A:275:A:N7	1:A:296:G:N2	2.48	0.60
1:A:1096:A:N6	1:A:1097:A:N3	2.49	0.60
1:A:617:G:N2	1:A:2060:A:OP2	2.34	0.60
1:A:2090:G:N2	1:A:2092:C:O4'	2.34	0.60
10:K:104:ARG:O	10:K:107:ARG:NH2	2.35	0.60
22:Y:66:PRO:C	22:Y:68:GLY:H	2.05	0.60
1:A:2122:G:N2	1:A:2226:U:O2	2.34	0.59
1:A:459:A:N6	1:A:2442:G:OP1	2.34	0.59
1:A:1094:A:N6	1:A:2780:G:N1	2.39	0.59
1:A:297:G:H2'	1:A:298:U:C6	2.38	0.59
1:A:2153:G:H5'	22:Y:43:GLU:OE2	2.03	0.59
5:F:149:ILE:HD12	5:F:149:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:C:H2'	1:A:873:U:C6	2.37	0.59
1:A:2267:G:H4'	1:A:2268:G:OP2	2.03	0.59
5:F:105:VAL:HG22	5:F:115:GLU:HG3	1.84	0.59
18:T:31:PRO:HB3	18:T:50:ASN:N	2.18	0.59
1:A:1526:G:C8	1:A:1526:G:H5''	2.38	0.59
1:A:305:A:H2'	1:A:306:C:H5'	1.83	0.59
1:A:1783:C:H5	10:K:97:ARG:HH21	1.49	0.59
1:A:1458:U:H1'	1:A:1460:G:C6	2.38	0.59
2:C:145:GLU:HB3	2:C:188:CYS:HB3	1.84	0.59
1:A:1527:C:O2'	1:A:1528:U:H5''	2.03	0.58
1:A:1362:G:O2'	1:A:1363:G:OP1	2.17	0.58
5:F:22:ASN:O	5:F:37:THR:OG1	2.20	0.58
1:A:1497:G:O6	1:A:1505:U:O4	2.22	0.58
1:A:309:U:H4'	1:A:407:A:N6	2.19	0.58
1:A:1097:A:N6	1:A:1156:G:N3	2.51	0.58
12:M:99:LYS:HG3	12:M:101:ASN:HB2	1.84	0.58
20:V:124:LEU:HD13	20:V:170:LEU:HD23	1.86	0.58
1:A:2152:A:C5'	22:Y:172:HIS:CD2	2.87	0.58
1:A:2560:A:N6	1:A:2691:A:H61	2.02	0.58
1:A:2195:G:H1	1:A:2200:A:H3'	1.67	0.58
1:A:5:A:H2'	1:A:6:A:C8	2.39	0.57
5:F:18:THR:HG22	5:F:26:ALA:HB3	1.85	0.57
15:P:93:VAL:HG12	15:P:100:VAL:HA	1.84	0.57
21:W:176:ILE:HD11	21:W:225:PHE:CD1	2.39	0.57
22:Y:59:ILE:HD12	22:Y:201:PRO:HG3	1.81	0.57
5:F:138:ASP:HB2	5:F:141:ARG:HG2	1.86	0.57
1:A:1310:C:H5''	1:A:1311:G:H5'	1.87	0.57
1:A:1568:G:N2	1:A:1569:A:O2'	2.38	0.57
22:Y:101:ILE:CD1	22:Y:124:VAL:HG23	2.33	0.57
1:A:1478:G:H2'	1:A:1479:G:C8	2.40	0.57
4:E:132:ASP:OD1	4:E:133:THR:N	2.38	0.57
21:W:26:GLU:HG2	21:W:250:ARG:HH22	1.70	0.57
1:A:896:A:H2'	1:A:897:G:H8	1.70	0.57
1:A:2090:G:H4'	1:A:2091:A:OP1	2.04	0.57
7:H:63:VAL:HG21	7:H:102:VAL:HG22	1.86	0.57
21:W:44:SER:OG	21:W:45:SER:N	2.38	0.57
1:A:1460:G:N2	1:A:1631:A:C5	2.72	0.57
1:A:2553:G:H1	1:A:2568:C:H41	1.52	0.57
3:D:100:GLU:N	3:D:100:GLU:OE1	2.38	0.57
8:I:90:GLU:OE1	8:I:92:THR:N	2.38	0.57
21:W:33:ASP:HB2	21:W:35:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:121:MET:HA	22:Y:124:VAL:HG12	1.87	0.57
1:A:688:G:H4'	1:A:692:A:H62	1.70	0.57
1:A:2059:A:H4'	1:A:2060:A:C8	2.40	0.57
1:A:259:A:H2'	1:A:260:A:H8	1.70	0.56
1:A:278:A:H2'	1:A:279:A:H8	1.69	0.56
22:Y:59:ILE:HD11	22:Y:201:PRO:HG2	1.79	0.56
1:A:279:A:H2'	1:A:280:G:C8	2.40	0.56
1:A:462:A:O2'	1:A:463:U:OP1	2.22	0.56
22:Y:49:GLY:HA2	22:Y:210:LYS:HE3	1.87	0.56
1:A:350:U:O2'	1:A:1251:U:OP1	2.23	0.56
1:A:2576:U:O2'	1:A:2577:G:O5'	2.23	0.56
1:A:2858:U:H4'	1:A:2859:G:O5'	2.05	0.56
16:R:10:THR:O	16:R:13:GLU:HG3	2.05	0.56
1:A:89:U:H2'	1:A:90:A:C8	2.41	0.56
21:W:116:LEU:HD11	21:W:136:LEU:HD12	1.86	0.56
1:A:2473:G:OP1	4:E:74:ARG:NH1	2.38	0.56
1:A:823:G:H3'	1:A:824:G:H5'	1.88	0.56
1:A:869:U:N3	1:A:870:A:N7	2.53	0.56
21:W:21:ASN:HD22	21:W:30:ILE:HD11	1.71	0.56
22:Y:201:PRO:CD	22:Y:208:TYR:CE1	2.88	0.56
1:A:288:C:H2'	1:A:289:C:C2	2.40	0.56
1:A:288:C:O2'	1:A:289:C:OP1	2.24	0.56
1:A:2780:G:H3'	1:A:2781:C:H6	1.71	0.56
21:W:41:ARG:HG2	21:W:58:THR:HG22	1.87	0.56
1:A:682:G:OP2	8:I:129:SER:OG	2.20	0.56
1:A:2882:G:N2	1:A:2885:A:OP2	2.34	0.56
1:A:1002:G:O6	1:A:1004:U:O2'	2.23	0.56
1:A:1774:A:H3'	1:A:1775:G:H8	1.70	0.56
1:A:1837:U:O2'	1:A:1838:A:OP1	2.22	0.56
1:A:1213:G:H2'	1:A:1214:U:C6	2.41	0.55
1:A:1526:G:H4'	1:A:1526:G:OP1	2.06	0.55
20:V:29:GLU:OE1	20:V:53:ARG:NH1	2.39	0.55
1:A:5:A:H2'	1:A:6:A:H8	1.72	0.55
1:A:465:U:H2'	1:A:466:C:C6	2.42	0.55
1:A:1465:A:H2'	1:A:1467:G:N7	2.21	0.55
3:D:6:LEU:HD21	3:D:81:LYS:CG	2.36	0.55
1:A:342:A:N3	1:A:363:C:O2'	2.38	0.55
21:W:62:ASP:O	21:W:73:ARG:NH2	2.37	0.55
1:A:1065:U:H3	1:A:1188:A:H62	1.54	0.55
1:A:2131:U:H2'	1:A:2132:A:C8	2.42	0.55
1:A:2197:G:H2'	1:A:2198:G:N2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:132:ASP:N	22:Y:137:MET:HE3	2.21	0.55
1:A:1001:U:O4	1:A:1004:U:O2'	2.23	0.55
1:A:2104:U:O2'	1:A:2105:U:H5'	2.05	0.55
8:I:90:GLU:OE1	8:I:92:THR:HG23	2.06	0.55
1:A:316:G:H2'	1:A:317:G:H8	1.70	0.55
1:A:2102:C:O2	1:A:2465:G:N2	2.39	0.55
22:Y:73:GLN:O	22:Y:157:LYS:NZ	2.39	0.55
1:A:2628:G:O2'	1:A:2629:A:H8	1.90	0.55
16:R:8:ASP:OD1	16:R:9:LEU:N	2.40	0.55
21:W:97:THR:HG22	22:Y:52:PRO:HD2	1.87	0.55
1:A:303:G:O2'	1:A:304:G:OP1	2.24	0.55
1:A:349:C:H2'	1:A:350:U:C6	2.42	0.55
1:A:2686:A:O4'	1:A:2694:A:N6	2.40	0.54
21:W:272:ILE:HG22	21:W:274:GLN:H	1.71	0.54
1:A:682:G:N7	8:I:110:LYS:NZ	2.53	0.54
1:A:1082:G:O6	1:A:1165:U:O2	2.25	0.54
1:A:309:U:O2'	1:A:407:A:N7	2.39	0.54
1:A:1250:G:H5''	1:A:1251:U:H3'	1.89	0.54
5:F:45:LYS:HE2	5:F:52:THR:HG23	1.89	0.54
1:A:2712:C:OP1	10:K:54:ARG:NH2	2.38	0.54
1:A:2788:G:N2	5:F:140:GLU:OE2	2.40	0.54
21:W:32:GLU:OE2	21:W:32:GLU:N	2.40	0.54
21:W:97:THR:HG23	22:Y:55:ASN:CB	2.36	0.54
1:A:2783:U:O2'	1:A:2785:U:OP1	2.18	0.54
1:A:2911:G:H2'	1:A:2912:A:H8	1.71	0.54
8:I:117:LEU:HD12	8:I:118:GLU:H	1.71	0.54
1:A:278:A:H2'	1:A:279:A:C8	2.43	0.54
1:A:2777:A:H2'	1:A:2778:A:C8	2.42	0.54
22:Y:175:ILE:HB	22:Y:188:ASN:HB3	1.89	0.54
1:A:687:U:H3'	1:A:688:G:C8	2.43	0.54
1:A:1426:A:H5'	1:A:1515:C:H1'	1.90	0.54
1:A:2109:G:O2'	1:A:2110:C:OP1	2.25	0.54
1:A:2582:G:C6	1:A:2584:U:H5'	2.42	0.54
5:F:85:GLU:O	5:F:86:ARG:HD2	2.07	0.54
22:Y:121:MET:CE	22:Y:121:MET:CA	2.86	0.54
20:V:266:ASP:OD1	20:V:267:ILE:N	2.41	0.54
22:Y:59:ILE:HD13	22:Y:201:PRO:CG	2.34	0.54
22:Y:104:ILE:HA	22:Y:108:TRP:HB2	1.90	0.54
1:A:1516:A:H62	1:A:1568:G:H8	1.55	0.53
1:A:2149:G:H2'	1:A:2150:G:C8	2.43	0.53
20:V:27:VAL:HG11	20:V:48:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:A:H2'	1:A:1075:A:H8	1.73	0.53
1:A:1075:A:H3'	1:A:1076:G:H8	1.74	0.53
5:F:59:GLN:HG3	5:F:61:GLU:OE1	2.09	0.53
16:R:11:THR:HA	16:R:14:ILE:HD12	1.91	0.53
16:R:20:SER:O	16:R:24:GLU:HG3	2.08	0.53
1:A:692:A:H3'	1:A:693:G:H8	1.74	0.53
2:C:5:LYS:HG2	2:C:17:THR:HG22	1.89	0.53
1:A:1455:C:O2'	1:A:1456:A:OP1	2.26	0.53
1:A:1540:A:H2'	1:A:1541:A:C8	2.44	0.53
1:A:1859:C:O2'	1:A:1860:G:H8	1.91	0.53
1:A:275:A:H61	1:A:297:G:H1'	1.72	0.53
1:A:439:U:O2'	1:A:440:U:OP1	2.25	0.53
3:D:180:ASP:OD1	3:D:185:LEU:HB2	2.08	0.53
22:Y:117:THR:N	22:Y:121:MET:SD	2.82	0.53
1:A:513:A:OP1	19:U:34:ARG:NH1	2.42	0.53
1:A:1214:U:H2'	1:A:1215:U:C6	2.44	0.53
1:A:1448:U:O2	1:A:1449:C:N4	2.40	0.53
12:M:28:GLU:N	12:M:31:GLU:OE1	2.41	0.53
1:A:106:G:H1'	1:A:337:A:H8	1.73	0.53
1:A:1656:C:O2'	1:A:1657:C:O5'	2.27	0.53
1:A:63:G:H21	14:O:66:VAL:HG11	1.74	0.53
1:A:1245:G:H1'	1:A:1246:G:H5'	1.90	0.53
1:A:2201:U:H1'	1:A:2203:C:C2	2.43	0.53
1:A:2022:U:H2'	1:A:2023:C:H5'	1.90	0.52
1:A:2778:A:OP2	1:A:2779:A:O2'	2.21	0.52
5:F:45:LYS:H	5:F:53:VAL:HG22	1.73	0.52
1:A:284:C:HO2'	1:A:288:C:HO2'	1.58	0.52
1:A:626:G:H2'	1:A:627:G:H8	1.73	0.52
1:A:1528:U:H4'	1:A:1529:G:H4'	1.91	0.52
1:A:1018:G:H3'	1:A:1019:A:H5''	1.92	0.52
22:Y:121:MET:CE	22:Y:121:MET:HA	2.34	0.52
1:A:58:G:O2'	1:A:59:G:OP1	2.26	0.52
1:A:1074:A:H2'	1:A:1075:A:C8	2.44	0.52
1:A:1339:A:H4'	1:A:1340:A:O5'	2.09	0.52
22:Y:80:LYS:HZ2	22:Y:120:MET:HB2	1.72	0.52
1:A:2062:A:O2'	1:A:2064:G:OP2	2.22	0.52
1:A:2123:A:N6	1:A:2224:U:O4	2.43	0.52
21:W:302:ASP:O	21:W:305:THR:OG1	2.26	0.52
1:A:416:U:O2'	1:A:470:A:OP2	2.25	0.52
1:A:264:G:C2	1:A:265:A:C8	2.98	0.52
1:A:867:A:H4'	1:A:883:G:N2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:191:VAL:HG22	20:V:205:VAL:HG13	1.92	0.52
5:F:110:TYR:HD1	5:F:112:HIS:CD2	2.29	0.52
5:F:149:ILE:HD12	5:F:149:ILE:N	2.25	0.52
1:A:314:A:H1'	1:A:316:G:C2	2.46	0.51
1:A:1438:C:O2'	1:A:1439:U:OP1	2.28	0.51
1:A:1519:C:H42	1:A:1565:U:H3	1.58	0.51
1:A:1782:G:N2	1:A:1785:G:OP2	2.41	0.51
4:E:117:LYS:NZ	4:E:186:VAL:O	2.37	0.51
9:J:91:TYR:OH	9:J:120:VAL:O	2.21	0.51
13:N:73:GLN:HB2	13:N:106:VAL:HB	1.93	0.51
20:V:53:ARG:NH1	20:V:55:MET:SD	2.83	0.51
21:W:234:ARG:CG	21:W:235:LYS:H	2.23	0.51
21:W:396:VAL:HG22	21:W:431:PHE:HB3	1.92	0.51
1:A:314:A:H1'	1:A:316:G:C4	2.45	0.51
1:A:674:G:H2'	1:A:675:C:C6	2.44	0.51
1:A:688:G:C2	1:A:690:A:H5''	2.44	0.51
1:A:698:C:H2'	1:A:698:C:O2	2.11	0.51
2:C:39:LYS:NZ	2:C:57:GLY:O	2.42	0.51
1:A:871:G:O2'	1:A:872:C:H5''	2.11	0.51
8:I:110:LYS:HG3	8:I:127:LYS:HG3	1.93	0.51
21:W:364:MET:HA	21:W:367:VAL:HG12	1.90	0.51
22:Y:120:MET:O	22:Y:120:MET:HG2	2.10	0.51
22:Y:197:LEU:O	22:Y:198:LYS:C	2.47	0.51
1:A:1480:A:H62	1:A:1606:A:H61	1.59	0.51
1:A:2124:A:H2'	1:A:2125:U:C6	2.45	0.51
1:A:2582:G:C5	1:A:2584:U:H5'	2.46	0.51
3:D:146:MET:HG2	3:D:158:LYS:HE2	1.92	0.51
1:A:304:G:H2'	1:A:305:A:C8	2.45	0.51
1:A:1526:G:C2	1:A:1559:C:C2	2.98	0.51
1:A:2209:U:H2'	1:A:2210:G:C8	2.45	0.51
21:W:162:HIS:O	21:W:164:LYS:NZ	2.39	0.51
1:A:461:C:HO2'	1:A:462:A:H8	1.59	0.51
1:A:637:A:H2'	1:A:638:U:C6	2.46	0.51
1:A:1528:U:C4'	1:A:1529:G:H4'	2.41	0.51
1:A:2193:C:H3'	1:A:2194:G:H8	1.76	0.51
1:A:403:C:H2'	1:A:404:C:C6	2.46	0.51
1:A:1096:A:C6	1:A:1097:A:H1'	2.46	0.51
1:A:2429:G:H2'	1:A:2430:U:C6	2.46	0.51
1:A:2694:A:H5''	1:A:2695:C:C5	2.46	0.51
1:A:1220:G:H2'	1:A:1221:A:C8	2.45	0.51
1:A:2909:U:H2'	1:A:2910:C:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:66:PRO:O	22:Y:68:GLY:N	2.44	0.51
1:A:313:U:H4'	1:A:314:A:H5''	1.92	0.51
1:A:327:G:OP1	1:A:327:G:H4'	2.09	0.51
1:A:1618:A:H2'	1:A:1619:A:C8	2.46	0.51
1:A:688:G:N3	1:A:690:A:H5''	2.26	0.50
1:A:2132:A:H2'	1:A:2133:C:C6	2.45	0.50
1:A:2155:A:N6	22:Y:39:ASP:N	2.59	0.50
1:A:870:A:C2'	1:A:871:G:H5'	2.40	0.50
1:A:1263:G:N7	12:M:70:LYS:NZ	2.60	0.50
21:W:319:PHE:CZ	21:W:320:LEU:HD22	2.46	0.50
22:Y:67:ASN:ND2	22:Y:67:ASN:H	2.08	0.50
1:A:172:U:H2'	1:A:173:A:H8	1.74	0.50
1:A:2138:U:H3	1:A:2209:U:H3	1.60	0.50
1:A:1213:G:H2'	1:A:1214:U:H6	1.76	0.50
1:A:2857:U:OP1	3:D:59:LYS:NZ	2.43	0.50
21:W:25:GLY:HA3	21:W:27:ARG:CZ	2.41	0.50
1:A:896:A:H2'	1:A:897:G:C8	2.45	0.50
1:A:1000:G:H22	1:A:1009:U:H3	1.58	0.50
1:A:1093:G:H2'	1:A:1157:A:N6	2.26	0.50
1:A:1476:C:H2'	1:A:1477:A:C8	2.46	0.50
1:A:2149:G:H2'	1:A:2150:G:H8	1.77	0.50
5:F:104:LEU:N	5:F:116:ILE:O	2.42	0.50
1:A:699:A:H2'	1:A:700:U:C5	2.46	0.50
1:A:1496:G:H22	1:A:1507:U:H3	1.58	0.50
1:A:1774:A:H3'	1:A:1775:G:C8	2.47	0.50
1:A:2128:U:H1'	1:A:2220:A:C2	2.46	0.50
4:E:32:VAL:HG12	4:E:109:ALA:HB2	1.94	0.50
8:I:71:ARG:HB3	8:I:73:GLU:OE2	2.11	0.50
1:A:90:A:H4'	1:A:91:A:O5'	2.12	0.50
20:V:206:ALA:HB2	20:V:260:THR:HG23	1.94	0.50
1:A:78:U:H2'	1:A:79:C:C6	2.47	0.50
1:A:675:C:H2'	1:A:676:G:H8	1.77	0.50
1:A:1515:C:H2'	1:A:1516:A:H8	1.77	0.50
1:A:1556:A:OP2	1:A:1556:A:H3'	2.11	0.50
1:A:2198:G:H2'	1:A:2199:G:C4	2.46	0.50
1:A:2610:G:H8	1:A:2612:G:N7	2.10	0.50
3:D:72:ALA:HB2	3:D:93:VAL:HG12	1.93	0.50
20:V:122:ARG:HG2	20:V:168:GLU:HB2	1.93	0.50
21:W:176:ILE:HD11	21:W:225:PHE:HD1	1.74	0.50
22:Y:65:LEU:HD13	22:Y:66:PRO:HD2	1.94	0.50
22:Y:121:MET:SD	22:Y:145:VAL:HG13	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:121:MET:N	22:Y:121:MET:HE3	2.27	0.50
1:A:626:G:H2'	1:A:627:G:C8	2.47	0.50
1:A:2494:C:H2'	1:A:2495:C:C6	2.47	0.50
1:A:873:U:H3	1:A:879:G:H1	1.59	0.49
1:A:2585:C:H4'	1:A:2586:G:O5'	2.12	0.49
8:I:96:LEU:HB2	8:I:102:ILE:HG22	1.94	0.49
15:P:69:MET:SD	15:P:78:VAL:HB	2.52	0.49
16:R:36:GLN:N	16:R:36:GLN:OE1	2.45	0.49
3:D:98:LYS:HB3	3:D:100:GLU:OE1	2.11	0.49
13:N:28:GLN:HB2	13:N:31:GLU:HG3	1.94	0.49
1:A:1096:A:N3	1:A:2780:G:O2'	2.43	0.49
1:A:1491:A:N6	1:A:1512:G:C6	2.80	0.49
1:A:462:A:H2'	1:A:463:U:C6	2.47	0.49
1:A:805:G:H21	1:A:2010:A:H62	1.60	0.49
1:A:1019:A:OP1	1:A:1019:A:H8	1.95	0.49
1:A:1092:A:O3'	1:A:1093:G:H8	1.95	0.49
1:A:1477:A:H2'	1:A:1478:G:C8	2.48	0.49
1:A:2566:U:H2'	1:A:2567:C:C6	2.47	0.49
21:W:33:ASP:N	21:W:33:ASP:OD1	2.45	0.49
21:W:124:THR:O	21:W:127:ARG:HB3	2.12	0.49
1:A:202:A:H1'	1:A:2462:A:C6	2.48	0.49
1:A:317:G:O2'	1:A:318:A:OP1	2.30	0.49
16:R:2:LYS:O	16:R:6:ILE:HG12	2.12	0.49
17:S:17:GLU:OE1	17:S:20:ARG:NH2	2.46	0.49
18:T:31:PRO:HB3	18:T:50:ASN:H	1.78	0.49
1:A:1811:C:O2	1:A:2637:G:O2'	2.16	0.49
1:A:2659:G:H2'	1:A:2660:G:H8	1.77	0.49
