



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:54 AM UTC

PDB ID : 8P09 / pdb_00008p09
EMDB ID : EMD-17330
Title : 48S late-stage initiation complex with non methylated mRNA
Authors : Guca, E.; Lima, L.H.F.; Boissier, F.; Hashem, Y.
Deposited on : 2023-05-09
Resolution : 3.30 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:

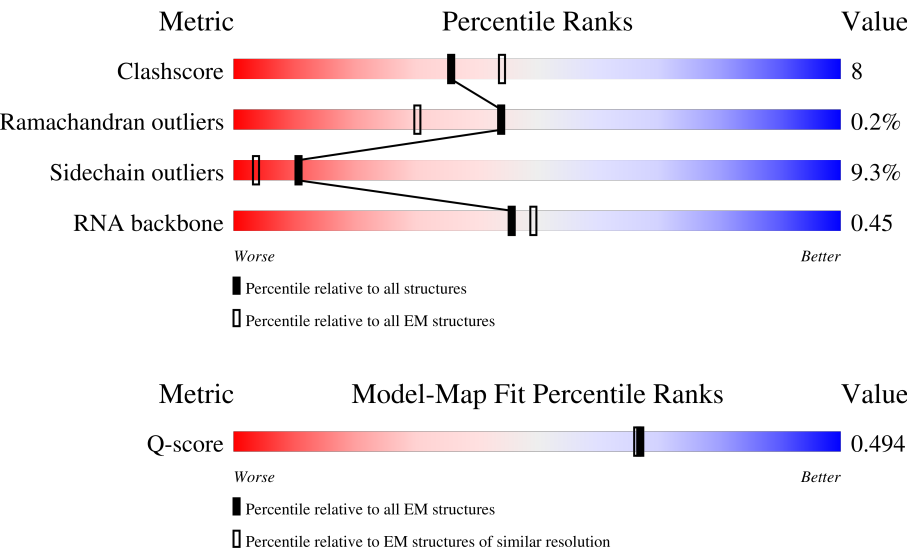
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	1	75	
2	2	1863	
3	3	9	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A	284	
5	C	207	
6	D	215	
7	E	270	
8	F	227	
9	G	263	
10	H	191	
11	I	237	
12	J	190	
13	K	206	
14	L	194	
15	M	98	
16	N	158	
17	O	132	
18	P	150	
19	Q	151	
20	R	145	
21	S	141	
22	T	135	
23	U	152	
24	V	141	
25	W	119	
26	X	83	
27	Y	130	
28	Z	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	a	133	
30	b	115	
31	c	84	
32	d	69	
33	e	56	
34	f	71	
35	g	313	
36	i	133	
37	j	111	
38	k	595	
39	l	25	
40	n	124	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 86284 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 initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1617	722	299	521	75		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1741	Total	C	N	O	P	0	0
			37147	16585	6650	12172	1740		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	9	Total	C	N	O	P	0	0
			192	86	36	61	9		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			2146	1354	376	405	11		

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	207	Total	C	N	O	S	0	0
			1637	1042	288	299	8		

- Molecule 6 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	215	Total	C	N	O	S	0	0
			1741	1107	309	310	15		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	226	Total	C	N	O	S	0	0
			1754	1139	298	310	7		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 9 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	187	Total	C	N	O	S	0	0
			1482	928	279	268	7		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	237	Total	C	N	O	S	0	0
			1924	1199	387	331	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	130	THR	PRO	conflict	UNP A0A5K1UJS7

- Molecule 12 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	188	Total	C	N	O	S	0	0
			1542	979	309	251	3		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 18 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 19 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 20 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	140	Total	C	N	O	S	0	0
			1154	733	219	195	7		

- Molecule 21 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 22 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	126	Total	C	N	O	S	0	0
			1019	639	188	187	5		

- Molecule 23 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	145	Total	C	N	O	S	0	0
			1194	747	243	203	1		

- Molecule 24 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 25 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 27 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 28 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	126	Total	C	N	O	S	0	0
			1021	645	198	173	5		

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	99	Total	C	N	O	S	0	0
			789	491	162	130	6		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 34 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 35 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	58	Total	C	N	O	S	0	0
			464	287	102	74	1		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	108	Total	C	N	O	S	0	0
			874	543	166	161	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	39	ILE	VAL	conflict	UNP G1SYS4
j	76	ILE	VAL	conflict	UNP G1SYS4

- Molecule 38 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total	C	N	O	S	0	0
			4693	2995	802	865	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	538	ILE	VAL	conflict	UNP G1SG72

- Molecule 39 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 40 is a protein called 40S ribosomal protein S25.

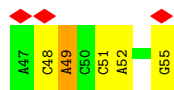
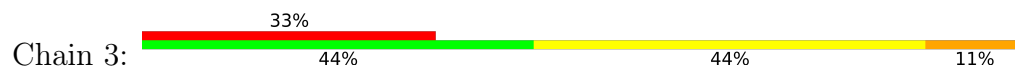
Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

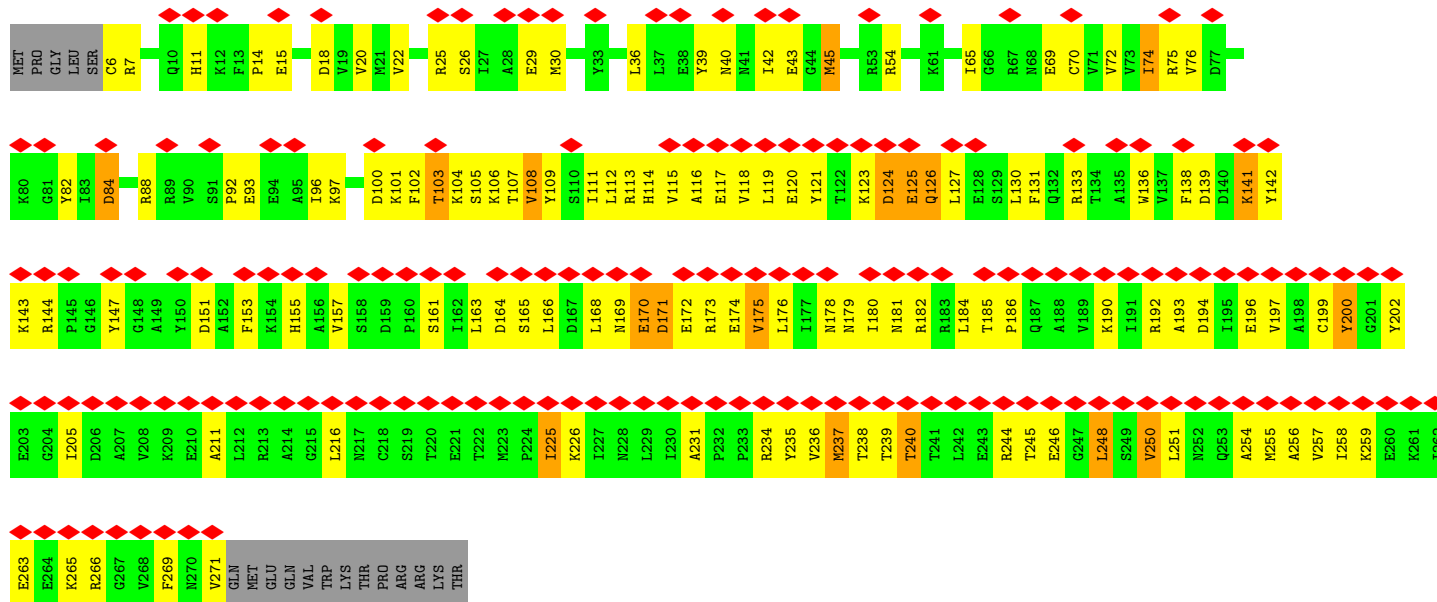
Mol	Chain	Residues	Atoms		AltConf
41	2	220	Total	Mg	0
			220	220	
41	3	3	Total	Mg	0
			3	3	
41	G	2	Total	Mg	0
			2	2	
41	I	2	Total	Mg	0
			2	2	
41	K	1	Total	Mg	0
			1	1	
41	L	1	Total	Mg	0
			1	1	
41	Z	1	Total	Mg	0
			1	1	

U1815	A1726	G1635	G1543	G1447	U1367	A1254	A1140	A1030	G929	A865	U829	U	C	U632
A1816	G1727	G1643	U1546	A1448	C1370	A1255	A1141	A1031	G932	A866	G	G	G	A633
A1818	G1731	G1643	U1546	A1449	C1370	A1256	A1145	A1032	C933	U867	U	U	A	G649
A1819	G1732	A1450	C1548	A1450	G1371	C1260	U1150	G1030	A934	A868	C	C	G	C650
G1820	C1733	A1451	C1549	G1452	A1372	A1261	U1151	G1039	U935	G870	C	C	C	U651
A1828	G1739	C1650	U1550	U1453	U1373	C1267	G1154	A1045	U936	A871	G	A	A	G652
A1829	A1740	A1551	U1550	G1454	A1374	C1267	G1154	A1045	G937	C972	C	C	C	G653
G1830	U1741	C1552	C1552	G1455	A1375	G1270	G1160	U1052	U938	C973	C	G	C	A654
G1831	C1742	G1653	C1553	G1456	A1376	G1271	G1161	A1054	U940	G874	G	G	G	G655
U1832	C1742	U1654	C1553	G1457	G1377	A1272	G1162	A1055	U941	C975	C	C	C	A656
C1835	G1747	C1655	C1557	U1458	C1380	A1273	G1166	A1056	G945	G876	U878	U878	C	A658
C1836	G1748	A1656	G1558	U1459	G1381	A1274	A1166	A1057	C946	C977	C786	C786	C	A661
G1837	C1749	C1559	C1558	C1460	A1382	C1275	G1167	A1058	U946	C978	C787	C787	C	A662
G1843	G1751	G1561	C1560	A1461	G1383	G1276	U1168	C1059	A951	G879	C788	C788	C	G663
A1844	G1752	C1562	G1561	C1464	A1392	A1277	U1169	C1060	G954	C880	C789	C789	C	C664
A1845	G1753	C1563	C1563	C1464	U1393	C1279	U1170	G1061	G954	U881	A790	A790	C	U665
C1846	G1754	U1666	A1564	A1472	U1394	A1280	A1177	C1074	G957	U883	A791	A791	C	U668
G1852	U1755	U1667	G1565	U1473	G1399	G1281	A1178	C1075	C957	U884	G792	G792	C	G673
A1853	C	A1476	G1566	A1476	U1400	G1282	A1179	A1076	A958	U885	C793	C793	C	G677
A1854	G	A1480	G1570	A1480	A1401	G1286	G1183	U1077	U961	U886	C794	C794	C	C677
G1855	G	A1483	G1571	A1483	G1402	A1289	A1191	A1078	U962	U887	C795	C795	C	U678
G1856	C	C1484	G1572	C1484	U1403	G1298	A1195	A1079	U962	U888	C796	C796	C	U679
A1857	C	A1485	U1573	A1485	A1404	G1299	A1195	A1080	U962	U889	C797	C797	C	G680
U1858	C	G1486	A1574	G1486	A1405	C1299	A1195	C1081	U962	G966	C798	C798	C	U681
A1859	C	C1486	C1575	C1486	G1407	U1300	A1195	C1090	U962	G967	C799	C799	C	G682
U1860	C	U1688	C1576	C1486	G1408	U1304	G1203	G1095	U962	A968	A807	A807	C	G683
A1861	G	U1689	U1581	G1491	C1409	C1304	G1203	G1095	U962	U982	A807	A807	C	A684
U1862	C1766	U1690	G1582	U1492	A1410	C1305	G1206	A1096	A977	U893	U810	U810	C	G685
A1863	C1767	A1583	A1583	A1493	C1411	U1306	G1207	U1097	G978	U894	U811	U811	C	G686
C1768	C1768	A1584	A1584	A1494	C1412	G1310	G1208	G1098	G981	C986	A812	A812	C	G687
U1769	G1769	U1590	U1590	A1502	C1414	C1311	G1211	G1103	G981	C987	G817	G817	C	U688
G1770	G1770	U1591	U1591	G1503	C1415	C1312	G1212	G1104	C985	C988	C827	C827	C	G
C1771	C1771	C1592	C1592	G1506	G1416	U1313	G1217	C1105	A986	U899	C828	C828	C	C
G1773	G1773	G1593	G1593	U1507	G1417	G1316	G1220	G1106	A988	C901	C829	C829	C	U
G1774	G1774	A1596	A1596	C1508	A1418	G1317	G1220	U1110	A988	C902	C829	C829	C	A
A1775	U1705	U1597	U1597	G1509	C1419	G1321	G1223	C1112	A997	G903	C829	C829	C	G
G1776	U1706	G1598	G1598	G1510	G1420	U1322	A1224	C1113	U998	A904	C830	C830	C	G
C1777	A1707	G1599	G1599	G1511	G1420	U1322	G1225	C1114	G1001	G905	C831	C831	C	C
U1709	C1708	G1600	G1600	C1515	U1422	U1325	G1231	A1115	G1001	C906	C832	C832	C	G
G1778	U1709	A1601	A1601	C1516	U1422	G1326	A1236	U1116	A1004	C907	A833	A833	C	G
C1782	A1710	A1517	A1517	A1517	C1424	A1328	A1237	U1116	A1005	C908	C834	C834	C	G
A1795	U1715	A1526	U1611	A1526	G1426	U1329	U1237	C1120	A1006	A909	C835	C835	C	G
G1799	U1716	C1527	G1612	C1527	C1426	U1329	U1238	C1121	A1007	C909	C836	C836	C	G
A1800	G1717	A1528	U1616	A1528	U1427	G1334	G1234	G1126	A1008	C910	C837	C837	C	U
A1803	A1718	C1529	U1617	C1529	C1429	U1339	I2T1244	U1125	U1009	U913	C838	C838	C	U
U1804	G1720	U1530	U1617	U1530	C1430	U1339	A1246	U1133	U1012	U914	C839	C839	C	C
C1805	G1721	G1531	A1618	A1531	C1431	U1343	A1247	C1134	U1013	A915	C840	C840	C	G
U1806	G1722	A1532	A1625	A1532	C1432	U1344	G1252	C1135	A1019	A916	C841	C841	C	C
A1807	U1723	G1535	U1632	G1535	C1433	G1346	G1252	G1136	U1019	A916	C842	C842	C	G
G1808	U1724	U1536	A1632	G1536	A1434	U1346	G1253	G1136	G1029	C920	A843	A843	C	C
G1814	U1725	U1536	A1632	G1536	C1435	U1346	G1253	G1136	G1029	A922	C847	C847	C	G
					U1437					C923	G848	G848	C	A
										G925	G864	G864	C	G

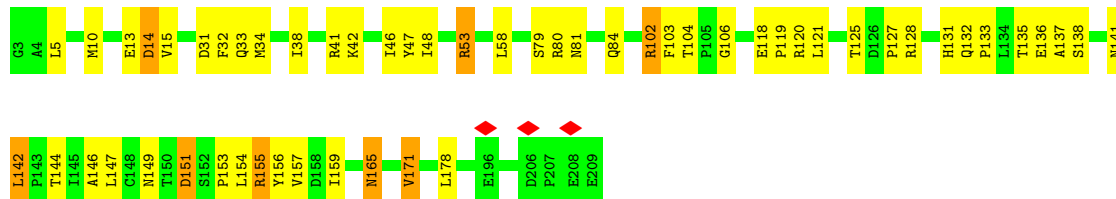
- Molecule 3: mRNA



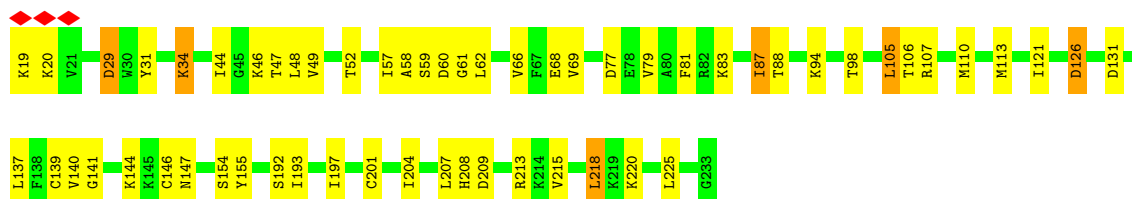
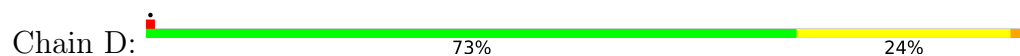
- Molecule 4: Eukaryotic translation initiation factor 2 subunit 1



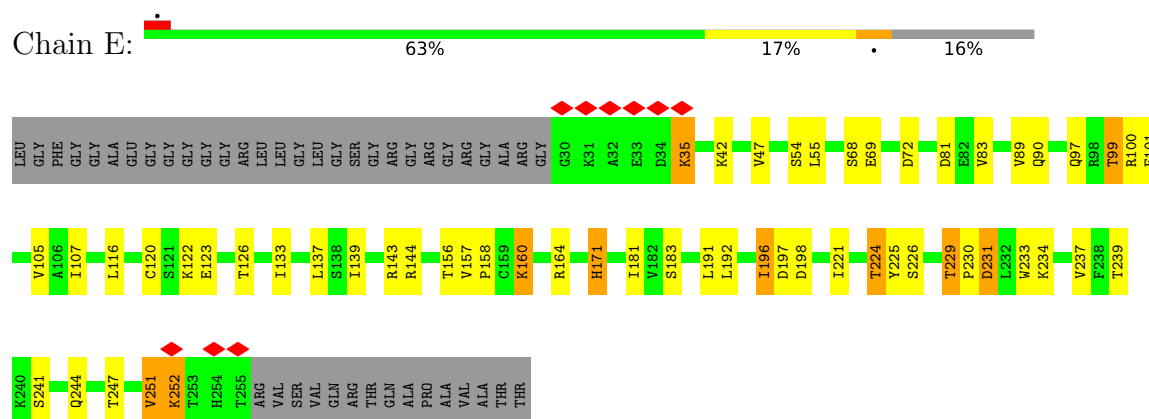
- Molecule 5: 40S ribosomal protein SA



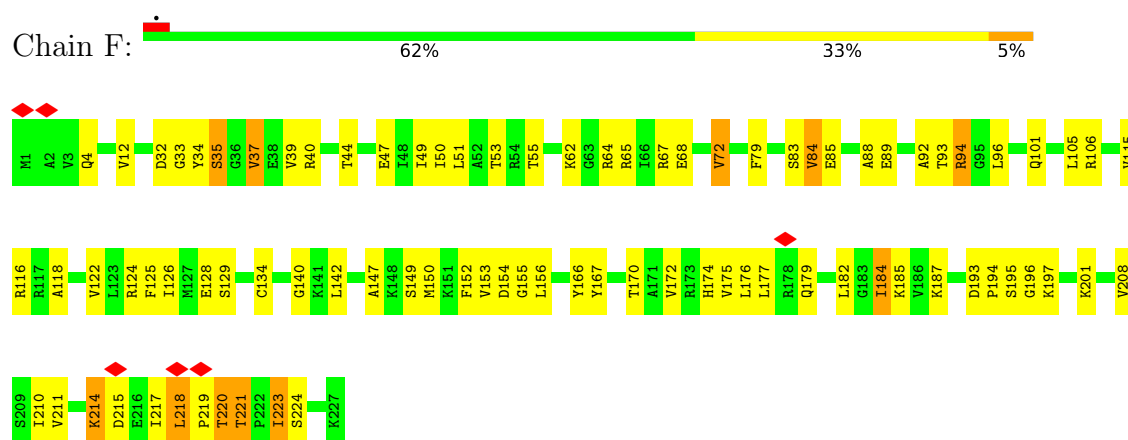
- Molecule 6: ribosomal protein eS1



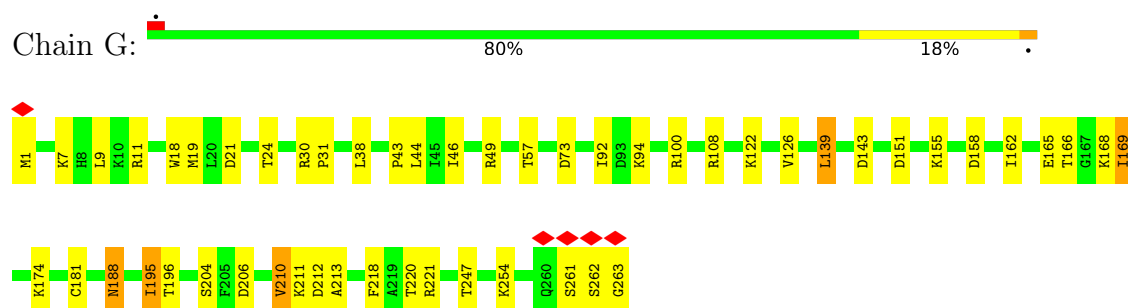
- Molecule 7: 40S ribosomal protein S2



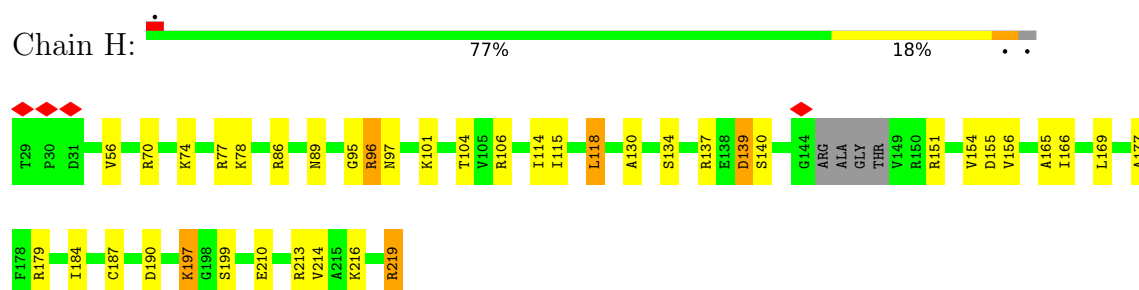
- Molecule 8: Ribosomal protein S3



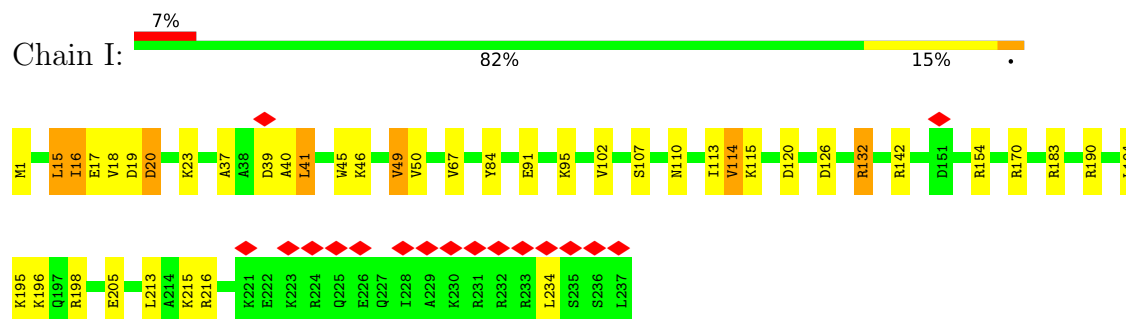
- Molecule 9: 40S ribosomal protein S4



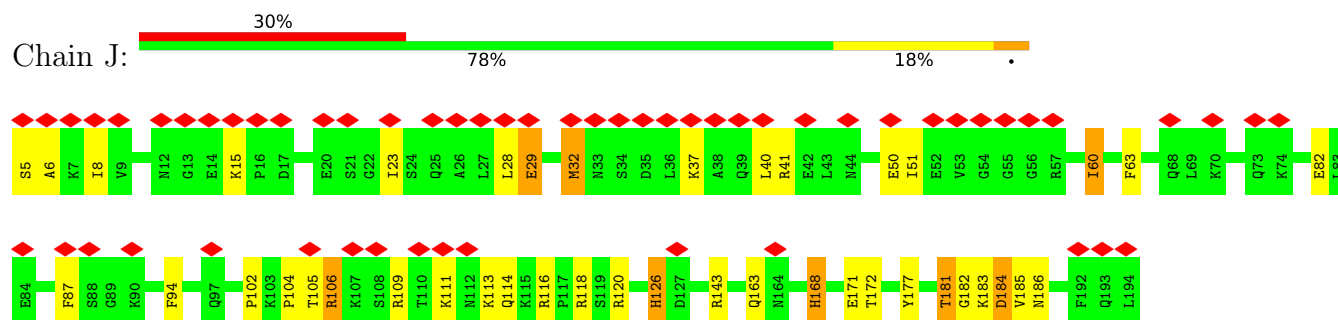
- Molecule 10: Ribosomal protein S5



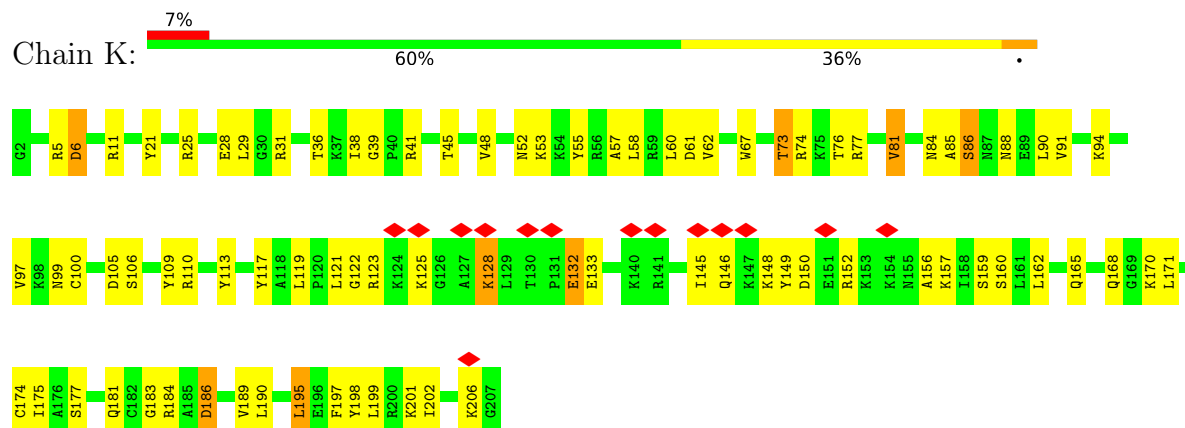
- Molecule 11: 40S ribosomal protein S6



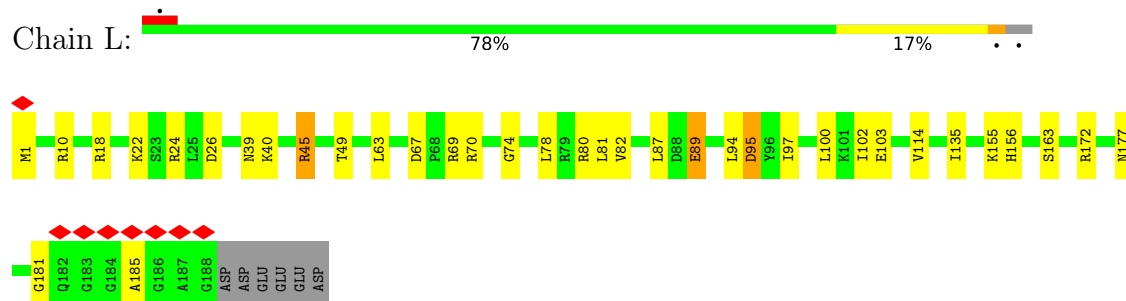
- Molecule 12: ribosomal protein eS7



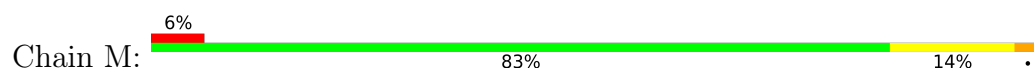
- Molecule 13: 40S ribosomal protein S8



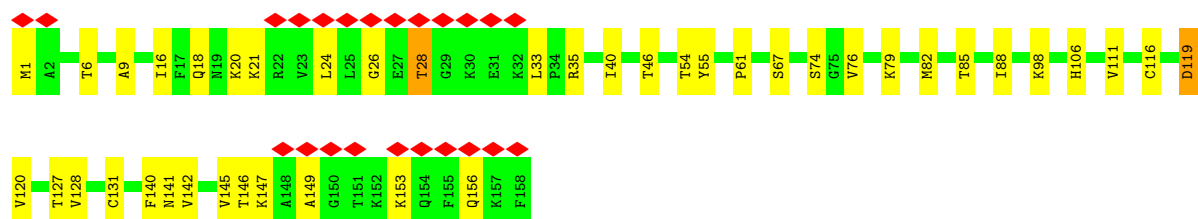
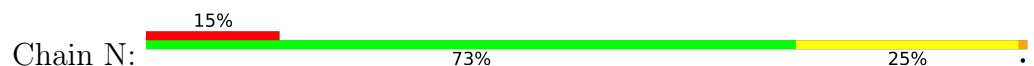
- Molecule 14: 40S ribosomal protein S9



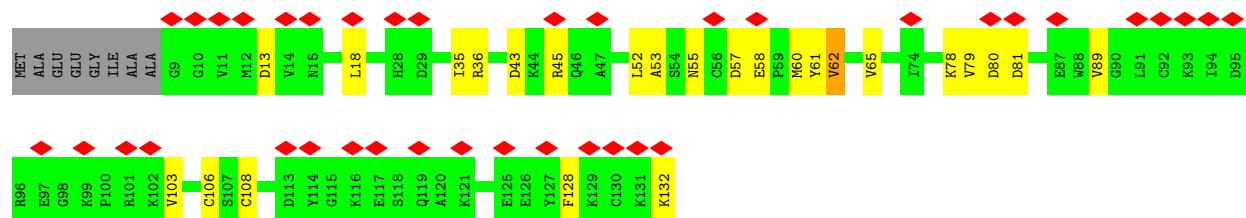
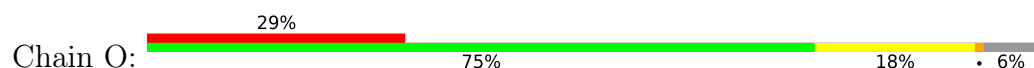
- Molecule 15: 40S ribosomal protein eS10



