



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:14 AM UTC

PDB ID : 6QDW / pdb_00006qdw
EMDB ID : EMD-4531
Title : Cryo-EM structure of the 50S ribosomal subunit at 2.83 Angstroms with modeled GBC SecM peptide
Authors : Schulte, L.; Reitz, J.; Hodirnau, V.V.; Kudlinzki, D.; Mao, J.; Glaubitz, C.; Frangakis, A.; Schwalbe, H.
Deposited on : 2019-01-03
Resolution : 2.83 Å(reported)
Based on initial model : 3JBU

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:

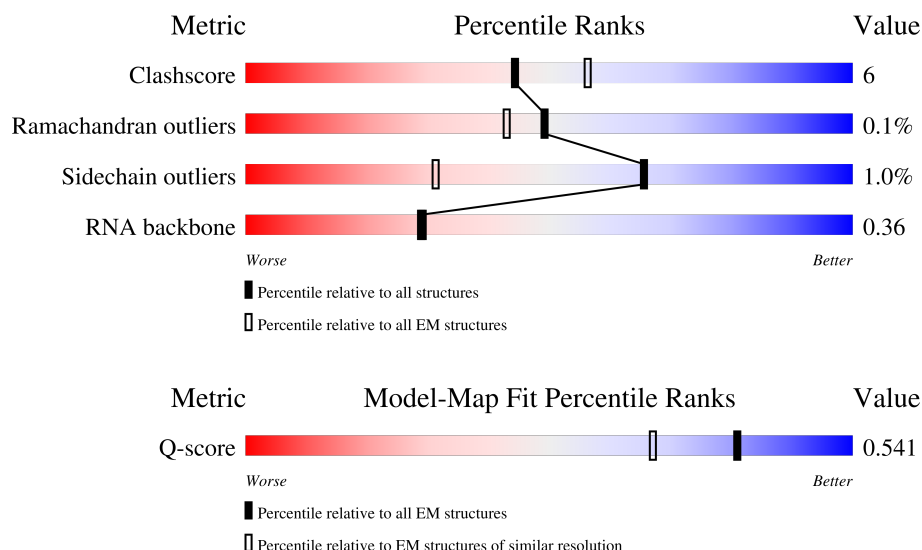
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



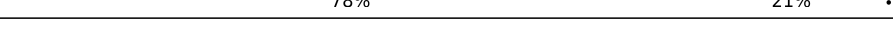
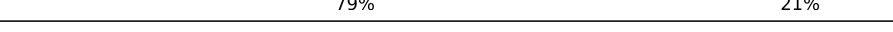
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	0	78	
2	1	63	
3	2	59	

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Mol	Chain	Length	Quality of chain
4	3	57	 75% 21% .
5	4	55	 73% 15% . 9%
6	6	46	 80% 20%
7	7	65	 82% 15% . .
8	8	38	 92% 8%
9	a	120	 58% 28% 12% .
10	b	2906	 61% 32% 6% .
11	c	273	 81% 18% .
12	d	209	 89% 11% .
13	e	201	 88% 11% .
14	f	179	 68% 28% . .
15	g	177	 84% 15% . .
16	h	149	 20% 5% . 74%
17	j	142	 84% 16%
18	k	123	 77% 22% .
19	l	144	 78% 21% .
20	m	136	 79% 21%
21	n	127	 84% 10% 6%
22	o	117	 75% 23% . .
23	p	115	 86% 12% .
24	q	118	 88% 11% .
25	r	103	 81% 16% .
26	s	110	 68% 31% .
27	t	100	 74% 18% . 7%
28	u	104	 85% 13% .