1:A:307:A:C5	1:A:308:C:C4	3.01	0.49
1:A:674:G:H4'	1:A:697:G:H4'	1.94	0.49
1:A:2794:A:OP2	1:A:2795:G:N2	2.44	0.49
5:F:76:MET:O	5:F:80:VAL:N	2.42	0.49
18:T:27:MET:SD	18:T:36:MET:SD	3.11	0.49
1:A:306:C:N4	1:A:307:A:H62	2.11	0.49
1:A:1520:A:N6	1:A:1564:C:H42	2.04	0.49
1:A:1425:C:H2'	1:A:1426:A:H8	1.77	0.48
11:L:95:LEU:HD12	12:M:4:ILE:HD13	1.95	0.48
1:A:674:G:H2'	1:A:675:C:H6	1.78	0.48
1:A:868:A:H5''	1:A:869:U:C6	2.48	0.48
1:A:2096:G:H2'	1:A:2098:G:H8	1.77	0.48
1:A:2254:A:H1'	1:A:2255:C:OP2	2.13	0.48
1:A:2655:C:H2'	1:A:2656:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:U:H5'	1:A:90:A:OP2	2.13	0.48
1:A:407:A:C2	1:A:408:G:H1'	2.48	0.48
1:A:767:U:C4	1:A:768:G:C5	3.01	0.48
1:A:1578:G:H1'	1:A:1588:A:H62	1.77	0.48
1:A:1712:G:O2'	1:A:2020:U:O4	2.27	0.48
1:A:2106:A:H2'	1:A:2107:C:C6	2.47	0.48
1:A:2207:C:O4'	22:Y:47:ARG:CB	2.62	0.48
1:A:2561:G:O2'	1:A:2686:A:N1	2.36	0.48
8:I:79:LEU:HB2	8:I:113:GLY:HA2	1.96	0.48
14:O:52:ASP:HB3	14:O:84:THR:HG22	1.95	0.48
1:A:1100:A:H2'	1:A:1151:U:H3	1.79	0.48
18:T:35:GLU:OE1	18:T:45:ALA:N	2.46	0.48
21:W:379:ARG:O	21:W:381:LYS:NZ	2.46	0.48
22:Y:67:ASN:HD21	22:Y:187:GLU:CB	2.17	0.48
1:A:115:C:O2'	1:A:125:A:N3	2.44	0.48
1:A:297:G:H4'	1:A:304:G:O2'	2.13	0.48
1:A:419:G:N2	1:A:448:A:OP2	2.40	0.48
1:A:1504:A:H4'	1:A:1505:U:O4'	2.14	0.48
15:P:40:MET:HE3	15:P:40:MET:HA	1.94	0.48
21:W:85:VAL:HG21	21:W:159:VAL:HG13	1.94	0.48
1:A:2110:C:O2'	1:A:2111:A:H5'	2.13	0.48
1:A:2522:U:O2'	21:W:433:ARG:NH1	2.47	0.48
1:A:2560:A:H61	1:A:2691:A:H61	1.62	0.48
5:F:86:ARG:HG3	5:F:142:VAL:HG13	1.95	0.48
8:I:35:HIS:O	8:I:35:HIS:ND1	2.47	0.48
1:A:351:G:N2	1:A:354:A:OP2	2.44	0.48
1:A:580:U:H2'	1:A:581:C:C6	2.48	0.48
1:A:897:G:H2'	1:A:898:U:C6	2.48	0.48
1:A:1518:G:N2	1:A:1566:G:H22	2.11	0.48
1:A:2131:U:H2'	1:A:2132:A:H8	1.77	0.48
21:W:87:ILE:HD11	21:W:155:LEU:HD21	1.95	0.48
1:A:202:A:C2	1:A:2462:A:H2'	2.49	0.48
1:A:304:G:H2'	1:A:305:A:H8	1.79	0.48
1:A:580:U:H5'	11:L:42:SER:HB2	1.96	0.48
1:A:1526:G:N2	1:A:1559:C:C2	2.82	0.48
1:A:1559:C:H2'	1:A:1560:U:C6	2.48	0.48
1:A:2572:G:H2'	1:A:2573:G:C8	2.49	0.48
21:W:184:PRO:HD3	21:W:233:MET:O	2.13	0.48
1:A:2619:A:H5'	1:A:2620:C:OP2	2.13	0.48
1:A:2911:G:H2'	1:A:2912:A:C8	2.49	0.48
11:L:50:ARG:O	11:L:54:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:C:H2'	1:A:307:A:C8	2.49	0.48
1:A:275:A:N6	1:A:297:G:H1'	2.29	0.47
1:A:1015:G:H2'	1:A:1016:U:C6	2.48	0.47
1:A:1476:C:H2'	1:A:1477:A:H8	1.79	0.47
16:R:10:THR:O	16:R:14:ILE:HG13	2.13	0.47
1:A:424:G:O6	1:A:444:U:C2	2.66	0.47
10:K:18:THR:O	10:K:18:THR:OG1	2.32	0.47
14:O:89:GLU:HA	14:O:89:GLU:OE1	2.15	0.47
21:W:240:TYR:CD2	21:W:240:TYR:O	2.67	0.47
22:Y:201:PRO:HG2	22:Y:208:TYR:CE1	2.44	0.47
1:A:807:G:H2'	1:A:808:A:O4'	2.14	0.47
1:A:1656:C:O2'	1:A:1657:C:H6	1.96	0.47
1:A:2125:U:H2'	1:A:2126:G:C8	2.43	0.47
1:A:2197:G:H2'	1:A:2198:G:H21	1.78	0.47
1:A:1046:A:H2'	1:A:1047:A:C8	2.49	0.47
1:A:1494:G:H2'	1:A:1495:C:O4'	2.15	0.47
1:A:1559:C:H2'	1:A:1560:U:H6	1.80	0.47
1:A:352:G:N2	1:A:524:A:N7	2.62	0.47
1:A:662:U:H2'	1:A:663:G:H8	1.78	0.47
1:A:1553:A:H3'	1:A:1554:U:C6	2.50	0.47
1:A:1819:C:O2'	2:C:208:ALA:HB2	2.15	0.47
1:A:2889:A:H2'	1:A:2890:U:C6	2.50	0.47
16:R:54:LYS:O	16:R:57:ILE:HG12	2.14	0.47
20:V:48:LEU:HD21	20:V:53:ARG:HD3	1.96	0.47
22:Y:59:ILE:HD13	22:Y:201:PRO:HG3	1.94	0.47
22:Y:104:ILE:HG12	22:Y:108:TRP:CD1	2.50	0.47
22:Y:118:PRO:HG3	22:Y:145:VAL:HG12	1.97	0.47
1:A:805:G:H21	1:A:2010:A:N6	2.13	0.47
1:A:1218:U:H2'	1:A:1220:G:N3	2.30	0.47
1:A:1557:G:H2'	1:A:1558:C:O4'	2.13	0.47
1:A:315:C:H4'	1:A:316:G:O4'	2.14	0.47
1:A:579:G:H2'	1:A:580:U:C6	2.50	0.47
1:A:1306:G:O5'	13:N:15:ARG:NH2	2.48	0.47
1:A:1552:C:H2'	1:A:1553:A:C8	2.50	0.47
1:A:2780:G:H3'	1:A:2781:C:C6	2.48	0.47
1:A:675:C:H1'	1:A:685:U:H3	1.79	0.47
1:A:687:U:H3'	1:A:688:G:H8	1.78	0.47
1:A:696:C:H2'	1:A:697:G:H5'	1.97	0.47
1:A:1096:A:C2'	1:A:1097:A:H4'	2.40	0.47
1:A:1244:A:C8	8:I:4:HIS:HB3	2.50	0.47
1:A:2697:G:H1'	5:F:113:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2831:A:H2'	1:A:2832:G:C8	2.50	0.47
20:V:64:ASP:HB3	20:V:67:VAL:HG12	1.97	0.47
1:A:759:G:H3'	1:A:760:G:C8	2.50	0.46
1:A:2234:C:H2'	1:A:2235:G:H8	1.80	0.46
10:K:32:HIS:NE2	10:K:88:GLU:OE1	2.47	0.46
1:A:63:G:H8	1:A:63:G:P	2.37	0.46
1:A:377:G:O2'	1:A:378:C:OP1	2.28	0.46
1:A:1079:U:O2'	1:A:1080:G:H5''	2.15	0.46
5:F:104:LEU:HD13	5:F:116:ILE:HB	1.97	0.46
5:F:149:ILE:H	5:F:149:ILE:CD1	2.28	0.46
20:V:133:LYS:HG3	23:V:301:GNP:O1B	2.15	0.46
1:A:198:A:H2'	1:A:253:G:H21	1.80	0.46
1:A:465:U:H2'	1:A:466:C:H6	1.79	0.46
1:A:1098:C:N3	1:A:1154:U:C4	2.84	0.46
1:A:1214:U:H2'	1:A:1215:U:C5	2.49	0.46
1:A:1696:G:O2'	1:A:1697:A:H8	1.97	0.46
1:A:2107:C:O2'	1:A:2462:A:N3	2.49	0.46
1:A:2111:A:H2'	1:A:2112:G:C8	2.50	0.46
1:A:2122:G:C2	1:A:2254:A:C5	3.03	0.46
8:I:102:ILE:HD12	8:I:109:VAL:HB	1.98	0.46
1:A:305:A:C8	1:A:306:C:C5	3.04	0.46
1:A:1445:A:H2'	1:A:1446:C:H6	1.80	0.46
1:A:2567:C:H2'	1:A:2568:C:O2	2.15	0.46
17:S:8:LEU:HB2	17:S:28:LEU:HD13	1.97	0.46
1:A:279:A:H2'	1:A:280:G:H8	1.79	0.46
1:A:1244:A:O2'	1:A:1245:G:O5'	2.34	0.46
1:A:2149:G:C2	1:A:2150:G:C5	3.04	0.46
1:A:2150:G:O2'	1:A:2151:U:OP1	2.29	0.46
21:W:189:SER:OG	23:W:501:GNP:O1G	2.30	0.46
1:A:296:G:HO2'	1:A:297:G:P	2.36	0.46
1:A:630:A:N1	1:A:856:G:O2'	2.46	0.46
1:A:1343:C:O2'	1:A:1344:C:O5'	2.33	0.46
1:A:2828:G:H2'	1:A:2829:G:C8	2.51	0.46
5:F:3:ARG:O	5:F:7:LYS:NZ	2.42	0.46
8:I:79:LEU:HB3	8:I:115:GLY:H	1.80	0.46
21:W:265:LEU:HB2	21:W:293:VAL:HG12	1.98	0.46
22:Y:64:VAL:HG12	22:Y:155:GLU:HB2	1.97	0.46
1:A:878:G:H2'	1:A:879:G:C8	2.51	0.46
1:A:1071:G:N7	1:A:1181:C:H1'	2.31	0.46
8:I:69:ILE:HD12	8:I:70:ASN:H	1.80	0.46
16:R:1:MET:HA	16:R:4:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:C:H1'	1:A:177:G:N2	2.30	0.46
1:A:332:G:H2'	1:A:333:A:H8	1.81	0.46
1:A:416:U:O4'	1:A:417:G:N2	2.48	0.46
1:A:698:C:H3'	1:A:699:A:H8	1.81	0.46
20:V:125:ILE:HD13	20:V:137:ILE:HD11	1.98	0.46
20:V:159:GLN:N	20:V:171:ASP:OD1	2.49	0.46
1:A:1002:G:O2'	1:A:1005:A:N6	2.40	0.45
1:A:2778:A:H5''	1:A:2779:A:H2'	1.97	0.45
1:A:2825:C:H5''	1:A:2826:A:N7	2.32	0.45
1:A:567:U:H2'	1:A:568:G:C8	2.51	0.45
1:A:1334:C:H2'	1:A:1335:A:H8	1.80	0.45
1:A:1396:C:H2'	1:A:1397:G:O4'	2.16	0.45
1:A:1445:A:H2'	1:A:1446:C:C6	2.52	0.45
4:E:120:ASP:OD1	4:E:120:ASP:N	2.46	0.45
5:F:88:LEU:HB2	5:F:132:VAL:HB	1.98	0.45
1:A:575:A:N3	1:A:576:G:N2	2.64	0.45
1:A:638:U:H2'	1:A:639:C:H6	1.81	0.45
1:A:744:C:H2'	1:A:745:C:C6	2.52	0.45
1:A:1343:C:HO2'	1:A:1344:C:C5'	2.30	0.45
1:A:2264:G:H2'	1:A:2265:U:O4'	2.17	0.45
1:A:2440:A:C6	1:A:2441:A:H1'	2.51	0.45
1:A:2576:U:H5'	1:A:2595:A:C2	2.52	0.45
1:A:2727:U:H2'	1:A:2728:U:C6	2.52	0.45
21:W:296:TRP:HH2	21:W:306:MET:SD	2.39	0.45
1:A:852:G:H21	1:A:878:G:H1'	1.81	0.45
1:A:1150:C:H3'	1:A:1151:U:H5''	1.97	0.45
1:A:1438:C:HO2'	1:A:1439:U:P	2.39	0.45
1:A:1696:G:C4	1:A:1697:A:C8	3.05	0.45
1:A:1846:G:HO2'	1:A:1847:U:P	2.38	0.45
1:A:688:G:H1'	1:A:691:U:OP1	2.17	0.45
1:A:759:G:C6	1:A:760:G:C6	3.04	0.45
1:A:2127:U:H2'	1:A:2128:U:O4'	2.17	0.45
1:A:2875:A:N7	1:A:2893:A:O2'	2.35	0.45
21:W:158:ALA:O	21:W:161:GLU:HG2	2.16	0.45
1:A:304:G:N7	1:A:411:G:N2	2.65	0.45
1:A:415:C:H5''	1:A:416:U:OP1	2.16	0.45
1:A:767:U:H2'	1:A:768:G:O4'	2.17	0.45
1:A:1216:C:H2'	1:A:1217:U:H5'	1.99	0.45
1:A:1684:U:H2'	1:A:1685:A:H5''	1.98	0.45
1:A:1832:A:H2	1:A:1852:G:H1'	1.82	0.45
1:A:1855:C:OP1	2:C:223:SER:OG	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:131:VAL:HG13	20:V:133:LYS:HG2	1.99	0.45
1:A:280:G:C6	1:A:281:A:C6	3.05	0.45
1:A:332:G:H2'	1:A:333:A:C8	2.51	0.45
1:A:414:C:HO2'	1:A:415:C:P	2.40	0.45
1:A:1550:C:H2'	1:A:1551:C:C6	2.52	0.45
1:A:2059:A:H5'	1:A:2060:A:OP1	2.16	0.45
1:A:2819:A:H4'	1:A:2820:U:H5''	1.99	0.45
5:F:28:LYS:HG2	5:F:29:GLY:H	1.82	0.45
1:A:428:A:H3'	1:A:434:U:O4	2.17	0.45
1:A:675:C:C2	1:A:676:G:C8	3.05	0.45
1:A:1094:A:C8	1:A:1157:A:C6	3.05	0.45
1:A:1345:U:O2'	1:A:1346:A:O5'	2.32	0.45
1:A:1619:A:H2'	1:A:1620:A:C8	2.52	0.45
1:A:1696:G:H5''	9:J:35:THR:OG1	2.17	0.45
1:A:2625:U:O2'	1:A:2626:G:N7	2.50	0.45
1:A:2820:U:H2'	1:A:2821:U:C6	2.51	0.45
20:V:224:ARG:HG3	20:V:225:TYR:H	1.81	0.45
1:A:305:A:N6	1:A:411:G:H21	2.13	0.45
1:A:689:A:H5''	1:A:690:A:OP2	2.17	0.45
1:A:1862:C:N3	1:A:1863:U:O2'	2.43	0.45
1:A:2555:G:H5'	1:A:2556:C:OP2	2.17	0.45
1:A:2655:C:H2'	1:A:2656:G:C8	2.52	0.45
1:A:2694:A:H3'	1:A:2695:C:C6	2.52	0.45
1:A:302:A:OP1	1:A:302:A:H3'	2.17	0.44
1:A:303:G:HO2'	1:A:304:G:P	2.41	0.44
1:A:327:G:H2'	1:A:328:G:C8	2.52	0.44
1:A:679:A:C5	1:A:680:G:H1'	2.52	0.44
1:A:1011:C:H2'	1:A:1012:G:H8	1.82	0.44
1:A:1579:A:H3'	1:A:1580:A:C8	2.52	0.44
1:A:2018:A:H2'	1:A:2019:C:O4'	2.17	0.44
1:A:90:A:H61	1:A:503:C:H41	1.64	0.44
1:A:2010:A:N3	1:A:2010:A:H2'	2.32	0.44
15:P:88:GLY:O	15:P:89:LYS:HD2	2.17	0.44
22:Y:66:PRO:C	22:Y:68:GLY:N	2.70	0.44
1:A:287:G:N1	1:A:289:C:OP1	2.51	0.44
1:A:1244:A:H8	8:I:4:HIS:HB3	1.81	0.44
1:A:1513:U:H3	1:A:1572:G:H1	1.66	0.44
1:A:2442:G:H2'	1:A:2443:G:O4'	2.17	0.44
4:E:103:LYS:HA	4:E:106:ARG:HE	1.83	0.44
5:F:59:GLN:CD	5:F:60:LYS:H	2.20	0.44
1:A:49:A:H2	1:A:119:U:H3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:A:H1'	1:A:2462:A:C5	2.53	0.44
1:A:776:G:O2'	1:A:810:G:H4'	2.17	0.44
1:A:1080:G:C5	1:A:1168:G:C2	3.06	0.44
1:A:1425:C:H2'	1:A:1426:A:C8	2.53	0.44
1:A:2543:U:H2'	1:A:2544:C:C6	2.52	0.44
1:A:2917:G:OP2	1:A:2917:G:N2	2.33	0.44
20:V:230:ILE:O	20:V:230:ILE:HG13	2.16	0.44
20:V:261:GLU:O	20:V:265:ARG:N	2.51	0.44
21:W:322:TYR:HB2	21:W:425:GLY:H	1.82	0.44
21:W:340:MET:O	21:W:344:ILE:HG12	2.17	0.44
2:C:68:LYS:HB3	2:C:70:ASP:OD1	2.17	0.44
3:D:121:GLY:HA2	3:D:161:PRO:HB3	1.98	0.44
1:A:310:C:N3	1:A:406:G:H2'	2.32	0.44
1:A:760:G:H2'	1:A:761:U:C6	2.53	0.44
1:A:2147:U:OP2	1:A:2147:U:H3'	2.18	0.44
1:A:2204:U:H2'	1:A:2205:A:O4'	2.16	0.44
1:A:2439:G:H2'	1:A:2440:A:C8	2.52	0.44
2:C:125:LYS:HE2	2:C:125:LYS:HB3	1.88	0.44
5:F:30:PRO:HD2	5:F:80:VAL:HG12	1.99	0.44
8:I:96:LEU:HB2	8:I:102:ILE:CG2	2.47	0.44
9:J:20:LEU:HB3	9:J:40:LEU:HD11	1.98	0.44
21:W:183:ARG:CZ	21:W:272:ILE:CD1	2.96	0.44
22:Y:194:ASP:O	22:Y:198:LYS:HB2	2.17	0.44
1:A:202:A:H1'	1:A:2462:A:N6	2.32	0.44
1:A:430:C:H42	1:A:437:A:H62	1.65	0.44
1:A:624:C:H2'	1:A:625:C:C6	2.53	0.44
1:A:2254:A:H4'	1:A:2255:C:O5'	2.18	0.44
1:A:2492:C:H2'	1:A:2493:C:C6	2.52	0.44
1:A:2682:U:H3'	1:A:2683:A:C8	2.53	0.44
1:A:2778:A:OP1	5:F:4:VAL:N	2.51	0.44
1:A:2823:C:H3'	1:A:2824:G:C8	2.47	0.44
5:F:139:LYS:HA	5:F:142:VAL:HG12	1.99	0.44
8:I:79:LEU:HB3	8:I:115:GLY:N	2.32	0.44
16:R:10:THR:HG23	16:R:11:THR:H	1.83	0.44
16:R:38:GLU:HG2	16:R:39:ASN:N	2.33	0.44
21:W:380:LEU:HD12	21:W:381:LYS:H	1.82	0.44
1:A:455:G:H2'	1:A:456:A:C8	2.53	0.44
1:A:1220:G:O2'	1:A:1221:A:O5'	2.35	0.44
1:A:2605:G:N3	1:A:2605:G:H2'	2.33	0.44
5:F:45:LYS:HB2	5:F:53:VAL:HA	2.00	0.44
10:K:91:ARG:HG2	10:K:115:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:41:ASN:HB3	20:V:44:ILE:HG22	1.99	0.44
20:V:222:LYS:HB3	20:V:222:LYS:HE3	1.86	0.44
20:V:273:GLY:O	20:V:275:LEU:HD23	2.18	0.44
1:A:1011:C:H2'	1:A:1012:G:C8	2.52	0.43
1:A:1343:C:H41	1:A:1652:C:N4	2.15	0.43
1:A:2786:A:N3	1:A:2786:A:H2'	2.32	0.43
5:F:108:VAL:HA	5:F:153:ARG:CZ	2.47	0.43
22:Y:58:GLN:OE1	22:Y:60:ARG:HB3	2.18	0.43
1:A:78:U:H2'	1:A:79:C:H6	1.83	0.43
1:A:150:A:H61	1:A:179:A:H2	1.65	0.43
1:A:151:U:H2'	1:A:152:C:H6	1.83	0.43
1:A:340:U:H2'	1:A:341:G:O4'	2.18	0.43
1:A:879:G:H2'	1:A:880:C:C6	2.53	0.43
1:A:1460:G:HO2'	1:A:1461:A:H8	1.62	0.43
1:A:1551:C:H2'	1:A:1552:C:O4'	2.18	0.43
1:A:1759:U:H5	1:A:1773:G:C4	2.36	0.43
1:A:2129:G:H2'	1:A:2130:G:H8	1.82	0.43
11:L:61:TRP:CZ2	11:L:94:MET:HB2	2.53	0.43
21:W:297:ASP:OD2	23:W:501:GNP:N2	2.43	0.43
21:W:350:HIS:CE1	21:W:391:LYS:CB	3.02	0.43
1:A:316:G:O2'	1:A:317:G:H5'	2.18	0.43
1:A:331:C:H2'	1:A:332:G:H8	1.82	0.43
1:A:662:U:H2'	1:A:663:G:C8	2.53	0.43
1:A:2122:G:N1	1:A:2254:A:N7	2.66	0.43
1:A:2672:G:H2'	1:A:2673:A:H8	1.83	0.43
1:A:2829:G:H2'	1:A:2830:A:C8	2.54	0.43
14:O:56:ILE:HD13	14:O:77:ARG:HH21	1.83	0.43
1:A:607:G:N2	11:L:37:GLN:OE1	2.39	0.43