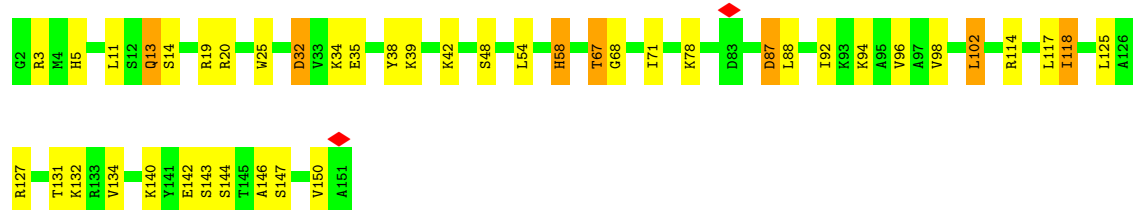
- Molecule 16: 40S ribosomal protein S11



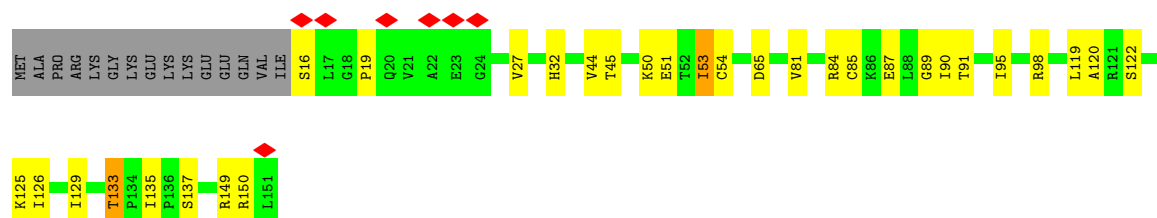
- Molecule 17: 40S ribosomal protein S12



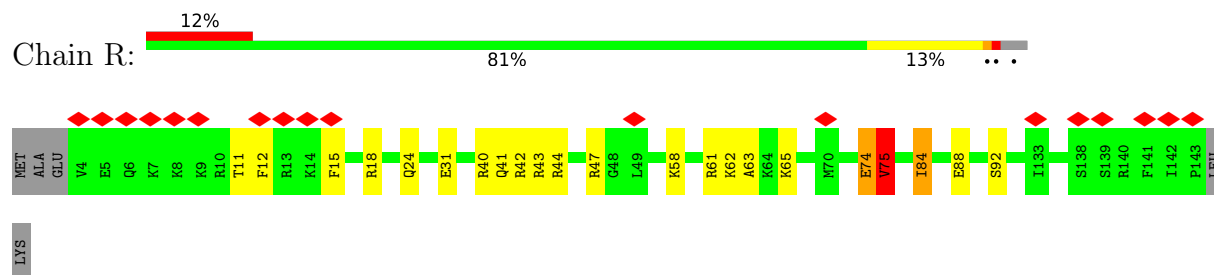
- Molecule 18: ribosomal protein uS15



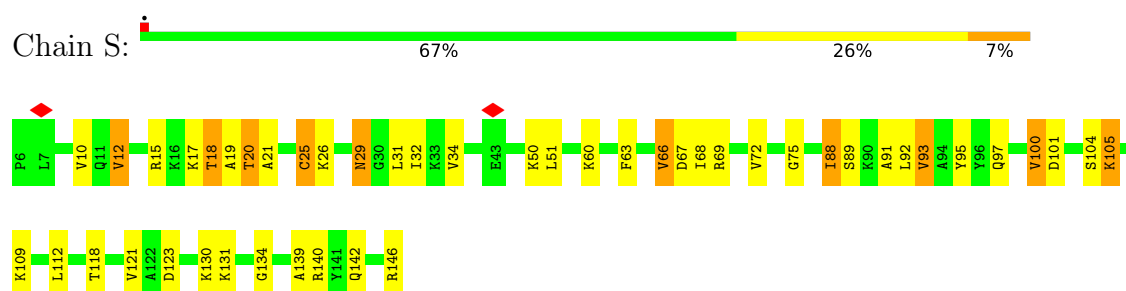
- Molecule 19: 40S ribosomal protein uS11



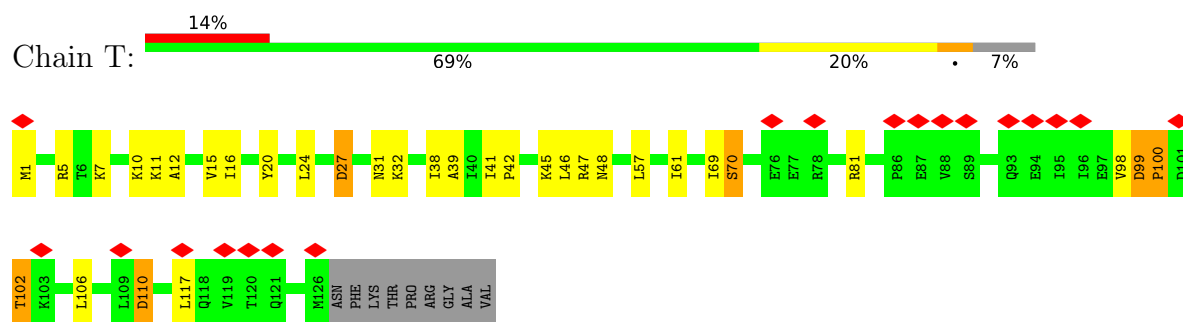
- Molecule 20: 40S ribosomal protein uS19



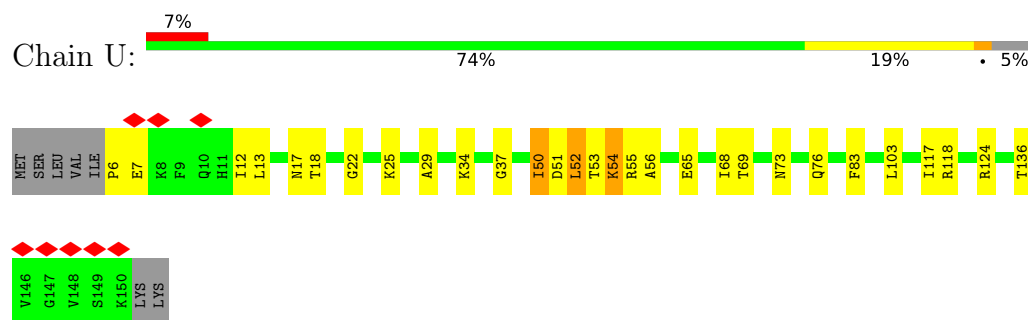
- Molecule 21: 40S ribosomal protein uS9



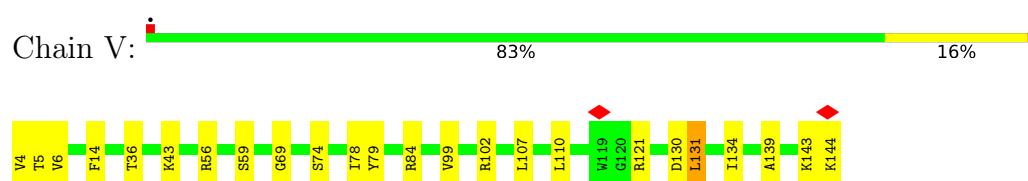
- Molecule 22: 40S ribosomal protein eS17



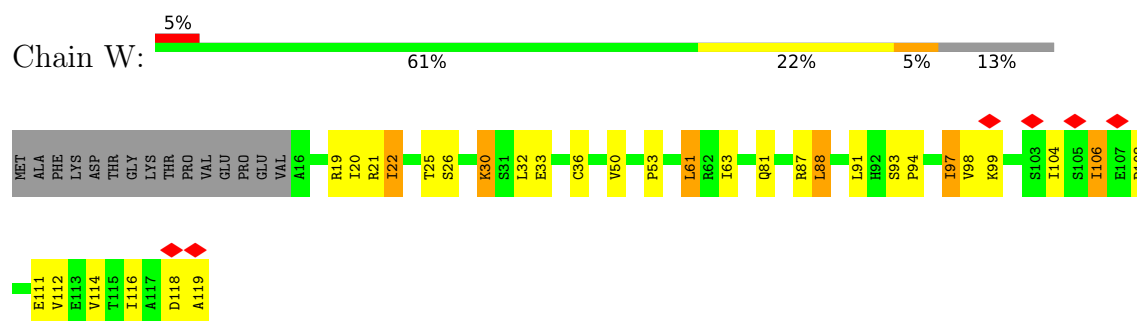
- Molecule 23: 40S ribosomal protein uS13



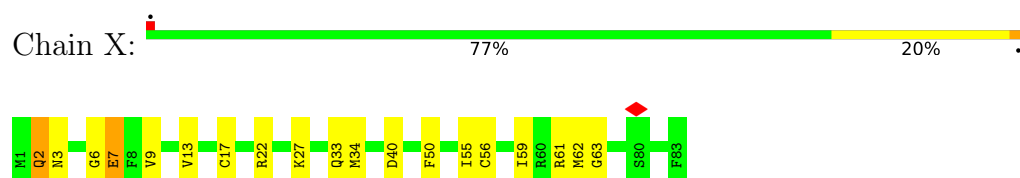
- Molecule 24: 40S ribosomal protein eS19



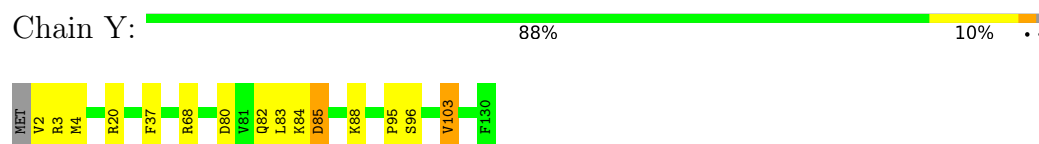
- Molecule 25: 40S ribosomal protein uS10



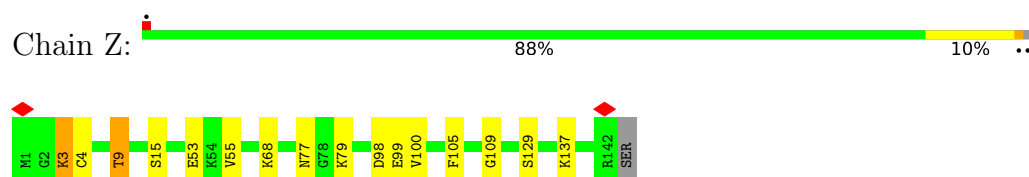
- Molecule 26: 40S ribosomal protein S21



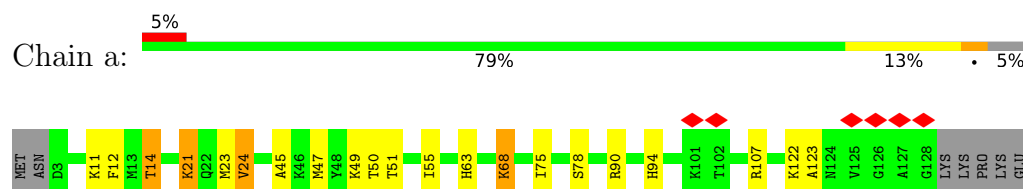
- Molecule 27: Ribosomal protein S15a



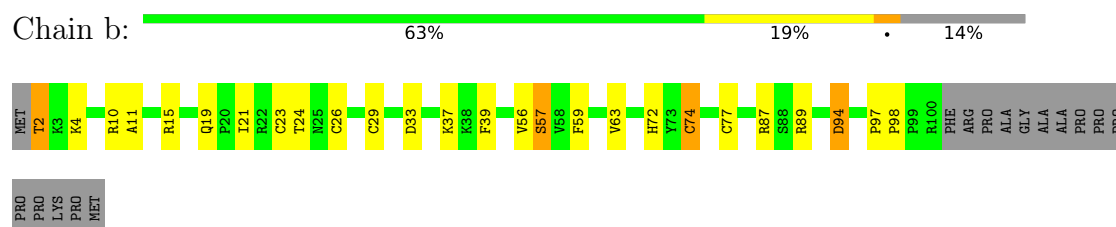
- Molecule 28: 40S ribosomal protein S23



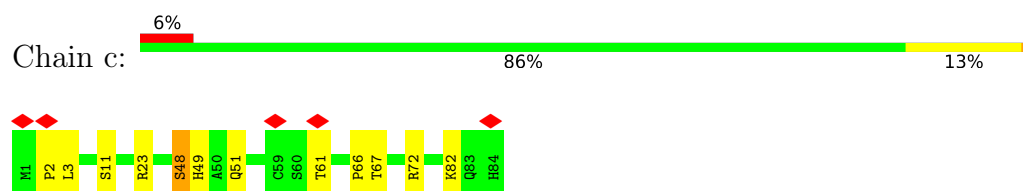
- Molecule 29: 40S ribosomal protein S24



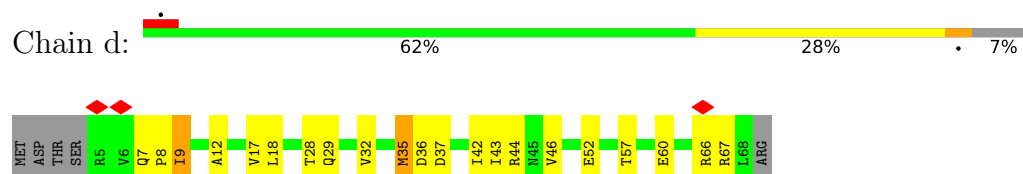
- Molecule 30: 40S ribosomal protein S26



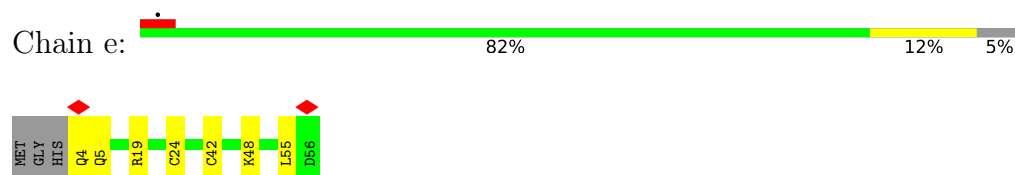
- Molecule 31: 40S ribosomal protein S27



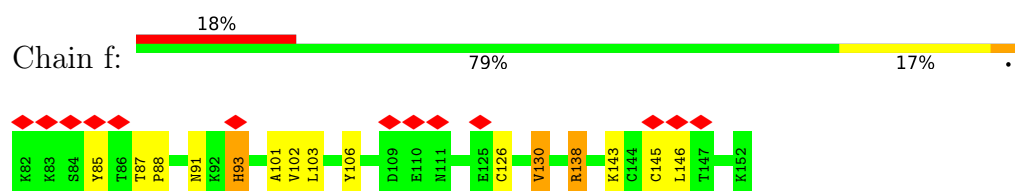
- Molecule 32: 40S ribosomal protein S28



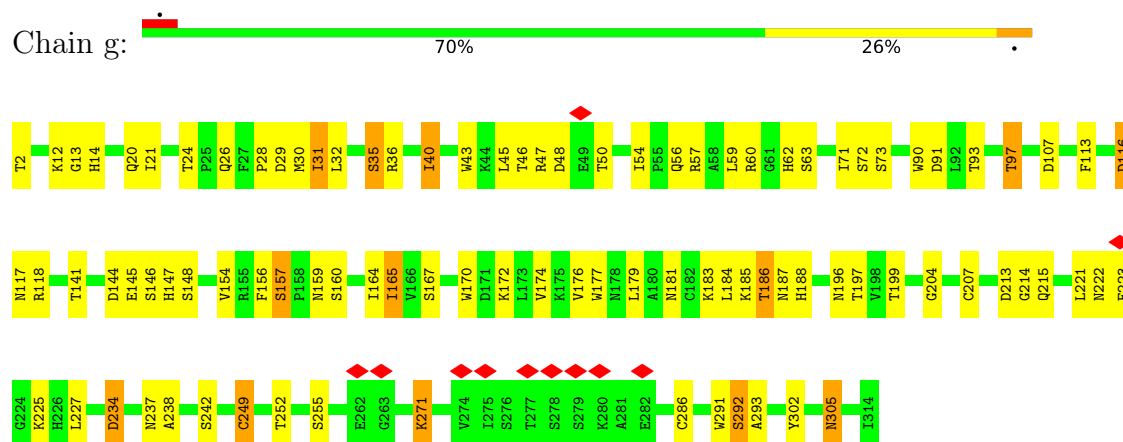
- Molecule 33: 40S ribosomal protein S29



- Molecule 34: ribosomal protein eS31

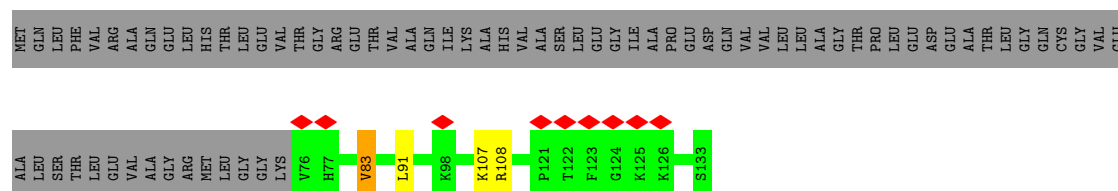


- Molecule 35: Ribosomal protein RACK1

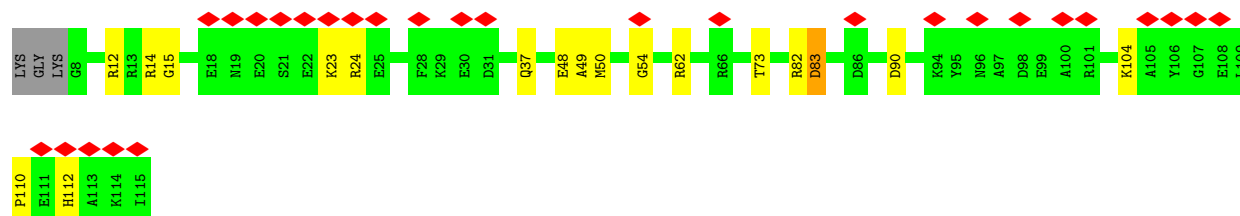
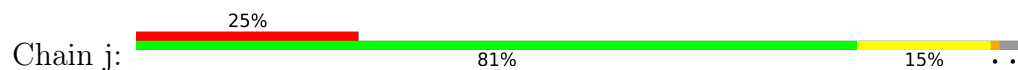


- Molecule 36: 40S ribosomal protein S30

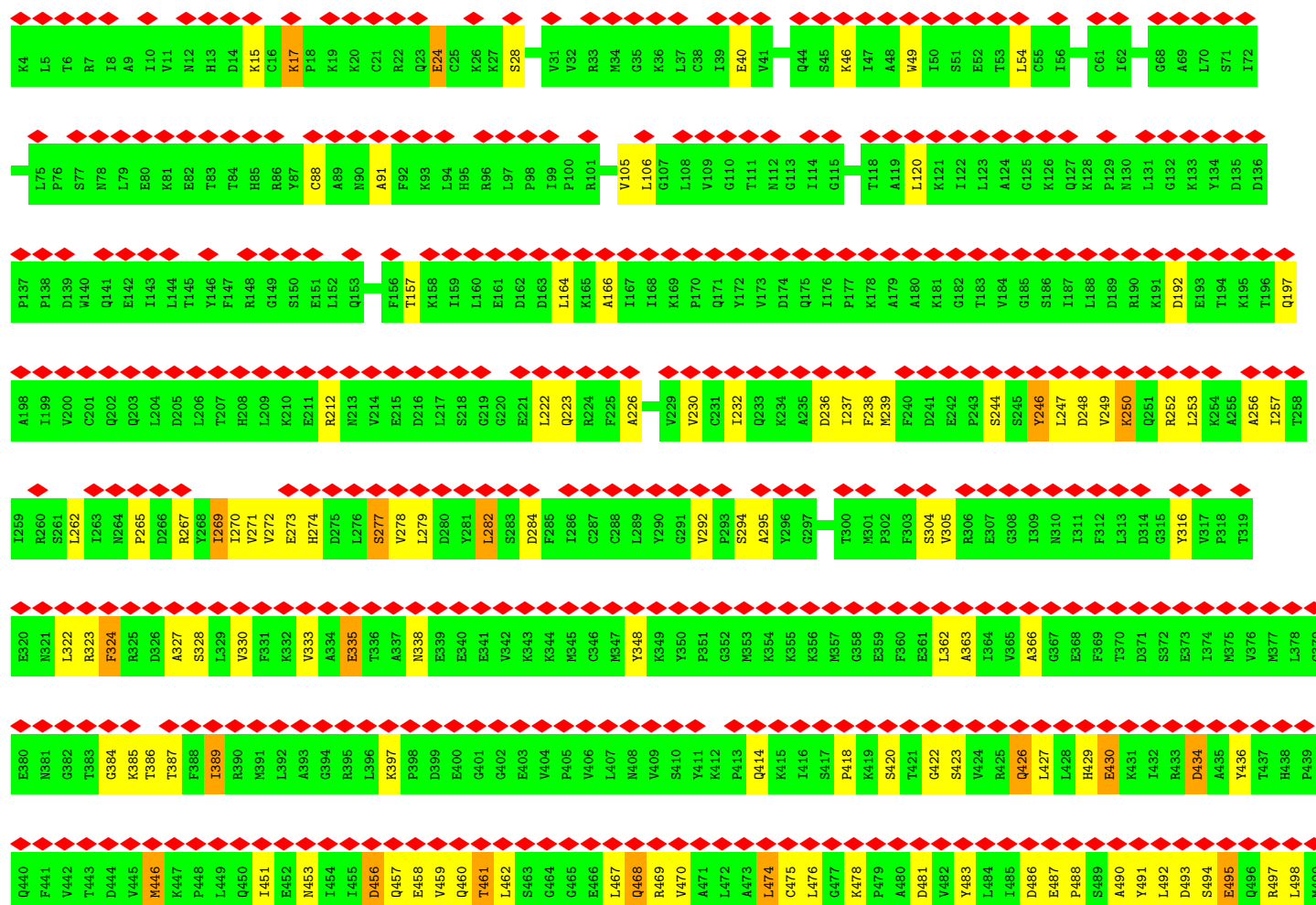
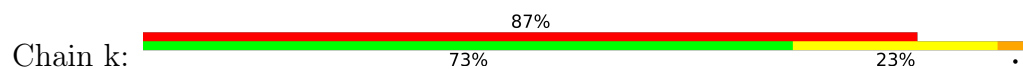


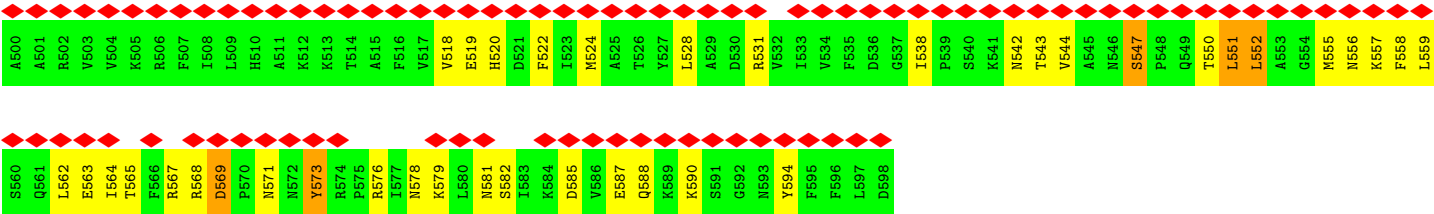


• Molecule 37: Eukaryotic translation initiation factor 4C



• Molecule 38: ATP binding cassette subfamily E member 1

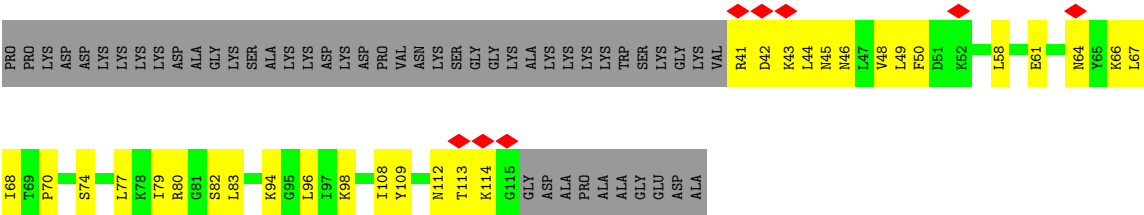
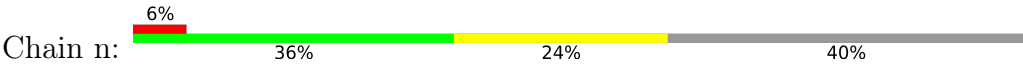




• Molecule 39: 60S ribosomal protein L41



• Molecule 40: 40S ribosomal protein S25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.060	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, MG, I2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.60	3/1773 (0.2%)	0.91	10/2763 (0.4%)
2	2	0.67	2/41502 (0.0%)	0.78	86/64679 (0.1%)
3	3	0.89	0/214	1.26	1/331 (0.3%)
4	A	0.36	0/2177	0.67	1/2935 (0.0%)
5	C	0.64	0/1674	0.93	3/2275 (0.1%)
6	D	0.50	0/1769	0.73	3/2367 (0.1%)
7	E	0.61	0/1794	0.87	3/2430 (0.1%)
8	F	0.47	0/1792	0.67	0/2412
9	G	0.54	0/2125	0.77	3/2856 (0.1%)
10	H	0.62	0/1503	0.98	4/2020 (0.2%)
11	I	0.60	0/1946	0.98	2/2588 (0.1%)
12	J	0.53	0/1553	1.01	3/2079 (0.1%)
13	K	0.59	0/1709	0.93	7/2278 (0.3%)
14	L	0.69	0/1567	1.03	4/2092 (0.2%)
15	M	0.58	0/852	1.05	0/1147
16	N	0.51	0/1319	0.59	0/1761
17	O	0.66	0/968	1.26	0/1296
18	P	0.54	0/1232	0.74	2/1656 (0.1%)
19	Q	0.62	0/1029	1.00	2/1380 (0.1%)
20	R	0.76	0/1177	1.30	6/1571 (0.4%)
21	S	0.58	0/1142	0.82	1/1528 (0.1%)
22	T	0.61	0/1031	1.06	5/1383 (0.4%)
23	U	0.47	0/1212	0.76	0/1621
24	V	0.62	0/1133	0.99	2/1517 (0.1%)
25	W	0.49	0/832	0.71	0/1117
26	X	0.57	0/643	0.85	0/860
27	Y	0.69	0/1051	0.95	0/1406
28	Z	0.67	0/1124	1.13	1/1500 (0.1%)
29	a	0.71	0/1038	1.13	2/1380 (0.1%)
30	b	0.71	0/802	1.06	2/1076 (0.2%)
31	c	0.62	0/673	1.12	3/902 (0.3%)
32	d	0.54	0/508	0.83	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.67	0/454	1.07	1/603 (0.2%)
34	f	0.63	0/594	1.09	1/786 (0.1%)
35	g	0.47	0/2494	0.79	0/3394
36	i	0.79	0/469	1.38	0/617
37	j	0.63	0/884	1.19	5/1175 (0.4%)
38	k	0.63	0/4780	1.15	13/6452 (0.2%)
39	l	0.51	0/241	0.59	0/305
40	n	0.35	0/604	0.56	0/810
All	All	0.63	5/91384 (0.0%)	0.87	176/132028 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
2	2	0	131
3	3	0	1
4	A	0	1
5	C	0	1
7	E	0	1
9	G	0	1
10	H	0	1
11	I	0	3
13	K	0	3
19	Q	0	2
24	V	0	2
27	Y	0	1
29	a	0	1
32	d	0	1
34	f	0	1
38	k	0	4
All	All	0	156

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	72	U	O3'-P	-12.66	1.42	1.61
2	2	1245	C	O3'-P	-12.24	1.42	1.61
2	2	1708	C	P-OP1	6.26	1.61	1.49
1	1	2	A	P-OP1	6.22	1.61	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2	A	P-OP2	6.17	1.61	1.49