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Mol	Chain	Length	Quality of chain
29	v	75	32% 53% 15%
30	w	94	86% 14%
31	y	85	68% 18% • 13%
32	z	61	25% 15% • 57%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90690 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 protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2888	Total	C	N	O	P	0	0
			62008	27660	11413	20047	2888		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1042	648	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	99	Total	C	N	O	S	0	0
			791	500	149	140	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	u	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	75	Total	C	N	O	P	0	0
			1583	707	270	531	75		

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	74	Total	C	N	O	S	0	0
			559	348	112	98	1		

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	26	Total	C	N	O	S	26	0
			412	266	74	70	2		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-32	MET	-	initiating methionine	UNP P02526
z	-31	GLY	-	expression tag	UNP P02526
z	-30	HIS	-	expression tag	UNP P02526
z	-29	HIS	-	expression tag	UNP P02526
z	-28	HIS	-	expression tag	UNP P02526
z	-27	HIS	-	expression tag	UNP P02526
z	-26	HIS	-	expression tag	UNP P02526
z	-25	HIS	-	expression tag	UNP P02526
z	-24	HIS	-	expression tag	UNP P02526
z	-23	HIS	-	expression tag	UNP P02526
z	-22	HIS	-	expression tag	UNP P02526
z	-21	HIS	-	expression tag	UNP P02526

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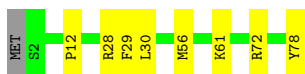
Chain	Residue	Modelled	Actual	Comment	Reference
z	13	PHE	ASN	conflict	UNP P02526
z	15	THR	ILE	conflict	UNP P02526
z	16	PRO	ARG	conflict	UNP P02526
z	18	TRP	-	expression tag	UNP P02526
z	19	ILE	-	expression tag	UNP P02526
z	20	SER	-	expression tag	UNP P02526
z	21	GLN	-	expression tag	UNP P02526
z	22	ALA	-	expression tag	UNP P02526
z	23	GLN	-	expression tag	UNP P02526
z	24	GLY	-	expression tag	UNP P02526
z	25	ILE	-	expression tag	UNP P02526
z	26	ARG	-	expression tag	UNP P02526
z	27	ALA	-	expression tag	UNP P02526
z	28	GLY	-	expression tag	UNP P02526

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

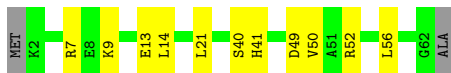
- Molecule 1: 50S ribosomal protein L28

Chain 0:  88% 10% .



- Molecule 2: 50S ribosomal protein L29

Chain 1:  79% 17% .



- Molecule 3: 50S ribosomal protein L30

Chain 2:  85% 12% .



- Molecule 4: 50S ribosomal protein L32

Chain 3:  75% 21% .



- Molecule 5: 50S ribosomal protein L33

Chain 4:  73% 15% . 9%



- Molecule 6: 50S ribosomal protein L34

Chain 6:  80% 20%



- Molecule 7: 50S ribosomal protein L35

Chain 7:  82% 15% ..