1:A:2669:G:OP1	6:G:100:LYS:NZ	2.48	0.43
8:I:83:ASN:HA	8:I:117:LEU:HD13	1.99	0.43
20:V:213:LEU:HB3	20:V:221:LEU:HG	1.99	0.43
21:W:338:THR:C	21:W:341:PRO:HD2	2.39	0.43
1:A:339:A:H2'	1:A:340:U:C6	2.54	0.43
1:A:462:A:C6	1:A:2438:G:N1	2.86	0.43
1:A:1552:C:O2'	1:A:1553:A:H5'	2.18	0.43
1:A:1557:G:C4	1:A:1558:C:C6	3.07	0.43
11:L:97:ASP:C	11:L:97:ASP:OD1	2.57	0.43
20:V:144:ASN:O	20:V:144:ASN:ND2	2.51	0.43
1:A:312:G:H2'	1:A:313:U:O4'	2.18	0.43
5:F:69:THR:OG1	5:F:70:ARG:N	2.52	0.43
5:F:88:LEU:HD23	5:F:88:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:132:ASP:OD2	22:Y:139:ASN:ND2	2.51	0.43
1:A:327:G:N2	1:A:400:U:O2	2.44	0.43
1:A:1572:G:H8	1:A:1572:G:OP2	2.02	0.43
1:A:2206:C:H2'	1:A:2207:C:C6	2.54	0.43
1:A:2465:G:H8	1:A:2465:G:O5'	2.02	0.43
1:A:2560:A:H1'	5:F:158:TYR:CE2	2.54	0.43
5:F:48:ASP:OD1	5:F:49:ASN:N	2.52	0.43
21:W:189:SER:H	23:W:501:GNP:HNB3	1.67	0.43
21:W:414:GLU:OE2	21:W:418:ARG:NH2	2.36	0.43
22:Y:200:LYS:HD2	22:Y:200:LYS:HA	1.71	0.43
1:A:1557:G:C5	1:A:1558:C:C5	3.07	0.43
1:A:2193:C:H3'	1:A:2194:G:C8	2.54	0.43
1:A:2431:U:O2'	1:A:2432:C:H3'	2.19	0.43
1:A:2433:C:O2	1:A:2443:G:N1	2.51	0.43
13:N:21:MET:HE3	13:N:76:VAL:HG23	2.01	0.43
1:A:283:G:C2	1:A:288:C:O2	2.72	0.43
1:A:822:G:OP1	1:A:824:G:O2'	2.37	0.43
1:A:1571:G:C2'	1:A:1572:G:H5'	2.49	0.43
1:A:2103:U:O2'	1:A:2626:G:H1'	2.19	0.43
1:A:2119:A:C6	1:A:2259:G:O6	2.72	0.43
1:A:2432:C:H2'	1:A:2443:G:H1	1.84	0.43
7:H:9:LYS:NZ	7:H:9:LYS:HB2	2.34	0.43
10:K:36:VAL:HA	10:K:40:ARG:O	2.19	0.43
1:A:259:A:H2'	1:A:260:A:C8	2.52	0.43
1:A:294:G:C6	1:A:295:G:N7	2.87	0.43
1:A:1177:G:N2	1:A:1178:U:O4	2.45	0.43
1:A:1734:A:H2'	1:A:1735:A:C8	2.54	0.43
1:A:2428:G:N3	1:A:2428:G:H2'	2.34	0.43
1:A:2670:A:H2'	1:A:2671:G:H8	1.83	0.43
1:A:421:A:H62	1:A:447:G:H21	1.67	0.42
1:A:683:A:C6	1:A:698:C:H1'	2.54	0.42
1:A:1166:G:H2'	1:A:1167:C:C6	2.54	0.42
1:A:1394:G:H2'	1:A:1395:C:C6	2.54	0.42
1:A:2131:U:C2	1:A:2132:A:C8	3.07	0.42
2:C:205:ILE:HG23	2:C:210:ARG:HB3	2.00	0.42
11:L:74:LEU:HD11	11:L:114:LYS:HG3	2.00	0.42
21:W:32:GLU:O	21:W:32:GLU:HG2	2.19	0.42
1:A:194:A:H2'	1:A:195:C:C6	2.54	0.42
1:A:2137:U:H2'	1:A:2138:U:C6	2.54	0.42
1:A:2443:G:H2'	1:A:2444:G:H8	1.83	0.42
21:W:350:HIS:ND1	21:W:391:LYS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:G:C4	1:A:305:A:C8	3.08	0.42
1:A:765:A:H2'	1:A:766:C:O4'	2.19	0.42
1:A:1507:U:H2'	1:A:1508:C:C6	2.54	0.42
1:A:1528:U:H4'	1:A:1529:G:H5'	2.00	0.42
1:A:1557:G:C6	1:A:1558:C:C4	3.07	0.42
1:A:2494:C:O2'	1:A:2495:C:O4'	2.35	0.42
2:C:105:LEU:CD1	2:C:156:ARG:HB2	2.49	0.42
20:V:69:GLN:HE22	20:V:73:GLU:CD	2.23	0.42
21:W:97:THR:CG2	22:Y:52:PRO:HD2	2.48	0.42
22:Y:194:ASP:HA	22:Y:197:LEU:CG	2.48	0.42
1:A:283:G:N1	1:A:288:C:N3	2.49	0.42
1:A:1515:C:H2'	1:A:1516:A:C8	2.54	0.42
1:A:2220:A:H2'	1:A:2221:C:O4'	2.20	0.42
1:A:2448:U:H2'	1:A:2449:C:C6	2.54	0.42
1:A:2716:U:H2'	1:A:2717:G:O4'	2.19	0.42
1:A:2775:U:H3'	1:A:2776:G:H8	1.84	0.42
20:V:200:ILE:HD11	20:V:202:LEU:HD13	2.02	0.42
22:Y:65:LEU:HD22	22:Y:65:LEU:HA	1.85	0.42
1:A:202:A:H5''	1:A:2272:U:H1'	2.00	0.42
1:A:430:C:H42	1:A:437:A:N6	2.18	0.42
1:A:488:U:O2'	4:E:46:GLN:OE1	2.26	0.42
1:A:1075:A:H2'	1:A:1076:G:O4'	2.20	0.42
20:V:23:LEU:O	20:V:122:ARG:NH1	2.44	0.42
1:A:297:G:H2'	1:A:298:U:C5	2.55	0.42
1:A:638:U:H2'	1:A:639:C:C6	2.54	0.42
1:A:873:U:O2	1:A:879:G:N2	2.52	0.42
1:A:1173:A:O2'	1:A:1174:A:OP1	2.31	0.42
1:A:1555:A:O3'	1:A:1556:A:C8	2.73	0.42
1:A:1557:G:O2'	1:A:1558:C:H5'	2.19	0.42
1:A:1808:U:OP2	1:A:1813:A:N6	2.50	0.42
1:A:1819:C:H2'	1:A:1820:A:C8	2.55	0.42
1:A:1846:G:O2'	1:A:1847:U:OP1	2.32	0.42
1:A:2432:C:H1'	1:A:2444:G:N1	2.34	0.42
1:A:2686:A:H2'	1:A:2687:C:O4'	2.19	0.42
20:V:221:LEU:HD23	20:V:221:LEU:HA	1.87	0.42
1:A:254:A:O5'	1:A:254:A:H8	2.03	0.42
1:A:759:G:C2'	1:A:760:G:H5'	2.50	0.42
1:A:1253:A:H2'	1:A:1254:A:H8	1.84	0.42
1:A:1315:G:OP2	1:A:1690:G:O2'	2.26	0.42
1:A:1557:G:H2'	1:A:1558:C:H6	1.85	0.42
1:A:2114:C:H42	1:A:2262:A:N6	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2820:U:H2'	1:A:2821:U:H6	1.84	0.42
5:F:23:ASN:HB2	5:F:38:PHE:H	1.83	0.42
21:W:219:THR:HA	21:W:224:GLU:HA	2.01	0.42
1:A:90:A:N6	1:A:503:C:H41	2.17	0.42
1:A:418:A:H2	1:A:448:A:H5''	1.84	0.42
1:A:688:G:O2'	1:A:692:A:N7	2.50	0.42
1:A:868:A:H5''	1:A:869:U:H6	1.85	0.42
1:A:2439:G:H2'	1:A:2440:A:H8	1.85	0.42
21:W:132:ASP:CG	22:Y:139:ASN:ND2	2.73	0.42
22:Y:194:ASP:OD1	22:Y:197:LEU:HD21	2.20	0.42
1:A:75:G:H22	1:A:110:A:H2	1.67	0.42
1:A:1016:U:H2'	1:A:1017:C:C6	2.55	0.42
1:A:1080:G:H2'	1:A:1081:U:O4'	2.20	0.42
1:A:1303:U:H2'	1:A:1304:G:C8	2.55	0.42
1:A:2785:U:O2'	1:A:2786:A:OP2	2.35	0.42
5:F:55:ARG:HD2	5:F:57:SER:O	2.19	0.42
1:A:677:A:O2'	1:A:678:A:OP1	2.32	0.42
1:A:2559:U:O3'	1:A:2563:C:N4	2.53	0.42
5:F:39:HIS:HD2	5:F:41:ASP:H	1.67	0.42
10:K:7:LEU:HD23	10:K:7:LEU:HA	1.88	0.42
20:V:138:ASN:HD21	20:V:146:ALA:HB3	1.84	0.42
21:W:391:LYS:HB2	21:W:391:LYS:HE3	1.40	0.42
1:A:66:C:C2	1:A:67:A:C8	3.08	0.41
1:A:1495:C:N4	1:A:1508:C:H42	2.17	0.41
1:A:1588:A:H3'	1:A:1589:G:H8	1.84	0.41
1:A:1617:A:H2'	1:A:1618:A:C8	2.55	0.41
1:A:2111:A:H2'	1:A:2112:G:H8	1.84	0.41
1:A:2143:A:O5'	1:A:2143:A:H8	2.03	0.41
1:A:2207:C:OP1	22:Y:211:ASN:CB	2.67	0.41
1:A:2209:U:H2'	1:A:2210:G:H8	1.85	0.41
1:A:525:A:O2'	1:A:526:A:OP1	2.36	0.41
1:A:1210:A:H2'	1:A:1211:C:C6	2.54	0.41
1:A:2130:G:H2'	1:A:2131:U:H6	1.84	0.41
1:A:2153:G:OP1	22:Y:43:GLU:OE1	2.38	0.41
1:A:2626:G:O2'	1:A:2627:A:O4'	2.23	0.41
1:A:2773:G:H2'	1:A:2774:C:C6	2.55	0.41
2:C:105:LEU:HD11	2:C:156:ARG:HB2	2.02	0.41
8:I:89:THR:OG1	8:I:122:THR:O	2.33	0.41
21:W:158:ALA:HA	21:W:161:GLU:OE1	2.20	0.41
1:A:2559:U:H2'	5:F:175:GLY:HA2	2.02	0.41
8:I:93:PRO:O	8:I:97:LEU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:40:LEU:HD22	9:J:117:ILE:HD13	2.00	0.41
1:A:7:G:N2	1:A:2921:U:C2	2.89	0.41
1:A:697:G:N3	1:A:698:C:H5	2.18	0.41
1:A:792:G:O2'	1:A:795:G:O2'	2.23	0.41
1:A:1080:G:H8	1:A:1080:G:O5'	2.04	0.41
1:A:2119:A:H2'	1:A:2120:U:C6	2.56	0.41
1:A:2130:G:O6	1:A:2217:U:O4	2.37	0.41
1:A:2553:G:H22	1:A:2568:C:H5	1.69	0.41
1:A:2584:U:H6	1:A:2586:G:OP2	2.03	0.41
20:V:97:VAL:N	20:V:98:PRO:HD2	2.35	0.41
21:W:41:ARG:HA	21:W:57:ASP:O	2.21	0.41
22:Y:78:PHE:O	22:Y:120:MET:CE	2.68	0.41
1:A:284:C:H1'	1:A:288:C:O2	2.20	0.41
1:A:2216:A:C6	1:A:2217:U:C4	3.08	0.41
1:A:2543:U:H2'	1:A:2544:C:H6	1.85	0.41
3:D:51:LEU:O	3:D:80:VAL:HA	2.20	0.41
20:V:217:TYR:HB3	20:V:220:ARG:HB2	2.02	0.41
21:W:124:THR:HA	21:W:127:ARG:NH1	2.35	0.41
22:Y:121:MET:HG3	22:Y:145:VAL:HG11	2.02	0.41
1:A:194:A:H2'	1:A:195:C:H6	1.83	0.41
1:A:677:A:H61	1:A:2432:C:H4'	1.86	0.41
1:A:1306:G:O2'	1:A:2041:G:O6	2.31	0.41
1:A:1831:A:H2'	1:A:1832:A:C8	2.56	0.41
1:A:2093:C:H2'	1:A:2094:C:H6	1.86	0.41
11:L:61:TRP:CH2	11:L:94:MET:HB2	2.55	0.41
21:W:21:ASN:ND2	21:W:30:ILE:HD11	2.33	0.41
21:W:55:LEU:HD12	21:W:55:LEU:HA	1.84	0.41
21:W:350:HIS:CE1	21:W:391:LYS:HB3	2.56	0.41
1:A:759:G:H2'	1:A:760:G:H5'	2.03	0.41
1:A:1632:G:H2'	1:A:1633:G:H8	1.85	0.41
1:A:1696:G:HO2'	1:A:1697:A:P	2.43	0.41
1:A:1713:A:N3	1:A:1715:C:N4	2.69	0.41
1:A:2076:C:H2'	1:A:2077:G:H8	1.85	0.41
1:A:2644:U:H2'	1:A:2645:C:H6	1.84	0.41
3:D:47:GLU:HB3	3:D:88:MET:HG3	2.02	0.41
21:W:266:ASP:CG	21:W:295:LYS:HE3	2.41	0.41
21:W:306:MET:O	21:W:310:GLU:HB2	2.20	0.41
1:A:305:A:C2'	1:A:306:C:H5'	2.49	0.41
1:A:420:U:O2'	1:A:470:A:N3	2.44	0.41
1:A:769:A:H2'	1:A:770:A:H8	1.86	0.41
1:A:2691:A:O5'	1:A:2691:A:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2785:U:O2'	1:A:2786:A:P	2.78	0.41
20:V:5:TRP:CD1	20:V:7:PRO:HD3	2.55	0.41
21:W:145:SER:O	21:W:149:GLY:N	2.50	0.41
21:W:393:PRO:HB2	21:W:395:PHE:CZ	2.56	0.41
1:A:230:A:H4'	1:A:231:A:O5'	2.20	0.41
1:A:331:C:H2'	1:A:332:G:C8	2.55	0.41
1:A:675:C:H1'	1:A:685:U:N3	2.35	0.41
1:A:871:G:OP2	1:A:871:G:H2'	2.20	0.41
1:A:2095:C:H2'	1:A:2096:G:C8	2.55	0.41
1:A:2138:U:H2'	1:A:2139:G:H8	1.77	0.41
1:A:2140:U:O2'	1:A:2147:U:O2'	2.35	0.41
1:A:2228:A:N6	1:A:2254:A:C8	2.89	0.41
1:A:2569:C:H2'	1:A:2570:A:O4'	2.21	0.41
1:A:2674:G:H4'	1:A:2761:G:O2'	2.20	0.41
3:D:25:VAL:HG11	3:D:187:LEU:HD23	2.03	0.41
7:H:76:TYR:O	10:K:75:ARG:HG3	2.21	0.41
20:V:23:LEU:HD13	21:W:369:MET:HG2	2.03	0.41
21:W:41:ARG:HD3	21:W:75:GLN:O	2.20	0.41
1:A:276:C:O2'	1:A:306:C:O5'	2.37	0.41
1:A:278:A:N6	1:A:294:G:C6	2.88	0.41
1:A:681:C:H3'	1:A:682:G:H8	1.84	0.41
1:A:1075:A:H3'	1:A:1076:G:C8	2.55	0.41
1:A:1279:C:H2'	1:A:1280:G:C8	2.56	0.41
1:A:1349:G:N2	1:A:1352:U:C4	2.89	0.41
1:A:2268:G:OP1	1:A:2268:G:H3'	2.20	0.41
21:W:210:THR:HB	21:W:231:ALA:HA	2.02	0.41
1:A:303:G:H8	1:A:303:G:O5'	2.04	0.40
1:A:418:A:H4'	1:A:419:G:H4'	2.02	0.40
1:A:621:G:O2'	1:A:1294:A:OP1	2.38	0.40
1:A:1094:A:C8	1:A:1157:A:C5	3.09	0.40
1:A:1210:A:H2'	1:A:1211:C:H6	1.86	0.40
5:F:145:ILE:HD13	5:F:145:ILE:HA	1.92	0.40
7:H:93:PRO:HG3	7:H:114:ILE:HG13	2.03	0.40
8:I:93:PRO:HG3	8:I:105:LEU:HD22	2.03	0.40
22:Y:129:ARG:HG2	22:Y:129:ARG:O	2.21	0.40
22:Y:202:ALA:O	22:Y:203:ALA:HB3	2.20	0.40
1:A:268:A:N6	1:A:474:U:O2'	2.54	0.40
1:A:560:A:H2'	1:A:561:A:H8	1.86	0.40
1:A:766:C:H2'	1:A:767:U:H5''	2.03	0.40
1:A:971:A:C6	1:A:972:U:C2	3.09	0.40
1:A:1003:A:N6	1:A:2528:C:OP2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:G:H2'	1:A:1526:G:O4'	2.20	0.40
1:A:1681:U:O2'	1:A:1789:A:N3	2.41	0.40
1:A:2029:G:C2	1:A:2030:A:C8	3.09	0.40
1:A:2111:A:H2'	1:A:2112:G:O4'	2.21	0.40
1:A:2471:C:H2'	1:A:2472:C:C6	2.56	0.40
1:A:2779:A:H1'	1:A:2781:C:H41	1.86	0.40
1:A:2812:A:O2'	1:A:2813:U:OP1	2.36	0.40
2:C:168:GLU:OE1	2:C:171:TYR:HB2	2.21	0.40
5:F:92:GLY:HA3	5:F:95:TYR:CD1	2.57	0.40
15:P:71:LEU:HD23	15:P:71:LEU:HA	1.88	0.40
21:W:283:HIS:ND1	21:W:322:TYR:OH	2.49	0.40
1:A:184:G:H4'	1:A:185:A:O5'	2.21	0.40
1:A:2122:G:O2'	1:A:2123:A:O4'	2.38	0.40
1:A:2473:G:H2'	1:A:2474:G:C8	2.55	0.40
4:E:38:LEU:HD12	4:E:38:LEU:HA	1.91	0.40
8:I:10:GLU:HA	8:I:10:GLU:OE2	2.22	0.40
11:L:90:VAL:HG12	12:M:11:GLN:HE22	1.84	0.40
12:M:50:ASN:HB2	12:M:51:PRO:CD	2.48	0.40
1:A:93:C:H2'	1:A:94:A:C8	2.55	0.40
1:A:1070:G:C5'	1:A:1071:G:H5''	2.51	0.40
1:A:1078:A:H2	1:A:1168:G:H22	1.69	0.40
1:A:1098:C:N3	1:A:1099:C:C4	2.90	0.40
1:A:1824:C:H2'	1:A:1825:U:C6	2.57	0.40
1:A:2054:C:H2'	1:A:2055:U:C6	2.57	0.40
13:N:14:PRO:O	13:N:15:ARG:HB3	2.22	0.40
21:W:15:GLY:HA2	23:W:502:GNP:PA	2.60	0.40
1:A:303:G:H2'	1:A:304:G:O4'	2.21	0.40
1:A:462:A:HO2'	1:A:463:U:P	2.43	0.40
1:A:1244:A:C4	1:A:1245:G:N2	2.90	0.40
1:A:1467:G:O2'	1:A:1540:A:N6	2.54	0.40
1:A:1576:G:C2	1:A:1577:C:C2	3.09	0.40
3:D:80:VAL:O	3:D:81:LYS:HD2	2.21	0.40
14:O:91:GLU:O	14:O:91:GLU:CD	2.59	0.40
21:W:132:ASP:OD1	22:Y:137:MET:CE	2.70	0.40
21:W:325:ILE:HG22	21:W:327:PHE:CE1	2.57	0.40
22:Y:123:GLU:O	22:Y:127:ILE:HG22	2.21	0.40
22:Y:201:PRO:CG	22:Y:208:TYR:HE1	2.32	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	
2	C	242/277 (87%)	234 (97%)	8 (3%)	0	100	100
3	D	205/209 (98%)	198 (97%)	7 (3%)	0	100	100
4	E	196/207 (95%)	188 (96%)	8 (4%)	0	100	100
5	F	173/179 (97%)	159 (92%)	14 (8%)	0	100	100
6	G	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
7	H	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
8	I	100/146 (68%)	94 (94%)	6 (6%)	0	100	100
9	J	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
10	K	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
11	L	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
12	M	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
13	N	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
14	O	90/95 (95%)	87 (97%)	3 (3%)	0	100	100
15	P	94/103 (91%)	89 (95%)	5 (5%)	0	100	100
16	R	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
17	S	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
18	T	52/59 (88%)	49 (94%)	3 (6%)	0	100	100
19	U	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
20	V	263/282 (93%)	253 (96%)	10 (4%)	0	100	100
21	W	409/436 (94%)	392 (96%)	17 (4%)	0	100	100
22	Y	168/232 (72%)	148 (88%)	17 (10%)	3 (2%)	7	29
All	All	2962/3229 (92%)	2819 (95%)	140 (5%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	Y	66	PRO
22	Y	67	ASN
22	Y	130	VAL