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	72	U	OP2-P-O3'	-29.25	20.26	108.00
1	1	28	U	P-O3'-C3'	-9.55	105.87	120.20
2	2	73	C	C2'-C3'-O3'	9.47	123.71	109.50
1	1	2	A	P-O5'-C5'	-9.34	106.88	120.90
24	V	143	LYS	O-C-N	-9.32	110.99	122.55
2	2	1245	C	OP2-P-O3'	8.51	133.52	108.00
2	2	1551	A	C1'-O4'-C4'	-8.48	101.42	109.90
2	2	572	U	C5'-C4'-C3'	-8.34	103.48	116.00
9	G	1	MET	CA-C-N	8.26	134.59	122.86
9	G	1	MET	C-N-CA	8.26	134.59	122.86
1	1	72	U	OP1-P-O3'	8.18	132.53	108.00
2	2	1515	G	C2'-C3'-O3'	-7.93	101.80	113.70
2	2	1547	G	C4'-C3'-O3'	7.65	120.88	109.40
2	2	1245	C	OP1-P-O3'	-7.58	85.27	108.00
7	E	171	HIS	CA-CB-CG	7.50	121.30	113.80
20	R	42	ARG	NE-CZ-NH2	7.48	125.93	119.20
2	2	67	C	C2'-C3'-O3'	7.32	120.49	109.50
37	j	83	ASP	CA-CB-CG	7.26	119.86	112.60
2	2	540	C	C5'-C4'-C3'	-7.13	105.31	116.00
2	2	78	C	O4'-C1'-N1	7.12	118.88	108.20
38	k	495	GLU	O-C-N	-7.00	114.70	122.12
13	K	6	ASP	CA-CB-CG	6.94	119.54	112.60
13	K	150	ASP	CA-CB-CG	6.87	119.47	112.60
1	1	35	A	C5'-C4'-C3'	-6.77	105.85	116.00
2	2	1547	G	P-O3'-C3'	6.76	130.34	120.20
2	2	524	G	C3'-C2'-C1'	6.75	108.05	101.30
2	2	1550	U	C1'-O4'-C4'	-6.63	103.07	109.70
2	2	598	C	C5'-C4'-C3'	-6.60	106.10	116.00
2	2	85	A	C4'-C3'-C2'	-6.59	96.01	102.60
2	2	17	C	C4'-C3'-C2'	-6.46	96.14	102.60
2	2	72	C	C2'-C3'-O3'	6.46	119.19	109.50
20	R	15	PHE	CA-CB-CG	6.45	120.25	113.80
2	2	74	G	O4'-C1'-N9	6.36	118.04	108.50
2	2	654	A	C4'-C3'-C2'	-6.36	96.25	102.60
2	2	915	A	O4'-C1'-N9	6.33	117.69	108.20
2	2	1831	G	C2'-C3'-O3'	-6.28	104.27	113.70
2	2	614	C	C5'-C4'-C3'	-6.27	106.60	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1549	C	C3'-C2'-C1'	6.26	107.56	101.30
33	e	19	ARG	NE-CZ-NH2	6.24	124.81	119.20
12	J	94	PHE	CA-CB-CG	6.22	120.02	113.80
2	2	987	G	O4'-C4'-C3'	6.19	110.19	104.00
24	V	121	ARG	NE-CZ-NH2	6.18	124.77	119.20
1	1	34	C	C4'-C3'-O3'	-6.17	103.74	113.00
2	2	541	U	C5'-C4'-C3'	-6.13	106.80	116.00
2	2	746	C	C4'-C3'-C2'	-6.10	96.50	102.60
2	2	1550	U	C3'-C2'-C1'	-6.07	95.43	101.50
10	H	151	ARG	NE-CZ-NH2	6.03	124.62	119.20
38	k	323	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	2	1207	G	C5'-C4'-C3'	-6.02	106.97	116.00
37	j	24	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	1	41	C	C3'-C2'-C1'	6.00	107.30	101.30
2	2	1549	C	C5'-C4'-C3'	-5.98	107.03	116.00
2	2	820	C	C4'-C3'-C2'	-5.98	96.62	102.60
37	j	82	ARG	NE-CZ-NH2	5.96	124.57	119.20
2	2	1106	G	C5'-C4'-C3'	-5.96	107.06	116.00
10	H	139	ASP	O-C-N	-5.96	114.78	122.94
31	c	61	THR	CA-C-N	5.95	128.77	122.11
31	c	61	THR	C-N-CA	5.95	128.77	122.11
38	k	28	SER	N-CA-C	5.93	117.41	110.41
2	2	1305	C	C4'-C3'-C2'	-5.92	96.68	102.60
20	R	44	ARG	NE-CZ-NH2	5.92	124.53	119.20
14	L	156	HIS	CB-CA-C	5.87	118.54	109.03
7	E	171	HIS	CB-CG-CD2	-5.85	123.59	131.20
19	Q	65	ASP	CA-CB-CG	5.83	118.43	112.60
2	2	1054	A	O4'-C1'-N9	5.82	117.24	108.50
2	2	1120	C	C3'-C2'-C1'	5.81	107.11	101.30
2	2	1120	C	C5'-C4'-C3'	-5.80	107.30	116.00
38	k	469	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	2	1550	U	O4'-C1'-C2'	-5.76	100.04	105.80
14	L	80	ARG	NE-CZ-NH2	5.76	124.38	119.20
2	2	38	A	N9-C1'-C2'	-5.75	105.37	114.00
2	2	1325	U	C4'-C3'-C2'	-5.75	96.86	102.60
1	1	29	G	C4'-C3'-C2'	-5.74	96.86	102.60
2	2	1237	A	C3'-C2'-C1'	5.73	107.03	101.30
2	2	76	U	C4'-C3'-C2'	-5.72	96.88	102.60
2	2	498	A	C5'-C4'-C3'	-5.67	107.49	116.00
29	a	63	HIS	CB-CG-CD2	-5.64	123.87	131.20
2	2	428	G	C5'-C4'-C3'	-5.63	107.56	116.00
38	k	446	MET	N-CA-C	5.63	118.27	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	987	G	C3'-C2'-C1'	5.62	106.92	101.30
2	2	841	G	C4'-C3'-C2'	-5.62	96.98	102.60
13	K	25	ARG	NE-CZ-NH2	5.62	124.25	119.20
2	2	1562	G	O4'-C1'-N9	5.59	116.88	108.50
5	C	151	ASP	CA-C-N	-5.55	111.70	122.70
5	C	151	ASP	C-N-CA	-5.55	111.70	122.70
14	L	26	ASP	CA-CB-CG	5.55	118.15	112.60
9	G	108	ARG	NE-CZ-NH2	5.52	124.17	119.20
13	K	146	GLN	OE1-CD-NE2	-5.50	117.09	122.60
2	2	71	G	C2'-C3'-O3'	5.50	117.75	109.50
14	L	45	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	2	1103	G	O3'-P-O5'	5.47	112.20	104.00
20	R	43	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	1	34	C	C5'-C4'-C3'	-5.46	107.80	116.00
30	b	15	ARG	NE-CZ-NH2	5.46	124.11	119.20
31	c	23	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	2	74	G	N9-C1'-C2'	-5.44	103.84	112.00
2	2	1570	G	C4'-C3'-C2'	-5.43	97.17	102.60
2	2	1054	A	C3'-C2'-C1'	5.43	106.73	101.30
18	P	19	ARG	NE-CZ-NH2	5.43	124.08	119.20
2	2	954	G	C5'-C4'-C3'	-5.42	107.87	116.00
2	2	1231	G	C4'-C3'-C2'	-5.42	97.19	102.60
19	Q	32	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	2	499	G	C4'-C3'-C2'	-5.39	97.20	102.60
2	2	954	G	C3'-C2'-C1'	5.39	106.69	101.30
38	k	324	PHE	CA-CB-CG	5.39	119.19	113.80
22	T	99	ASP	CA-C-N	5.38	126.57	119.84
22	T	99	ASP	C-N-CA	5.38	126.57	119.84
2	2	1684	C	C4'-C3'-C2'	-5.38	97.22	102.60
38	k	434	ASP	CA-CB-CG	5.37	117.97	112.60
5	C	53	ARG	NE-CZ-NH2	5.36	124.02	119.20
38	k	531	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	2	1321	G	O3'-P-O5'	-5.32	96.02	104.00
22	T	81	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	2	71	G	P-O3'-C3'	5.30	128.15	120.20
2	2	1792	C	C5'-C4'-C3'	-5.29	108.06	116.00
38	k	397	LYS	CB-CA-C	5.28	115.60	111.00
2	2	1056	A	O4'-C1'-C2'	-5.28	100.53	105.80
2	2	191	C	O4'-C4'-C3'	5.26	109.26	104.00
38	k	24	GLU	CA-C-N	5.25	127.27	120.44
38	k	24	GLU	C-N-CA	5.25	127.27	120.44
2	2	65	C	O4'-C4'-C3'	5.25	109.25	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	78	C	C2'-C3'-O3'	5.23	117.34	109.50
12	J	63	PHE	CA-CB-CG	5.23	119.03	113.80
37	j	23	LYS	N-CA-C	5.21	118.78	111.90
2	2	504	U	C4'-C3'-C2'	-5.20	97.40	102.60
2	2	200	U	C4'-C3'-C2'	-5.20	97.40	102.60
6	D	147	ASN	CA-C-N	5.20	130.97	122.65
6	D	147	ASN	C-N-CA	5.20	130.97	122.65
2	2	1380	C	C4'-C3'-C2'	-5.19	97.41	102.60
6	D	126	ASP	CA-CB-CG	5.19	117.79	112.60
7	E	164	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	2	539	C	O3'-P-O5'	-5.16	96.26	104.00
30	b	10	ARG	N-CA-CB	-5.16	103.04	111.66
3	3	49	A	O4'-C1'-N9	5.15	116.23	108.50
2	2	915	A	O4'-C1'-C2'	-5.14	100.66	105.80
13	K	28	GLU	CA-C-N	5.14	128.14	120.90
13	K	28	GLU	C-N-CA	5.14	128.14	120.90
12	J	168	HIS	CB-CG-CD2	-5.13	124.53	131.20
20	R	47	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	2	1121	C	C4'-C3'-C2'	-5.12	97.48	102.60
34	f	138	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	2	78	C	C3'-C2'-C1'	-5.12	96.38	101.50
11	I	132	ARG	NE-CZ-NH2	5.12	123.81	119.20
38	k	323	ARG	NE-CZ-NH1	-5.12	116.38	121.50
2	2	478	U	C4'-C3'-C2'	-5.11	97.49	102.60
2	2	1162	G	C4'-C3'-C2'	-5.11	97.49	102.60
2	2	1208	G	C4'-C3'-C2'	-5.10	97.50	102.60
11	I	142	ARG	NE-CZ-NH2	5.10	123.79	119.20
29	a	107	ARG	NE-CZ-NH2	5.10	123.79	119.20
21	S	146	ARG	NE-CZ-NH2	5.09	123.78	119.20
38	k	17	LYS	CB-CG-CD	5.09	123.01	111.30
2	2	1304	U	C5'-C4'-C3'	-5.09	107.57	115.20
4	A	54	ARG	NE-CZ-NH2	5.08	123.78	119.20
2	2	1343	U	C3'-C2'-C1'	5.08	106.38	101.30
37	j	62	ARG	NE-CZ-NH2	5.08	123.77	119.20
22	T	117	LEU	O-C-N	-5.08	117.94	123.52
2	2	596	G	C1'-O4'-C4'	-5.07	104.63	109.70
2	2	73	C	C4'-C3'-C2'	-5.07	97.53	102.60
28	Z	98	ASP	CA-CB-CG	5.07	117.67	112.60
2	2	78	C	C4'-C3'-C2'	-5.06	97.54	102.60
1	1	41	C	O3'-P-O5'	5.06	111.59	104.00
2	2	915	A	C3'-C2'-C1'	-5.06	96.44	101.50
2	2	73	C	P-O3'-C3'	5.05	127.78	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	100	PRO	CA-N-CD	-5.05	104.93	112.00
13	K	29	LEU	N-CA-C	5.05	117.36	110.24
2	2	954	G	O4'-C1'-N9	5.05	116.07	108.50
2	2	439	A	O4'-C1'-C2'	-5.04	100.75	105.80
2	2	341	G	C4'-C3'-C2'	-5.04	97.56	102.60
20	R	18	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	2	67	C	P-O3'-C3'	5.04	127.76	120.20
18	P	20	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	2	800	U	C4'-C3'-C2'	-5.02	97.58	102.60
10	H	70	ARG	CA-C-N	5.01	127.26	120.44
10	H	70	ARG	C-N-CA	5.01	127.26	120.44
2	2	395	G	C4'-C3'-C2'	-5.01	97.59	102.60
2	2	1511	G	C4'-C3'-C2'	-5.00	97.60	102.60

There are no chirality outliers.

All (156) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	32	C	Sidechain
2	2	1012	U	Sidechain
2	2	1052	U	Sidechain
2	2	1090	C	Sidechain
2	2	1104	G	Sidechain
2	2	1105	C	Sidechain
2	2	1154	G	Sidechain
2	2	1160	G	Sidechain
2	2	1161	G	Sidechain
2	2	1206	G	Sidechain
2	2	1212	C	Sidechain
2	2	1231	G	Sidechain
2	2	1236	A	Sidechain
2	2	1247	A	Sidechain
2	2	1253	G	Sidechain
2	2	1260	C	Sidechain
2	2	1280	A	Sidechain
2	2	1286	G	Sidechain
2	2	1289	A	Sidechain
2	2	1304	U	Sidechain
2	2	1322	U	Sidechain
2	2	1334	G	Sidechain
2	2	1339	U	Sidechain
2	2	1381	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	2	1382	A	Sidechain
2	2	1383	G	Sidechain
2	2	142	C	Sidechain
2	2	1454	G	Sidechain
2	2	146	G	Sidechain
2	2	1476	A	Sidechain
2	2	1480	A	Sidechain
2	2	1483	A	Sidechain
2	2	1486	G	Sidechain
2	2	1491	G	Sidechain
2	2	150	A	Sidechain
2	2	1510	G	Sidechain
2	2	1536	G	Sidechain
2	2	1548	C	Sidechain
2	2	1551	A	Sidechain
2	2	1552	C	Sidechain
2	2	1557	C	Sidechain
2	2	1558	G	Sidechain
2	2	1560	C	Sidechain
2	2	1561	G	Sidechain
2	2	1564	A	Sidechain
2	2	1566	G	Sidechain
2	2	1573	U	Sidechain
2	2	1574	A	Sidechain
2	2	1611	U	Sidechain
2	2	1612	G	Sidechain
2	2	1635	A	Sidechain
2	2	1655	C	Sidechain
2	2	1656	A	Sidechain
2	2	1697	G	Sidechain
2	2	170	A	Sidechain
2	2	1792	C	Sidechain
2	2	1816	A	Sidechain
2	2	1817	A	Sidechain
2	2	1818	A	Sidechain
2	2	1819	A	Sidechain
2	2	1832	U	Sidechain
2	2	1852	G	Sidechain
2	2	1853	A	Sidechain
2	2	1854	A	Sidechain
2	2	1860	A	Sidechain
2	2	191	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	2	193	C	Sidechain
2	2	198	U	Sidechain
2	2	26	U	Sidechain
2	2	306	C	Sidechain
2	2	307	G	Sidechain
2	2	338	A	Sidechain
2	2	339	A	Sidechain
2	2	357	U	Sidechain
2	2	360	G	Sidechain
2	2	370	G	Sidechain
2	2	371	C	Sidechain
2	2	373	G	Sidechain
2	2	377	C	Sidechain
2	2	38	A	Sidechain
2	2	422	G	Sidechain
2	2	428	G	Sidechain
2	2	434	G	Sidechain
2	2	436	G	Sidechain
2	2	44	U	Sidechain
2	2	45	A	Sidechain
2	2	456	G	Sidechain
2	2	470	G	Sidechain
2	2	472	G	Sidechain
2	2	483	A	Sidechain
2	2	493	C	Sidechain
2	2	496	G	Sidechain
2	2	497	G	Sidechain
2	2	512	A	Sidechain
2	2	518	A	Sidechain
2	2	541	U	Sidechain
2	2	561	U	Sidechain
2	2	564	A	Sidechain
2	2	570	U	Sidechain
2	2	572	U	Sidechain
2	2	580	A	Sidechain
2	2	604	G	Sidechain
2	2	605	C	Sidechain
2	2	606	A	Sidechain
2	2	615	G	Sidechain
2	2	625	G	Sidechain
2	2	629	C	Sidechain
2	2	654	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	2	67	C	Sidechain
2	2	69	C	Sidechain
2	2	70	G	Sidechain
2	2	71	G	Sidechain
2	2	74	G	Sidechain
2	2	75	G	Sidechain
2	2	76	U	Sidechain
2	2	78	C	Sidechain
2	2	784	G	Sidechain
2	2	785	G	Sidechain
2	2	79	A	Sidechain
2	2	80	G	Sidechain
2	2	800	U	Sidechain
2	2	819	U	Sidechain
2	2	820	C	Sidechain
2	2	841	G	Sidechain
2	2	910	U	Sidechain
2	2	914	U	Sidechain
2	2	916	A	Sidechain
2	2	954	G	Sidechain
2	2	957	G	Sidechain
2	2	959	A	Sidechain
2	2	97	U	Sidechain
2	2	987	G	Sidechain
3	3	49	A	Sidechain
4	A	88	ARG	Sidechain
5	C	41	ARG	Sidechain
7	E	171	HIS	Sidechain
9	G	100	ARG	Sidechain
10	H	86	ARG	Sidechain
11	I	132	ARG	Sidechain
11	I	154	ARG	Sidechain
11	I	170	ARG	Sidechain
13	K	11	ARG	Sidechain
13	K	21	TYR	Sidechain
13	K	5	ARG	Sidechain
19	Q	150	ARG	Mainchain
19	Q	98	ARG	Sidechain
24	V	102	ARG	Sidechain
24	V	79	TYR	Sidechain
27	Y	3	ARG	Sidechain
29	a	90	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
32	d	66	ARG	Sidechain
34	f	106	TYR	Sidechain
38	k	212	ARG	Sidechain
38	k	246	TYR	Sidechain
38	k	348	TYR	Sidechain
38	k	491	TYR	Sidechain