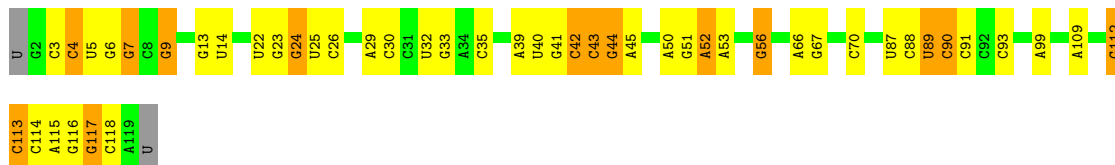
- Molecule 8: 50S ribosomal protein L36

Chain 8:  92% 8%



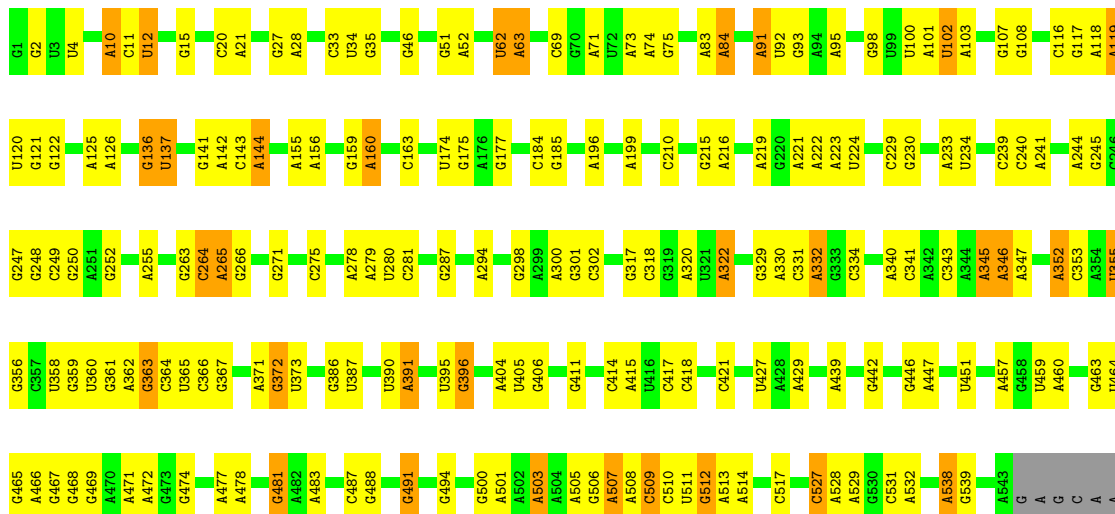
- Molecule 9: 5S rRNA

Chain a:  58% 28% 12% .