5.3.2 Protein sidechains [i](#)

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	
2	C	200/225 (89%)	197 (98%)	3 (2%)	60	80
3	D	168/170 (99%)	168 (100%)	0	100	100
4	E	162/170 (95%)	162 (100%)	0	100	100
5	F	131/151 (87%)	131 (100%)	0	100	100
6	G	120/123 (98%)	119 (99%)	1 (1%)	79	89
7	H	101/101 (100%)	96 (95%)	5 (5%)	20	50
8	I	71/110 (64%)	70 (99%)	1 (1%)	62	81
9	J	99/100 (99%)	99 (100%)	0	100	100
10	K	98/100 (98%)	98 (100%)	0	100	100
11	L	95/97 (98%)	93 (98%)	2 (2%)	48	72
12	M	83/84 (99%)	82 (99%)	1 (1%)	67	83
13	N	90/93 (97%)	89 (99%)	1 (1%)	70	84
14	O	82/85 (96%)	82 (100%)	0	100	100
15	P	82/87 (94%)	82 (100%)	0	100	100
16	R	56/57 (98%)	55 (98%)	1 (2%)	54	76
17	S	52/53 (98%)	52 (100%)	0	100	100
18	T	38/53 (72%)	37 (97%)	1 (3%)	41	68
19	U	39/39 (100%)	39 (100%)	0	100	100
20	V	227/244 (93%)	223 (98%)	4 (2%)	54	76
21	W	343/371 (92%)	338 (98%)	5 (2%)	60	80
22	Y	138/185 (75%)	125 (91%)	13 (9%)	7	27
All	All	2475/2698 (92%)	2437 (98%)	38 (2%)	60	80

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	87	ARG
2	C	103	TYR
2	C	273	ARG
6	G	97	TYR
7	H	8	LEU
7	H	20	LEU
7	H	73	ASP
7	H	90	ASP
7	H	110	ASN
8	I	126	ASN
11	L	97	ASP
11	L	102	ASP
12	M	50	ASN
13	N	65	ASP
16	R	30	PHE
18	T	27	MET
20	V	82	SER
20	V	133	LYS
20	V	214	GLU
20	V	275	LEU
21	W	45	SER
21	W	68	PHE
21	W	296	TRP
21	W	391	LYS
21	W	421	PHE
22	Y	56	ASP
22	Y	57	GLN
22	Y	59	ILE
22	Y	60	ARG
22	Y	65	LEU
22	Y	67	ASN
22	Y	121	MET
22	Y	123	GLU
22	Y	127	ILE
22	Y	130	VAL
22	Y	200	LYS
22	Y	205	LYS
22	Y	207	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	191	ASN
11	L	101	ASN
16	R	4	ASN
21	W	312	ASN
21	W	349	ASN
21	W	357	ASN
22	Y	55	ASN
22	Y	57	GLN
22	Y	67	ASN
22	Y	106	GLN
22	Y	188	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2396/2927 (81%)	711 (29%)	53 (2%)

All (711) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	28	A
1	A	34	U
1	A	36	G
1	A	39	C
1	A	43	G
1	A	51	G
1	A	55	G
1	A	59	G
1	A	60	G
1	A	63	G
1	A	67	A
1	A	71	A
1	A	75	G
1	A	87	U
1	A	90	A
1	A	91	A
1	A	92	G
1	A	94	A
1	A	98	U
1	A	99	U
1	A	100	U

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Mol	Chain	Res	Type
1	A	101	G
1	A	117	A
1	A	119	U
1	A	133	A
1	A	157	U
1	A	158	C
1	A	159	U
1	A	161	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	166	A
1	A	176	A
1	A	177	G
1	A	184	G
1	A	185	A
1	A	203	U
1	A	204	C
1	A	206	A
1	A	207	A
1	A	216	A
1	A	219	A
1	A	225	A
1	A	226	A
1	A	228	C
1	A	229	A
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	262	G
1	A	266	U
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	273	A
1	A	274	A

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Mol	Chain	Res	Type
1	A	275	A
1	A	276	C
1	A	277	C
1	A	278	A
1	A	280	G
1	A	281	A
1	A	282	G
1	A	287	G
1	A	288	C
1	A	289	C
1	A	290	U
1	A	291	C
1	A	293	U
1	A	294	G
1	A	297	G
1	A	298	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	303	G
1	A	304	G
1	A	306	C
1	A	307	A
1	A	309	U
1	A	314	A
1	A	315	C
1	A	316	G
1	A	317	G
1	A	318	A
1	A	321	U
1	A	322	A
1	A	324	A
1	A	327	G
1	A	328	G
1	A	329	A
1	A	330	A
1	A	337	A
1	A	338	G
1	A	344	G
1	A	345	A
1	A	346	G