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	1	1617	0	821	0	0
2	2	37147	0	18655	431	0
3	3	192	0	99	0	0
4	A	2146	0	2191	91	0
5	C	1637	0	1641	30	0
6	D	1741	0	1815	27	0
7	E	1754	0	1834	28	0
8	F	1764	0	1863	57	0
9	G	2083	0	2189	33	0
10	H	1482	0	1534	20	0
11	I	1924	0	2089	23	0
12	J	1530	0	1627	26	0
13	K	1680	0	1762	46	0
14	L	1542	0	1659	19	0
15	M	828	0	854	11	0
16	N	1296	0	1374	22	0
17	O	958	0	993	16	0
18	P	1208	0	1294	26	0
19	Q	1016	0	1039	14	0
20	R	1154	0	1213	11	0
21	S	1124	0	1193	29	0
22	T	1019	0	1075	22	0
23	U	1194	0	1253	16	0
24	V	1113	0	1149	9	0
25	W	822	0	887	16	0
26	X	636	0	637	10	0
27	Y	1034	0	1080	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Z	1106	0	1179	8	0
29	a	1021	0	1085	13	0
30	b	789	0	839	15	0
31	c	659	0	683	8	0
32	d	506	0	536	9	0
33	e	444	0	442	4	0
34	f	582	0	599	8	0
35	g	2437	0	2393	55	0
36	i	464	0	511	3	0
37	j	874	0	893	6	0
38	k	4693	0	4826	88	0
39	l	240	0	289	5	0
40	n	598	0	656	22	0
41	2	220	0	0	0	0
41	3	3	0	0	0	0
41	G	2	0	0	0	0
41	I	2	0	0	0	0
41	K	1	0	0	0	0
41	L	1	0	0	0	0
41	Z	1	0	0	0	0
All	All	86284	0	68751	1175	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 (1175) 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)
7:E:247:THR:O	7:E:251:VAL:HG23	1.45	1.16
2:2:1417:A:N6	2:2:1423:C:N4	2.13	0.96
2:2:124:U:H3	2:2:330:C:N4	1.63	0.95
6:D:49:VAL:HG11	6:D:62:LEU:HD11	1.47	0.95
2:2:1407:G:N1	2:2:1431:C:N3	2.14	0.95
2:2:1276:G:H1	2:2:1313:U:H3	1.16	0.93
2:2:318:U:H2'	2:2:319:G:C8	2.03	0.92
2:2:1717:G:H1	2:2:1806:U:H3	1.17	0.91
2:2:1417:A:H61	2:2:1423:C:N4	1.69	0.90
4:A:103:THR:HA	4:A:106:LYS:HE2	1.53	0.88
2:2:1407:G:N2	2:2:1431:C:O2	2.06	0.88
40:n:112:ASN:HB3	40:n:114:LYS:HG2	1.55	0.86
2:2:515:A:N6	2:2:579:G:O6	2.06	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1417:A:N6	2:2:1423:C:C4	2.45	0.84
2:2:1747:C:N3	2:2:1775:A:N6	2.26	0.84
2:2:1344:G:H1	2:2:1377:G:H22	1.25	0.83
4:A:211:ALA:HB1	4:A:258:ILE:HG13	1.60	0.83
2:2:1374:A:OP2	5:C:102:ARG:NH1	2.11	0.83
2:2:1416:G:N1	2:2:1423:C:N3	2.27	0.82
2:2:832:G:N2	2:2:834:G:OP2	2.13	0.81
4:A:180:ILE:O	4:A:184:LEU:N	2.11	0.81
2:2:1416:G:N2	2:2:1423:C:O2	2.10	0.81
6:D:144:LYS:HB2	6:D:208:HIS:HB3	1.62	0.80
2:2:740:G:O2'	2:2:741:C:OP1	1.99	0.80
38:k:292:VAL:HG23	38:k:295:ALA:HB3	1.62	0.79
25:W:19:ARG:HG2	25:W:119:ALA:HB3	1.65	0.79
7:E:231:ASP:OD1	7:E:231:ASP:N	2.16	0.79
2:2:985:C:OP2	6:D:155:TYR:OH	2.00	0.78
26:X:3:ASN:ND2	26:X:7:GLU:OE1	2.15	0.78
2:2:1407:G:N2	2:2:1431:C:C2	2.51	0.78
4:A:123:LYS:HD2	4:A:125:GLU:HB3	1.64	0.78
12:J:37:LYS:O	12:J:41:ARG:NH2	2.17	0.77
2:2:1503:G:OP2	34:f:93:HIS:NE2	2.18	0.77
40:n:68:ILE:HB	40:n:109:TYR:HB2	1.66	0.77
10:H:219:ARG:NE	32:d:60:GLU:OE2	2.16	0.77
2:2:164:A:H3'	2:2:165:G:H21	1.49	0.76
18:P:32:ASP:OD1	18:P:32:ASP:N	2.18	0.76
2:2:683:G:O6	2:2:732:C:N4	2.19	0.76
30:b:23:CYS:SG	30:b:74:CYS:N	2.52	0.75
2:2:550:A:OP2	14:L:177:ASN:ND2	2.20	0.75
12:J:8:ILE:HA	12:J:15:LYS:HE2	1.66	0.75
8:F:67:ARG:HD2	15:M:93:THR:HG23	1.68	0.75
17:O:78:LYS:NZ	17:O:80:ASP:OD1	2.19	0.75
40:n:98:LYS:NZ	40:n:112:ASN:OD1	2.19	0.75
2:2:1417:A:C6	2:2:1423:C:C4	2.75	0.74
2:2:1267:C:O2	33:e:5:GLN:NE2	2.20	0.74
38:k:492:LEU:HB2	38:k:497:ARG:HG3	1.69	0.73
2:2:1449:C:H42	2:2:1472:A:H61	1.36	0.73
4:A:25:ARG:NH1	4:A:43:GLU:OE1	2.22	0.73
35:g:249:CYS:SG	35:g:291:TRP:NE1	2.61	0.73
10:H:96:ARG:O	10:H:97:ASN:ND2	2.21	0.72
4:A:29:GLU:HG2	4:A:30:MET:HG3	1.71	0.72
38:k:567:ARG:NH2	38:k:578:ASN:OD1	2.23	0.72
21:S:31:LEU:HD21	21:S:69:ARG:HH22	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:487:GLU:HG3	38:k:490:ALA:HB2	1.71	0.72
7:E:221:ILE:O	7:E:224:THR:OG1	2.08	0.71
2:2:577:A:OP2	14:L:172:ARG:NH2	2.23	0.71
38:k:486:ASP:HA	38:k:518:VAL:HB	1.71	0.71
2:2:966:G:OP1	2:2:966:G:N2	2.23	0.71
4:A:114:HIS:HA	4:A:117:GLU:HG3	1.73	0.71
13:K:110:ARG:NH2	13:K:122:GLY:O	2.22	0.71
16:N:147:LYS:NZ	16:N:149:ALA:O	2.23	0.71
25:W:33:GLU:OE1	25:W:87:ARG:NH2	2.24	0.71
6:D:34:LYS:O	6:D:98:THR:OG1	2.09	0.71
38:k:559:LEU:O	38:k:563:GLU:N	2.22	0.70
2:2:1408:C:H3'	2:2:1409:G:H8	1.55	0.70
4:A:231:ALA:HB3	4:A:234:ARG:HB2	1.73	0.70
4:A:175:VAL:HG22	4:A:179:ASN:HD21	1.56	0.70
2:2:126:G:O6	11:I:196:LYS:NZ	2.23	0.70
38:k:565:THR:OG1	38:k:588:GLN:OE1	2.10	0.70
8:F:170:THR:HG22	8:F:187:LYS:HG2	1.73	0.69
2:2:182:C:OP1	2:2:183:G:N2	2.25	0.69
2:2:409:G:O3'	27:Y:88:LYS:NZ	2.25	0.69
4:A:157:VAL:HG11	4:A:180:ILE:HB	1.73	0.69
2:2:899:A:H2'	2:2:900:A:C8	2.27	0.69
2:2:920:G:OP2	18:P:3:ARG:NH2	2.26	0.69
38:k:24:GLU:OE1	38:k:24:GLU:N	2.26	0.69
2:2:1413:C:N3	2:2:1415:C:N4	2.41	0.69
4:A:193:ALA:HB3	4:A:236:VAL:HA	1.74	0.69
35:g:31:ILE:HG23	35:g:43:TRP:HB2	1.74	0.69
2:2:740:G:H1'	12:J:109:ARG:HB2	1.74	0.68
4:A:84:ASP:OD1	10:H:213:ARG:NH2	2.26	0.68
35:g:35:SER:OG	35:g:36:ARG:N	2.26	0.68
2:2:318:U:H2'	2:2:319:G:H8	1.53	0.68
2:2:1731:G:H2'	2:2:1732:G:H8	1.57	0.68
38:k:271:VAL:HG21	38:k:282:LEU:HD12	1.75	0.68
2:2:828:G:O2'	9:G:261:SER:O	2.10	0.68
2:2:902:U:H2'	2:2:903:G:C8	2.27	0.68
35:g:187:ASN:O	35:g:188:HIS:ND1	2.27	0.68
18:P:87:ASP:OD1	18:P:87:ASP:N	2.18	0.68
2:2:411:G:O3'	16:N:98:LYS:NZ	2.27	0.67
2:2:829:C:O2'	9:G:263:GLY:OXT	2.11	0.67
29:a:12:PHE:HZ	29:a:21:LYS:HE2	1.59	0.67
6:D:105:LEU:HD13	6:D:213:ARG:HA	1.75	0.67
8:F:64:ARG:NH1	15:M:95:ARG:O	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:526:A:H62	2:2:537:G:H21	1.40	0.67
2:2:632:U:O4	36:i:107:LYS:NZ	2.23	0.67
18:P:142:GLU:O	18:P:146:ALA:N	2.28	0.67
2:2:526:A:H62	2:2:537:G:N2	1.92	0.67
2:2:308:C:H5	11:I:183:ARG:HH12	1.42	0.67
6:D:139:CYS:SG	6:D:140:VAL:N	2.67	0.67
13:K:84:ASN:HD22	13:K:90:LEU:HB2	1.60	0.67
38:k:582:SER:HB2	38:k:585:ASP:H	1.58	0.67
2:2:579:G:N2	2:2:581:U:O2	2.28	0.66
18:P:35:GLU:HG3	18:P:39:LYS:HE3	1.76	0.66
2:2:649:G:HO2'	2:2:652:G:HO2'	1.38	0.66
9:G:11:ARG:NH2	9:G:21:ASP:OD1	2.29	0.66
29:a:94:HIS:O	29:a:94:HIS:ND1	2.27	0.66
12:J:126:HIS:HD2	12:J:183:LYS:HE2	1.60	0.66
35:g:176:VAL:HG13	35:g:185:LYS:HB3	1.78	0.66
2:2:1643:G:N2	2:2:1670:A:OP2	2.22	0.66
5:C:10:MET:HE3	5:C:15:VAL:HG22	1.78	0.66
13:K:117:TYR:HD1	13:K:152:ARG:HB3	1.60	0.66
2:2:668:U:OP1	18:P:127:ARG:NH1	2.29	0.66
12:J:50:GLU:HB2	12:J:60:ILE:HG22	1.78	0.66
13:K:57:ALA:HB2	13:K:183:GLY:HA2	1.78	0.66
9:G:168:LYS:NZ	11:I:205:GLU:OE2	2.25	0.66
2:2:124:U:H3	2:2:330:C:H42	0.82	0.65
35:g:174:VAL:HB	35:g:188:HIS:HB2	1.76	0.65
2:2:1306:U:H5''	34:f:130:VAL:HG23	1.79	0.65
5:C:42:LYS:HG3	5:C:48:ILE:HD11	1.78	0.65
2:2:1417:A:C6	2:2:1423:C:N3	2.65	0.65
14:L:18:ARG:O	14:L:24:ARG:NH2	2.30	0.65
19:Q:16:SER:OG	19:Q:87:GLU:O	2.15	0.65
4:A:142:TYR:HB3	4:A:147:TYR:HB2	1.78	0.65
5:C:165:ASN:HA	5:C:171:VAL:HG22	1.77	0.65
2:2:1731:G:H2'	2:2:1732:G:C8	2.31	0.65
35:g:237:ASN:ND2	35:g:286:CYS:O	2.27	0.65
38:k:363:ALA:HB3	38:k:544:VAL:HG22	1.79	0.65
8:F:50:ILE:HG22	8:F:88:ALA:HA	1.79	0.64
29:a:55:ILE:HG12	29:a:75:ILE:HG12	1.79	0.64
4:A:74:ILE:HG13	4:A:75:ARG:HG3	1.79	0.64
2:2:1751:G:H1	2:2:1769:U:H3	1.45	0.64
35:g:252:THR:OG1	35:g:255:SER:O	2.15	0.64
2:2:1245:C:C2'	2:2:1246:A:OP1	2.46	0.64
2:2:1668:U:OP2	21:S:17:LYS:NZ	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1098:G:H22	2:2:1126:G:N2	1.96	0.64
2:2:1688:G:H21	2:2:1828:A:H8	1.44	0.64
2:2:681:U:H3	2:2:733:G:H1	1.46	0.64
2:2:1167:G:O2'	2:2:1183:G:O6	2.16	0.64
2:2:649:G:O2'	2:2:652:G:O2'	2.10	0.63
38:k:456:ASP:N	38:k:456:ASP:OD1	2.29	0.63
4:A:7:ARG:HA	4:A:40:ASN:HD21	1.62	0.63
7:E:99:THR:O	7:E:122:LYS:NZ	2.31	0.63
35:g:40:ILE:HD11	35:g:59:LEU:HD12	1.80	0.63
40:n:45:ASN:O	40:n:46:ASN:ND2	2.31	0.63
2:2:1413:C:H2'	2:2:1415:C:H5	1.64	0.63
2:2:1415:C:O4'	24:V:4:VAL:N	2.31	0.63
38:k:389:ILE:HD12	38:k:389:ILE:H	1.63	0.63
2:2:876:G:OP2	2:2:876:G:N2	2.25	0.63
2:2:1450:A:N6	22:T:1:MET:SD	2.71	0.63
4:A:118:VAL:HG23	4:A:119:LEU:HD12	1.81	0.63
38:k:487:GLU:OE2	38:k:490:ALA:N	2.32	0.62
2:2:533:C:H3'	2:2:534:G:H8	1.65	0.62
2:2:1414:C:O2'	2:2:1416:G:OP2	2.12	0.62
17:O:55:ASN:ND2	17:O:57:ASP:O	2.32	0.62
2:2:317:G:H1'	2:2:318:U:C6	2.34	0.62
2:2:1414:C:N4	2:2:1421:G:OP2	2.24	0.62
35:g:159:ASN:OD1	35:g:160:SER:N	2.33	0.62
4:A:120:GLU:O	4:A:126:GLN:NE2	2.33	0.62
2:2:578:G:H4'	2:2:579:G:H5'	1.82	0.62
2:2:220:C:H2'	2:2:221:A:C8	2.35	0.61
2:2:847:C:O2'	2:2:848:G:N2	2.33	0.61
2:2:1408:C:H42	2:2:1430:C:H42	1.46	0.61
2:2:744:C:H2'	2:2:745:U:C2	2.34	0.61
2:2:1344:G:H22	2:2:1377:G:N2	1.98	0.61
8:F:166:TYR:HD2	8:F:167:TYR:HD2	1.48	0.61
25:W:20:ILE:HD13	25:W:98:VAL:HG21	1.82	0.61
16:N:35:ARG:HH22	16:N:55:TYR:H	1.48	0.61
2:2:1195:A:H5''	30:b:2:THR:HB	1.82	0.61
4:A:151:ASP:O	4:A:155:HIS:ND1	2.33	0.61
4:A:109:TYR:HE1	4:A:113:ARG:HH11	1.48	0.61
12:J:109:ARG:O	12:J:113:LYS:NZ	2.26	0.61
9:G:262:SER:OG	9:G:263:GLY:N	2.33	0.61
2:2:545:A:H2'	2:2:546:U:C1'	2.31	0.61
2:2:977:A:H2'	2:2:978:G:C8	2.36	0.61
5:C:33:GLN:NE2	26:X:63:GLY:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:2:GLN:NE2	26:X:6:GLY:O	2.31	0.61
2:2:868:A:O2'	2:2:869:G:O5'	2.19	0.61
4:A:36:LEU:HD12	4:A:42:ILE:HG23	1.83	0.61
4:A:100:ASP:OD1	4:A:101:LYS:N	2.34	0.61
14:L:89:GLU:CD	14:L:89:GLU:H	2.05	0.61
5:C:156:TYR:OH	26:X:61:ARG:NH2	2.34	0.60
38:k:238:PHE:HE1	38:k:267:ARG:HD2	1.67	0.60
2:2:1135:C:H2'	2:2:1136:G:O4'	2.01	0.60
2:2:1281:G:H21	34:f:101:ALA:C	2.09	0.60
6:D:137:LEU:HG	6:D:215:VAL:HG22	1.83	0.60
8:F:214:LYS:HG3	8:F:215:ASP:H	1.66	0.60
2:2:1029:G:N1	2:2:1076:A:O2'	2.28	0.60
4:A:226:LYS:HB2	4:A:238:THR:HB	1.83	0.60
7:E:35:LYS:HD2	7:E:35:LYS:O	2.02	0.60
2:2:581:U:O2'	2:2:582:C:H3'	2.02	0.60
2:2:1750:C:H2'	2:2:1751:G:H8	1.66	0.60
12:J:5:SER:OG	12:J:6:ALA:N	2.35	0.60
14:L:87:LEU:HD13	14:L:100:LEU:HD11	1.84	0.60
2:2:1857:A:OP2	30:b:4:LYS:NZ	2.34	0.60
20:R:88:GLU:N	20:R:88:GLU:OE1	2.34	0.60
2:2:275:C:N3	2:2:887:G:O2'	2.33	0.60
2:2:1224:A:H2'	2:2:1225:G:C8	2.37	0.60
13:K:128:LYS:HE2	13:K:128:LYS:H	1.67	0.60
19:Q:53:ILE:HG22	19:Q:54:CYS:H	1.66	0.59
27:Y:84:LYS:NZ	27:Y:85:ASP:OD1	2.35	0.59
16:N:18:GLN:O	16:N:20:LYS:NZ	2.24	0.59
38:k:250:LYS:HG2	38:k:564:ILE:HD11	1.84	0.59
2:2:107:A:H2'	2:2:108:G:C8	2.36	0.59
2:2:544:A:H2'	2:2:545:A:C8	2.38	0.59
38:k:105:VAL:HG22	38:k:269:ILE:HD13	1.84	0.59
38:k:256:ALA:HA	38:k:282:LEU:HD23	1.83	0.59
2:2:1716:U:H4'	2:2:1717:G:H5''	1.83	0.59
21:S:100:VAL:HG12	21:S:101:ASP:H	1.68	0.59
22:T:57:LEU:HD13	22:T:69:ILE:HD11	1.84	0.59
2:2:744:C:H42	2:2:790:A:H61	1.50	0.59
8:F:211:VAL:O	22:T:20:TYR:OH	2.18	0.59
38:k:565:THR:HG23	38:k:578:ASN:HB2	1.83	0.59
4:A:130:LEU:HA	4:A:133:ARG:HE	1.68	0.59
2:2:868:A:O2'	2:2:869:G:O4'	2.21	0.58
2:2:1688:G:N2	2:2:1828:A:H8	2.01	0.58
13:K:117:TYR:CD1	13:K:152:ARG:HB3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:15:LYS:HE2	38:k:17:LYS:HB2	1.85	0.58
38:k:551:LEU:HD23	38:k:551:LEU:H	1.68	0.58
4:A:256:ALA:HA	4:A:259:LYS:HE3	1.84	0.58
2:2:1141:A:O3'	30:b:89:ARG:NH1	2.36	0.58
2:2:1406:C:C2	2:2:1407:G:N7	2.72	0.58
2:2:486:C:OP1	9:G:49:ARG:NH1	2.36	0.58
23:U:22:GLY:HA2	23:U:56:ALA:HB3	1.84	0.58
2:2:1179:A:OP1	39:l:15:ARG:NH1	2.36	0.58
22:T:106:LEU:O	22:T:110:ASP:N	2.36	0.58
40:n:70:PRO:O	40:n:74:SER:OG	2.19	0.58
38:k:420:SER:HB3	38:k:427:LEU:HD13	1.86	0.58
20:R:61:ARG:C	20:R:63:ALA:H	2.11	0.58
21:S:25:CYS:HB2	21:S:68:ILE:HG12	1.85	0.58
21:S:29:ASN:N	21:S:29:ASN:OD1	2.35	0.58
2:2:215:U:O2	13:K:184:ARG:NH2	2.33	0.58
2:2:1584:A:N3	2:2:1648:U:O2'	2.36	0.58
2:2:1526:A:OP1	24:V:84:ARG:NH1	2.37	0.57
2:2:1461:A:O3'	22:T:10:LYS:NZ	2.37	0.57
16:N:147:LYS:HG2	16:N:153:LYS:HG3	1.86	0.57
2:2:206:A:H2'	2:2:207:U:O4'	2.04	0.57
15:M:74:GLU:OE1	15:M:74:GLU:N	2.34	0.57
7:E:251:VAL:O	7:E:252:LYS:O	2.21	0.57
22:T:27:ASP:O	22:T:31:ASN:ND2	2.32	0.57
26:X:55:ILE:HG23	26:X:59:ILE:HD11	1.87	0.57
38:k:418:PRO:HG3	38:k:467:LEU:HD11	1.87	0.57
2:2:1277:G:H2'	2:2:1278:A:H8	1.69	0.57
2:2:1535:G:OP2	24:V:43:LYS:NZ	2.36	0.57
4:A:111:ILE:HG22	4:A:112:LEU:HD12	1.87	0.57
2:2:545:A:H2'	2:2:546:U:O4'	2.04	0.57
2:2:740:G:H2'	2:2:741:C:O4'	2.03	0.56
2:2:1412:C:H2'	2:2:1413:C:C6	2.41	0.56
4:A:124:ASP:HA	4:A:127:LEU:HD23	1.86	0.56
2:2:1419:C:H1'	2:2:1420:G:C8	2.40	0.56
7:E:181:ILE:HD12	7:E:192:LEU:HD23	1.86	0.56
38:k:568:ARG:NH2	38:k:573:TYR:O	2.38	0.56
2:2:1245:C:O2'	2:2:1246:A:OP1	2.21	0.56
35:g:165:ILE:HG13	35:g:177:TRP:HB2	1.88	0.56
2:2:31:U:OP1	28:Z:137:LYS:NZ	2.39	0.56
8:F:218:LEU:N	8:F:219:PRO:HD2	2.20	0.56
35:g:116:ASP:OD1	35:g:116:ASP:N	2.38	0.56
2:2:832:G:H2'	2:2:833:A:N7	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:552:LEU:HD23	38:k:552:LEU:H	1.71	0.56
2:2:681:U:H2'	2:2:682:G:C8	2.41	0.56
2:2:1774:G:H2'	2:2:1775:A:C8	2.41	0.56
33:e:4:GLN:HG3	33:e:5:GLN:H	1.70	0.56
4:A:175:VAL:HG22	4:A:179:ASN:ND2	2.20	0.56
5:C:103:PHE:O	5:C:104:THR:OG1	2.24	0.56
2:2:1426:C:N4	2:2:1427:G:O6	2.39	0.56
2:2:208:G:H2'	2:2:209:C:C6	2.40	0.56
2:2:868:A:H2'	2:2:869:G:C8	2.40	0.56
38:k:166:ALA:HA	38:k:237:ILE:HG23	1.87	0.56
2:2:879:U:H2'	2:2:880:C:C6	2.41	0.55
2:2:921:G:H1	2:2:1013:U:H3	1.53	0.55
14:L:89:GLU:OE1	14:L:89:GLU:N	2.38	0.55
38:k:338:ASN:OD1	38:k:338:ASN:N	2.39	0.55
38:k:494:SER:HA	38:k:497:ARG:HH11	1.72	0.55
2:2:837:G:OP2	29:a:14:THR:HG22	2.07	0.55
23:U:51:ASP:OD1	23:U:52:LEU:N	2.39	0.55
37:j:50:MET:HE1	37:j:54:GLY:HA2	1.88	0.55
2:2:147:A:O2'	2:2:148:U:OP2	2.22	0.55
6:D:57:ILE:HD12	6:D:60:ASP:H	1.70	0.55
2:2:1411:C:H2'	2:2:1412:C:C6	2.41	0.55
2:2:1418:G:H22	2:2:1420:G:H3'	1.70	0.55
6:D:107:ARG:NH1	19:Q:133:THR:O	2.32	0.55
13:K:48:VAL:HG22	13:K:52:ASN:O	2.07	0.55
6:D:44:ILE:HD12	6:D:69:VAL:HG21	1.89	0.55
21:S:19:ALA:HB2	21:S:75:GLY:HA3	1.87	0.55
2:2:533:C:H3'	2:2:534:G:C8	2.42	0.55
8:F:106:ARG:NH2	8:F:174:HIS:O	2.40	0.55
17:O:58:GLU:HG3	17:O:60:MET:H	1.72	0.55
28:Z:4:CYS:HB2	28:Z:9:THR:HG21	1.88	0.55
29:a:50:THR:OG1	29:a:51:THR:N	2.40	0.55
2:2:847:C:H5''	2:2:848:G:H5'	1.89	0.55
2:2:1115:A:O2'	31:c:72:ARG:NH2	2.40	0.55
4:A:69:GLU:OE2	4:A:70:CYS:N	2.36	0.55
20:R:74:GLU:HG2	20:R:75:VAL:H	1.71	0.55
2:2:182:C:N3	2:2:184:G:N1	2.55	0.54
2:2:897:G:H2'	2:2:898:G:C8	2.42	0.54
2:2:1406:C:H2'	2:2:1407:G:C8	2.41	0.54
2:2:217:U:H5'	13:K:177:SER:OG	2.08	0.54
2:2:896:C:H2'	2:2:897:G:H8	1.73	0.54
2:2:897:G:H2'	2:2:898:G:H8	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1407:G:C2	2:2:1432:C:C2	2.95	0.54
4:A:200:TYR:HB2	4:A:269:PHE:CZ	2.43	0.54
9:G:18:TRP:HH2	9:G:31:PRO:HD3	1.72	0.54
20:R:74:GLU:OE1	20:R:74:GLU:N	2.25	0.54
2:2:965:U:O2	6:D:20:LYS:NZ	2.40	0.54
9:G:220:THR:HG22	9:G:221:ARG:H	1.72	0.54
2:2:1717:G:O6	2:2:1806:U:O4	2.24	0.54
2:2:1774:G:H2'	2:2:1775:A:H8	1.72	0.54
11:I:84:TYR:OH	11:I:91:GLU:OE1	2.25	0.54
2:2:1392:A:O2'	2:2:1394:G:N7	2.38	0.54
16:N:20:LYS:C	16:N:21:LYS:HD2	2.33	0.54
2:2:1407:G:C2	2:2:1431:C:O2	2.61	0.54
32:d:37:ASP:OD1	32:d:37:ASP:N	2.40	0.54
38:k:248:ASP:O	38:k:252:ARG:HG3	2.08	0.54
2:2:155:G:H4'	11:I:15:LEU:HD13	1.89	0.54
4:A:14:PRO:HB3	4:A:39:TYR:CE1	2.42	0.54
21:S:93:VAL:HG21	21:S:109:LYS:HG3	1.90	0.54
11:I:49:VAL:HG12	11:I:115:LYS:HB3	1.90	0.54
2:2:728:U:H5''	2:2:729:C:C5	2.43	0.54
2:2:1701:G:H2'	2:2:1702:U:C6	2.43	0.54
5:C:128:ARG:NH1	5:C:153:PRO:HD3	2.23	0.54
10:H:177:ALA:HB2	10:H:187:CYS:SG	2.48	0.54
25:W:106:ILE:HD12	25:W:108:PRO:HD2	1.90	0.54
34:f:102:VAL:HG12	34:f:103:LEU:HB2	1.89	0.54
13:K:113:TYR:CD2	13:K:121:LEU:HG	2.43	0.54
14:L:181:GLY:HA2	14:L:185:ALA:HB3	1.90	0.54
22:T:47:ARG:HH11	22:T:48:ASN:HD21	1.54	0.54
35:g:56:GLN:HG3	35:g:57:ARG:HG3	1.90	0.54
38:k:106:LEU:HD23	38:k:270:ILE:HG23	1.88	0.54
13:K:84:ASN:HD21	13:K:90:LEU:HD12	1.73	0.53
17:O:61:TYR:O	17:O:65:VAL:HG13	2.08	0.53
38:k:192:ASP:OD2	38:k:232:ILE:HG13	2.08	0.53
2:2:1316:G:H2'	2:2:1317:G:O4'	2.08	0.53
2:2:1805:C:H2'	2:2:1806:U:C6	2.43	0.53
2:2:902:U:H2'	2:2:903:G:H8	1.70	0.53
2:2:1406:C:H2'	2:2:1407:G:H8	1.73	0.53
2:2:1427:G:HO2'	2:2:1428:U:P	2.32	0.53
35:g:24:THR:HG22	35:g:26:GLN:HG2	1.90	0.53
35:g:91:ASP:OD1	35:g:93:THR:OG1	2.26	0.53
2:2:127:C:O2'	2:2:212:G:OP2	2.24	0.53
2:2:794:G:N7	12:J:109:ARG:HA	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:832:G:H3'	2:2:832:G:N3	2.24	0.53
2:2:1223:G:C2	2:2:1224:A:C8	2.97	0.53
5:C:128:ARG:NH1	5:C:151:ASP:O	2.35	0.53
8:F:101:GLN:HG3	8:F:126:ILE:HG21	1.89	0.53
16:N:119:ASP:OD1	16:N:119:ASP:N	2.41	0.53
18:P:54:LEU:HD23	18:P:58:HIS:HD2	1.72	0.53
38:k:105:VAL:HA	38:k:269:ILE:HG23	1.89	0.53
2:2:906:G:O2'	2:2:907:C:O5'	2.25	0.53
2:2:1407:G:N1	2:2:1432:C:N3	2.56	0.53
7:E:181:ILE:HD12	7:E:192:LEU:CD2	2.38	0.53
38:k:587:GLU:O	38:k:590:LYS:HG3	2.07	0.53
21:S:130:LYS:HG2	21:S:131:LYS:N	2.23	0.53
2:2:732:C:H2'	2:2:733:G:C8	2.44	0.53
16:N:82:MET:HE3	16:N:85:THR:HG23	1.91	0.53
16:N:120:VAL:HG12	16:N:145:VAL:HG11	1.91	0.53
2:2:1803:A:H2'	2:2:1804:U:C6	2.44	0.53
8:F:210:ILE:HG13	22:T:39:ALA:HB2	1.91	0.53
11:I:19:ASP:OD1	11:I:19:ASP:N	2.41	0.53
11:I:215:LYS:C	11:I:215:LYS:HZ2	2.17	0.53
2:2:1110:U:H3	2:2:1115:A:H61	1.57	0.52
10:H:179:ARG:HH12	40:n:41:ARG:HD2	1.74	0.52
2:2:745:U:H2'	2:2:746:C:C6	2.44	0.52
6:D:121:ILE:HD12	6:D:207:LEU:HD11	1.91	0.52
9:G:158:ASP:OD2	9:G:174:LYS:HD2	2.10	0.52
2:2:794:G:H3'	2:2:795:U:H5'	1.91	0.52
2:2:873:C:H2'	2:2:874:G:H5''	1.92	0.52
5:C:32:PHE:HD1	5:C:32:PHE:H	1.56	0.52
21:S:100:VAL:HG12	21:S:101:ASP:OD1	2.09	0.52
2:2:220:C:H2'	2:2:221:A:H8	1.74	0.52
2:2:1766:C:H2'	2:2:1767:C:C6	2.44	0.52
17:O:58:GLU:HG3	17:O:61:TYR:H	1.74	0.52
26:X:59:ILE:HA	26:X:62:MET:HG2	1.91	0.52
2:2:536:G:H2'	2:2:537:G:O4'	2.08	0.52
2:2:903:G:H2'	2:2:904:A:C8	2.44	0.52
2:2:1592:C:H4'	2:2:1598:G:C6	2.45	0.52
2:2:1721:G:H2'	2:2:1722:G:H8	1.75	0.52
6:D:144:LYS:CB	6:D:208:HIS:HB3	2.37	0.52
6:D:193:ILE:O	6:D:197:ILE:HG13	2.09	0.52
8:F:51:LEU:HD13	8:F:89:GLU:HB3	1.91	0.52
8:F:166:TYR:CD2	8:F:167:TYR:HD2	2.27	0.52
23:U:34:LYS:HE3	23:U:103:LEU:HD23	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:87:ARG:HH12	30:b:94:ASP:HB2	1.74	0.52
40:n:77:LEU:HB2	40:n:79:ILE:HG12	1.91	0.52
40:n:79:ILE:HD12	40:n:83:LEU:HD23	1.91	0.52
2:2:834:G:H5''	2:2:835:C:H5''	1.92	0.52
2:2:874:G:OP1	2:2:874:G:H3'	2.10	0.52
2:2:1098:G:H1	2:2:1126:G:H22	1.58	0.52
6:D:68:GLU:HG2	6:D:83:LYS:HE3	1.92	0.52
2:2:1447:G:OP1	22:T:32:LYS:NZ	2.34	0.52
2:2:1750:C:H2'	2:2:1751:G:C8	2.44	0.52
2:2:1771:G:H2'	2:2:1772:C:C6	2.44	0.52
5:C:38:ILE:HG21	5:C:47:TYR:HD2	1.74	0.52
21:S:15:ARG:HG2	21:S:20:THR:HG23	1.90	0.52
21:S:32:ILE:HG13	21:S:68:ILE:HB	1.92	0.52
38:k:474:LEU:O	38:k:478:LYS:HG2	2.09	0.52
2:2:1405:A:H61	2:2:1432:C:H42	1.57	0.52
2:2:1282:G:O6	17:O:36:ARG:HB3	2.10	0.52
2:2:1407:G:N1	2:2:1431:C:C2	2.76	0.52
15:M:72:THR:OG1	15:M:73:ASN:N	2.43	0.52
21:S:101:ASP:OD1	21:S:101:ASP:N	2.43	0.52
30:b:26:CYS:HB2	30:b:77:CYS:SG	2.50	0.52
21:S:97:GLN:HG3	21:S:105:LYS:HD3	1.93	0.51
38:k:579:LYS:C	38:k:581:ASN:H	2.19	0.51
2:2:313:C:H2'	2:2:315:C:C2	2.44	0.51
2:2:1417:A:N6	2:2:1423:C:H42	2.03	0.51
2:2:125:C:O2'	11:I:198:ARG:NH1	2.43	0.51
2:2:185:C:H2'	2:2:186:G:C8	2.44	0.51
2:2:225:C:H42	2:2:882:A:H2'	1.76	0.51
2:2:1407:G:C2	2:2:1431:C:C2	2.99	0.51
4:A:131:PHE:HE2	4:A:136:TRP:HE1	1.59	0.51
9:G:210:VAL:HG12	9:G:211:LYS:H	1.74	0.51
10:H:74:LYS:HG3	10:H:77:ARG:HH11	1.75	0.51
2:2:313:C:H5''	2:2:315:C:C4	2.46	0.51
2:2:1343:U:H2'	2:2:1344:G:C8	2.45	0.51
2:2:1408:C:H3'	2:2:1409:G:C8	2.40	0.51
4:A:20:VAL:O	4:A:70:CYS:HA	2.11	0.51
38:k:284:ASP:O	38:k:305:VAL:HG23	2.09	0.51
32:d:12:ALA:HB1	32:d:32:VAL:HB	1.91	0.51
4:A:199:CYS:SG	4:A:235:TYR:OH	2.69	0.51
21:S:21:ALA:HB2	21:S:72:VAL:HG13	1.92	0.51
38:k:468:GLN:HE22	38:k:488:PRO:HA	1.76	0.51
2:2:545:A:H2'	2:2:546:U:H1'	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:678:U:H3	12:J:102:PRO:HA	1.75	0.51
2:2:1419:C:O2'	2:2:1420:G:H5''	2.11	0.51
4:A:104:LYS:O	4:A:108:VAL:HG13	2.11	0.51
4:A:175:VAL:O	4:A:179:ASN:ND2	2.44	0.51
23:U:65:GLU:O	23:U:69:THR:HG23	2.10	0.51
24:V:5:THR:OG1	24:V:6:VAL:N	2.44	0.51
29:a:45:ALA:O	29:a:49:LYS:N	2.37	0.51
2:2:744:C:H42	2:2:790:A:N6	2.09	0.51
9:G:195:ILE:O	9:G:196:THR:HG22	2.11	0.51
2:2:280:G:OP1	9:G:155:LYS:NZ	2.32	0.51
2:2:1299:C:H2'	2:2:1300:U:C6	2.45	0.51
4:A:161:SER:O	4:A:165:SER:OG	2.28	0.51
6:D:29:ASP:N	6:D:29:ASP:OD1	2.43	0.51
6:D:107:ARG:NH1	19:Q:133:THR:H	2.09	0.51
21:S:25:CYS:SG	21:S:95:TYR:HB2	2.51	0.51
2:2:1327:C:H41	37:j:15:GLY:HA2	1.76	0.50
15:M:12:TYR:CD1	15:M:79:LEU:HD21	2.47	0.50
2:2:1008:A:H2'	2:2:1009:U:O4'	2.10	0.50
4:A:138:PHE:HA	4:A:141:LYS:HE2	1.93	0.50
35:g:147:HIS:NE2	35:g:167:SER:OG	2.44	0.50
2:2:524:G:H2'	2:2:525:G:C8	2.46	0.50
2:2:1625:A:H5''	23:U:37:GLY:H	1.76	0.50
10:H:197:LYS:O	10:H:197:LYS:NZ	2.36	0.50
2:2:1031:A:H2'	2:2:1032:A:O4'	2.11	0.50
2:2:1421:G:H2'	2:2:1422:U:C6	2.46	0.50
2:2:1732:G:H2'	2:2:1733:C:H6	1.75	0.50
4:A:123:LYS:HD2	4:A:125:GLU:CB	2.38	0.50
6:D:58:ALA:O	6:D:61:GLY:N	2.43	0.50
8:F:34:TYR:OH	8:F:37:VAL:HG22	2.10	0.50
13:K:125:LYS:HB2	13:K:128:LYS:NZ	2.26	0.50
35:g:40:ILE:HG12	35:g:59:LEU:HB2	1.93	0.50
40:n:58:LEU:O	40:n:61:GLU:HG3	2.11	0.50
10:H:210:GLU:O	10:H:214:VAL:HG23	2.11	0.50
13:K:88:ASN:O	13:K:91:VAL:HG22	2.12	0.50
35:g:197:THR:HG21	35:g:238:ALA:HA	1.94	0.50
2:2:29:G:H4'	28:Z:129:SER:OG	2.12	0.50
5:C:147:LEU:O	5:C:165:ASN:ND2	2.45	0.50
2:2:118:C:H1'	2:2:435:A:C5	2.47	0.50
2:2:465:C:H5''	14:L:1:MET:CE	2.41	0.50
2:2:1773:G:H2'	2:2:1774:G:C8	2.47	0.50
11:I:20:ASP:O	11:I:23:LYS:HG2	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:131:CYS:SG	16:N:141:ASN:HB2	2.51	0.50
18:P:25:TRP:CD2	31:c:82:LYS:HE3	2.47	0.50
20:R:31:GLU:CD	20:R:31:GLU:H	2.19	0.50
22:T:98:VAL:HG22	22:T:99:ASP:H	1.76	0.50
35:g:72:SER:OG	35:g:73:SER:N	2.44	0.50
11:I:49:VAL:HG13	11:I:114:VAL:HG13	1.94	0.50
15:M:86:PRO:O	15:M:89:ILE:HG22	2.12	0.50
25:W:61:LEU:O	25:W:81:GLN:HA	2.12	0.50
2:2:741:C:H2'	2:2:742:C:C6	2.46	0.49
2:2:1277:G:H2'	2:2:1278:A:C8	2.47	0.49
18:P:34:LYS:HE3	18:P:67:THR:HG21	1.94	0.49
34:f:126:CYS:HB3	34:f:130:VAL:HG11	1.93	0.49
38:k:333:VAL:O	38:k:335:GLU:HG2	2.12	0.49
39:l:1:MET:SD	39:l:1:MET:N	2.67	0.49
2:2:292:A:N3	13:K:73:THR:HG21	2.26	0.49
2:2:737:C:H3'	2:2:738:U:H5''	1.95	0.49
2:2:1615:A:O2'	20:R:40:ARG:NH1	2.45	0.49
8:F:40:ARG:NH2	8:F:49:ILE:HD11	2.26	0.49
8:F:72:VAL:HG13	15:M:20:VAL:HG21	1.93	0.49
37:j:12:ARG:HA	37:j:14:ARG:HD2	1.93	0.49
2:2:520:U:H2'	2:2:521:A:H8	1.77	0.49
2:2:907:C:O2'	2:2:908:C:H5'	2.13	0.49
2:2:1653:G:C5	2:2:1654:U:C5	3.00	0.49
4:A:216:LEU:HD13	4:A:240:THR:HB	1.94	0.49
4:A:240:THR:HG22	4:A:250:VAL:HG11	1.93	0.49
17:O:18:LEU:HD11	17:O:79:VAL:HG21	1.94	0.49
31:c:48:SER:OG	31:c:49:HIS:N	2.45	0.49
2:2:520:U:H2'	2:2:521:A:C8	2.48	0.49
2:2:1749:C:H2'	2:2:1750:C:C6	2.48	0.49
7:E:251:VAL:C	7:E:252:LYS:O	2.55	0.49
35:g:157:SER:OG	35:g:164:ILE:O	2.21	0.49
2:2:297:C:H42	13:K:41:ARG:HH11	1.59	0.49
2:2:546:U:C4	2:2:547:U:C2	3.01	0.49
7:E:69:GLU:OE1	7:E:69:GLU:N	2.45	0.49
8:F:214:LYS:CG	8:F:215:ASP:H	2.25	0.49
12:J:185:VAL:O	12:J:186:ASN:ND2	2.46	0.49
17:O:128:PHE:CD1	17:O:132:LYS:HE3	2.48	0.49
29:a:12:PHE:HE1	29:a:23:MET:HE3	1.78	0.49
32:d:36:ASP:OD1	32:d:36:ASP:N	2.43	0.49
35:g:223:GLU:HB3	35:g:225:LYS:NZ	2.27	0.49
35:g:234:ASP:OD1	35:g:234:ASP:N	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:445:A:H2'	2:2:446:C:C6	2.48	0.49
2:2:1403:U:H2'	2:2:1404:U:C6	2.47	0.49
27:Y:37:PHE:CE2	27:Y:103:VAL:HG11	2.47	0.49
2:2:1409:G:C2	2:2:1410:A:C4	3.01	0.49
5:C:120:ARG:HH22	7:E:244:GLN:HB2	1.77	0.49
4:A:92:PRO:O	4:A:96:ILE:HG12	2.13	0.49
8:F:35:SER:O	8:F:35:SER:OG	2.25	0.49
15:M:17:LYS:HB3	15:M:17:LYS:HE3	1.58	0.49
21:S:139:ALA:O	21:S:140:ARG:NE	2.37	0.49
38:k:322:LEU:HD21	38:k:324:PHE:CE1	2.48	0.49
2:2:939:U:C2	2:2:940:A:C8	3.01	0.49
4:A:190:LYS:H	4:A:244:ARG:HD3	1.77	0.49
17:O:52:LEU:HD22	17:O:65:VAL:HG21	1.94	0.49
19:Q:95:ILE:HD11	19:Q:126:ILE:HD12	1.95	0.49
21:S:63:PHE:CZ	21:S:92:LEU:HD22	2.48	0.49
2:2:794:G:H5'	2:2:796:U:OP2	2.13	0.48
4:A:181:ASN:OD1	4:A:182:ARG:HD2	2.13	0.48
23:U:50:ILE:HG22	23:U:51:ASP:O	2.13	0.48
35:g:154:VAL:HG12	35:g:167:SER:HB2	1.93	0.48
38:k:40:GLU:HB3	38:k:49:TRP:HB3	1.95	0.48
4:A:7:ARG:HA	4:A:40:ASN:ND2	2.26	0.48
5:C:102:ARG:HG2	5:C:102:ARG:HH21	1.78	0.48
8:F:33:GLY:O	8:F:53:THR:HG23	2.13	0.48
8:F:140:GLY:HA3	8:F:182:LEU:HD22	1.95	0.48
8:F:224:SER:HG	35:g:188:HIS:CE1	2.30	0.48
38:k:316:TYR:CE1	38:k:327:ALA:HB2	2.47	0.48
38:k:522:PHE:CE1	38:k:555:MET:HE1	2.48	0.48
2:2:833:A:H5'	29:a:47:MET:SD	2.53	0.48
2:2:878:U:H2'	2:2:879:U:H6	1.79	0.48
8:F:68:GLU:O	8:F:72:VAL:HG22	2.12	0.48
13:K:60:LEU:HD23	13:K:60:LEU:HA	1.63	0.48
2:2:320:G:N1	2:2:321:C:C4	2.80	0.48
2:2:1078:A:H5'	2:2:1837:G:H4'	1.96	0.48
2:2:1506:G:H2'	2:2:1506:G:N3	2.28	0.48
2:2:554:A:H2'	2:2:555:G:O4'	2.14	0.48
2:2:1741:U:H2'	2:2:1742:C:H6	1.78	0.48
12:J:105:THR:O	12:J:106:ARG:NE	2.47	0.48
15:M:86:PRO:O	15:M:88:GLU:N	2.46	0.48
23:U:52:LEU:HD12	23:U:52:LEU:HA	1.62	0.48
2:2:936:U:H3	2:2:998:U:H3	1.61	0.48
13:K:81:VAL:HG21	13:K:94:LYS:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:48:VAL:HG23	40:n:49:LEU:HD12	1.95	0.48
2:2:751:C:H2'	2:2:752:C:C6	2.48	0.48
10:H:89:ASN:HD21	10:H:101:LYS:NZ	2.12	0.48
13:K:195:LEU:O	13:K:199:LEU:HG	2.14	0.48
21:S:130:LYS:NZ	21:S:134:GLY:O	2.38	0.48
22:T:110:ASP:N	22:T:110:ASP:OD1	2.46	0.48
2:2:486:C:P	9:G:49:ARG:HH12	2.37	0.48
4:A:105:SER:O	4:A:108:VAL:HG22	2.14	0.48
13:K:85:ALA:HB1	16:N:9:ALA:HB2	1.96	0.48
18:P:5:HIS:HD2	18:P:117:LEU:HB3	1.79	0.48
2:2:182:C:H4'	2:2:183:G:C6	2.49	0.47
2:2:1408:C:H42	2:2:1430:C:N4	2.10	0.47
4:A:178:ASN:O	4:A:182:ARG:HD3	2.14	0.47
35:g:242:SER:HA	35:g:291:TRP:CD1	2.49	0.47
2:2:158:A:H2'	2:2:159:A:O4'	2.13	0.47
2:2:310:G:C6	2:2:311:C:C5	3.02	0.47
2:2:833:A:H2'	2:2:834:G:C8	2.48	0.47
2:2:1281:G:N3	34:f:102:VAL:N	2.62	0.47
5:C:106:GLY:N	5:C:136:GLU:OE2	2.35	0.47
19:Q:54:CYS:SG	19:Q:81:VAL:HG13	2.54	0.47
35:g:223:GLU:HB3	35:g:225:LYS:HZ3	1.79	0.47
38:k:164:LEU:HB2	38:k:236:ASP:HB3	1.96	0.47
2:2:900:A:H2'	2:2:901:C:C6	2.49	0.47
4:A:130:LEU:HD23	4:A:133:ARG:HE	1.80	0.47
18:P:92:ILE:O	18:P:96:VAL:HG13	2.14	0.47
21:S:18:THR:O	21:S:18:THR:OG1	2.30	0.47
40:n:112:ASN:HD22	40:n:114:LYS:HD3	1.79	0.47
2:2:526:A:N6	2:2:537:G:H21	2.09	0.47
2:2:1217:G:O2'	2:2:1671:U:O2	2.32	0.47
7:E:160:LYS:HE3	27:Y:95:PRO:HA	1.95	0.47
2:2:1720:U:C2	2:2:1721:G:C8	3.02	0.47
2:2:1741:U:H2'	2:2:1742:C:C6	2.49	0.47
18:P:67:THR:HG22	18:P:68:GLY:H	1.79	0.47
2:2:92:A:H4'	2:2:93:U:OP2	2.15	0.47
2:2:313:C:O2'	2:2:315:C:O4'	2.25	0.47
2:2:1748:G:C6	2:2:1749:C:N4	2.83	0.47
4:A:199:CYS:HA	4:A:269:PHE:HE2	1.79	0.47
8:F:224:SER:OG	35:g:188:HIS:ND1	2.41	0.47
2:2:1401:A:H2'	2:2:1402:G:O4'	2.15	0.47
4:A:65:ILE:HD12	4:A:65:ILE:H	1.79	0.47
4:A:120:GLU:HB3	4:A:126:GLN:NE2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:229:THR:HG22	7:E:230:PRO:HD2	1.97	0.47
13:K:67:TRP:HA	13:K:189:VAL:HG12	1.97	0.47
16:N:40:ILE:HD11	16:N:61:PRO:O	2.15	0.47
30:b:26:CYS:HB2	30:b:77:CYS:HG	1.80	0.47
34:f:88:PRO:HG2	34:f:91:ASN:OD1	2.15	0.47
35:g:170:TRP:C	35:g:172:LYS:H	2.23	0.47
2:2:1417:A:C8	2:2:1418:G:C8	3.03	0.47
2:2:1688:G:N2	2:2:1828:A:C8	2.80	0.47
4:A:185:THR:OG1	4:A:186:PRO:HD3	2.14	0.47
20:R:11:THR:HG22	20:R:12:PHE:H	1.80	0.47
35:g:207:CYS:SG	35:g:221:LEU:HD21	2.55	0.47
38:k:524:MET:HB3	38:k:524:MET:HE3	1.76	0.47
4:A:102:PHE:O	4:A:106:LYS:HG3	2.15	0.47
8:F:55:THR:HG22	8:F:88:ALA:HB1	1.97	0.47
35:g:176:VAL:HG13	35:g:186:THR:H	1.80	0.47
2:2:72:C:H4'	2:2:73:C:C4	2.50	0.47
2:2:1583:A:H2'	2:2:1584:A:C8	2.50	0.47
2:2:1804:U:H2'	2:2:1805:C:C6	2.50	0.47
12:J:5:SER:O	12:J:28:LEU:HD13	2.15	0.47
12:J:113:LYS:HG3	12:J:114:GLN:H	1.80	0.47
12:J:181:THR:OG1	12:J:182:GLY:N	2.48	0.47
12:J:184:ASP:OD1	12:J:184:ASP:N	2.48	0.47
29:a:12:PHE:HD1	29:a:23:MET:HB3	1.79	0.47
38:k:542:ASN:OD1	38:k:543:THR:N	2.48	0.47
40:n:94:LYS:HB3	40:n:96:LEU:HG	1.97	0.47
2:2:233:A:H2'	2:2:234:C:O4'	2.15	0.46
2:2:897:G:C2	2:2:898:G:C5	3.03	0.46
2:2:1413:C:C2	2:2:1415:C:N4	2.83	0.46
4:A:139:ASP:O	4:A:143:LYS:HB2	2.15	0.46
8:F:79:PHE:CD2	8:F:84:VAL:HG22	2.50	0.46
13:K:84:ASN:ND2	13:K:90:LEU:HD12	2.30	0.46
19:Q:19:PRO:HG2	19:Q:27:VAL:HG21	1.96	0.46
35:g:305:ASN:OD1	35:g:305:ASN:N	2.48	0.46
2:2:107:A:H2'	2:2:108:G:H8	1.80	0.46
2:2:543:U:H2'	2:2:544:A:N3	2.31	0.46
2:2:1169:A:H2'	2:2:1170:U:O4'	2.15	0.46
13:K:132:GLU:OE1	13:K:133:GLU:N	2.47	0.46
38:k:495:GLU:O	38:k:498:LEU:HG	2.16	0.46
2:2:145:G:H2'	2:2:146:G:C8	2.50	0.46
2:2:358:U:H4'	2:2:359:C:O5'	2.15	0.46
2:2:839:C:H2'	2:2:840:U:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1531:G:H2'	2:2:1532:A:C8	2.50	0.46
9:G:21:ASP:OD2	9:G:24:THR:OG1	2.29	0.46
25:W:94:PRO:HD2	25:W:97:ILE:HD11	1.98	0.46
32:d:7:GLN:NE2	32:d:8:PRO:HD2	2.30	0.46
38:k:579:LYS:HE2	38:k:579:LYS:HB2	1.68	0.46
2:2:320:G:C6	2:2:321:C:N4	2.84	0.46
2:2:830:C:H2'	2:2:831:C:C6	2.50	0.46
2:2:1407:G:N1	2:2:1432:C:C2	2.83	0.46
2:2:1717:G:N1	2:2:1806:U:N3	2.45	0.46
10:H:165:ALA:O	10:H:169:LEU:HG	2.15	0.46
17:O:52:LEU:HD11	17:O:62:VAL:HG12	1.97	0.46
18:P:132:LYS:HB3	18:P:134:VAL:HG23	1.96	0.46
18:P:147:SER:O	18:P:150:VAL:HG12	2.16	0.46
26:X:17:CYS:SG	26:X:56:CYS:N	2.82	0.46
38:k:246:TYR:C	38:k:247:LEU:HD12	2.40	0.46
2:2:1418:G:N2	2:2:1419:C:O2'	2.48	0.46
5:C:31:ASP:OD1	5:C:151:ASP:HA	2.16	0.46
6:D:141:GLY:HA2	6:D:209:ASP:O	2.16	0.46
8:F:124:ARG:O	8:F:128:GLU:HG2	2.16	0.46
9:G:143:ASP:OD1	9:G:143:ASP:N	2.35	0.46
9:G:188:ASN:ND2	9:G:218:PHE:HB2	2.31	0.46
13:K:106:SER:HA	13:K:109:TYR:HD2	1.81	0.46
13:K:157:LYS:HA	13:K:157:LYS:HD2	1.70	0.46
18:P:143:SER:OG	18:P:144:SER:N	2.49	0.46
21:S:29:ASN:N	21:S:67:ASP:OD1	2.48	0.46
23:U:143:GLY:HA2	23:U:144:ARG:NH2	2.31	0.46
28:Z:77:ASN:HB3	28:Z:79:LYS:HG2	1.98	0.46
38:k:422:GLY:N	38:k:458:GLU:OE2	2.46	0.46
8:F:172:VAL:HA	8:F:184:ILE:O	2.16	0.46
10:H:74:LYS:HG3	10:H:77:ARG:NH1	2.31	0.46
23:U:54:LYS:HB3	23:U:54:LYS:HE3	1.68	0.46
27:Y:82:GLN:C	27:Y:84:LYS:H	2.23	0.46
35:g:28:PRO:O	35:g:47:ARG:NH1	2.46	0.46
35:g:222:ASN:OD1	35:g:222:ASN:N	2.48	0.46
2:2:525:G:H2'	2:2:526:A:H8	1.80	0.46
2:2:1402:G:H2'	2:2:1403:U:C6	2.51	0.46
5:C:132:GLN:HB3	5:C:133:PRO:HD3	1.98	0.46
13:K:45:THR:HG22	13:K:55:TYR:HD1	1.81	0.46
13:K:113:TYR:OH	13:K:156:ALA:HB1	2.15	0.46
22:T:16:ILE:HG22	22:T:24:LEU:HD11	1.97	0.46
37:j:104:LYS:HB3	37:j:104:LYS:HE2	1.68	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:547:U:C4	2:2:548:G:N7	2.84	0.46
2:2:553:G:O2'	2:2:554:A:O5'	2.33	0.46
2:2:1531:G:H2'	2:2:1532:A:H8	1.81	0.46
2:2:1709:U:H2'	2:2:1710:A:C8	2.50	0.46
4:A:104:LYS:O	4:A:107:THR:HG22	2.16	0.46
6:D:31:TYR:CD2	6:D:94:LYS:HA	2.51	0.46
13:K:197:PHE:CZ	13:K:201:LYS:HE3	2.51	0.46
14:L:63:LEU:O	14:L:70:ARG:NH2	2.48	0.46
25:W:53:PRO:HA	25:W:88:LEU:O	2.16	0.46
35:g:12:LYS:HG2	35:g:13:GLY:N	2.30	0.46
35:g:148:SER:O	35:g:148:SER:OG	2.33	0.46
38:k:550:THR:OG1	38:k:551:LEU:N	2.48	0.46
2:2:546:U:H2'	2:2:547:U:O4'	2.16	0.46
7:E:68:SER:HB2	7:E:133:ILE:HG23	1.98	0.46
8:F:208:VAL:HG11	22:T:12:ALA:HB2	1.98	0.46
10:H:139:ASP:OD1	10:H:140:SER:N	2.49	0.46
14:L:74:GLY:O	14:L:78:LEU:HG	2.15	0.46
18:P:38:TYR:O	18:P:42:LYS:HG2	2.16	0.46
35:g:292:SER:OG	35:g:293:ALA:N	2.48	0.46
38:k:468:GLN:NE2	38:k:488:PRO:O	2.48	0.46
2:2:225:C:O5'	2:2:884:U:H4'	2.16	0.46
2:2:1224:A:H2'	2:2:1225:G:H8	1.81	0.46
2:2:1411:C:N4	2:2:1427:G:H1	2.14	0.46
2:2:1770:G:H2'	2:2:1771:G:H8	1.78	0.46
2:2:1862:U:O4	30:b:98:PRO:HG2	2.16	0.46
21:S:101:ASP:OD1	21:S:104:SER:OG	2.26	0.46
35:g:184:LEU:H	35:g:184:LEU:HD23	1.81	0.46
38:k:249:VAL:HA	38:k:252:ARG:HD2	1.97	0.46
4:A:216:LEU:HD22	4:A:225:ILE:HD12	1.97	0.45
8:F:221:THR:O	8:F:223:ILE:HG23	2.16	0.45
9:G:162:ILE:HG22	9:G:169:ILE:HG22	1.99	0.45
16:N:33:LEU:HD23	16:N:33:LEU:HA	1.74	0.45
18:P:13:GLN:H	18:P:13:GLN:HG2	1.47	0.45
18:P:114:ARG:O	18:P:118:ILE:HD12	2.16	0.45
38:k:277:SER:OG	38:k:576:ARG:HA	2.16	0.45
38:k:430:GLU:O	38:k:478:LYS:NZ	2.49	0.45
2:2:542:G:C5	2:2:543:U:C4	3.04	0.45
2:2:1427:G:O2'	2:2:1428:U:O5'	2.22	0.45
2:2:1772:C:H2'	2:2:1773:G:C8	2.51	0.45
7:E:123:GLU:OE2	7:E:126:THR:OG1	2.30	0.45
18:P:140:LYS:HD2	18:P:140:LYS:HA	1.76	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:310:G:C2	2:2:322:G:C2	3.03	0.45
2:2:1409:G:C6	2:2:1410:A:C6	3.04	0.45
2:2:1776:G:O5'	2:2:1776:G:H8	1.99	0.45
4:A:181:ASN:HA	4:A:184:LEU:HB3	1.99	0.45
16:N:40:ILE:HD13	16:N:40:ILE:HA	1.76	0.45
38:k:328:SER:O	38:k:328:SER:OG	2.31	0.45
38:k:478:LYS:HD3	38:k:478:LYS:HA	1.65	0.45
2:2:165:G:H1'	11:I:110:ASN:HD22	1.81	0.45
2:2:525:G:H2'	2:2:526:A:C8	2.52	0.45
2:2:883:U:O2'	2:2:884:U:H5''	2.17	0.45
2:2:945:G:H2'	2:2:946:C:C6	2.52	0.45
5:C:131:HIS:O	5:C:135:THR:HG23	2.16	0.45
8:F:62:LYS:O	8:F:64:ARG:NH1	2.48	0.45
9:G:212:ASP:OD1	9:G:213:ALA:N	2.44	0.45
17:O:43:ASP:O	17:O:45:ARG:NH2	2.49	0.45
35:g:30:MET:HE2	35:g:30:MET:HB3	1.71	0.45
38:k:222:LEU:HD13	38:k:222:LEU:C	2.41	0.45
2:2:1370:C:H2'	2:2:1371:G:O4'	2.15	0.45
2:2:1376:C:H2'	2:2:1377:G:O4'	2.16	0.45
2:2:1767:C:H2'	2:2:1768:C:C6	2.51	0.45
2:2:1799:G:H2'	2:2:1800:A:H8	1.82	0.45
4:A:263:GLU:HA	4:A:269:PHE:CD1	2.51	0.45
16:N:1:MET:HA	16:N:1:MET:HE2	1.99	0.45
22:T:5:ARG:HB2	22:T:10:LYS:HE2	1.98	0.45
40:n:64:ASN:OD1	40:n:64:ASN:N	2.48	0.45
2:2:831:C:H2'	2:2:832:G:N2	2.32	0.45
2:2:923:C:O2	31:c:51:GLN:NE2	2.49	0.45
2:2:1705:C:H2'	2:2:1706:U:C6	2.51	0.45
8:F:208:VAL:HG23	22:T:41:ILE:HG13	1.97	0.45
11:I:110:ASN:OD1	11:I:110:ASN:N	2.48	0.45
15:M:72:THR:O	15:M:76:ILE:HG13	2.16	0.45
35:g:116:ASP:O	35:g:118:ARG:HG2	2.16	0.45
38:k:559:LEU:HD13	38:k:594:TYR:HB2	1.99	0.45
2:2:1408:C:N4	2:2:1430:C:H42	2.14	0.45
13:K:113:TYR:CE1	13:K:117:TYR:HD2	2.34	0.45
22:T:7:LYS:O	22:T:11:LYS:HG3	2.17	0.45
4:A:172:GLU:O	4:A:176:LEU:HD13	2.17	0.45
12:J:29:GLU:HA	12:J:32:MET:HG2	1.98	0.45
16:N:111:VAL:HG12	16:N:140:PHE:HB2	1.98	0.45
25:W:111:GLU:OE2	25:W:112:VAL:N	2.50	0.45
8:F:92:ALA:O	8:F:93:THR:OG1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:155:ASP:N	10:H:155:ASP:OD1	2.36	0.45
12:J:181:THR:OG1	12:J:183:LYS:HG3	2.17	0.45
38:k:226:ALA:O	38:k:230:VAL:HG12	2.16	0.45
38:k:265:PRO:HG2	38:k:267:ARG:NE	2.32	0.45
2:2:684:A:H2'	2:2:685:G:C8	2.52	0.45
10:H:114:ILE:HG23	40:n:67:LEU:HD13	1.99	0.45
11:I:16:ILE:HG12	11:I:17:GLU:H	1.82	0.45
13:K:186:ASP:OD1	13:K:186:ASP:N	2.48	0.45
18:P:94:LYS:O	18:P:98:VAL:HG23	2.17	0.45
35:g:204:GLY:C	35:g:221:LEU:HD12	2.42	0.45
38:k:244:SER:N	38:k:273:GLU:OE2	2.50	0.45
38:k:486:ASP:OD1	38:k:486:ASP:N	2.48	0.45
13:K:165:GLN:NE2	13:K:170:LYS:O	2.50	0.44
25:W:87:ARG:C	25:W:88:LEU:HD23	2.42	0.44
2:2:1039:G:H2'	2:2:1040:G:O4'	2.18	0.44
8:F:150:MET:HE2	8:F:152:PHE:CZ	2.52	0.44
9:G:31:PRO:HB3	9:G:43:PRO:HG3	1.98	0.44
14:L:81:LEU:HD23	14:L:81:LEU:HA	1.73	0.44
16:N:147:LYS:HD2	16:N:147:LYS:HA	1.75	0.44
35:g:181:ASN:OD1	35:g:183:LYS:HG2	2.16	0.44
40:n:48:VAL:C	40:n:83:LEU:HD22	2.41	0.44
2:2:876:G:H21	2:2:876:G:P	2.37	0.44
4:A:120:GLU:HB3	4:A:126:GLN:HE21	1.82	0.44
12:J:168:HIS:CD2	12:J:168:HIS:H	2.35	0.44
20:R:65:LYS:HB2	20:R:65:LYS:HE3	1.63	0.44
21:S:26:LYS:O	21:S:66:VAL:HA	2.17	0.44
23:U:73:ASN:HB3	23:U:76:GLN:HG2	1.99	0.44
32:d:35:MET:HB3	32:d:35:MET:HE3	1.71	0.44
35:g:90:TRP:CE3	35:g:97:THR:HG22	2.53	0.44
2:2:740:G:HO2'	2:2:741:C:P	2.37	0.44
12:J:37:LYS:HG2	12:J:41:ARG:HH12	1.82	0.44
21:S:118:THR:HA	21:S:121:VAL:O	2.17	0.44
30:b:57:SER:OG	30:b:59:PHE:N	2.50	0.44
30:b:94:ASP:OD1	30:b:94:ASP:N	2.50	0.44
38:k:239:MET:HA	38:k:270:ILE:O	2.17	0.44
2:2:209:C:H2'	2:2:210:G:H8	1.83	0.44
2:2:366:A:N3	13:K:86:SER:HB3	2.33	0.44
4:A:196:GLU:HG2	4:A:234:ARG:HE	1.83	0.44
18:P:98:VAL:HG12	18:P:102:LEU:HD23	1.99	0.44
22:T:41:ILE:HG23	22:T:46:LEU:HD23	2.00	0.44
35:g:227:LEU:HD23	35:g:227:LEU:HA	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1571:G:H2'	2:2:1572:G:H8	1.83	0.44
7:E:191:LEU:HD23	7:E:221:ILE:HD11	2.00	0.44
8:F:118:ALA:O	8:F:122:VAL:HG22	2.18	0.44
11:I:50:VAL:HG12	11:I:113:ILE:HA	2.00	0.44
29:a:68:LYS:HB2	29:a:68:LYS:HE3	1.59	0.44
35:g:286:CYS:HB2	35:g:302:TYR:CE2	2.53	0.44
38:k:238:PHE:CE1	38:k:267:ARG:HD2	2.48	0.44
2:2:319:G:C5	2:2:320:G:C8	3.06	0.44
2:2:445:A:H2'	2:2:446:C:H6	1.83	0.44
2:2:1411:C:H2'	2:2:1412:C:H6	1.82	0.44
2:2:1451:A:C2	2:2:1452:G:C8	3.06	0.44
2:2:1724:U:H2'	2:2:1725:U:C5	2.53	0.44
2:2:1752:G:H2'	2:2:1753:G:C8	2.53	0.44
5:C:118:GLU:OE2	7:E:42:LYS:HG3	2.16	0.44
5:C:159:ILE:HD11	26:X:34:MET:HE3	2.00	0.44
6:D:110:MET:HA	6:D:113:MET:HE2	2.00	0.44
8:F:217:ILE:O	8:F:217:ILE:HG13	2.18	0.44
18:P:88:LEU:HD12	18:P:88:LEU:HA	1.76	0.44
19:Q:95:ILE:HD12	19:Q:126:ILE:HG23	2.00	0.44
22:T:70:SER:O	22:T:70:SER:OG	2.31	0.44
2:2:552:U:H2'	2:2:553:G:C8	2.53	0.44
2:2:1701:G:H2'	2:2:1702:U:H6	1.83	0.44
2:2:1720:U:N3	2:2:1721:G:N7	2.65	0.44
4:A:22:VAL:HG12	4:A:36:LEU:HD23	2.00	0.44
13:K:190:LEU:HD23	13:K:190:LEU:HA	1.70	0.44
20:R:84:ILE:HD12	20:R:84:ILE:H	1.83	0.44
25:W:30:LYS:H	25:W:30:LYS:HD2	1.83	0.44
30:b:11:ALA:HB3	30:b:33:ASP:HB2	2.00	0.44
38:k:362:LEU:HD13	38:k:384:GLY:HA3	1.99	0.44
2:2:426:G:OP2	2:2:461:G:O2'	2.34	0.44
6:D:52:THR:HG23	6:D:57:ILE:HA	1.99	0.44
9:G:44:LEU:HD12	9:G:44:LEU:HA	1.66	0.44
12:J:126:HIS:O	12:J:177:TYR:OH	2.36	0.44
24:V:139:ALA:O	24:V:144:LYS:N	2.51	0.44
35:g:213:ASP:OD1	35:g:214:GLY:N	2.51	0.44
40:n:42:ASP:CG	40:n:43:LYS:H	2.25	0.44
2:2:1862:U:C5	30:b:97:PRO:HB2	2.53	0.43
11:I:50:VAL:HG12	11:I:113:ILE:HG12	1.99	0.43
39:l:19:LYS:HZ2	39:l:19:LYS:C	2.26	0.43
2:2:811:U:C2	2:2:812:A:C8	3.06	0.43
2:2:864:G:H5''	16:N:156:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:868:A:N6	2:2:911:G:C5	2.86	0.43
2:2:1061:G:OP1	19:Q:149:ARG:HD2	2.17	0.43
2:2:1134:C:P	5:C:155:ARG:HH12	2.41	0.43
4:A:76:VAL:HA	4:A:82:TYR:O	2.18	0.43
7:E:197:ASP:N	7:E:197:ASP:OD1	2.51	0.43
8:F:193:ASP:CG	8:F:196:GLY:HA3	2.43	0.43
14:L:78:LEU:HD21	14:L:94:LEU:HD23	1.99	0.43
18:P:102:LEU:HD13	18:P:102:LEU:HA	1.80	0.43
40:n:113:THR:HG22	40:n:113:THR:O	2.17	0.43
2:2:231:C:N4	2:2:891:G:O6	2.51	0.43
2:2:864:G:H5''	16:N:156:GLN:HE22	1.84	0.43
2:2:951:A:C2	2:2:968:A:C5	3.06	0.43
2:2:1116:U:H5'	31:c:72:ARG:NH2	2.32	0.43
2:2:1374:A:H4'	2:2:1375:A:O5'	2.19	0.43
4:A:254:ALA:HB3	4:A:255:MET:HE2	2.00	0.43
5:C:34:MET:HE2	5:C:149:ASN:O	2.18	0.43
20:R:61:ARG:O	20:R:62:LYS:HB3	2.18	0.43
23:U:25:LYS:O	23:U:29:ALA:N	2.52	0.43
38:k:414:GLN:N	38:k:486:ASP:OD2	2.51	0.43
2:2:96:C:OP1	14:L:1:MET:HA	2.18	0.43
2:2:1799:G:H2'	2:2:1800:A:C8	2.53	0.43
2:2:1836:C:OP1	39:l:3:ALA:HB3	2.19	0.43
7:E:123:GLU:N	7:E:123:GLU:OE1	2.51	0.43
10:H:216:LYS:HG3	10:H:219:ARG:NH2	2.34	0.43
13:K:198:TYR:O	13:K:202:ILE:HG13	2.17	0.43
17:O:35:ILE:HD13	17:O:61:TYR:HD2	1.83	0.43
35:g:97:THR:O	35:g:97:THR:OG1	2.33	0.43
2:2:1464:C:OP2	22:T:1:MET:HE1	2.19	0.43
2:2:1717:G:H2'	2:2:1718:G:O4'	2.18	0.43
4:A:15:GLU:N	4:A:15:GLU:OE1	2.52	0.43
7:E:90:GLN:HB3	7:E:99:THR:HB	2.01	0.43
17:O:52:LEU:HD12	17:O:53:ALA:H	1.83	0.43
21:S:63:PHE:CE1	21:S:92:LEU:HD22	2.54	0.43
23:U:51:ASP:OD1	23:U:53:THR:N	2.51	0.43
25:W:22:ILE:HG23	25:W:114:VAL:HB	1.99	0.43
30:b:24:THR:HG23	30:b:72:HIS:O	2.18	0.43
35:g:213:ASP:CG	35:g:215:GLN:H	2.26	0.43
2:2:126:G:OP2	11:I:195:LYS:HE3	2.18	0.43
2:2:209:C:H2'	2:2:210:G:C8	2.53	0.43
4:A:100:ASP:O	4:A:104:LYS:HG2	2.19	0.43
8:F:150:MET:HE2	8:F:152:PHE:HZ	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:151:ASP:OD2	11:I:216:ARG:NH1	2.48	0.43
11:I:37:ALA:HA	11:I:49:VAL:HG23	2.00	0.43
12:J:126:HIS:NE2	12:J:181:THR:HB	2.33	0.43
13:K:73:THR:O	13:K:74:ARG:HD2	2.18	0.43
35:g:32:LEU:HD12	35:g:32:LEU:HA	1.81	0.43
35:g:73:SER:OG	35:g:117:ASN:ND2	2.51	0.43
38:k:250:LYS:HE3	38:k:250:LYS:HB2	1.65	0.43
2:2:320:G:O6	2:2:321:C:N4	2.52	0.43
2:2:1060:C:H5''	19:Q:149:ARG:HG3	1.99	0.43
2:2:1526:A:H4'	2:2:1600:G:H4'	2.01	0.43
9:G:94:LYS:HD2	9:G:94:LYS:HA	1.77	0.43
27:Y:37:PHE:CZ	27:Y:103:VAL:HG11	2.53	0.43
37:j:48:GLU:HG3	37:j:49:ALA:N	2.34	0.43
38:k:253:LEU:O	38:k:257:ILE:HG12	2.19	0.43
38:k:461:THR:O	38:k:461:THR:OG1	2.34	0.43
2:2:297:C:O2'	2:2:298:G:H3'	2.18	0.43
2:2:319:G:C6	2:2:320:G:C5	3.07	0.43
2:2:1593:G:O2'	40:n:80:ARG:O	2.29	0.43
2:2:1601:G:HO2'	2:2:1602:A:P	2.42	0.43
5:C:119:PRO:HG2	5:C:142:LEU:HD11	2.01	0.43
26:X:22:ARG:HE	26:X:22:ARG:HB3	1.67	0.43
32:d:44:ARG:HD2	32:d:44:ARG:HA	1.87	0.43
38:k:569:ASP:OD1	38:k:569:ASP:N	2.52	0.43
2:2:1721:G:H2'	2:2:1722:G:C8	2.51	0.43
4:A:115:VAL:HB	4:A:172:GLU:OE1	2.18	0.43
4:A:168:LEU:HD12	4:A:168:LEU:HA	1.88	0.43
7:E:101:PHE:O	7:E:120:CYS:HA	2.18	0.43
10:H:95:GLY:C	10:H:97:ASN:H	2.27	0.43
24:V:74:SER:O	24:V:78:ILE:HG13	2.19	0.43
32:d:9:ILE:H	32:d:9:ILE:HG12	1.63	0.43
39:l:1:MET:HG2	39:l:4:LYS:HD3	2.01	0.43
2:2:528:U:C2	2:2:536:G:C2	3.07	0.43
8:F:154:ASP:OD1	8:F:155:GLY:N	2.52	0.43
9:G:73:ASP:OD1	9:G:73:ASP:N	2.52	0.43
21:S:88:ILE:HG13	21:S:89:SER:N	2.34	0.43
30:b:26:CYS:HB2	30:b:74:CYS:SG	2.59	0.43
35:g:271:LYS:HE2	35:g:271:LYS:HB3	1.83	0.43
2:2:738:U:HO2'	2:2:740:G:P	2.42	0.42
2:2:879:U:H2'	2:2:880:C:H6	1.83	0.42
2:2:1133:U:O2'	2:2:1134:C:H5''	2.19	0.42
6:D:81:PHE:HB3	6:D:106:THR:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:54:SER:OG	7:E:55:LEU:N	2.49	0.42
16:N:26:GLY:C	16:N:28:THR:H	2.27	0.42
20:R:58:LYS:O	20:R:61:ARG:HG2	2.18	0.42
33:e:48:LYS:HE2	33:e:48:LYS:HB3	1.86	0.42
2:2:182:C:N3	2:2:184:G:C2	2.86	0.42
2:2:272:C:H2'	2:2:273:G:H8	1.84	0.42
2:2:418:U:H2'	2:2:418:U:O2	2.18	0.42
2:2:664:C:H2'	2:2:665:U:C6	2.54	0.42
2:2:1392:A:O2'	2:2:1394:G:C8	2.72	0.42
4:A:20:VAL:HG11	4:A:36:LEU:HD22	2.02	0.42
4:A:200:TYR:HB2	4:A:269:PHE:HZ	1.81	0.42
6:D:218:LEU:HD12	6:D:218:LEU:HA	1.66	0.42
7:E:97:GLN:HE21	7:E:97:GLN:HB2	1.63	0.42
9:G:165:GLU:OE1	9:G:165:GLU:N	2.51	0.42
13:K:148:LYS:HE3	13:K:149:TYR:CE1	2.54	0.42
2:2:938:G:H2'	2:2:939:U:C6	2.54	0.42
2:2:1404:U:H2'	2:2:1405:A:O4'	2.20	0.42
2:2:1770:G:H2'	2:2:1771:G:C8	2.53	0.42
5:C:121:LEU:HD12	5:C:121:LEU:HA	1.82	0.42
22:T:45:LYS:HB2	22:T:45:LYS:HE2	1.71	0.42
23:U:6:PRO:HD2	40:n:50:PHE:HB2	2.02	0.42
28:Z:68:LYS:HE2	36:i:83:VAL:HG12	2.01	0.42
31:c:51:GLN:HA	31:c:66:PRO:HB3	2.02	0.42
2:2:163:U:H2'	2:2:164:A:H8	1.85	0.42
2:2:181:A:OP2	2:2:181:A:H3'	2.19	0.42
9:G:166:THR:O	9:G:168:LYS:HG2	2.19	0.42
19:Q:44:VAL:HG11	19:Q:85:CYS:SG	2.60	0.42
38:k:557:LYS:HE3	38:k:557:LYS:HB2	1.83	0.42
38:k:563:GLU:HA	38:k:563:GLU:OE1	2.19	0.42
2:2:165:G:C8	2:2:166:A:C8	3.08	0.42
2:2:198:U:C5	2:2:199:G:C5	3.07	0.42
2:2:596:G:C3'	2:2:597:U:H5''	2.49	0.42
2:2:934:A:N1	2:2:1001:G:C6	2.87	0.42
2:2:1717:G:N2	2:2:1806:U:O2	2.46	0.42
6:D:197:ILE:HG22	6:D:201:CYS:SG	2.59	0.42
8:F:4:GLN:H	8:F:4:GLN:CD	2.28	0.42
8:F:105:LEU:HD23	8:F:184:ILE:HG21	2.00	0.42
19:Q:120:ALA:HB1	30:b:56:VAL:HG21	2.01	0.42
2:2:828:G:H21	9:G:263:GLY:N	2.17	0.42
2:2:1416:G:O6	2:2:1423:C:N4	2.31	0.42
2:2:1417:A:N1	2:2:1423:C:C4	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1592:C:H4'	2:2:1598:G:O6	2.19	0.42
2:2:1662:U:H2'	2:2:1663:U:C6	2.54	0.42
4:A:153:PHE:HB3	4:A:180:ILE:HD13	2.01	0.42
4:A:194:ASP:OD1	4:A:234:ARG:NH1	2.49	0.42
9:G:169:ILE:O	9:G:169:ILE:HG13	2.19	0.42
11:I:41:LEU:HD23	11:I:45:TRP:CE3	2.55	0.42
13:K:171:LEU:HD13	13:K:189:VAL:HG21	2.02	0.42
13:K:175:ILE:H	13:K:175:ILE:HG12	1.72	0.42
33:e:24:CYS:SG	33:e:42:CYS:SG	3.16	0.42
2:2:793:C:C2'	2:2:794:G:H4'	2.49	0.42
2:2:1273:C:H2'	2:2:1274:A:H8	1.84	0.42
2:2:1393:U:O4	21:S:12:VAL:HG12	2.20	0.42
2:2:1700:C:H2'	2:2:1701:G:C8	2.54	0.42
4:A:115:VAL:HB	4:A:172:GLU:CD	2.45	0.42
7:E:83:VAL:HG22	7:E:105:VAL:HG22	2.01	0.42
8:F:47:GLU:HG3	8:F:85:GLU:HB3	2.02	0.42
14:L:114:VAL:HG21	14:L:135:ILE:CD1	2.49	0.42
31:c:2:PRO:O	31:c:3:LEU:HB3	2.20	0.42
35:g:60:ARG:HB2	35:g:60:ARG:CZ	2.49	0.42
37:j:110:PRO:HB2	37:j:112:HIS:CG	2.55	0.42
38:k:88:CYS:H	38:k:91:ALA:HB3	1.84	0.42
2:2:546:U:N3	2:2:547:U:C2	2.88	0.42
2:2:940:A:C6	2:2:941:U:C4	3.08	0.42
2:2:961:U:H2'	2:2:962:U:H5'	2.02	0.42
2:2:1410:A:H2'	2:2:1411:C:H6	1.85	0.42
2:2:1672:U:OP2	10:H:78:LYS:NZ	2.33	0.42
2:2:1778:G:OP2	2:2:1778:G:H3'	2.20	0.42
4:A:248:LEU:H	4:A:248:LEU:HD22	1.85	0.42
13:K:76:THR:HG22	13:K:77:ARG:O	2.20	0.42
13:K:105:ASP:OD1	13:K:106:SER:N	2.53	0.42
2:2:320:G:C6	2:2:321:C:C4	3.08	0.42
2:2:1345:G:H2'	2:2:1346:U:C6	2.55	0.42
2:2:1413:C:O2	2:2:1415:C:C5	2.72	0.42
2:2:1748:G:C6	2:2:1749:C:C4	3.08	0.42
4:A:6:CYS:O	4:A:40:ASN:ND2	2.51	0.42
9:G:19:MET:HB2	9:G:19:MET:HE3	1.75	0.42
9:G:122:LYS:NZ	9:G:143:ASP:OD2	2.39	0.42
9:G:139:LEU:HA	9:G:139:LEU:HD23	1.83	0.42
14:L:22:LYS:HA	14:L:22:LYS:HD3	1.76	0.42
16:N:128:VAL:HG12	16:N:142:VAL:HA	2.02	0.42
17:O:52:LEU:HD22	17:O:65:VAL:CG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:132:LYS:HD2	18:P:132:LYS:HA	1.90	0.42
2:2:585:U:H2'	2:2:586:U:C6	2.54	0.42
2:2:1098:G:H1	2:2:1126:G:N2	2.18	0.42
2:2:1098:G:N2	2:2:1126:G:N2	2.65	0.42
2:2:1411:C:C2	2:2:1427:G:N2	2.88	0.42
2:2:1732:G:H2'	2:2:1733:C:C6	2.53	0.42
4:A:115:VAL:HG11	4:A:130:LEU:HD13	2.02	0.42
4:A:163:LEU:HD23	4:A:163:LEU:H	1.84	0.42
4:A:237:MET:HB3	4:A:237:MET:HE2	1.80	0.42
5:C:137:ALA:HB1	5:C:142:LEU:HB3	2.01	0.42
7:E:143:ARG:O	7:E:158:PRO:HD3	2.19	0.42
17:O:62:VAL:O	17:O:65:VAL:HG22	2.19	0.42
23:U:117:ILE:C	23:U:118:ARG:HG2	2.44	0.42
35:g:48:ASP:OD2	35:g:50:THR:OG1	2.30	0.42
2:2:152:U:C2	2:2:153:G:C8	3.08	0.41
2:2:193:C:H2'	2:2:194:C:C6	2.55	0.41
2:2:847:C:O3'	2:2:848:G:N2	2.52	0.41
2:2:1006:G:H2'	2:2:1007:A:C8	2.55	0.41
2:2:1582:G:O2'	24:V:78:ILE:HA	2.20	0.41
4:A:45:MET:HE3	4:A:45:MET:HB3	1.78	0.41
4:A:116:ALA:O	4:A:121:TYR:HB3	2.20	0.41
5:C:14:ASP:OD1	5:C:14:ASP:N	2.52	0.41
5:C:165:ASN:OD1	5:C:165:ASN:C	2.63	0.41
8:F:32:ASP:OD2	8:F:65:ARG:NH2	2.41	0.41
12:J:104:PRO:HD3	12:J:116:ARG:HD3	2.02	0.41
16:N:79:LYS:HB2	16:N:79:LYS:HE3	1.86	0.41
2:2:190:A:H3'	2:2:191:C:H5''	2.01	0.41
2:2:1807:A:H2'	2:2:1808:G:O4'	2.20	0.41
4:A:69:GLU:CD	4:A:70:CYS:H	2.26	0.41
8:F:67:ARG:NH1	15:M:97:SER:OG	2.53	0.41
8:F:187:LYS:HB3	8:F:187:LYS:HE3	1.90	0.41
8:F:195:SER:H	8:F:201:LYS:HG2	1.85	0.41
9:G:31:PRO:HG2	9:G:38:LEU:HG	2.03	0.41
11:I:194:LEU:HD23	11:I:194:LEU:HA	1.86	0.41
14:L:40:LYS:HE3	36:i:108:ARG:HH22	1.86	0.41
23:U:124:ARG:HD2	23:U:124:ARG:HA	1.76	0.41
26:X:27:LYS:HD3	26:X:27:LYS:HA	1.84	0.41
2:2:540:C:H2'	2:2:541:U:C6	2.56	0.41
2:2:631:A:OP1	14:L:40:LYS:NZ	2.43	0.41
2:2:1006:G:H2'	2:2:1007:A:H8	1.85	0.41
5:C:81:ASN:HA	5:C:84:GLN:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:151:ASP:OD1	5:C:151:ASP:N	2.49	0.41
7:E:156:THR:OG1	7:E:157:VAL:N	2.53	0.41
9:G:9:LEU:HB2	9:G:30:ARG:HD3	2.02	0.41
28:Z:99:GLU:O	28:Z:100:VAL:HG13	2.21	0.41
38:k:475:CYS:HB3	38:k:483:TYR:CE1	2.55	0.41
2:2:291:U:H2'	2:2:292:A:H8	1.85	0.41
2:2:967:G:H1	6:D:20:LYS:NZ	2.18	0.41
2:2:1255:A:H2'	2:2:1256:A:H5''	2.02	0.41
4:A:93:GLU:O	4:A:97:LYS:HG2	2.20	0.41
13:K:76:THR:HG23	13:K:105:ASP:CG	2.45	0.41
23:U:12:ILE:HD12	23:U:12:ILE:H	1.84	0.41
29:a:12:PHE:CE1	29:a:23:MET:HE3	2.54	0.41
38:k:274:HIS:ND1	38:k:493:ASP:HA	2.36	0.41
38:k:558:PHE:CZ	38:k:562:LEU:HD11	2.54	0.41
2:2:553:G:O2'	2:2:554:A:H8	2.03	0.41
2:2:1456:C:H2'	2:2:1457:G:H5''	2.01	0.41
12:J:109:ARG:HD2	12:J:111:LYS:HE2	2.02	0.41
13:K:119:LEU:HD23	13:K:119:LEU:HA	1.80	0.41
18:P:78:LYS:HD2	18:P:78:LYS:HA	1.81	0.41
28:Z:53:GLU:OE1	28:Z:55:VAL:HG13	2.20	0.41
40:n:98:LYS:HE2	40:n:112:ASN:O	2.21	0.41
2:2:125:C:H2'	11:I:198:ARG:NE	2.35	0.41
2:2:141:A:C5	2:2:178:C:H1'	2.55	0.41
2:2:291:U:H2'	2:2:292:A:C8	2.55	0.41
2:2:546:U:C4	2:2:547:U:N3	2.89	0.41
2:2:895:U:H2'	2:2:896:C:C6	2.56	0.41
4:A:36:LEU:HD23	4:A:36:LEU:HA	1.86	0.41
9:G:126:VAL:HG13	9:G:139:LEU:HD21	2.02	0.41
10:H:187:CYS:HA	10:H:190:ASP:OD2	2.20	0.41
13:K:106:SER:HA	13:K:109:TYR:CD2	2.55	0.41
19:Q:125:LYS:HE3	19:Q:125:LYS:HB3	1.88	0.41
28:Z:3:LYS:HB2	28:Z:3:LYS:HE2	1.84	0.41
35:g:45:LEU:HA	35:g:45:LEU:HD23	1.77	0.41
38:k:271:VAL:HG11	38:k:282:LEU:HD11	2.02	0.41
2:2:160:U:O2'	2:2:162:C:H5'	2.21	0.41
2:2:186:G:H2'	2:2:187:C:C6	2.56	0.41
2:2:740:G:N2	2:2:794:G:H1'	2.35	0.41
2:2:1116:U:H5'	31:c:72:ARG:HH22	1.85	0.41
2:2:1223:G:N3	2:2:1223:G:H2'	2.35	0.41
2:2:1419:C:O3'	2:2:1420:G:H8	2.02	0.41
8:F:221:THR:O	8:F:223:ILE:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:84:ARG:HD3	19:Q:84:ARG:HA	1.84	0.41
22:T:41:ILE:HA	22:T:42:PRO:HD3	1.90	0.41
22:T:100:PRO:C	22:T:102:THR:H	2.27	0.41
2:2:317:G:H1'	2:2:318:U:C5	2.56	0.41
2:2:810:U:C4	2:2:811:U:C5	3.09	0.41
2:2:1548:C:C6	2:2:1548:C:H5'	2.56	0.41
2:2:1814:G:H2'	2:2:1815:U:C6	2.56	0.41
4:A:166:LEU:HD13	4:A:166:LEU:HA	1.92	0.41
8:F:105:LEU:HB2	8:F:122:VAL:HG11	2.03	0.41
11:I:39:ASP:OD1	11:I:40:ALA:N	2.54	0.41
38:k:446:MET:HG2	38:k:451:ILE:HG23	2.01	0.41
2:2:524:G:H2'	2:2:525:G:H8	1.83	0.41
2:2:541:U:H2'	2:2:542:G:C8	2.55	0.41
2:2:924:G:H2'	2:2:925:G:C8	2.55	0.41
2:2:1009:U:OP1	2:2:1125:G:O2'	2.39	0.41
2:2:1273:C:H2'	2:2:1274:A:C8	2.56	0.41
2:2:1400:U:OP1	25:W:21:ARG:NH1	2.53	0.41
2:2:1407:G:O6	2:2:1431:C:N4	2.48	0.41
2:2:1416:G:C2	2:2:1417:A:N7	2.89	0.41
2:2:1726:A:H2'	2:2:1727:G:H8	1.85	0.41
4:A:130:LEU:HA	4:A:133:ARG:NE	2.33	0.41
4:A:173:ARG:HA	4:A:176:LEU:HB2	2.02	0.41
8:F:106:ARG:HG3	8:F:175:VAL:HG22	2.02	0.41
8:F:194:PRO:O	8:F:195:SER:OG	2.34	0.41
12:J:23:ILE:HG13	12:J:87:PHE:CZ	2.56	0.41
12:J:109:ARG:NH2	12:J:113:LYS:HE2	2.36	0.41
17:O:106:CYS:C	17:O:108:CYS:H	2.28	0.41
18:P:125:LEU:HD12	18:P:125:LEU:HA	1.85	0.41
21:S:12:VAL:HG21	21:S:91:ALA:HA	2.03	0.41
21:S:112:LEU:HA	21:S:112:LEU:HD23	1.79	0.41
24:V:14:PHE:HZ	24:V:131:LEU:HD23	1.86	0.41
29:a:11:LYS:HG3	29:a:24:VAL:HG23	2.02	0.41
29:a:122:LYS:HG3	29:a:123:ALA:H	1.85	0.41
35:g:29:ASP:OD1	35:g:45:LEU:N	2.54	0.41
38:k:487:GLU:HG3	38:k:490:ALA:CB	2.47	0.41
2:2:871:A:O5'	2:2:871:A:H8	2.03	0.41
2:2:1329:U:H5'	8:F:147:ALA:HB2	2.03	0.41
2:2:1414:C:N3	2:2:1420:G:H5'	2.35	0.41
5:C:127:PRO:HG3	5:C:146:ALA:HB1	2.02	0.41
8:F:116:ARG:HG2	8:F:150:MET:HE1	2.03	0.41
12:J:113:LYS:H	12:J:113:LYS:HG2	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:45:ARG:O	14:L:49:THR:HG23	2.20	0.41
14:L:95:ASP:OD1	14:L:95:ASP:N	2.51	0.41
25:W:21:ARG:NH2	25:W:118:ASP:OD2	2.54	0.41
27:Y:20:ARG:HD2	27:Y:20:ARG:HA	1.82	0.41
34:f:145:CYS:C	34:f:146:LEU:HD23	2.46	0.41
40:n:74:SER:HA	40:n:79:ILE:HB	2.02	0.41
2:2:1515:G:N3	2:2:1515:G:H2'	2.36	0.40
2:2:1717:G:O6	2:2:1806:U:C4	2.75	0.40
4:A:102:PHE:CE2	4:A:106:LYS:HD3	2.56	0.40
7:E:144:ARG:HG2	7:E:196:ILE:HG13	2.04	0.40
8:F:64:ARG:NH1	8:F:67:ARG:HE	2.19	0.40
8:F:142:LEU:HD13	8:F:150:MET:SD	2.62	0.40
25:W:36:CYS:SG	25:W:53:PRO:HB3	2.61	0.40
32:d:18:LEU:HD12	32:d:29:GLN:HB3	2.04	0.40
2:2:210:G:C6	2:2:211:U:C4	3.09	0.40
2:2:905:G:C2	2:2:906:G:C5	3.09	0.40
2:2:1436:C:O2'	2:2:1437:U:H5'	2.22	0.40
2:2:1575:A:O2'	2:2:1576:C:H5'	2.21	0.40
4:A:170:GLU:C	4:A:172:GLU:H	2.29	0.40
4:A:190:LYS:N	4:A:244:ARG:HD3	2.36	0.40
8:F:214:LYS:HA	8:F:214:LYS:HD2	1.76	0.40
8:F:218:LEU:O	8:F:220:THR:OG1	2.32	0.40
10:H:130:ALA:O	10:H:134:SER:OG	2.37	0.40
13:K:121:LEU:O	13:K:123:ARG:HG2	2.20	0.40
13:K:168:GLN:N	13:K:168:GLN:OE1	2.54	0.40
24:V:107:LEU:HA	24:V:107:LEU:HD23	1.89	0.40
38:k:105:VAL:HG11	38:k:282:LEU:HD13	2.02	0.40
38:k:250:LYS:HG2	38:k:564:ILE:CD1	2.50	0.40
38:k:426:GLN:H	38:k:426:GLN:HG3	1.64	0.40
2:2:213:C:C2	2:2:214:A:C8	3.10	0.40
2:2:743:U:H1'	2:2:744:C:C1'	2.51	0.40
4:A:265:LYS:HD2	4:A:265:LYS:HA	1.79	0.40
8:F:94:ARG:HH21	8:F:125:PHE:HZ	1.69	0.40
8:F:218:LEU:HA	8:F:218:LEU:HD12	1.79	0.40
10:H:118:LEU:HA	10:H:118:LEU:HD12	1.80	0.40
21:S:60:LYS:HE3	21:S:60:LYS:HB3	1.86	0.40
25:W:21:ARG:HD2	25:W:118:ASP:OD2	2.21	0.40
38:k:462:LEU:HD23	38:k:467:LEU:HD13	2.03	0.40
38:k:556:ASN:HD22	38:k:556:ASN:HA	1.67	0.40
2:2:932:G:H2'	2:2:933:C:C6	2.57	0.40
2:2:1125:G:H5''	2:2:1126:G:OP2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:233:TRP:CZ2	27:Y:68:ARG:HB3	2.56	0.40
13:K:39:GLY:O	13:K:61:ASP:HB2	2.21	0.40
13:K:197:PHE:CE1	13:K:201:LYS:HG3	2.57	0.40
25:W:26:SER:OG	25:W:32:LEU:HB2	2.22	0.40
38:k:423:SER:HG	38:k:457:GLN:C	2.27	0.40
38:k:458:GLU:CD	38:k:460:GLN:HG2	2.46	0.40
2:2:232:A:H2'	2:2:233:A:C8	2.56	0.40
2:2:1593:G:OP2	40:n:82:SER:OG	2.30	0.40
4:A:169:ASN:HD22	4:A:172:GLU:HB2	1.86	0.40
4:A:171:ASP:O	4:A:174:GLU:HB3	2.21	0.40
6:D:66:VAL:HG22	6:D:87:ILE:HG23	2.03	0.40
35:g:156:PHE:HA	35:g:165:ILE:HG22	2.03	0.40
38:k:366:ALA:O	38:k:547:SER:OG	2.34	0.40
38:k:457:GLN:HE22	38:k:462:LEU:CB	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
4	A	264/284 (93%)	238 (90%)	26 (10%)	0	100	100
5	C	205/207 (99%)	179 (87%)	26 (13%)	0	100	100
6	D	213/215 (99%)	185 (87%)	28 (13%)	0	100	100
7	E	224/270 (83%)	192 (86%)	30 (13%)	2 (1%)	14	43
8	F	225/227 (99%)	200 (89%)	25 (11%)	0	100	100
9	G	261/263 (99%)	232 (89%)	29 (11%)	0	100	100
10	H	183/191 (96%)	162 (88%)	21 (12%)	0	100	100
11	I	235/237 (99%)	211 (90%)	24 (10%)	0	100	100
12	J	188/190 (99%)	163 (87%)	25 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	204/206 (99%)	178 (87%)	25 (12%)	1 (0%)	24	55
14	L	186/194 (96%)	172 (92%)	14 (8%)	0	100	100
15	M	96/98 (98%)	84 (88%)	11 (12%)	1 (1%)	12	40
16	N	156/158 (99%)	140 (90%)	16 (10%)	0	100	100
17	O	122/132 (92%)	105 (86%)	16 (13%)	1 (1%)	16	45
18	P	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
19	Q	134/151 (89%)	111 (83%)	22 (16%)	1 (1%)	18	49
20	R	138/145 (95%)	125 (91%)	12 (9%)	1 (1%)	18	49
21	S	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
22	T	124/135 (92%)	106 (86%)	18 (14%)	0	100	100
23	U	143/152 (94%)	128 (90%)	15 (10%)	0	100	100
24	V	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	18	49
25	W	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
26	X	81/83 (98%)	62 (76%)	19 (24%)	0	100	100
27	Y	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
28	Z	140/143 (98%)	128 (91%)	11 (8%)	1 (1%)	18	49
29	a	124/133 (93%)	109 (88%)	15 (12%)	0	100	100
30	b	97/115 (84%)	86 (89%)	11 (11%)	0	100	100
31	c	82/84 (98%)	70 (85%)	12 (15%)	0	100	100
32	d	62/69 (90%)	50 (81%)	12 (19%)	0	100	100
33	e	51/56 (91%)	43 (84%)	8 (16%)	0	100	100
34	f	69/71 (97%)	58 (84%)	11 (16%)	0	100	100
35	g	311/313 (99%)	275 (88%)	36 (12%)	0	100	100
36	i	56/133 (42%)	50 (89%)	6 (11%)	0	100	100
37	j	106/111 (96%)	91 (86%)	15 (14%)	0	100	100
38	k	593/595 (100%)	512 (86%)	81 (14%)	0	100	100
39	l	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
40	n	73/124 (59%)	66 (90%)	7 (10%)	0	100	100
All	All	5824/6191 (94%)	5129 (88%)	686 (12%)	9 (0%)	44	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	252	LYS
20	R	75	VAL
7	E	251	VAL
15	M	33	PRO
17	O	103	VAL
13	K	31	ARG
19	Q	89	GLY
28	Z	109	GLY
24	V	69	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	238/255 (93%)	203 (85%)	35 (15%)	3	14
5	C	173/173 (100%)	153 (88%)	20 (12%)	5	21
6	D	196/196 (100%)	175 (89%)	21 (11%)	6	24
7	E	190/214 (89%)	166 (87%)	24 (13%)	4	18
8	F	190/190 (100%)	163 (86%)	27 (14%)	3	14
9	G	225/225 (100%)	211 (94%)	14 (6%)	16	45
10	H	159/161 (99%)	145 (91%)	14 (9%)	9	32
11	I	207/207 (100%)	189 (91%)	18 (9%)	9	32
12	J	170/170 (100%)	154 (91%)	16 (9%)	8	30
13	K	177/177 (100%)	154 (87%)	23 (13%)	4	17
14	L	162/168 (96%)	150 (93%)	12 (7%)	13	38
15	M	89/89 (100%)	84 (94%)	5 (6%)	19	47
16	N	142/142 (100%)	127 (89%)	15 (11%)	6	24
17	O	104/108 (96%)	100 (96%)	4 (4%)	29	57
18	P	130/130 (100%)	118 (91%)	12 (9%)	8	30
19	Q	106/119 (89%)	94 (89%)	12 (11%)	5	21
20	R	126/130 (97%)	120 (95%)	6 (5%)	23	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	117/117 (100%)	101 (86%)	16 (14%)	3	16
22	T	114/121 (94%)	107 (94%)	7 (6%)	17	45
23	U	125/132 (95%)	113 (90%)	12 (10%)	8	29
24	V	113/113 (100%)	105 (93%)	8 (7%)	13	40
25	W	94/107 (88%)	80 (85%)	14 (15%)	3	13
26	X	67/67 (100%)	60 (90%)	7 (10%)	7	25
27	Y	112/113 (99%)	105 (94%)	7 (6%)	16	44
28	Z	114/115 (99%)	110 (96%)	4 (4%)	32	58
29	a	108/115 (94%)	103 (95%)	5 (5%)	24	53
30	b	87/99 (88%)	77 (88%)	10 (12%)	5	21
31	c	76/76 (100%)	73 (96%)	3 (4%)	28	56
32	d	57/62 (92%)	47 (82%)	10 (18%)	2	9
33	e	47/49 (96%)	46 (98%)	1 (2%)	47	67
34	f	64/64 (100%)	58 (91%)	6 (9%)	8	30
35	g	272/272 (100%)	241 (89%)	31 (11%)	5	21
36	i	48/106 (45%)	46 (96%)	2 (4%)	26	55
37	j	91/93 (98%)	87 (96%)	4 (4%)	25	54
38	k	523/523 (100%)	477 (91%)	46 (9%)	9	32
39	l	24/24 (100%)	22 (92%)	2 (8%)	10	34
40	n	66/102 (65%)	63 (96%)	3 (4%)	24	53
All	All	5103/5324 (96%)	4627 (91%)	476 (9%)	11	30