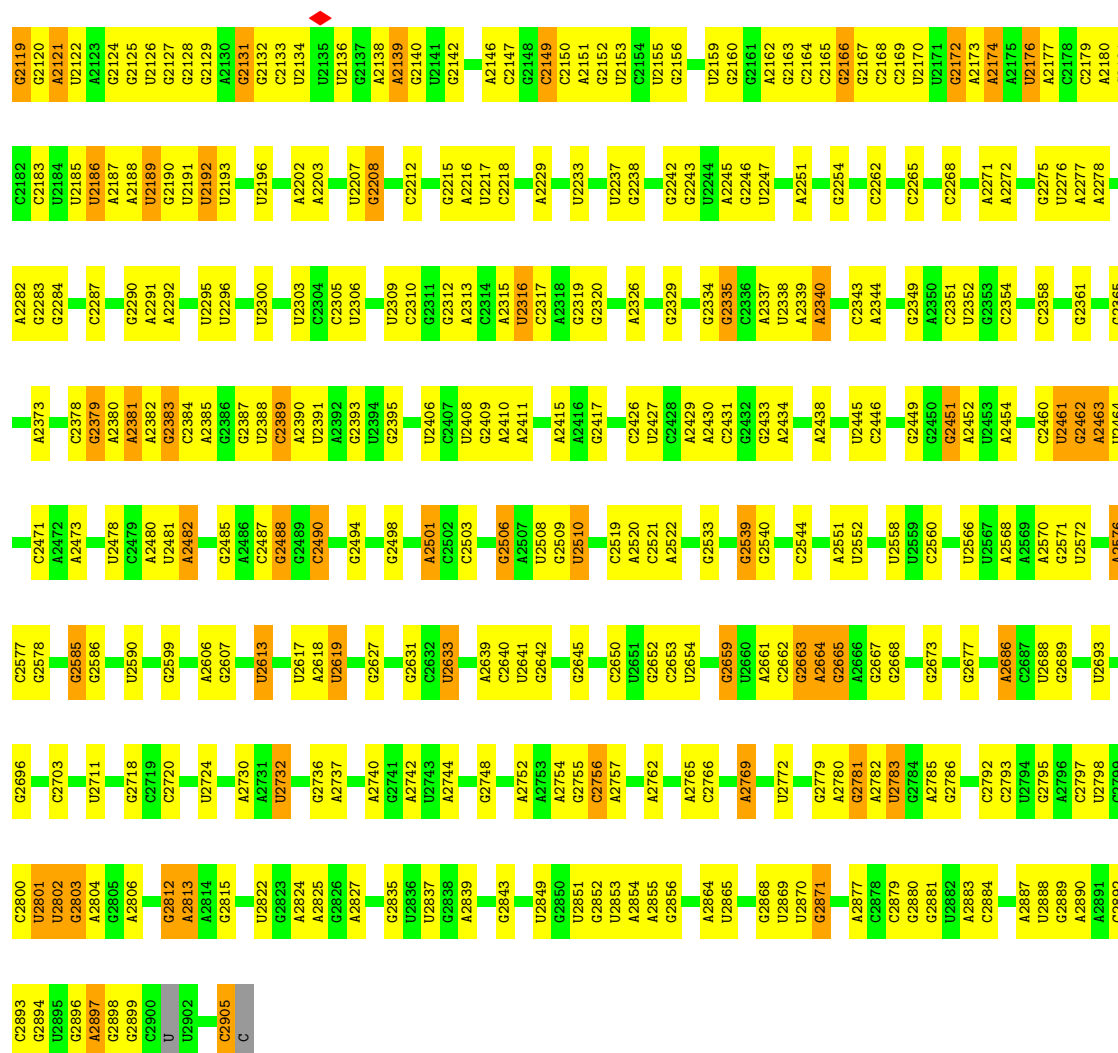


- Molecule 10: 23S rRNA

Chain b:  61% 32% 6% .