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Mol	Chain	Res	Type
1	A	348	U
1	A	355	A
1	A	360	C
1	A	361	G
1	A	368	G
1	A	374	A
1	A	378	C
1	A	382	G
1	A	386	U
1	A	388	A
1	A	392	C
1	A	393	U
1	A	396	G
1	A	399	C
1	A	402	U
1	A	405	U
1	A	408	G
1	A	410	G
1	A	412	A
1	A	413	U
1	A	414	C
1	A	415	C
1	A	416	U
1	A	418	A
1	A	419	G
1	A	420	U
1	A	424	G
1	A	426	G
1	A	431	A
1	A	433	G
1	A	434	U
1	A	435	G
1	A	437	A
1	A	438	A
1	A	439	U
1	A	440	U
1	A	445	C
1	A	446	G
1	A	449	A
1	A	450	U
1	A	453	G
1	A	459	A

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Mol	Chain	Res	Type
1	A	462	A
1	A	463	U
1	A	464	C
1	A	474	U
1	A	482	C
1	A	487	G
1	A	502	C
1	A	503	C
1	A	504	A
1	A	526	A
1	A	528	G
1	A	538	A
1	A	550	G
1	A	551	A
1	A	554	U
1	A	555	C
1	A	556	C
1	A	568	G
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	584	A
1	A	588	C
1	A	592	A
1	A	595	G
1	A	607	G
1	A	619	A
1	A	632	U
1	A	647	A
1	A	651	U
1	A	658	A
1	A	673	A
1	A	678	A
1	A	680	G
1	A	681	C
1	A	683	A
1	A	684	G
1	A	685	U
1	A	686	C
1	A	688	G
1	A	690	A

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Mol	Chain	Res	Type
1	A	691	U
1	A	692	A
1	A	694	G
1	A	696	C
1	A	697	G
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	715	A
1	A	722	A
1	A	732	A
1	A	733	U
1	A	734	C
1	A	735	U
1	A	760	G
1	A	761	U
1	A	762	A
1	A	765	A
1	A	766	C
1	A	767	U
1	A	768	G
1	A	777	C
1	A	793	U
1	A	794	U
1	A	795	G
1	A	799	A
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	837	U
1	A	838	C
1	A	839	G
1	A	841	A
1	A	848	G
1	A	852	G
1	A	858	U

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Mol	Chain	Res	Type
1	A	859	C
1	A	866	A
1	A	870	A
1	A	871	G
1	A	873	U
1	A	874	U
1	A	875	U
1	A	876	A
1	A	881	U
1	A	882	A
1	A	892	U
1	A	972	U
1	A	973	G
1	A	975	C
1	A	976	U
1	A	978	A
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1000	G
1	A	1002	G
1	A	1003	A
1	A	1004	U
1	A	1005	A
1	A	1010	C
1	A	1019	A
1	A	1020	A
1	A	1027	A
1	A	1029	A
1	A	1041	C
1	A	1042	A
1	A	1049	G
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1057	G
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1068	G
1	A	1069	U
1	A	1071	G

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Mol	Chain	Res	Type
1	A	1072	A
1	A	1073	A
1	A	1077	G
1	A	1078	A
1	A	1079	U
1	A	1081	U
1	A	1082	G
1	A	1084	A
1	A	1085	G
1	A	1086	U
1	A	1089	C
1	A	1090	U
1	A	1091	U
1	A	1093	G
1	A	1094	A
1	A	1095	C
1	A	1096	A
1	A	1097	A
1	A	1098	C
1	A	1099	C
1	A	1100	A
1	A	1101	G
1	A	1151	U
1	A	1152	G
1	A	1153	G
1	A	1156	G
1	A	1157	A
1	A	1158	G
1	A	1161	A
1	A	1165	U
1	A	1167	C
1	A	1172	A
1	A	1173	A
1	A	1174	A
1	A	1175	A
1	A	1176	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1185	G
1	A	1187	U
1	A	1188	A

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Mol	Chain	Res	Type
1	A	1192	G
1	A	1209	G
1	A	1215	U
1	A	1216	C
1	A	1217	U
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1245	G
1	A	1246	G
1	A	1247	G
1	A	1248	C
1	A	1251	U
1	A	1252	G
1	A	1260	A
1	A	1276	G
1	A	1278	G
1	A	1287	A
1	A	1289	U
1	A	1293	A
1	A	1294	A
1	A	1296	G
1	A	1312	A
1	A	1314	A
1	A	1315	G
1	A	1328	C
1	A	1339	A
1	A	1340	A
1	A	1344	C
1	A	1345	U
1	A	1346	A
1	A	1352	U
1	A	1360	A
1	A	1363	G
1	A	1364	C
1	A	1376	G
1	A	1380	U
1	A	1388	A
1	A	1391	U
1	A	1404	A
1	A	1405	A
1	A	1407	G

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Mol	Chain	Res	Type
1	A	1414	G
1	A	1418	U
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1428	G
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1439	U
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1452	C
1	A	1455	C
1	A	1456	A
1	A	1458	U
1	A	1459	U
1	A	1460	G
1	A	1462	G
1	A	1465	A
1	A	1467	G
1	A	1473	A
1	A	1474	C
1	A	1479	G
1	A	1480	A
1	A	1481	G
1	A	1483	A
1	A	1484	U
1	A	1491	A
1	A	1495	C
1	A	1496	G
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1501	U
1	A	1503	G
1	A	1504	A
1	A	1505	U
1	A	1506	A
1	A	1507	U
1	A	1513	U

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Mol	Chain	Res	Type
1	A	1516	A
1	A	1520	A
1	A	1521	G
1	A	1524	A
1	A	1526	G
1	A	1528	U
1	A	1529	G
1	A	1533	A
1	A	1534	A
1	A	1539	C
1	A	1540	A
1	A	1543	U
1	A	1547	U
1	A	1553	A
1	A	1554	U
1	A	1555	A
1	A	1556	A
1	A	1559	C
1	A	1561	G
1	A	1567	U
1	A	1571	G
1	A	1572	G
1	A	1573	C
1	A	1576	G
1	A	1577	C
1	A	1578	G
1	A	1580	A
1	A	1589	G
1	A	1596	U
1	A	1598	C
1	A	1600	G
1	A	1607	C
1	A	1614	A
1	A	1617	A
1	A	1626	U
1	A	1630	G
1	A	1631	A
1	A	1632	G
1	A	1634	U
1	A	1638	A
1	A	1652	C
1	A	1653	A

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Mol	Chain	Res	Type
1	A	1655	A
1	A	1657	C
1	A	1667	A
1	A	1677	A
1	A	1678	G
1	A	1679	A
1	A	1685	A
1	A	1692	U
1	A	1693	C
1	A	1697	A
1	A	1719	G
1	A	1728	C
1	A	1729	C
1	A	1733	U
1	A	1745	A
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1761	G
1	A	1774	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1787	G
1	A	1791	A
1	A	1792	G
1	A	1793	G
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1813	A
1	A	1829	C
1	A	1831	A
1	A	1834	C
1	A	1838	A
1	A	1847	U
1	A	1850	A
1	A	1858	A
1	A	1860	G
1	A	1861	C
1	A	1862	C
1	A	1863	U

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Mol	Chain	Res	Type
1	A	2005	C
1	A	2014	G
1	A	2020	U
1	A	2021	G
1	A	2022	U
1	A	2023	C
1	A	2024	U
1	A	2026	A
1	A	2050	G
1	A	2052	A
1	A	2055	U
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	U
1	A	2072	C
1	A	2085	G
1	A	2091	A
1	A	2092	C
1	A	2093	C
1	A	2096	G
1	A	2097	U
1	A	2098	G
1	A	2104	U
1	A	2105	U
1	A	2106	A
1	A	2108	U
1	A	2109	G
1	A	2110	C
1	A	2111	A
1	A	2114	C
1	A	2115	U
1	A	2117	A
1	A	2129	G
1	A	2134	A
1	A	2138	U
1	A	2140	U
1	A	2142	C
1	A	2144	G
1	A	2146	A
1	A	2147	U

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Mol	Chain	Res	Type
1	A	2149	G
1	A	2150	G
1	A	2151	U
1	A	2152	A
1	A	2153	G
1	A	2155	A
1	A	2156	G
1	A	2157	C
1	A	2189	G
1	A	2190	C
1	A	2193	C
1	A	2195	G
1	A	2196	U
1	A	2197	G
1	A	2198	G
1	A	2199	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2209	U
1	A	2211	G
1	A	2214	G
1	A	2216	A
1	A	2218	U
1	A	2222	C
1	A	2224	U
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2239	U
1	A	2240	U
1	A	2241	A
1	A	2243	C
1	A	2252	A
1	A	2253	G
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2262	A

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Mol	Chain	Res	Type
1	A	2263	G
1	A	2264	G
1	A	2266	G
1	A	2267	G
1	A	2268	G
1	A	2272	U
1	A	2428	G
1	A	2431	U
1	A	2432	C
1	A	2433	C
1	A	2434	G
1	A	2435	C
1	A	2437	U
1	A	2441	A
1	A	2442	G
1	A	2443	G
1	A	2449	C
1	A	2450	G
1	A	2462	A
1	A	2463	A
1	A	2464	A
1	A	2466	C
1	A	2474	G
1	A	2475	G
1	A	2489	U
1	A	2490	C
1	A	2492	C
1	A	2493	C
1	A	2494	C
1	A	2495	C
1	A	2516	G
1	A	2517	A
1	A	2518	G
1	A	2519	G
1	A	2522	U
1	A	2523	G
1	A	2525	C
1	A	2526	A
1	A	2527	C
1	A	2541	C
1	A	2542	A
1	A	2547	A

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Mol	Chain	Res	Type
1	A	2548	U
1	A	2549	C
1	A	2555	G
1	A	2556	C
1	A	2557	U
1	A	2560	A
1	A	2563	C
1	A	2577	G
1	A	2581	U
1	A	2582	G
1	A	2583	U
1	A	2584	U
1	A	2585	C
1	A	2586	G
1	A	2588	C
1	A	2595	A
1	A	2596	G
1	A	2601	A
1	A	2602	C
1	A	2611	G
1	A	2612	G
1	A	2613	U
1	A	2615	C
1	A	2616	A
1	A	2619	A
1	A	2620	C
1	A	2621	G
1	A	2625	U
1	A	2628	G
1	A	2629	A
1	A	2631	A
1	A	2632	G
1	A	2634	U
1	A	2639	C
1	A	2642	U
1	A	2648	U
1	A	2658	A
1	A	2660	G
1	A	2661	A
1	A	2668	A
1	A	2675	C
1	A	2681	U

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Mol	Chain	Res	Type
1	A	2684	G
1	A	2686	A
1	A	2689	A
1	A	2690	G
1	A	2693	G
1	A	2694	A
1	A	2696	C
1	A	2697	G
1	A	2698	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2731	G
1	A	2734	A
1	A	2736	G
1	A	2743	G
1	A	2755	U
1	A	2762	A
1	A	2766	G
1	A	2767	A
1	A	2773	G
1	A	2775	U
1	A	2776	G
1	A	2777	A
1	A	2780	G
1	A	2781	C
1	A	2782	A
1	A	2783	U
1	A	2784	C
1	A	2786	A
1	A	2787	A
1	A	2788	G
1	A	2794	A
1	A	2795	G
1	A	2796	C
1	A	2797	C
1	A	2807	A
1	A	2811	G
1	A	2813	U
1	A	2818	C
1	A	2819	A
1	A	2820	U

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Mol	Chain	Res	Type
1	A	2823	C
1	A	2825	C
1	A	2826	A
1	A	2837	A
1	A	2845	A
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2868	G
1	A	2874	G
1	A	2892	G
1	A	2897	G
1	A	2908	A
1	A	2910	C
1	A	2916	A
1	A	2924	A
1	A	2925	C

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	58	G
1	A	90	A
1	A	97	C
1	A	160	G
1	A	184	G
1	A	230	A
1	A	267	C
1	A	268	A
1	A	271	C
1	A	288	C
1	A	296	G
1	A	303	G
1	A	317	G
1	A	377	G
1	A	414	C
1	A	433	G
1	A	439	U
1	A	462	A
1	A	503	C
1	A	525	A
1	A	549	A

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Mol	Chain	Res	Type
1	A	578	A
1	A	677	A
1	A	682	G
1	A	837	U
1	A	1155	C
1	A	1173	A
1	A	1245	G
1	A	1250	G
1	A	1339	A
1	A	1351	U
1	A	1362	G
1	A	1434	A
1	A	1438	C
1	A	1455	C
1	A	1478	G
1	A	1526	G
1	A	1595	U
1	A	1652	C
1	A	1837	U
1	A	1846	G
1	A	2090	G
1	A	2091	A
1	A	2109	G
1	A	2150	G
1	A	2254	A
1	A	2583	U
1	A	2585	C
1	A	2683	A
1	A	2779	A
1	A	2785	U
1	A	2812	A
1	A	2858	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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GNP	W	502	-	29,34,34	1.65	7 (24%)	33,54,54	2.22	6 (18%)
23	GNP	W	501	-	29,34,34	1.62	7 (24%)	33,54,54	2.20	5 (15%)
23	GNP	V	301	-	29,34,34	1.56	7 (24%)	33,54,54	2.20	5 (15%)

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
23	GNP	W	502	-	-	5/14/38/38	0/3/3/3
23	GNP	W	501	-	-	6/14/38/38	0/3/3/3
23	GNP	V	301	-	-	6/14/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	502	GNP	PB-O3A	4.72	1.64	1.59
23	W	501	GNP	PB-O3A	4.49	1.64	1.59
23	V	301	GNP	PB-O3A	4.05	1.64	1.59
23	W	502	GNP	PB-O1B	3.22	1.51	1.46
23	W	501	GNP	PB-O1B	3.11	1.50	1.46
23	W	502	GNP	C6-N1	3.09	1.38	1.33
23	W	501	GNP	C6-N1	3.07	1.38	1.33
23	V	301	GNP	C6-N1	3.06	1.38	1.33
23	V	301	GNP	PB-O1B	2.97	1.50	1.46
23	W	502	GNP	PG-N3B	2.94	1.71	1.63
23	W	501	GNP	PG-N3B	2.87	1.70	1.63
23	W	501	GNP	PG-O1G	2.79	1.50	1.46
23	V	301	GNP	PG-N3B	2.73	1.70	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	V	301	GNP	PG-O1G	2.71	1.50	1.46
23	W	502	GNP	PG-O1G	2.67	1.50	1.46
23	V	301	GNP	PB-O2B	-2.27	1.50	1.56
23	W	502	GNP	PB-O2B	-2.27	1.50	1.56
23	W	501	GNP	PB-O2B	-2.23	1.50	1.56
23	W	502	GNP	C5-C6	2.11	1.45	1.41
23	W	501	GNP	C5-C6	2.01	1.44	1.41
23	V	301	GNP	C5-C6	2.00	1.44	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	501	GNP	C5-C6-N1	-8.60	111.92	123.42
23	W	502	GNP	C5-C6-N1	-8.60	111.93	123.42
23	V	301	GNP	C5-C6-N1	-8.55	111.98	123.42
23	W	501	GNP	C2-N1-C6	6.64	125.20	115.96
23	W	502	GNP	C2-N1-C6	6.64	125.19	115.96
23	V	301	GNP	C2-N1-C6	6.59	125.12	115.96
23	V	301	GNP	N3-C2-N1	-2.91	123.51	127.21
23	W	501	GNP	N3-C2-N1	-2.89	123.53	127.21
23	W	502	GNP	N3-C2-N1	-2.88	123.54	127.21
23	W	501	GNP	C2-N3-C4	-2.44	112.86	115.48
23	W	502	GNP	C2-N3-C4	-2.43	112.87	115.48
23	V	301	GNP	C2-N3-C4	-2.41	112.88	115.48
23	V	301	GNP	O1G-PG-N3B	-2.37	108.27	111.77
23	W	501	GNP	O1B-PB-N3B	-2.14	108.62	111.77
23	W	502	GNP	O1B-PB-N3B	-2.12	108.65	111.77
23	W	502	GNP	O2A-PA-O3A	2.04	112.78	107.27

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	V	301	GNP	PB-N3B-PG-O1G
23	V	301	GNP	PG-N3B-PB-O1B
23	V	301	GNP	PA-O3A-PB-O2B
23	V	301	GNP	C5'-O5'-PA-O3A
23	W	501	GNP	PG-N3B-PB-O1B
23	W	502	GNP	PB-N3B-PG-O1G
23	W	502	GNP	PG-N3B-PB-O1B
23	W	502	GNP	PG-N3B-PB-O3A
23	W	502	GNP	PA-O3A-PB-O2B