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	11	HIS
4	A	18	ASP
4	A	26	SER
4	A	45	MET
4	A	72	VAL
4	A	74	ILE
4	A	84	ASP
4	A	103	THR
4	A	108	VAL
4	A	124	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	125	GLU
4	A	126	GLN
4	A	141	LYS
4	A	144	ARG
4	A	164	ASP
4	A	170	GLU
4	A	171	ASP
4	A	175	VAL
4	A	192	ARG
4	A	197	VAL
4	A	200	TYR
4	A	202	TYR
4	A	205	ILE
4	A	225	ILE
4	A	237	MET
4	A	239	THR
4	A	240	THR
4	A	245	THR
4	A	246	GLU
4	A	248	LEU
4	A	250	VAL
4	A	251	LEU
4	A	257	VAL
4	A	266	ARG
4	A	271	VAL
5	C	5	LEU
5	C	13	GLU
5	C	14	ASP
5	C	46	ILE
5	C	53	ARG
5	C	58	LEU
5	C	79	SER
5	C	80	ARG
5	C	102	ARG
5	C	125	THR
5	C	138	SER
5	C	141	ASN
5	C	142	LEU
5	C	144	THR
5	C	154	LEU
5	C	155	ARG
5	C	157	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	165	ASN
5	C	171	VAL
5	C	178	LEU
6	D	19	LYS
6	D	29	ASP
6	D	34	LYS
6	D	46	LYS
6	D	47	THR
6	D	48	LEU
6	D	59	SER
6	D	77	ASP
6	D	79	VAL
6	D	87	ILE
6	D	88	THR
6	D	105	LEU
6	D	126	ASP
6	D	131	ASP
6	D	146	CYS
6	D	154	SER
6	D	192	SER
6	D	204	ILE
6	D	218	LEU
6	D	220	LYS
6	D	225	LEU
7	E	35	LYS
7	E	47	VAL
7	E	72	ASP
7	E	81	ASP
7	E	89	VAL
7	E	99	THR
7	E	100	ARG
7	E	107	ILE
7	E	116	LEU
7	E	137	LEU
7	E	139	ILE
7	E	160	LYS
7	E	183	SER
7	E	196	ILE
7	E	198	ASP
7	E	224	THR
7	E	225	TYR
7	E	226	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	229	THR
7	E	231	ASP
7	E	234	LYS
7	E	237	VAL
7	E	239	THR
7	E	241	SER
8	F	12	VAL
8	F	35	SER
8	F	37	VAL
8	F	39	VAL
8	F	44	THR
8	F	72	VAL
8	F	83	SER
8	F	84	VAL
8	F	94	ARG
8	F	96	LEU
8	F	115	VAL
8	F	129	SER
8	F	134	CYS
8	F	149	SER
8	F	153	VAL
8	F	156	LEU
8	F	176	LEU
8	F	177	LEU
8	F	179	GLN
8	F	184	ILE
8	F	185	LYS
8	F	197	LYS
8	F	214	LYS
8	F	218	LEU
8	F	220	THR
8	F	221	THR
8	F	223	ILE
9	G	7	LYS
9	G	46	ILE
9	G	57	THR
9	G	92	ILE
9	G	139	LEU
9	G	169	ILE
9	G	181	CYS
9	G	188	ASN
9	G	195	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	204	SER
9	G	206	ASP
9	G	210	VAL
9	G	247	THR
9	G	254	LYS
10	H	56	VAL
10	H	96	ARG
10	H	104	THR
10	H	106	ARG
10	H	115	ILE
10	H	118	LEU
10	H	137	ARG
10	H	154	VAL
10	H	156	VAL
10	H	166	ILE
10	H	184	ILE
10	H	197	LYS
10	H	199	SER
10	H	219	ARG
11	I	1	MET
11	I	15	LEU
11	I	16	ILE
11	I	18	VAL
11	I	20	ASP
11	I	41	LEU
11	I	46	LYS
11	I	49	VAL
11	I	67	VAL
11	I	95	LYS
11	I	102	VAL
11	I	107	SER
11	I	114	VAL
11	I	120	ASP
11	I	126	ASP
11	I	190	ARG
11	I	213	LEU
11	I	234	LEU
12	J	29	GLU
12	J	32	MET
12	J	40	LEU
12	J	51	ILE
12	J	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	82	GLU
12	J	106	ARG
12	J	118	ARG
12	J	120	ARG
12	J	126	HIS
12	J	143	ARG
12	J	163	GLN
12	J	171	GLU
12	J	172	THR
12	J	181	THR
12	J	184	ASP
13	K	6	ASP
13	K	36	THR
13	K	38	ILE
13	K	53	LYS
13	K	58	LEU
13	K	62	VAL
13	K	73	THR
13	K	81	VAL
13	K	86	SER
13	K	97	VAL
13	K	99	ASN
13	K	100	CYS
13	K	128	LYS
13	K	132	GLU
13	K	145	ILE
13	K	159	SER
13	K	160	SER
13	K	162	LEU
13	K	174	CYS
13	K	181	GLN
13	K	186	ASP
13	K	195	LEU
13	K	206	LYS
14	L	10	ARG
14	L	39	ASN
14	L	67	ASP
14	L	69	ARG
14	L	82	VAL
14	L	89	GLU
14	L	95	ASP
14	L	97	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	L	102	ILE
14	L	103	GLU
14	L	155	LYS
14	L	163	SER
15	M	21	MET
15	M	58	VAL
15	M	72	THR
15	M	89	ILE
15	M	97	SER
16	N	6	THR
16	N	16	ILE
16	N	24	LEU
16	N	28	THR
16	N	46	THR
16	N	54	THR
16	N	67	SER
16	N	74	SER
16	N	76	VAL
16	N	88	ILE
16	N	106	HIS
16	N	116	CYS
16	N	119	ASP
16	N	127	THR
16	N	146	THR
17	O	13	ASP
17	O	62	VAL
17	O	81	ASP
17	O	89	VAL
18	P	11	LEU
18	P	13	GLN
18	P	14	SER
18	P	32	ASP
18	P	48	SER
18	P	58	HIS
18	P	67	THR
18	P	71	ILE
18	P	87	ASP
18	P	102	LEU
18	P	118	ILE
18	P	131	THR
19	Q	45	THR
19	Q	50	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	51	GLU
19	Q	53	ILE
19	Q	90	ILE
19	Q	91	THR
19	Q	119	LEU
19	Q	122	SER
19	Q	129	ILE
19	Q	133	THR
19	Q	135	ILE
19	Q	137	SER
20	R	24	GLN
20	R	41	GLN
20	R	74	GLU
20	R	75	VAL
20	R	84	ILE
20	R	92	SER
21	S	10	VAL
21	S	12	VAL
21	S	18	THR
21	S	20	THR
21	S	25	CYS
21	S	29	ASN
21	S	34	VAL
21	S	50	LYS
21	S	51	LEU
21	S	66	VAL
21	S	88	ILE
21	S	93	VAL
21	S	100	VAL
21	S	105	LYS
21	S	123	ASP
21	S	142	GLN
22	T	15	VAL
22	T	27	ASP
22	T	38	ILE
22	T	61	ILE
22	T	70	SER
22	T	102	THR
22	T	110	ASP
23	U	7	GLU
23	U	13	LEU
23	U	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	18	THR
23	U	50	ILE
23	U	52	LEU
23	U	54	LYS
23	U	55	ARG
23	U	68	ILE
23	U	83	PHE
23	U	136	THR
23	U	138	THR
24	V	36	THR
24	V	56	ARG
24	V	59	SER
24	V	99	VAL
24	V	110	LEU
24	V	130	ASP
24	V	131	LEU
24	V	134	ILE
25	W	22	ILE
25	W	25	THR
25	W	30	LYS
25	W	50	VAL
25	W	61	LEU
25	W	63	ILE
25	W	88	LEU
25	W	91	LEU
25	W	93	SER
25	W	97	ILE
25	W	99	LYS
25	W	104	ILE
25	W	106	ILE
25	W	116	ILE
26	X	2	GLN
26	X	7	GLU
26	X	9	VAL
26	X	13	VAL
26	X	33	GLN
26	X	40	ASP
26	X	50	PHE
27	Y	2	VAL
27	Y	4	MET
27	Y	80	ASP
27	Y	83	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Y	85	ASP
27	Y	96	SER
27	Y	103	VAL
28	Z	3	LYS
28	Z	9	THR
28	Z	15	SER
28	Z	105	PHE
29	a	14	THR
29	a	21	LYS
29	a	24	VAL
29	a	68	LYS
29	a	78	SER
30	b	2	THR
30	b	19	GLN
30	b	21	ILE
30	b	29	CYS
30	b	37	LYS
30	b	39	PHE
30	b	57	SER
30	b	63	VAL
30	b	74	CYS
30	b	94	ASP
31	c	11	SER
31	c	48	SER
31	c	67	THR
32	d	9	ILE
32	d	17	VAL
32	d	28	THR
32	d	35	MET
32	d	42	ILE
32	d	43	ILE
32	d	46	VAL
32	d	52	GLU
32	d	57	THR
32	d	67	ARG
33	e	55	LEU
34	f	85	TYR
34	f	87	THR
34	f	93	HIS
34	f	130	VAL
34	f	138	ARG
34	f	143	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	g	2	THR
35	g	14	HIS
35	g	20	GLN
35	g	21	ILE
35	g	31	ILE
35	g	35	SER
35	g	40	ILE
35	g	46	THR
35	g	54	ILE
35	g	62	HIS
35	g	63	SER
35	g	71	ILE
35	g	97	THR
35	g	107	ASP
35	g	113	PHE
35	g	116	ASP
35	g	141	THR
35	g	144	ASP
35	g	145	GLU
35	g	146	SER
35	g	157	SER
35	g	165	ILE
35	g	179	LEU
35	g	186	THR
35	g	196	ASN
35	g	199	THR
35	g	234	ASP
35	g	249	CYS
35	g	271	LYS
35	g	292	SER
35	g	305	ASN
36	i	83	VAL
36	i	91	LEU
37	j	37	GLN
37	j	73	THR
37	j	83	ASP
37	j	90	ASP
38	k	46	LYS
38	k	54	LEU
38	k	120	LEU
38	k	157	THR
38	k	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	k	223	GLN
38	k	250	LYS
38	k	262	LEU
38	k	269	ILE
38	k	272	VAL
38	k	277	SER
38	k	278	VAL
38	k	279	LEU
38	k	282	LEU
38	k	294	SER
38	k	304	SER
38	k	330	VAL
38	k	335	GLU
38	k	385	LYS
38	k	386	THR
38	k	387	THR
38	k	389	ILE
38	k	426	GLN
38	k	429	HIS
38	k	430	GLU
38	k	434	ASP
38	k	436	TYR
38	k	453	ASN
38	k	456	ASP
38	k	459	VAL
38	k	461	THR
38	k	468	GLN
38	k	470	VAL
38	k	474	LEU
38	k	476	LEU
38	k	481	ASP
38	k	519	GLU
38	k	520	HIS
38	k	528	LEU
38	k	538	ILE
38	k	547	SER
38	k	551	LEU
38	k	552	LEU
38	k	569	ASP
38	k	571	ASN
38	k	573	TYR
39	l	12	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	l	22	GLN
40	n	44	LEU
40	n	66	LYS
40	n	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	23	ASN
4	A	40	ASN
4	A	41	ASN
4	A	169	ASN
4	A	179	ASN
4	A	228	ASN
5	C	24	HIS
5	C	110	ASN
5	C	131	HIS
5	C	149	ASN
6	D	43	ASN
6	D	149	GLN
6	D	208	HIS
7	E	97	GLN
7	E	254	HIS
8	F	207	HIS
9	G	50	ASN
9	G	67	GLN
9	G	98	ASN
9	G	142	HIS
9	G	157	ASN
9	G	209	HIS
9	G	216	ASN
10	H	66	HIS
10	H	89	ASN
10	H	97	ASN
10	H	98	ASN
10	H	129	ASN
10	H	218	ASN
11	I	186	GLN
11	I	225	GLN
12	J	73	GLN
12	J	91	HIS
12	J	126	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	168	HIS
12	J	186	ASN
13	K	35	ASN
13	K	44	HIS
13	K	52	ASN
13	K	84	ASN
13	K	99	ASN
13	K	155	ASN
13	K	165	GLN
13	K	181	GLN
14	L	156	HIS
15	M	73	ASN
16	N	106	HIS
16	N	112	HIS
18	P	58	HIS
18	P	69	ASN
18	P	90	HIS
18	P	101	HIS
19	Q	32	HIS
19	Q	79	GLN
20	R	114	HIS
20	R	137	HIS
21	S	8	GLN
21	S	24	HIS
22	T	48	ASN
22	T	74	GLN
22	T	121	GLN
23	U	19	ASN
25	W	81	GLN
27	Y	44	HIS
28	Z	63	ASN
28	Z	77	ASN
28	Z	92	ASN
30	b	86	ASN
31	c	9	HIS
31	c	19	HIS
31	c	49	HIS
31	c	51	GLN
32	d	7	GLN
33	e	10	HIS
33	e	28	HIS
33	e	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	f	151	ASN
35	g	14	HIS
35	g	56	GLN
35	g	76	GLN
35	g	117	ASN
35	g	178	ASN
35	g	196	ASN
36	i	118	ASN
36	i	130	ASN
36	i	132	ASN
37	j	37	GLN
38	k	23	GLN
38	k	74	ASN
38	k	95	HIS
38	k	154	ASN
38	k	321	ASN
38	k	381	ASN
38	k	440	GLN
38	k	468	GLN
38	k	556	ASN
40	n	46	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	16 (21%)	1 (1%)
2	2	1734/1863 (93%)	300 (17%)	24 (1%)
3	3	8/9 (88%)	4 (50%)	0
All	All	1816/1947 (93%)	320 (17%)	25 (1%)

All (320) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	11	G
1	1	13	G
1	1	14	C
1	1	17	C
1	1	18	G
1	1	19	G
1	1	20	A
1	1	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	22	G
1	1	48	C
1	1	49	G
1	1	58	A
1	1	72	U
1	1	73	A
1	1	74	C
1	1	76	A
2	2	4	C
2	2	11	A
2	2	33	G
2	2	37	C
2	2	41	G
2	2	42	A
2	2	46	A
2	2	56	G
2	2	67	C
2	2	68	A
2	2	72	C
2	2	73	C
2	2	74	G
2	2	75	G
2	2	76	U
2	2	77	A
2	2	78	C
2	2	79	A
2	2	80	G
2	2	91	A
2	2	102	A
2	2	103	A
2	2	113	G
2	2	115	U
2	2	126	G
2	2	127	C
2	2	143	U
2	2	147	A
2	2	148	U
2	2	155	G
2	2	163	U
2	2	181	A
2	2	182	C
2	2	183	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	191	C
2	2	197	U
2	2	202	U
2	2	223	A
2	2	226	A
2	2	273	G
2	2	277	U
2	2	278	U
2	2	285	U
2	2	286	C
2	2	296	U
2	2	297	C
2	2	299	G
2	2	300	G
2	2	315	C
2	2	316	C
2	2	317	G
2	2	318	U
2	2	322	G
2	2	325	G
2	2	333	A
2	2	337	G
2	2	347	C
2	2	352	C
2	2	354	A
2	2	358	U
2	2	359	C
2	2	367	G
2	2	372	C
2	2	374	U
2	2	375	G
2	2	376	C
2	2	399	C
2	2	407	C
2	2	408	A
2	2	431	C
2	2	438	A
2	2	440	C
2	2	455	A
2	2	462	C
2	2	464	G
2	2	472	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	477	U
2	2	482	C
2	2	515	A
2	2	516	A
2	2	541	U
2	2	542	G
2	2	543	U
2	2	546	U
2	2	547	U
2	2	548	G
2	2	553	G
2	2	554	A
2	2	555	G
2	2	579	G
2	2	582	C
2	2	583	C
2	2	584	A
2	2	588	G
2	2	590	G
2	2	598	C
2	2	604	G
2	2	618	A
2	2	633	A
2	2	649	G
2	2	650	C
2	2	658	A
2	2	659	A
2	2	661	A
2	2	662	A
2	2	673	G
2	2	678	U
2	2	679	U
2	2	680	G
2	2	681	U
2	2	682	G
2	2	729	C
2	2	734	C
2	2	735	C
2	2	736	C
2	2	737	C
2	2	738	U
2	2	739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	740	G
2	2	741	C
2	2	743	U
2	2	744	C
2	2	747	G
2	2	748	G
2	2	749	C
2	2	750	G
2	2	787	C
2	2	789	G
2	2	791	A
2	2	793	C
2	2	794	G
2	2	795	U
2	2	806	A
2	2	807	A
2	2	817	G
2	2	818	U
2	2	819	U
2	2	820	C
2	2	827	G
2	2	829	C
2	2	833	A
2	2	834	G
2	2	835	C
2	2	837	G
2	2	843	A
2	2	866	A
2	2	868	A
2	2	869	G
2	2	870	G
2	2	874	G
2	2	883	U
2	2	884	U
2	2	886	U
2	2	892	U
2	2	900	A
2	2	903	G
2	2	907	C
2	2	909	A
2	2	912	A
2	2	916	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	929	G
2	2	934	A
2	2	939	U
2	2	951	A
2	2	965	U
2	2	967	G
2	2	981	G
2	2	985	C
2	2	986	A
2	2	987	G
2	2	988	A
2	2	997	A
2	2	1004	A
2	2	1013	U
2	2	1019	A
2	2	1045	A
2	2	1057	U
2	2	1058	A
2	2	1074	C
2	2	1079	A
2	2	1081	C
2	2	1095	G
2	2	1096	A
2	2	1111	U
2	2	1113	C
2	2	1125	G
2	2	1134	C
2	2	1135	C
2	2	1136	G
2	2	1140	A
2	2	1145	A
2	2	1150	U
2	2	1151	U
2	2	1166	A
2	2	1177	A
2	2	1191	A
2	2	1203	G
2	2	1211	C
2	2	1220	G
2	2	1238	U
2	2	1247	A
2	2	1252	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1253	G
2	2	1255	A
2	2	1261	A
2	2	1270	G
2	2	1271	G
2	2	1280	A
2	2	1281	G
2	2	1282	G
2	2	1298	G
2	2	1311	U
2	2	1367	U
2	2	1371	G
2	2	1373	U
2	2	1374	A
2	2	1399	C
2	2	1406	C
2	2	1408	C
2	2	1414	C
2	2	1415	C
2	2	1420	G
2	2	1421	G
2	2	1424	G
2	2	1428	U
2	2	1433	C
2	2	1434	A
2	2	1450	A
2	2	1457	G
2	2	1458	U
2	2	1459	U
2	2	1472	A
2	2	1473	U
2	2	1485	A
2	2	1486	G
2	2	1493	G
2	2	1494	A
2	2	1502	A
2	2	1506	G
2	2	1507	U
2	2	1508	C
2	2	1515	G
2	2	1516	C
2	2	1517	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1528	A
2	2	1530	U
2	2	1543	G
2	2	1546	U
2	2	1547	G
2	2	1548	C
2	2	1549	C
2	2	1550	U
2	2	1551	A
2	2	1552	C
2	2	1553	C
2	2	1574	A
2	2	1575	A
2	2	1581	U
2	2	1583	A
2	2	1590	U
2	2	1596	A
2	2	1601	G
2	2	1616	U
2	2	1618	A
2	2	1632	A
2	2	1643	G
2	2	1649	G
2	2	1651	G
2	2	1655	C
2	2	1660	G
2	2	1666	G
2	2	1690	A
2	2	1694	A
2	2	1707	A
2	2	1710	A
2	2	1715	U
2	2	1716	U
2	2	1717	G
2	2	1739	G
2	2	1747	C
2	2	1748	G
2	2	1777	C
2	2	1778	G
2	2	1792	C
2	2	1795	A
2	2	1804	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1816	A
2	2	1820	G
2	2	1829	A
2	2	1831	G
2	2	1832	U
2	2	1835	C
2	2	1843	G
2	2	1845	A
2	2	1846	C
2	2	1855	G
2	2	1856	G
2	2	1857	A
2	2	1859	C
2	2	1863	A
3	3	48	C
3	3	51	C
3	3	52	A
3	3	55	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	72	U
2	2	67	C
2	2	71	G
2	2	73	C
2	2	74	G
2	2	76	U
2	2	102	A
2	2	191	C
2	2	596	G
2	2	597	U
2	2	677	C
2	2	740	G
2	2	1012	U
2	2	1161	G
2	2	1310	U
2	2	1427	G
2	2	1433	C
2	2	1472	A
2	2	1515	G
2	2	1547	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1548	C
2	2	1550	U
2	2	1552	C
2	2	1831	G
2	2	1855	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	I2T	2	1244	2	25,29,30	2.70	4 (16%)	28,42,45	1.26	4 (14%)
1	T6A	1	37	1	31,34,35	0.95	3 (9%)	43,49,52	1.62	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I2T	2	1244	2	-	1/16/34/35	0/2/2/2
1	T6A	1	37	1	-	5/23/41/42	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1244	I2T	CN1-N1	-9.62	1.27	1.46
2	2	1244	I2T	O2'-C2'	-7.53	1.24	1.43
2	2	1244	I2T	C33-N34	-4.08	1.27	1.48
1	1	37	T6A	ODA-C13	2.66	1.30	1.22
1	1	37	T6A	ODB-C13	-2.47	1.22	1.30
1	1	37	T6A	C6-N6	-2.35	1.34	1.39
2	2	1244	I2T	C4-N3	-2.05	1.36	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C14-C12-C13	3.85	116.75	110.03
1	1	37	T6A	ODB-C13-C12	3.69	126.95	114.15
2	2	1244	I2T	O3'-C3'-C4'	-3.63	100.65	111.08
1	1	37	T6A	C12-N11-C10	3.35	127.55	121.99
1	1	37	T6A	N6-C10-N11	3.24	118.23	113.77
1	1	37	T6A	O10-C10-N6	-3.05	118.22	123.64
2	2	1244	I2T	C3'-C2'-C1'	2.64	104.81	101.69
2	2	1244	I2T	O3'-C3'-C2'	2.63	120.24	111.82
1	1	37	T6A	ODA-C13-C12	-2.50	113.55	121.86
1	1	37	T6A	C15-C14-C12	2.17	116.59	112.29
1	1	37	T6A	O4'-C1'-N9	2.15	112.22	108.09
1	1	37	T6A	ODB-C13-ODA	-2.02	119.49	124.08
2	2	1244	I2T	C32-C31-N3	-2.01	108.64	112.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	N11-C12-C13-ODA
1	1	37	T6A	N11-C12-C13-ODB
1	1	37	T6A	C14-C12-C13-ODA
1	1	37	T6A	C14-C12-C13-ODB
1	1	37	T6A	C14-C12-N11-C10
2	2	1244	I2T	N34-C33-C34-O36