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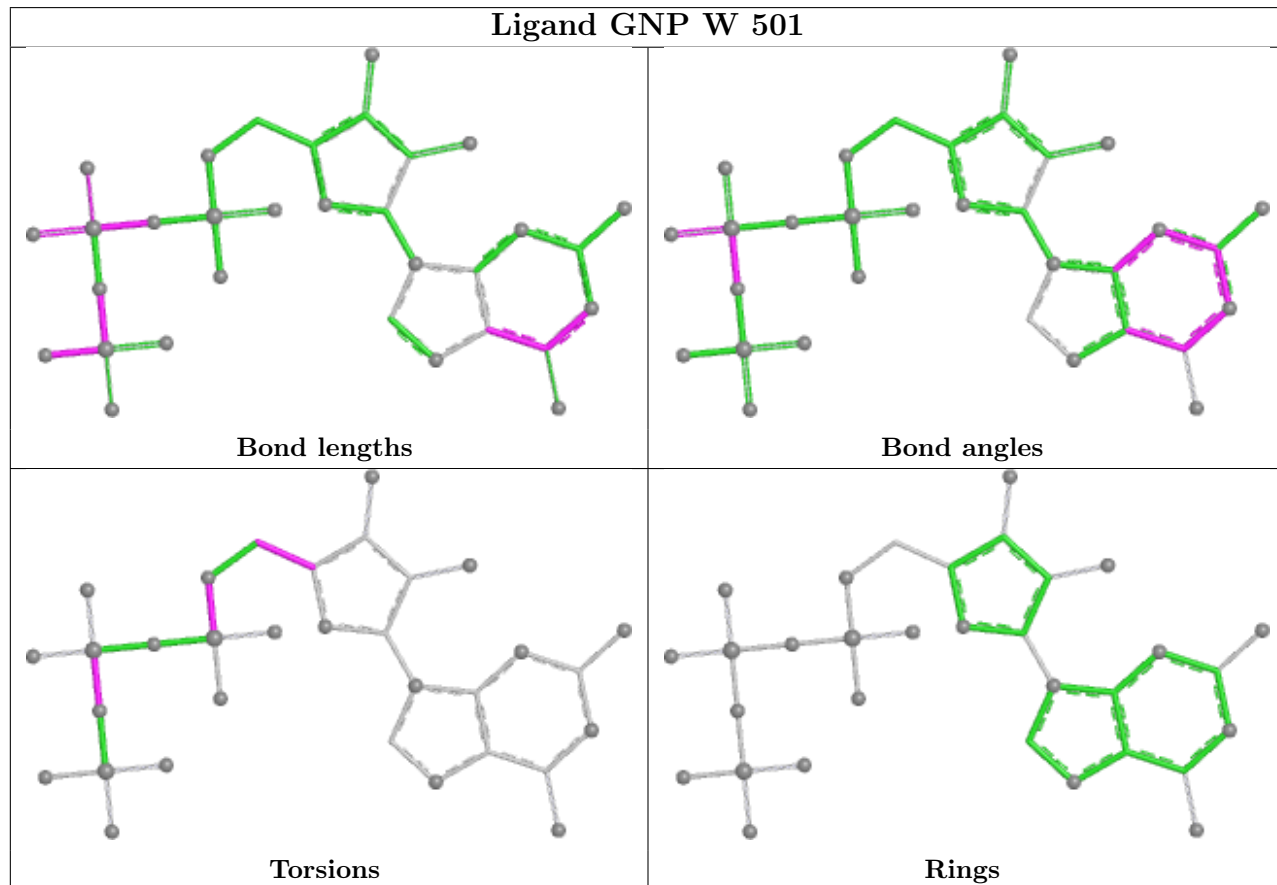
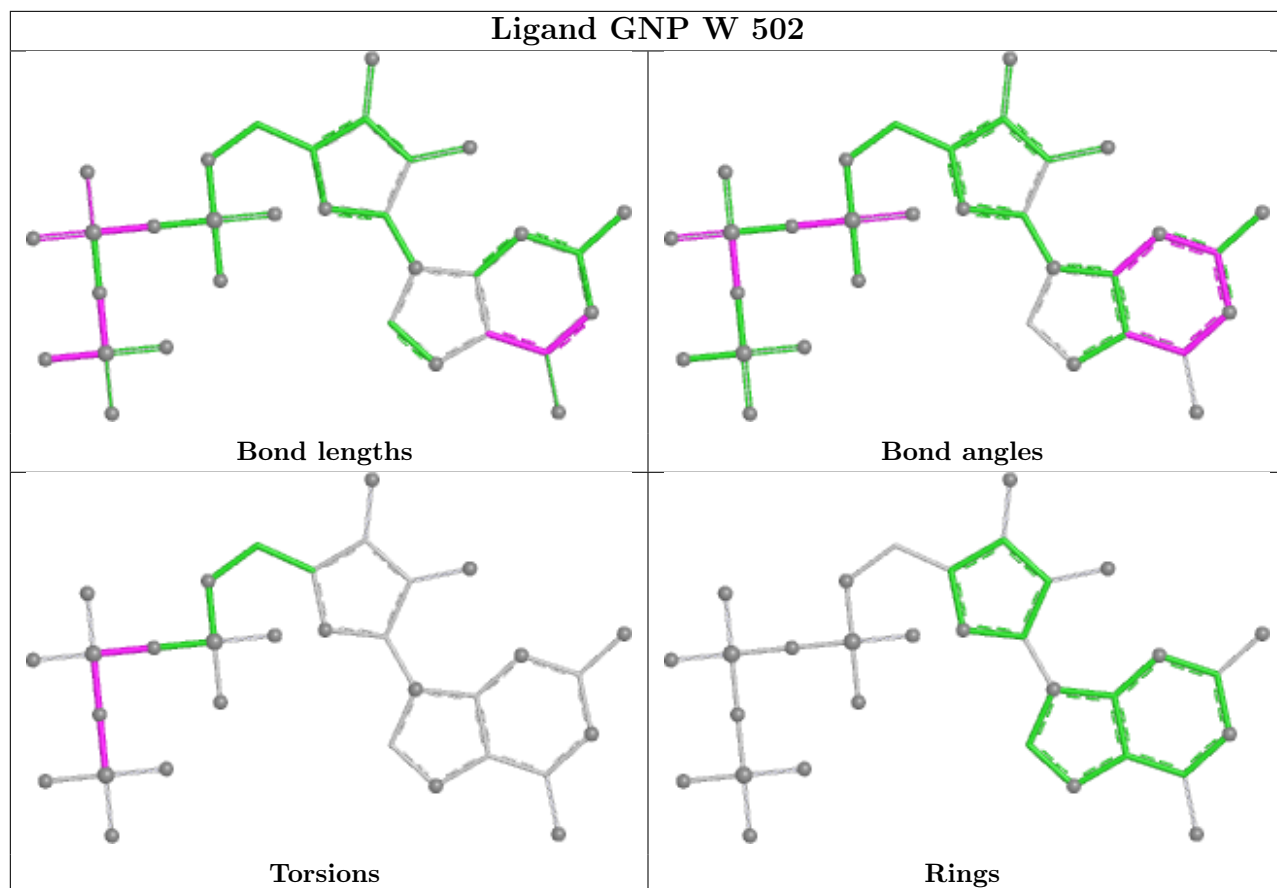
Mol	Chain	Res	Type	Atoms
23	W	501	GNP	O4'-C4'-C5'-O5'
23	W	501	GNP	C3'-C4'-C5'-O5'
23	V	301	GNP	C5'-O5'-PA-O1A
23	W	501	GNP	C5'-O5'-PA-O3A
23	W	501	GNP	C5'-O5'-PA-O1A
23	W	501	GNP	C5'-O5'-PA-O2A
23	V	301	GNP	PA-O3A-PB-O1B
23	W	502	GNP	PA-O3A-PB-O1B

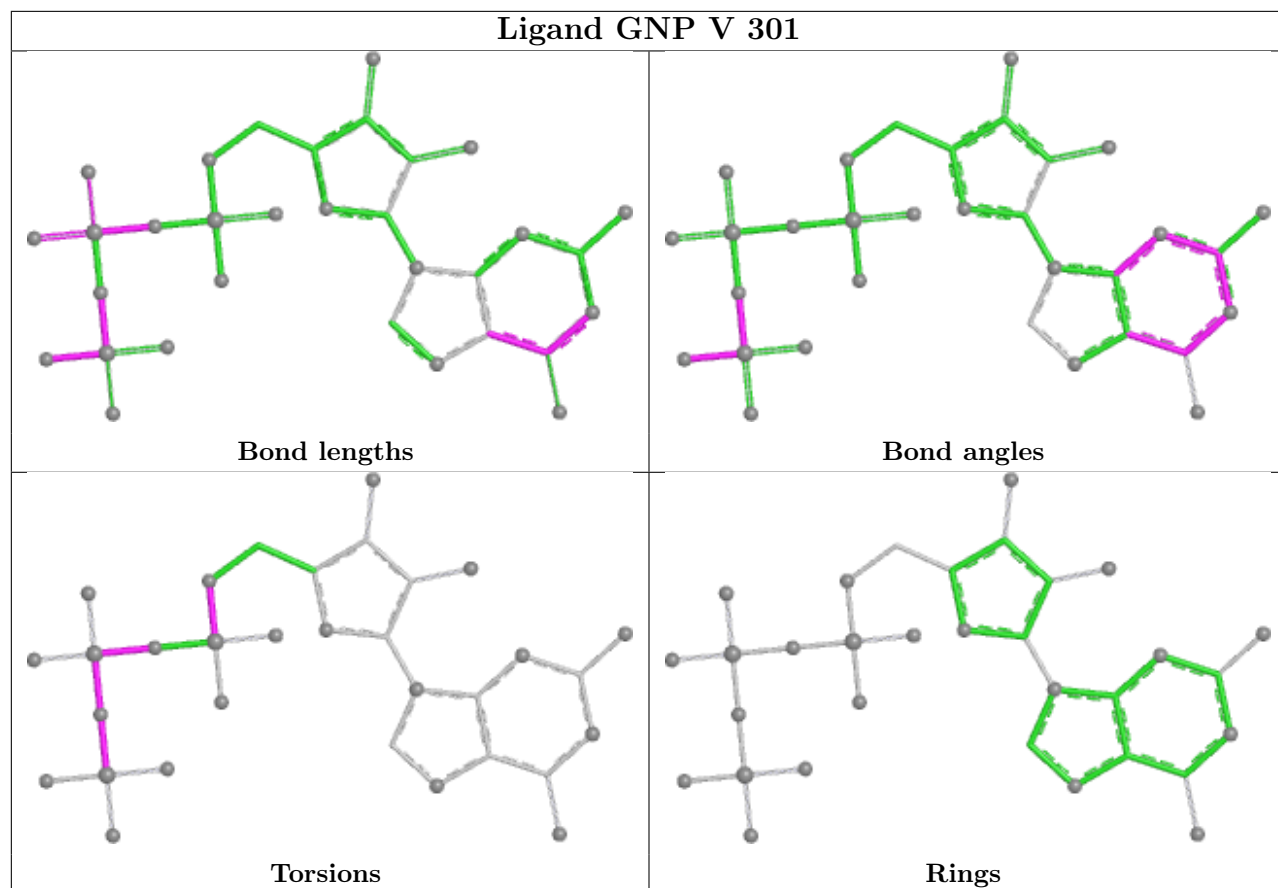
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	W	502	GNP	1	0
23	W	501	GNP	3	0
23	V	301	GNP	1	0

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.

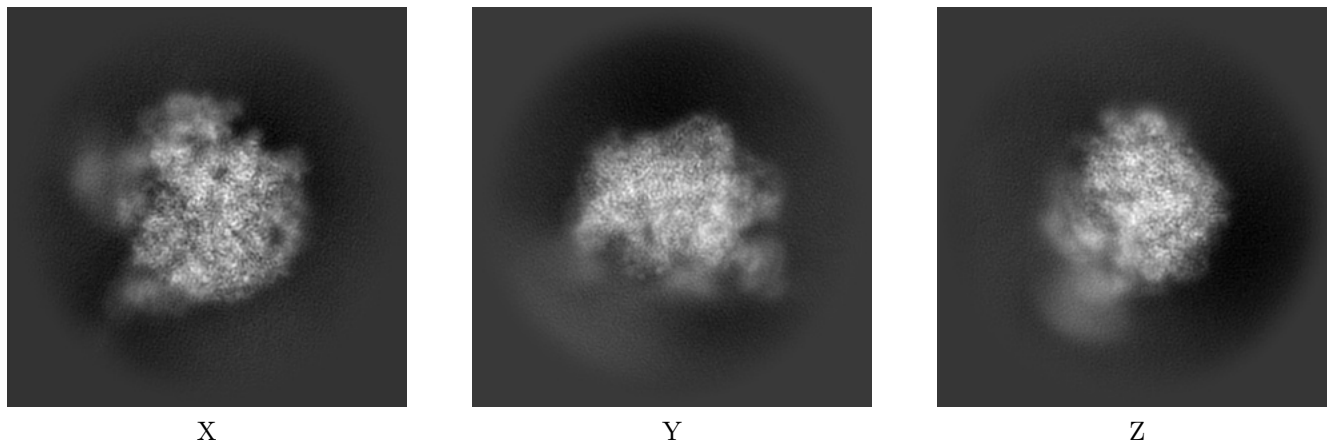
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44869. These allow visual inspection of the internal detail of the map and identification of artifacts.

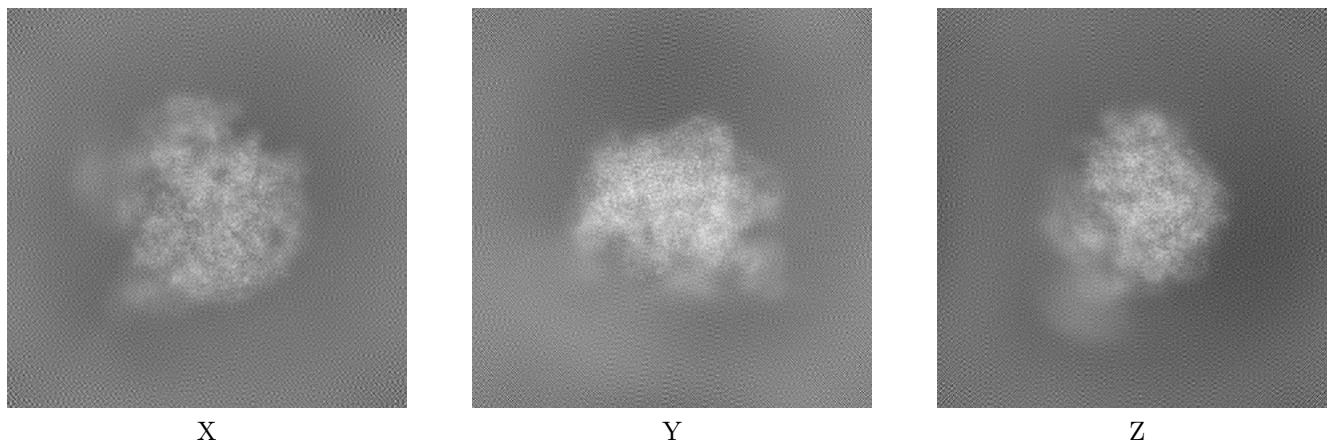
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



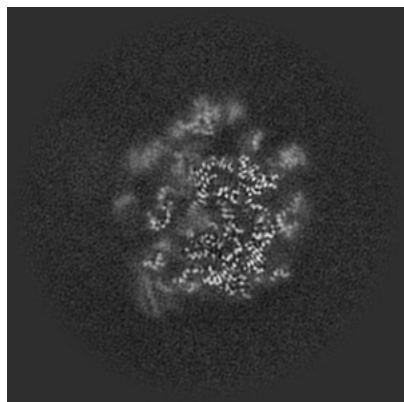
6.1.2 Raw map



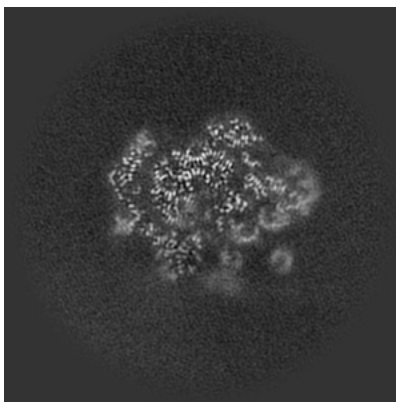
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

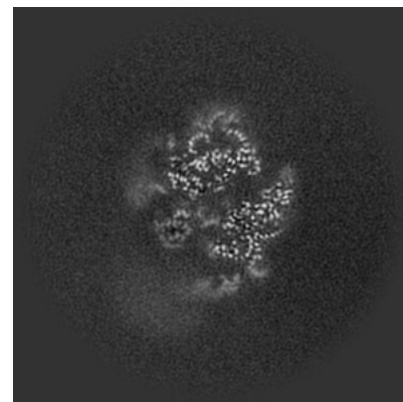
6.2.1 Primary map



X Index: 224

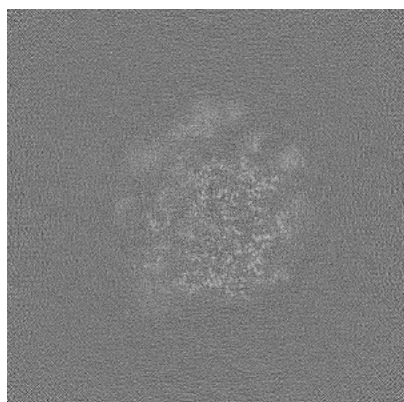


Y Index: 224

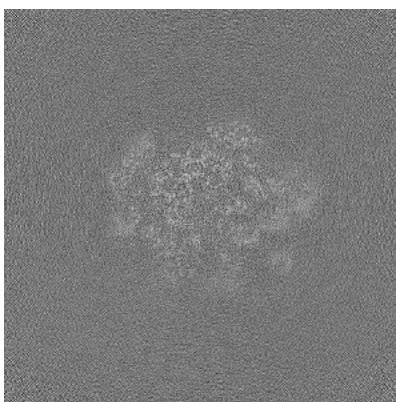


Z Index: 224

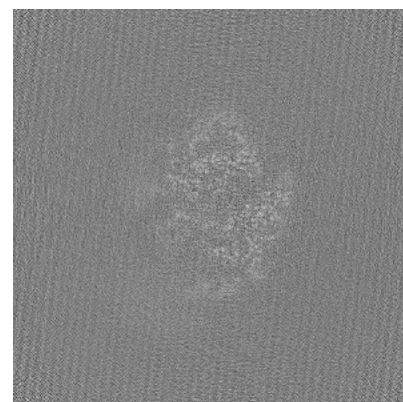
6.2.2 Raw map



X Index: 224



Y Index: 224

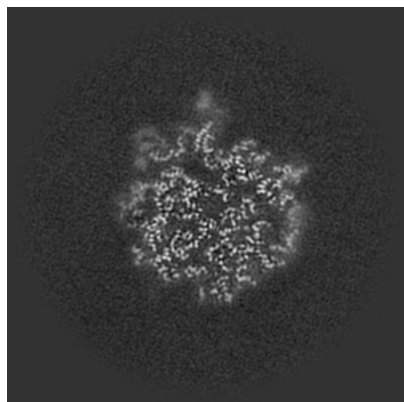


Z Index: 224

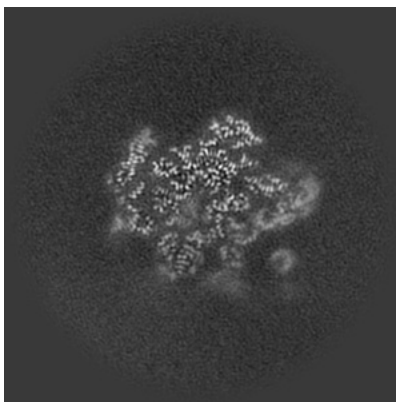
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

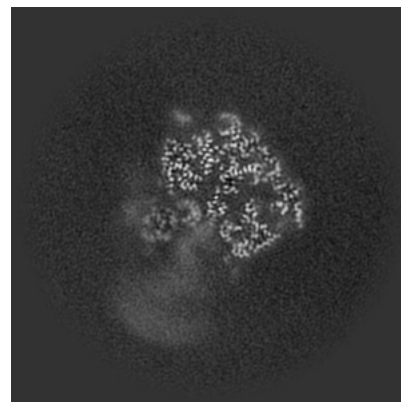
6.3.1 Primary map



X Index: 246

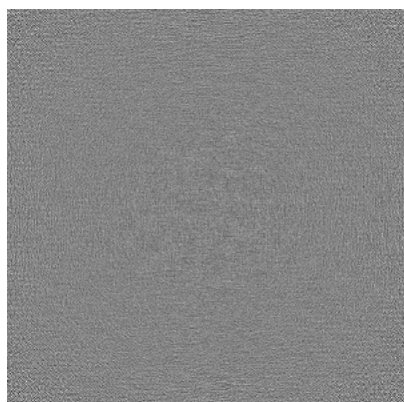


Y Index: 221

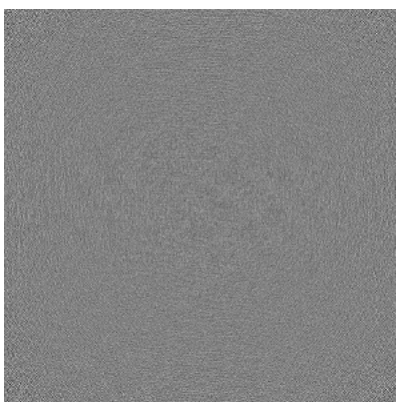


Z Index: 255

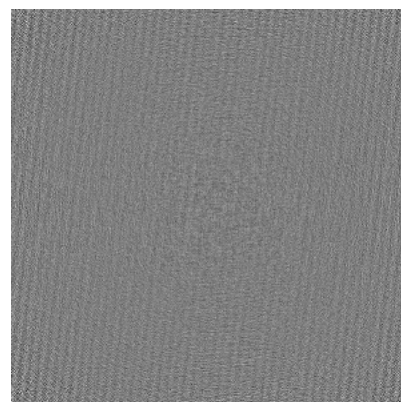
6.3.2 Raw map



X Index: 0



Y Index: 0

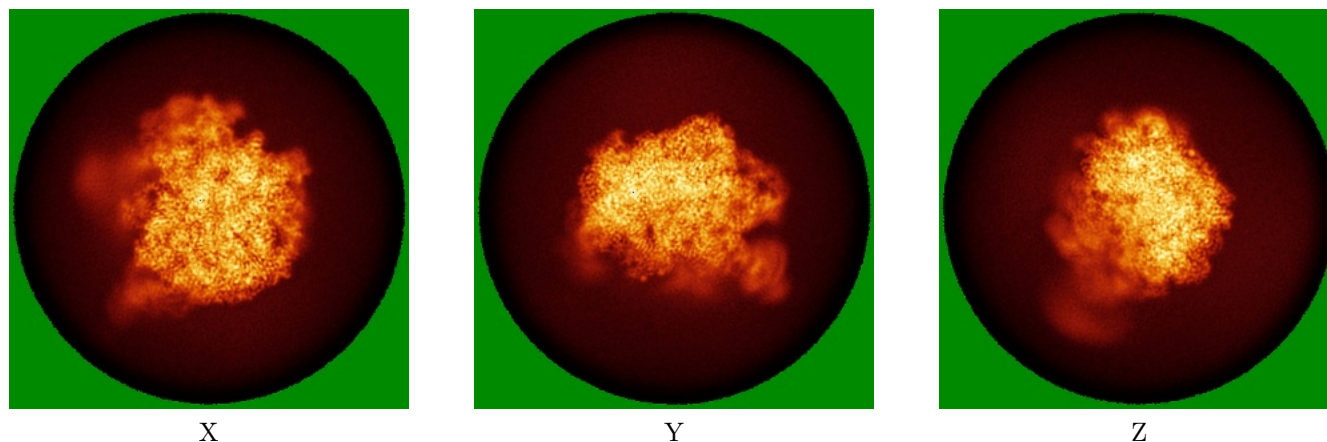


Z Index: 0

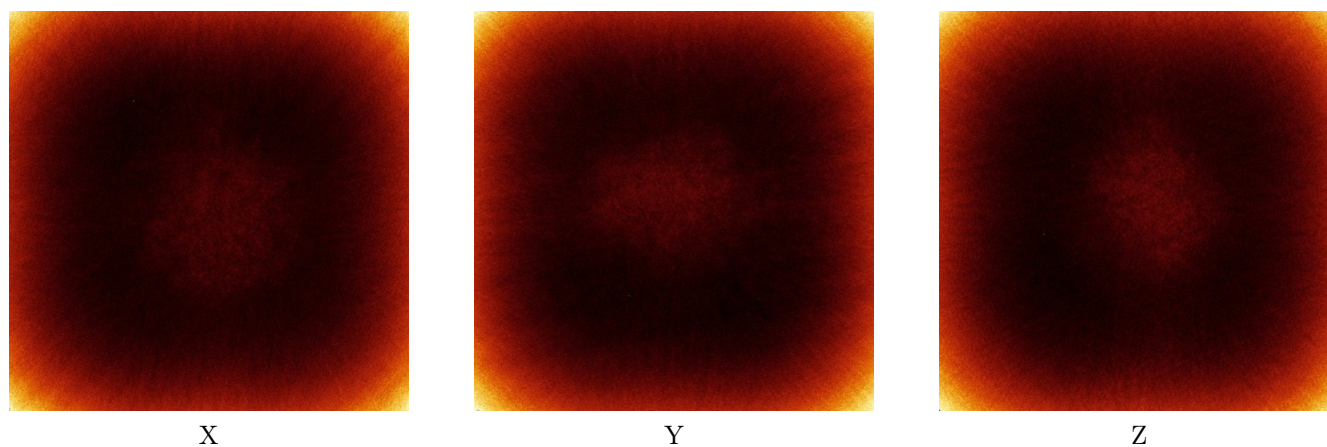
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



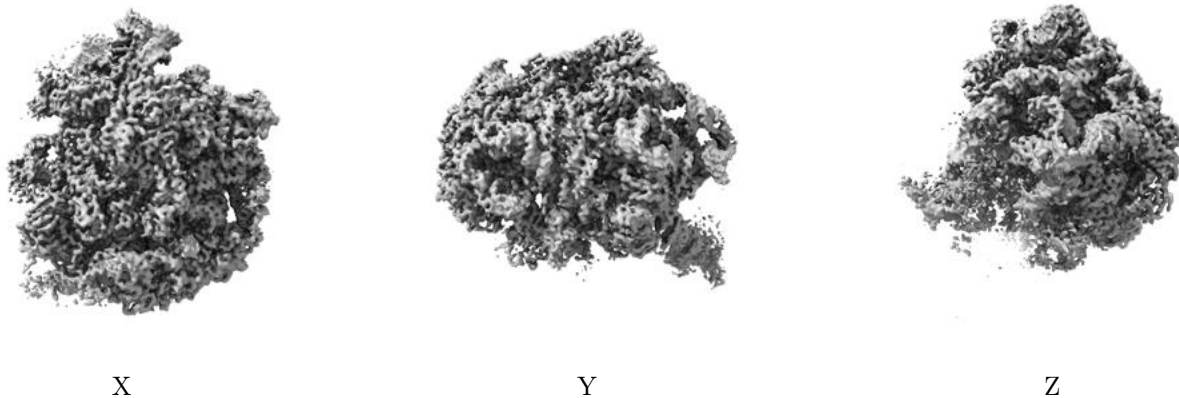
6.4.2 Raw map



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.

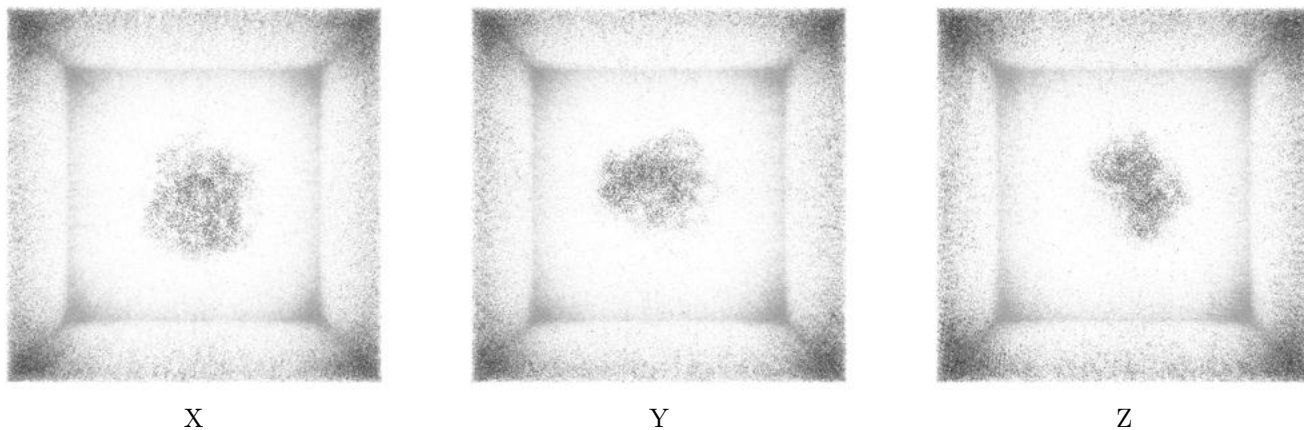
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.142. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

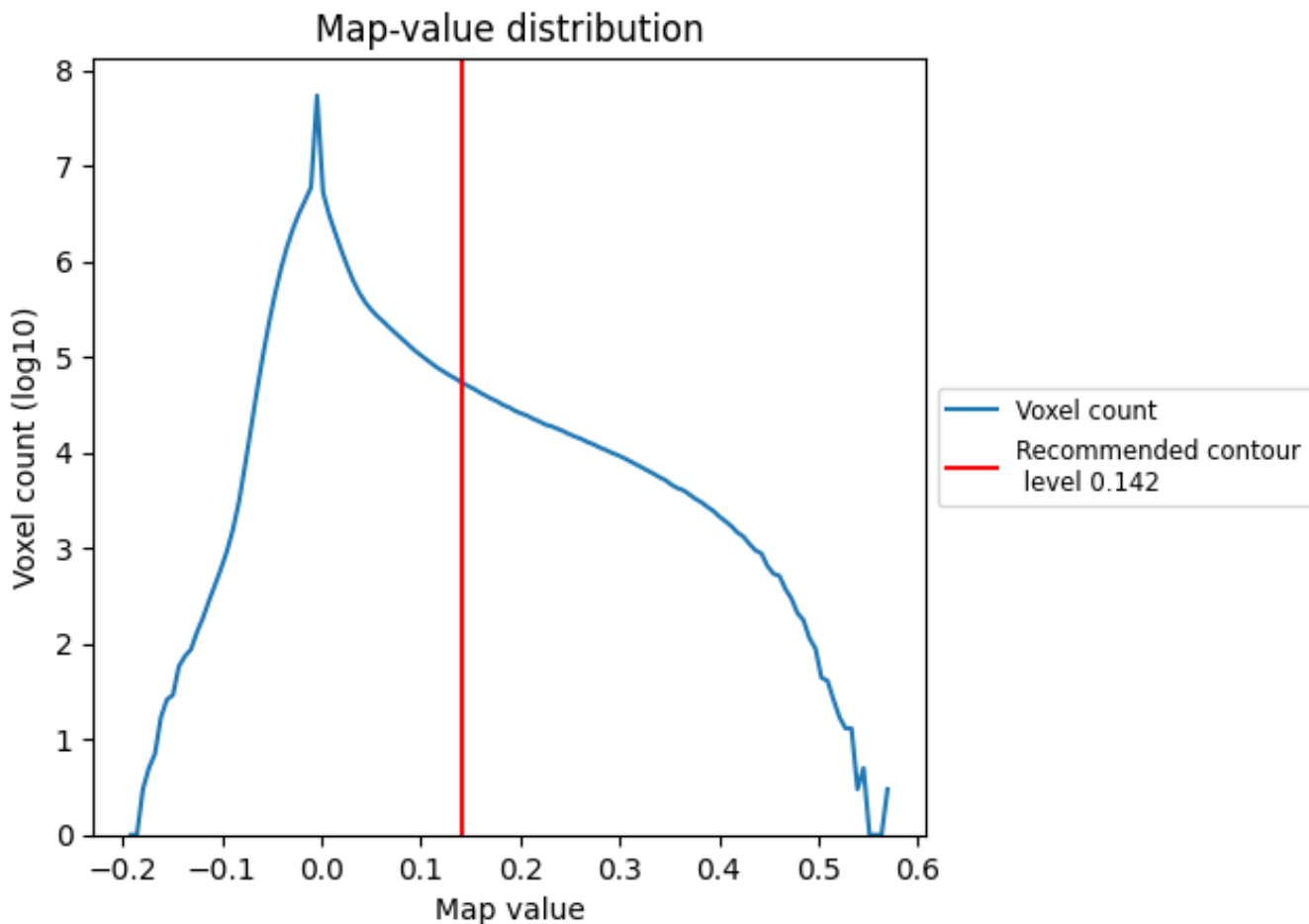
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

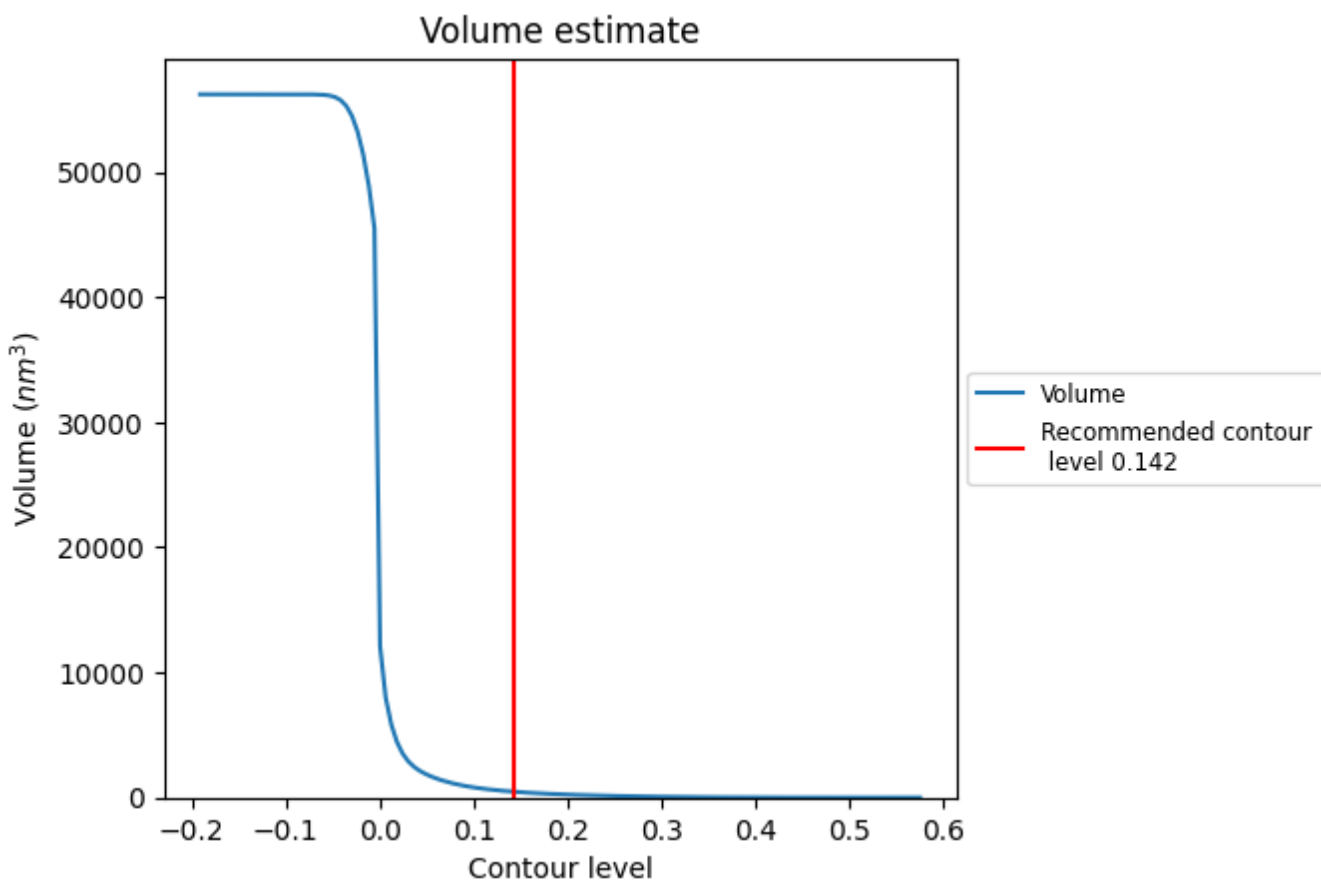
This section contains the results of statistical analysis of the map.