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 230 ligands modelled in this entry, 230 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	9.63

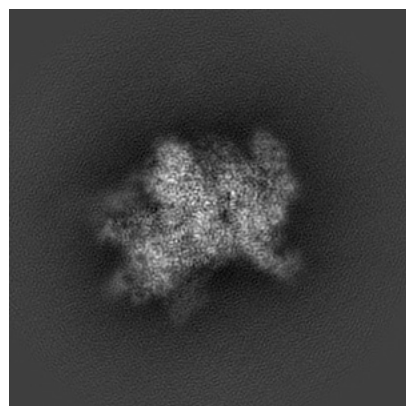
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17330. These allow visual inspection of the internal detail of the map and identification of artifacts.

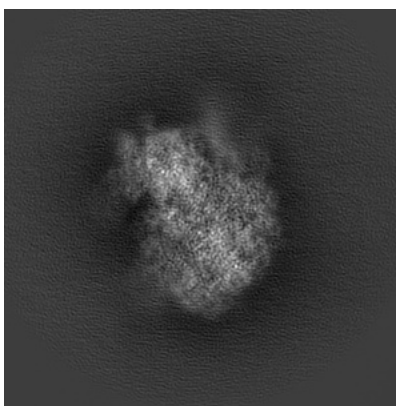
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

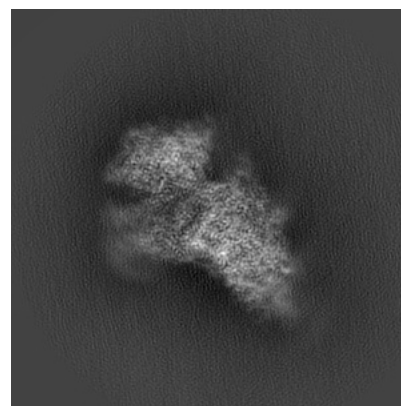
6.1.1 Primary map



X

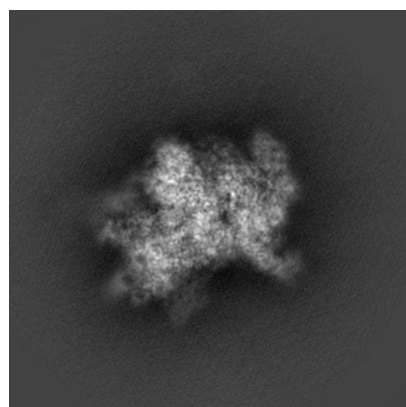


Y

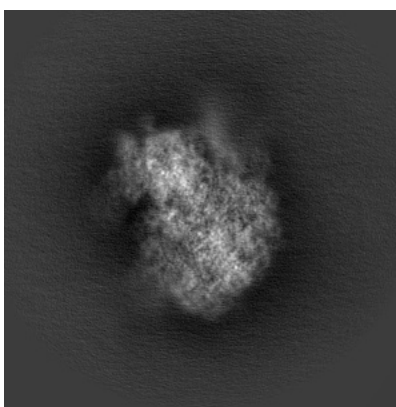


Z

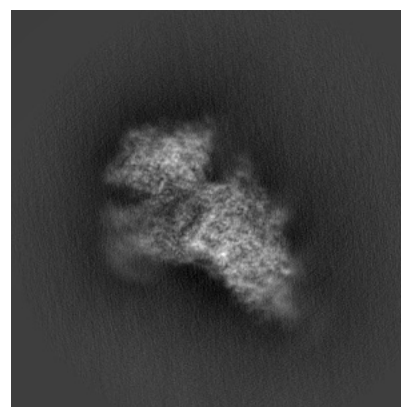
6.1.2 Raw map



X



Y

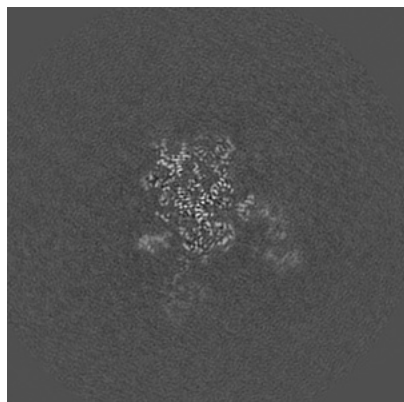


Z

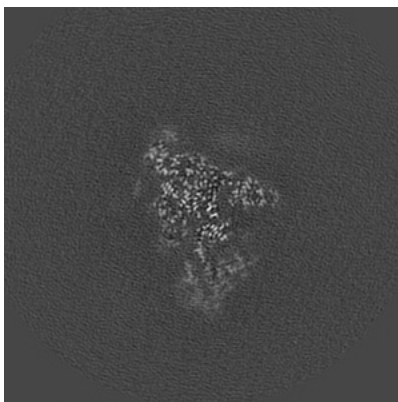
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

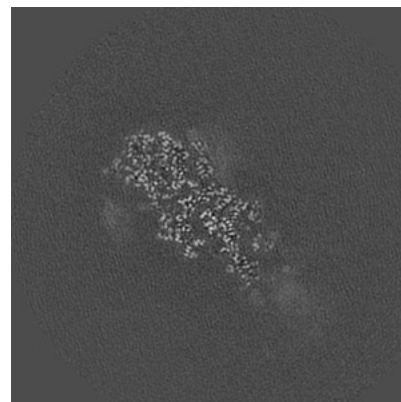
6.2.1 Primary map



X Index: 192

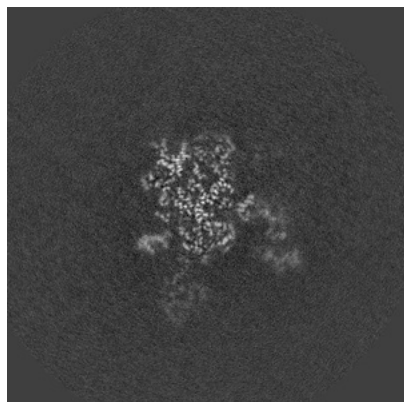


Y Index: 192

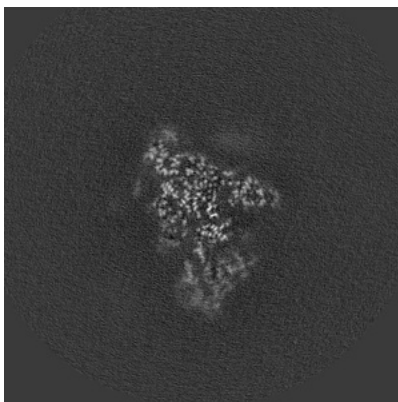


Z Index: 192

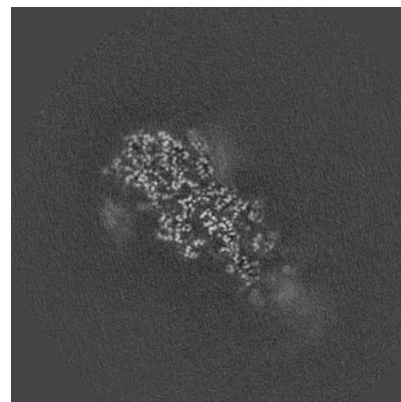
6.2.2 Raw map



X Index: 192



Y Index: 192

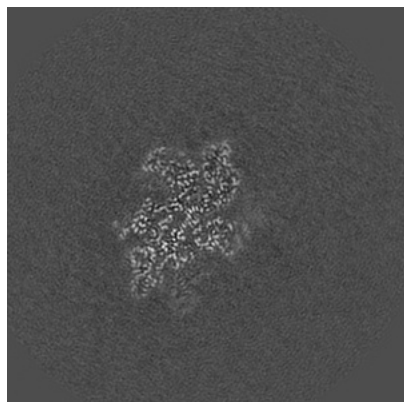


Z Index: 192

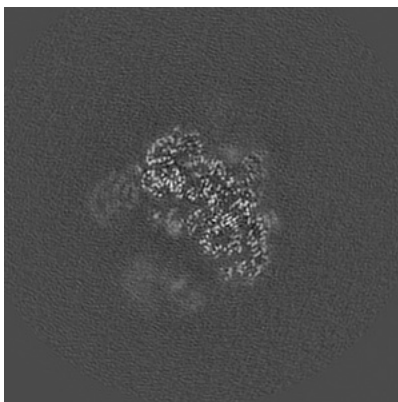
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