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.

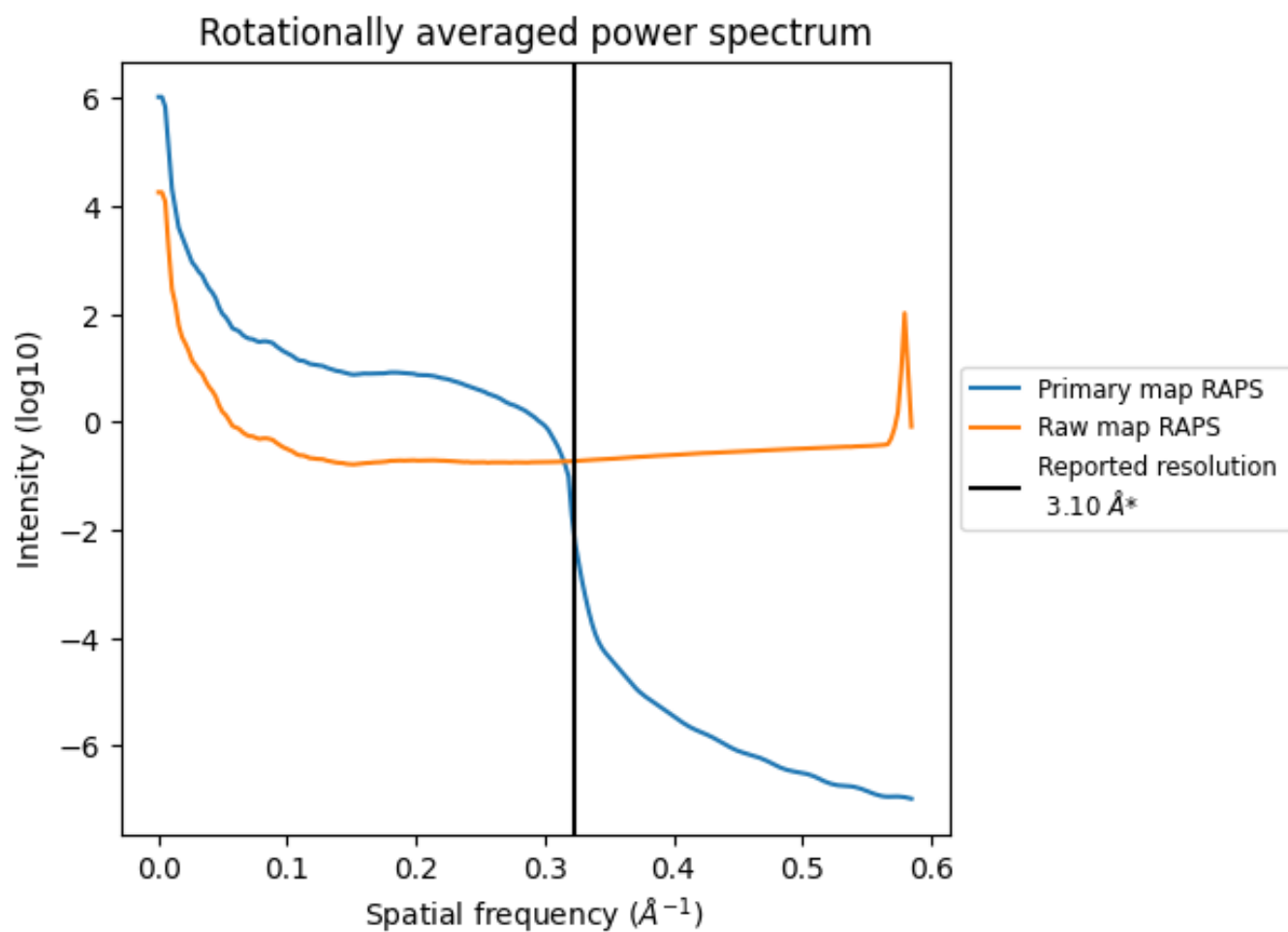
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 472 nm^3 ; this corresponds to an approximate mass of 426 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 [i](#)

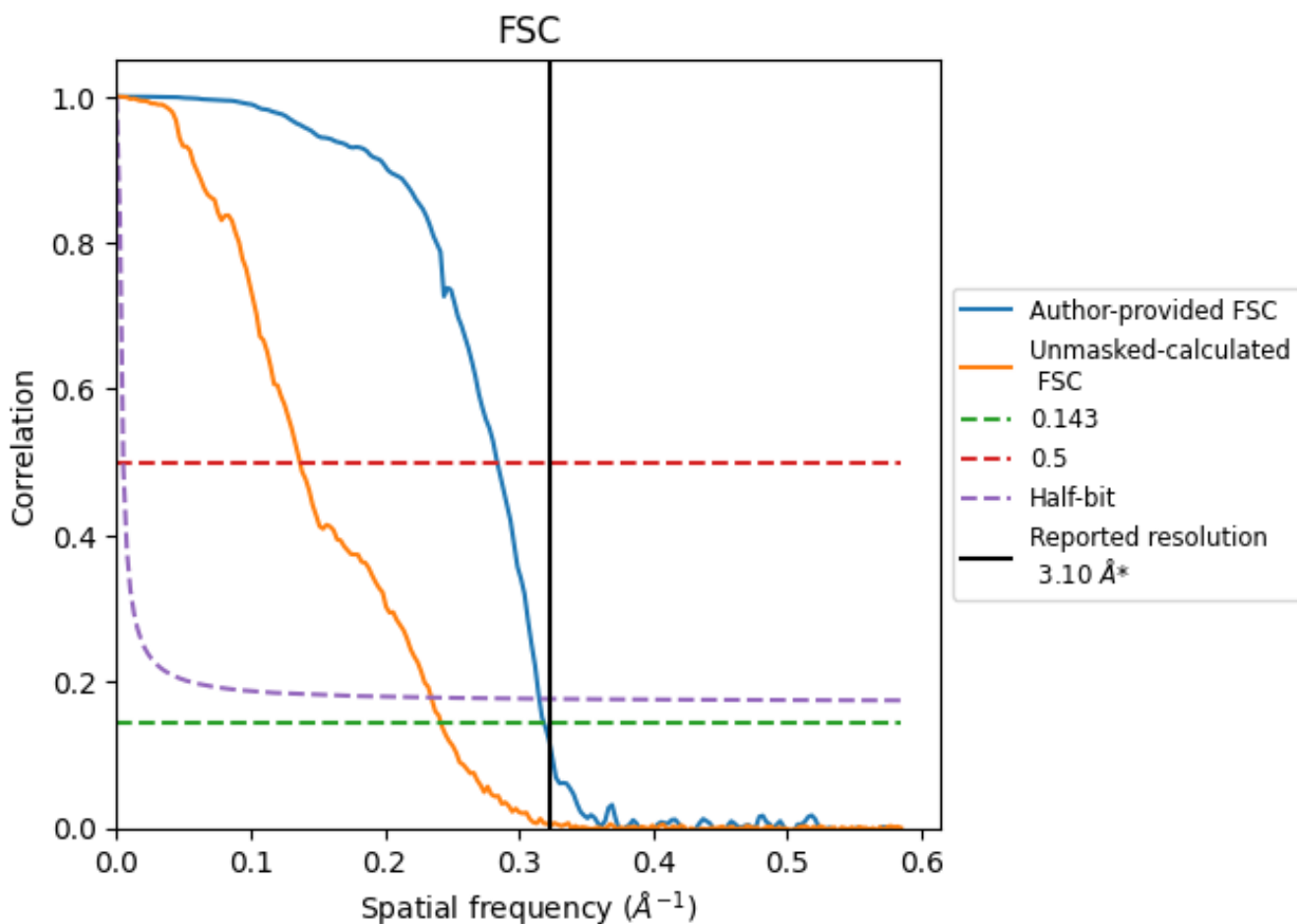


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

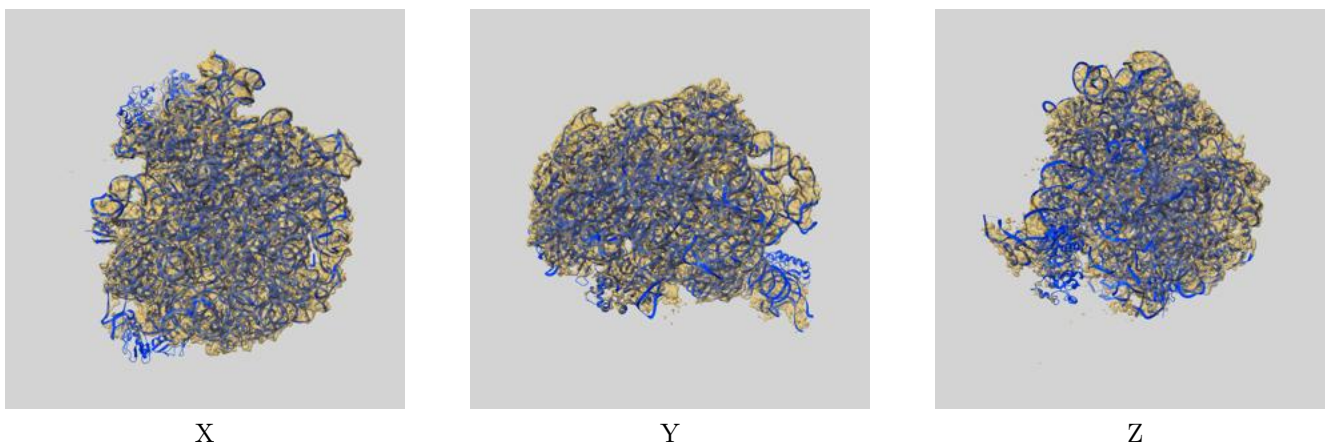
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.52	3.17
Unmasked-calculated*	4.13	7.32	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

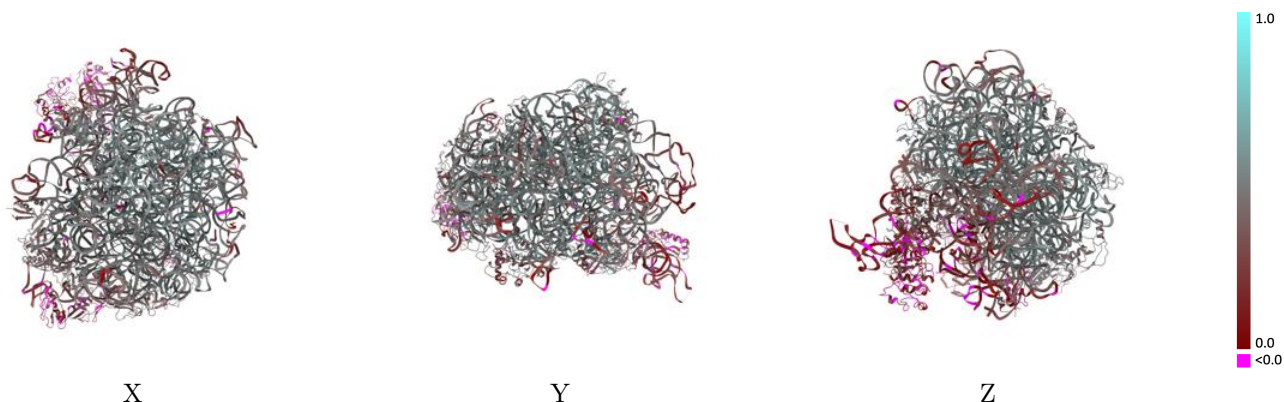
This section contains information regarding the fit between EMDB map EMD-44869 and PDB model 9BSL. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



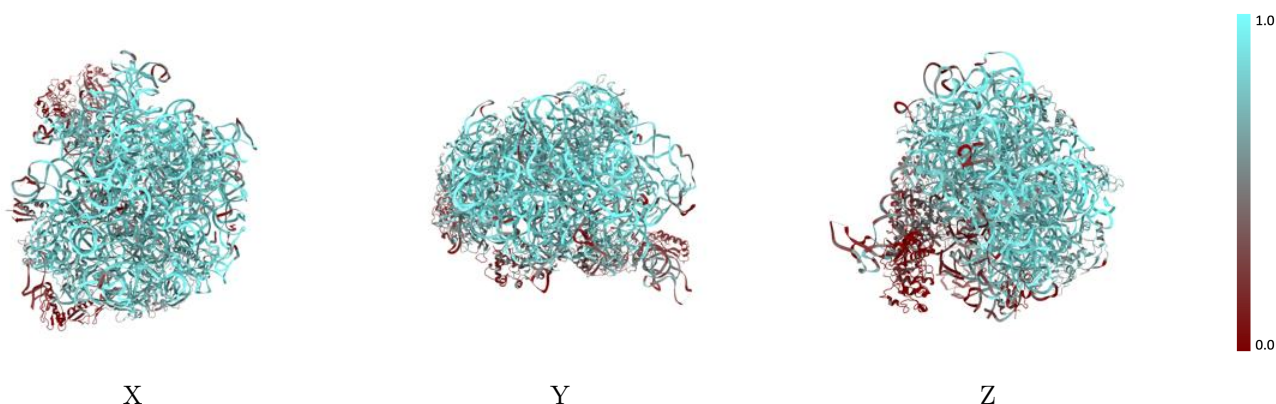
The images above show the 3D surface view of the map at the recommended contour level 0.142 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



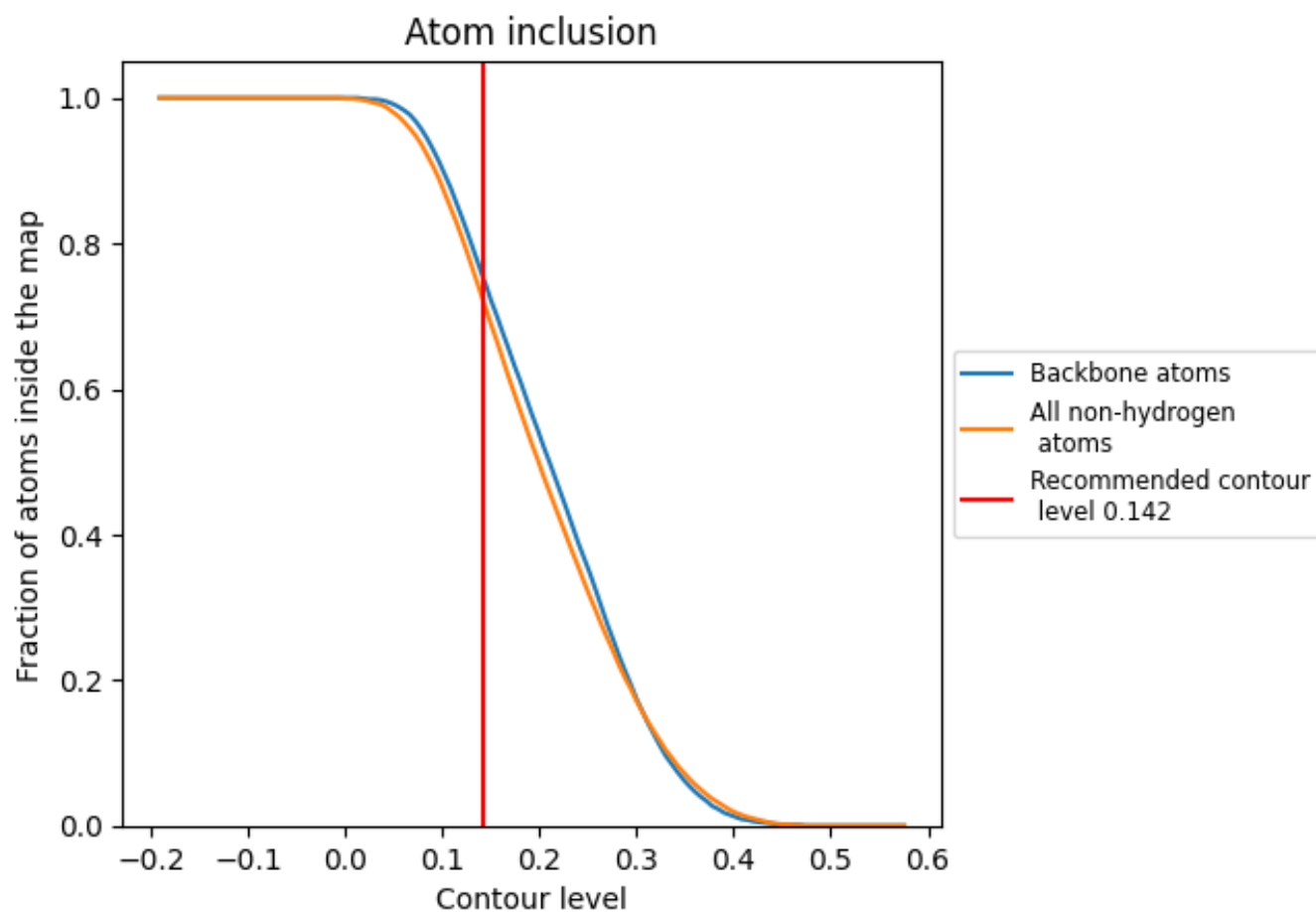
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.142).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.142) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.4140
A	 0.8020	 0.4260
C	 0.7320	 0.5150
D	 0.7280	 0.4610
E	 0.6990	 0.4840
F	 0.0370	 0.0990
G	 0.7370	 0.4410
H	 0.6300	 0.4650
I	 0.3110	 0.2860
J	 0.8140	 0.4970
K	 0.6660	 0.4490
L	 0.7770	 0.4670
M	 0.6690	 0.4600
N	 0.7790	 0.5070
O	 0.7540	 0.4990
P	 0.6950	 0.4810
R	 0.7240	 0.4400
S	 0.3820	 0.3840
T	 0.7060	 0.3680
U	 0.8290	 0.5510
V	 0.3820	 0.3580
W	 0.2940	 0.2870
Y	 0.0260	 0.0790