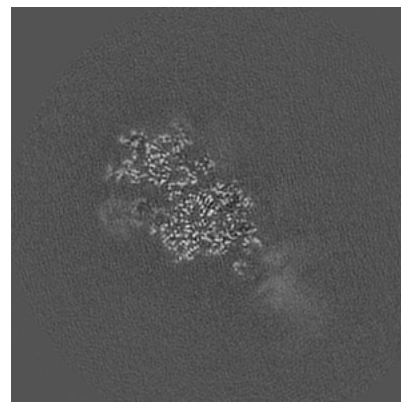
6.3.1 Primary map



X Index: 213

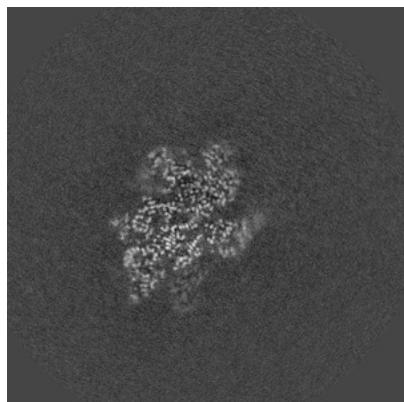


Y Index: 160

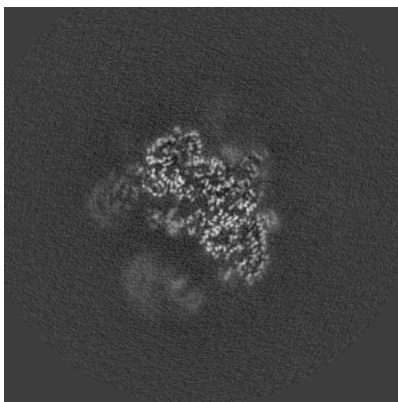


Z Index: 200

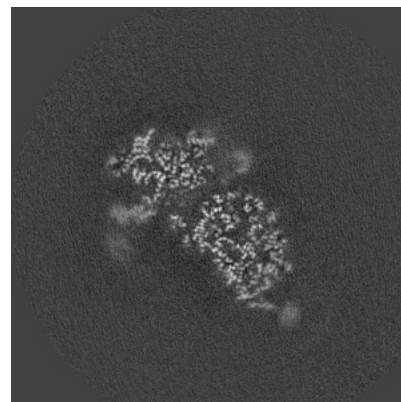
6.3.2 Raw map



X Index: 216



Y Index: 159

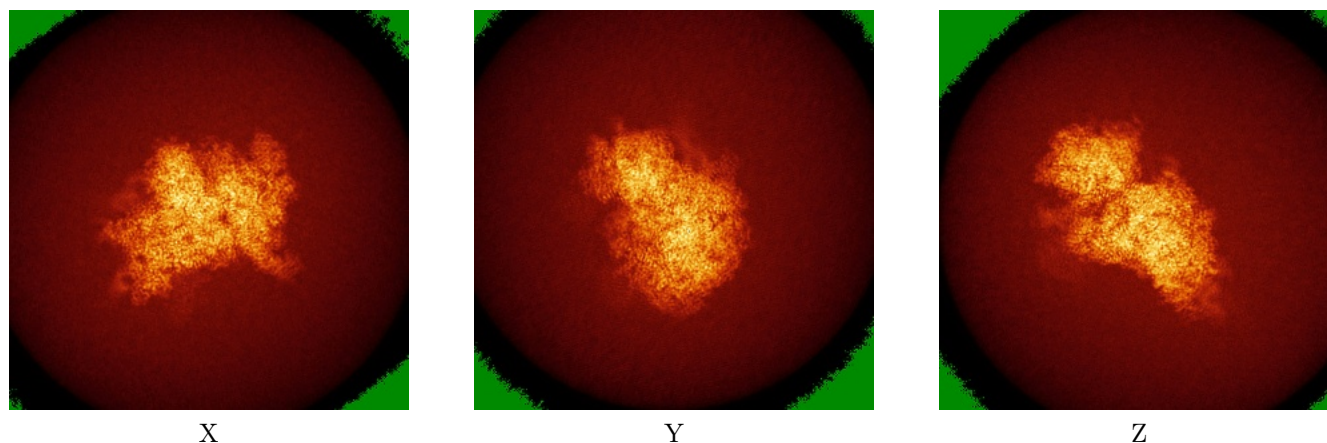


Z Index: 180

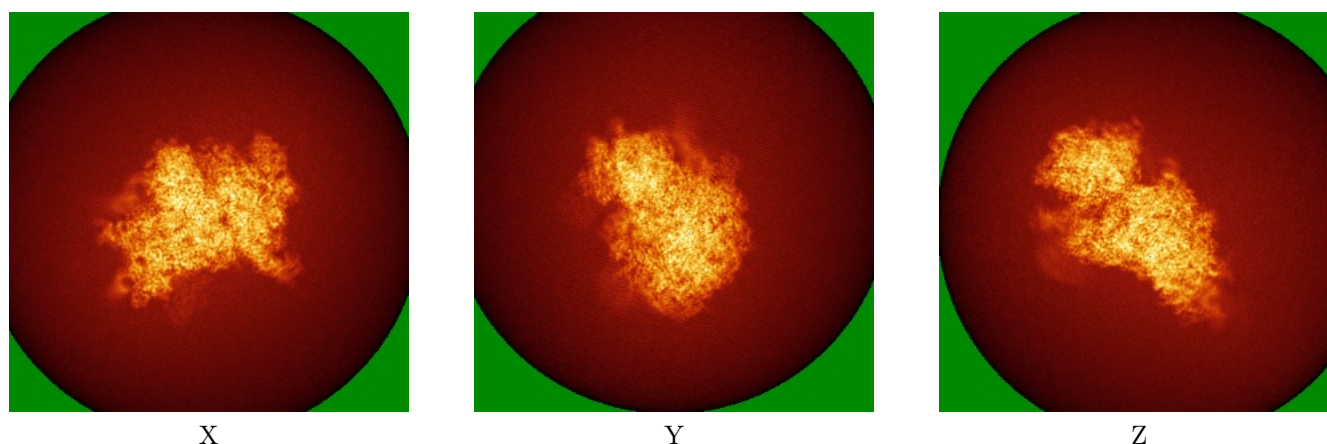
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

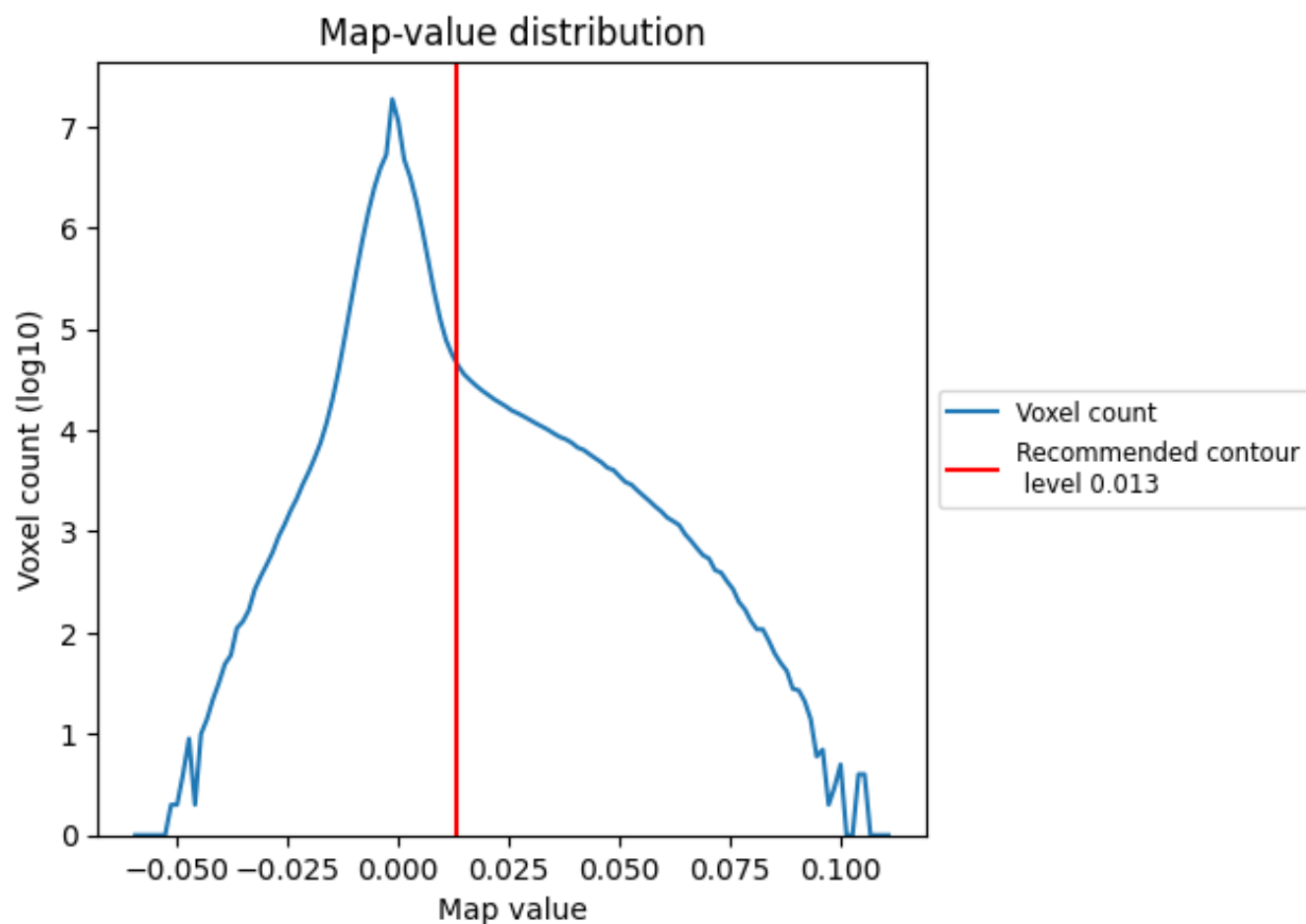
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

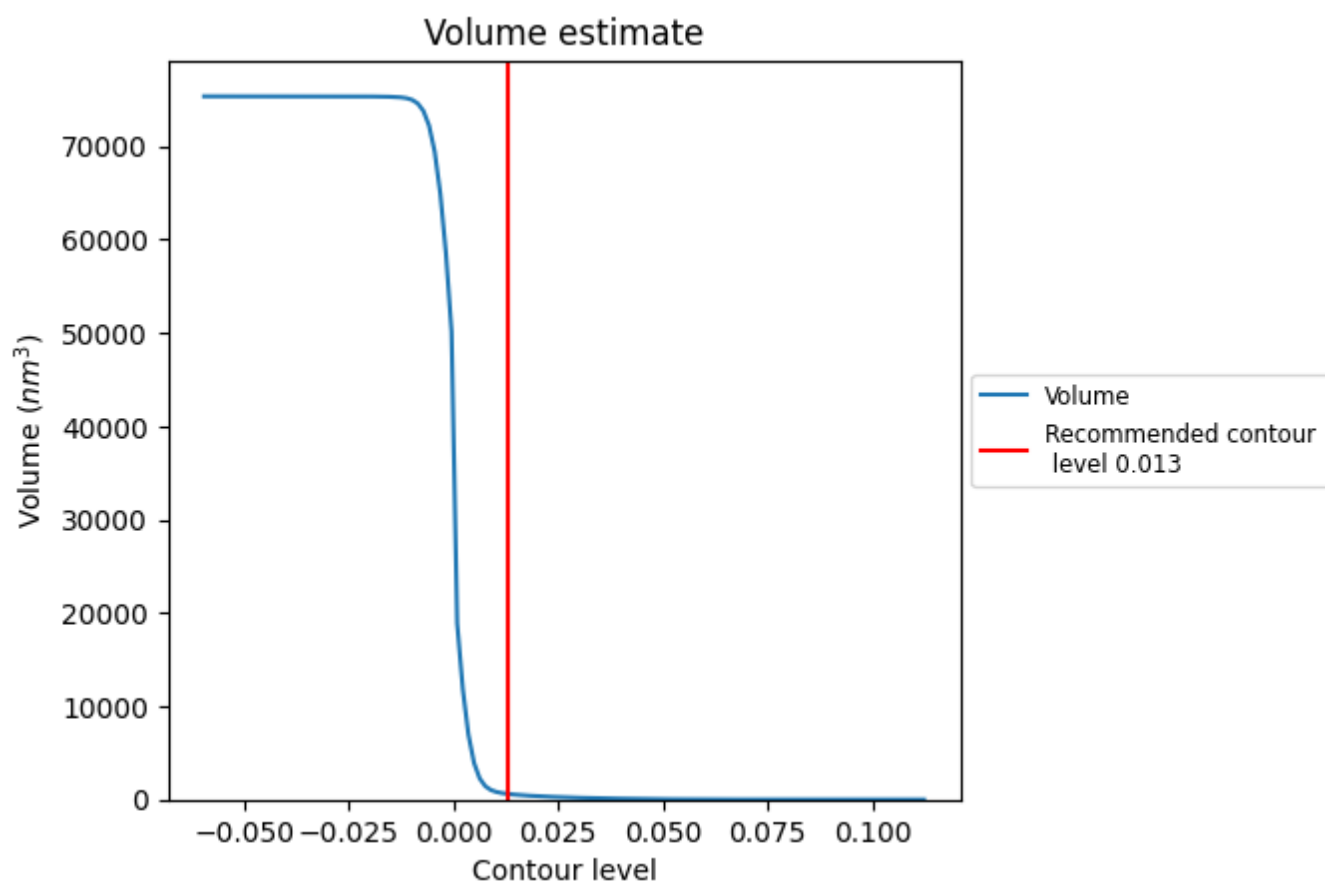
This section contains the results of statistical analysis of the map.

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.

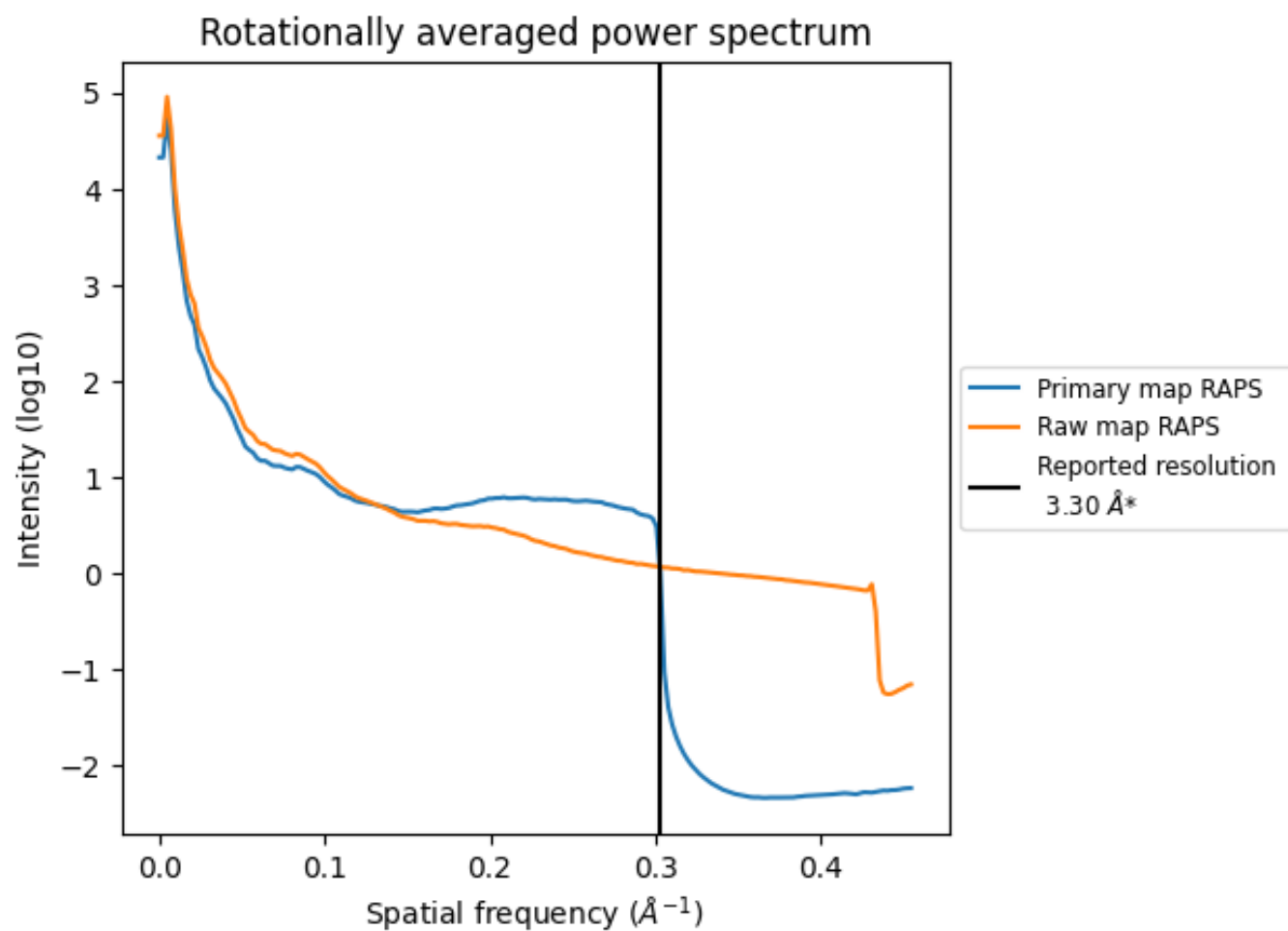
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm³; this corresponds to an approximate mass of 544 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

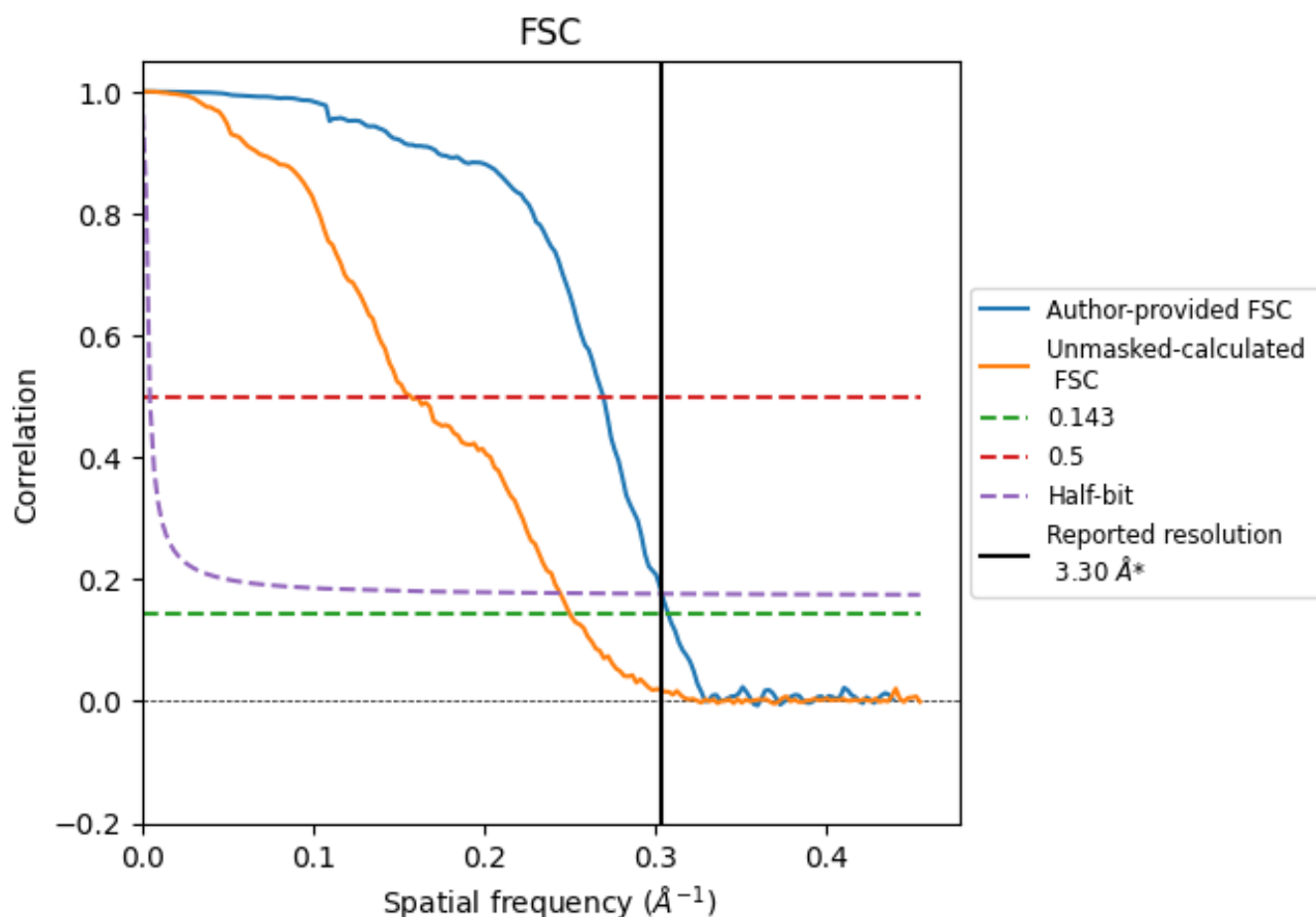


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

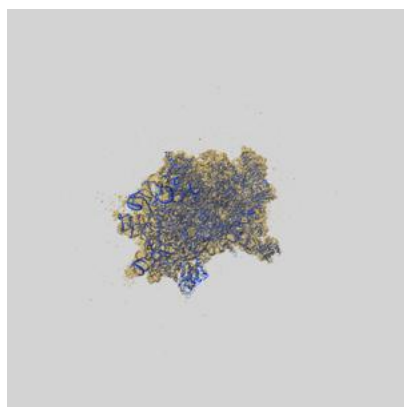
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.71	3.29
Unmasked-calculated*	4.00	6.37	4.09

*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 4.00 differs from the reported value 3.3 by more than 10 %

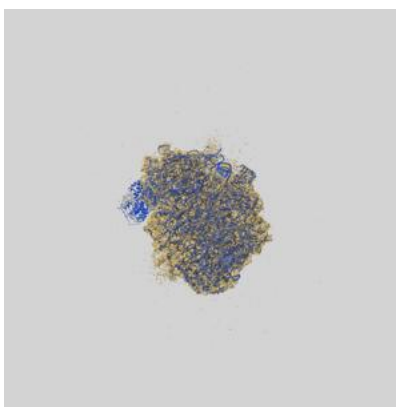
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17330 and PDB model 8P09. Per-residue inclusion information can be found in section 3 on page 12.

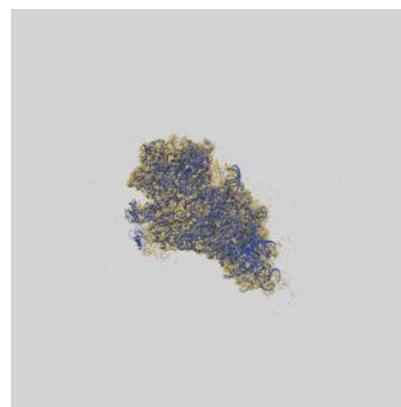
9.1 Map-model overlay [i](#)



X



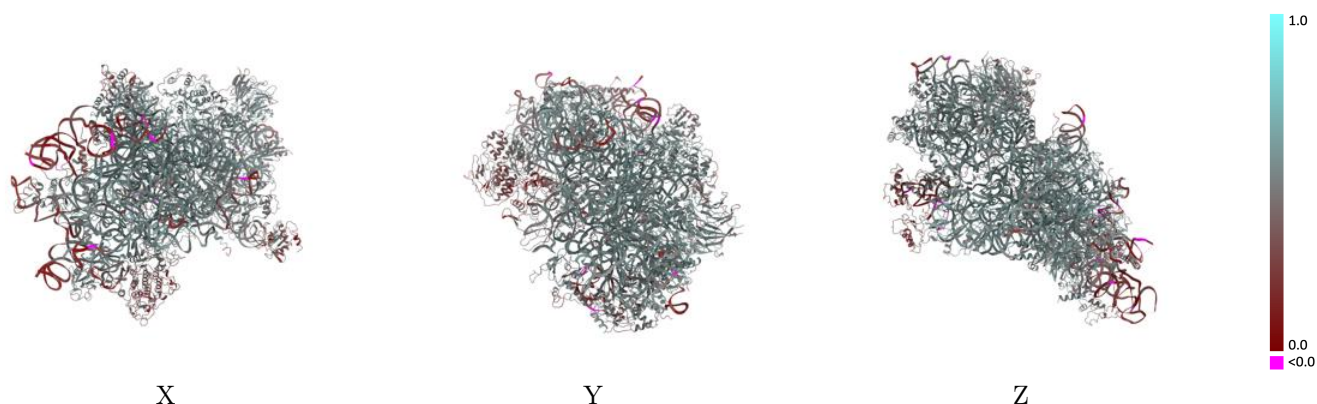
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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](#)

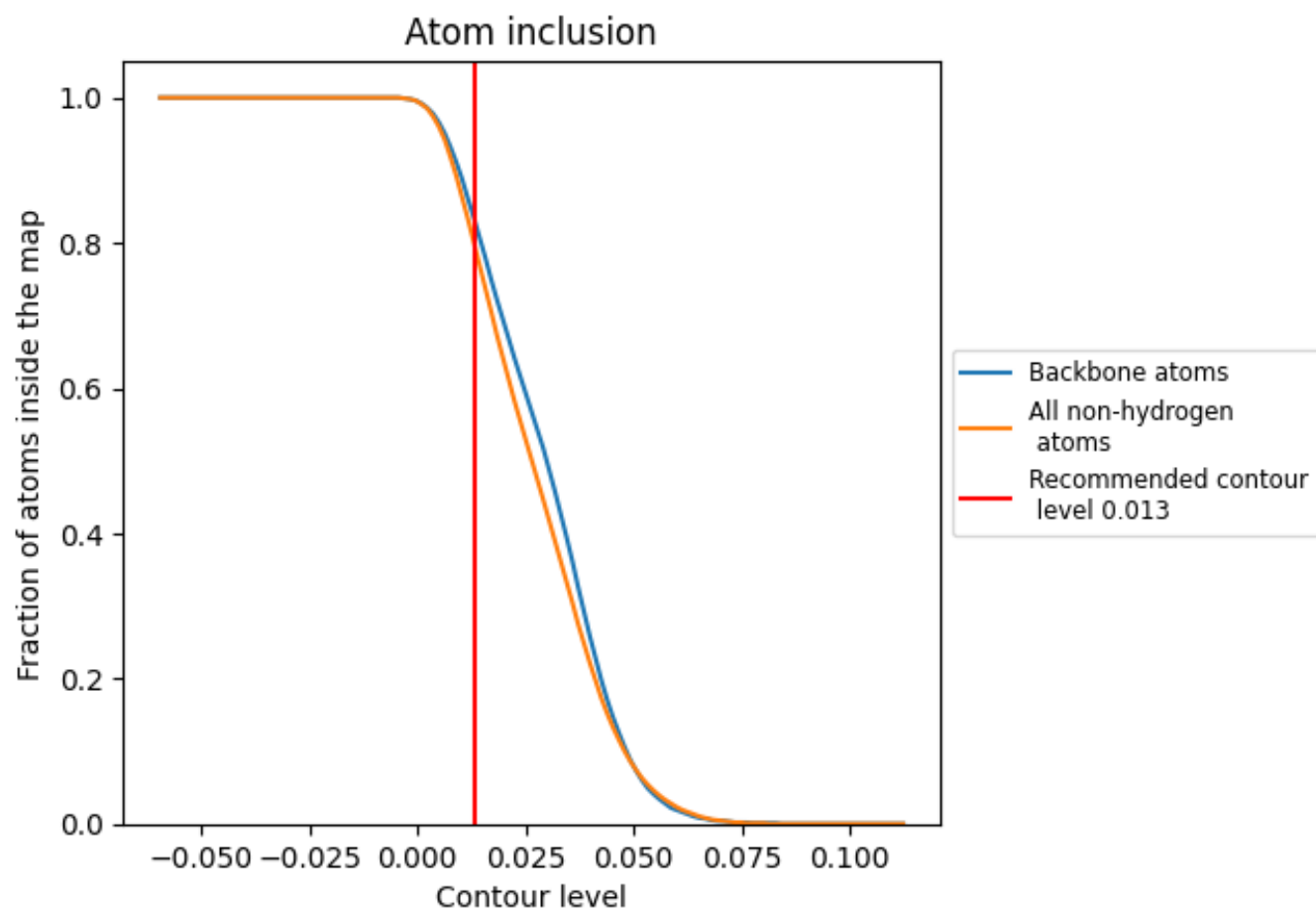


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8010	 0.4940
1	 0.5970	 0.2440
2	 0.9010	 0.5010
3	 0.6260	 0.4820
A	 0.2940	 0.3580
C	 0.8810	 0.5450
D	 0.8800	 0.5410
E	 0.8680	 0.5550
F	 0.8340	 0.5270
G	 0.8870	 0.5530
H	 0.8610	 0.5370
I	 0.7990	 0.4960
J	 0.5520	 0.4490
K	 0.8280	 0.5050
L	 0.8820	 0.5450
M	 0.8330	 0.4970
N	 0.7810	 0.5240
O	 0.5090	 0.3430
P	 0.8750	 0.5470
Q	 0.8610	 0.5390
R	 0.7510	 0.4870
S	 0.9010	 0.5570
T	 0.7390	 0.4960
U	 0.8110	 0.5090
V	 0.8670	 0.5310
W	 0.7790	 0.5130
X	 0.8790	 0.5490
Y	 0.9060	 0.5780
Z	 0.8810	 0.5610
a	 0.8670	 0.5140
b	 0.8960	 0.5640
c	 0.8130	 0.5130
d	 0.8090	 0.5440
e	 0.9080	 0.5580
f	 0.6630	 0.4080



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.8490	 0.5080
i	 0.7340	 0.4940
j	 0.5250	 0.4800
k	 0.1650	 0.3790
l	 0.7900	 0.5400
n	 0.7500	 0.4900