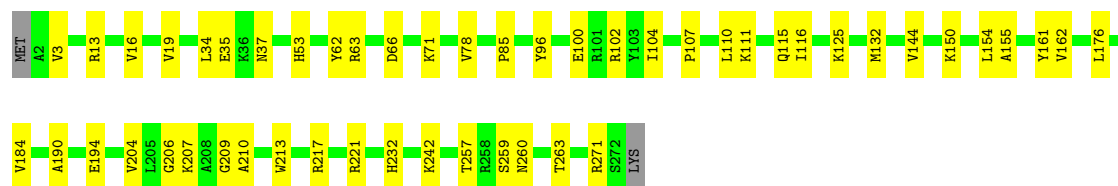


C2027	G1910	U1784	G1568	U1561	U1469	G1366	G1250	U1132	U1063	A986	G877	G759	U648	U
A2034	G1911	A1785	G1669	U1565	U1470	G1367	U1251	G1133	G1064	C989	C878	A763	G649	C
A2035	C1912	A1786	A1670	A1566	A1471	A1368	G1252	U1134	G1065	A899	A879	U764	A653	U
G2036	G1913	A1787	C1671	C1566	A1472	A1369	A1255	A1135	C1066	A890	A880	G653	A558	G
A2037	G1914	A1788	C1672	A1567	A1473	G1370	U1257	C1137	U1067	A991	G881	G765	G654	A
U2038	U1915	A1789	G1676	A1568	G1477	A1380	G1258	G1138	U1068	A992	G882	A766	U655	A
G2039	A1916	C1792	C1677	G1570	U1478	A1381	U1267	U1143	G1070	C997	G884	C767	C559	G
C2040	C1917	G1793	A1680	A1571	A1479	G1382	A1268	A1144	A1071	A998	G885	G777	A565	G
U2043	U1921	G1794	A1681	A1574	G1480	A1385	U1269	U1165	A1072	G999	U886	G778	U568	G
G2044	A1922	U1799	G1697	U1580	G1484	C1388	G1273	G1170	C1075	U1001	A888	A783	U569	G
C2047	C1923	G1800	G1705	U1583	U1488	C1389	A1274	A1171	G1076	A1002	U889	A784	U570	G
A2051	A1931	A1802	C1706	G1584	U1489	C1390	A1275	C1172	C1077	A1003	G890	A785	U571	G
G2052	C1932	A1803	A1707	C1585	C1495	A1394	U1276	A1173	C1078	G1004	G893	G786	G655	G
C2053	G1933	A1804	C1708	A1585	A1496	A1395	A1277	G1174	A1079	U1006	A894	G787	A670	G
G2054	G1934	A1810	G1709	C1586	A1497	U1396	A1278	C1175	U1080	C1007	G895	A791	U575	G
A2055	U1935	G1813	G1717	A1588	A1498	U1398	G1281	U1176	C1081	C1008	U896	U792	A576	G
A2056	A1940	C1818	G1720	U1591	U1499	U1402	A1286	A1177	A1083	C1009	U897	C793	U577	G
C2059	A1941	G1819	U1721	A1592	C1500	G1411	A1289	G1187	U1084	A1012	A795	G666	G579	G
G2060	U1942	U1820	G1722	A1593	A1506	G1412	G1290	G1189	U1085	G1013	A687	A796	G580	G
A2064	U1943	G1830	A1723	C1594	A1507	U1413	C1291	G1188	A1086	U1014	G581	C808	G582	G
G2065	U1944	A1831	G1725	A1595	A1507	U1414	G1292	G1189	A1087	C1015	U688	G689	C583	G
A2066	U1959	C1835	C1732	U1596	A1510	G1417	G1301	U1190	A1088	G909	A695	A695	A584	G
C2067	G1962	A1598	G1733	A1597	A1511	G1418	G1302	G1191	A1089	U1021	A912	C700	G587	G
U2071	U1967	U1601	G1734	U1525	U1526	U1421	A1303	G1197	A1090	A1022	A913	U704	A588	G
U2072	C1971	C1602	G1735	U1526	G1530	G1422	A1304	U1201	A1092	G1024	C914	U705	C589	G
G2073	U1974	A1605	G1736	G1531	A1530	G1423	G1313	A1206	U1096	G1028	U921	G706	U590	G
A2081	U1975	C1609	A1741	C1532	G1531	G1428	C1317	A1207	A1098	A1029	A922	U712	A604	G
G2084	G1976	A1610	C1750	A1533	C1532	A1429	G1321	U1208	A1099	A1030	U933	U715	A605	G
G2097	U1977	A1611	A1751	A1534	A1534	C1430	G1322	C1209	A1100	U1035	A943	G715	G606	G
A2100	C1978	A1612	G1752	C1535	G1535	G1431	A1323	G1212	G1101	G1036	G944	U719	G607	G
U2101	U1979	U1620	G1755	C1538	C1538	G1432	A1324	G1214	A1105	G	A947	C725	U608	G
A2102	A1984	A1621	A1756	G1539	G1540	G1434	U1328	U1226	C1106	G1039	C948	A723	A615	G
U2103	U1985	G1633	A1757	G1541	G1541	A1436	A1330	U1226	U1107	G1041	A949	A724	A616	G
G2104	U1986	A1636	G1758	G1542	G1542	A1441	U1331	G1229	G1108	A1042	C950	C725	U617	G
A2105	A2105	A1636	A1759	C1543	C1543	U1442	C1332	G1234	C1111	G1043	G954	A729	A623	G
G2106	G1996	A1637	U1760	C1544	C1544	G1443	G1333	U1234	G1112	C	U960	A730	A624	G
C2107	U1997	A1638	C1765	G1545	G1545	U1444	G1334	G1238	A1113	G1046	G858	G731	A629	G
U2108	C1998	A1639	C1766	C1549	C1549	U1445	G1335	A1239	G1114	C1047	G859	A732	G631	G
U2109	U1999	U1640	G1766	U1650	U1650	G1452	G1336	G1240	G1115	A1048	G860	G735	C836	G
G2110	C2000	U1651	U1771	G1651	C1552	C1453	U1342	G1241	C1116	G1049	G966	A736	G837	G
U2111	C2001	A1652	A1775	A1653	A1553	G1454	U1346	U1242	G1117	C1055	U965	G736	G638	G
A2112	U2112	U1886	A1775	A1654	A1554	G1455	U1346	A1243	C1119	A1056	A974	G740	A639	G
U2113	G1888	G1888	G1778	A1654	A1555	G1456	C1353	G1245	G1120	G1057	A975	U749	G640	G
G2114	A2009	U1556	G1778	U1556	U1556	G1457	U1353	C1245	U1121	G1058	G976	G750	C642	G
U2115	G2014	G1557	U1781	C1557	G1557	G1461	U1354	A1246	G1127	A1059	G980	A754	U643	G
G2116	U2116	C1558	U1782	C1558	C1558	U1462	A1355	G1247	A1128	U1060	C875	A754	U644	G
A2118	A2023	C1559	U1783	C1559	C1560	C1463	A1361	A1248	G1127	G1061	C875	A754	U645	G



• Molecule 11: 50S ribosomal protein L2

Chain c: 81% 18% .



• Molecule 12: 50S ribosomal protein L3

Chain d: 89% 11% .



• Molecule 13: 50S ribosomal protein L4

#1	T18	R21	R44	A45	Q46	V52	K58	R69	S70	G71	G82	R88	K106	R114	V121	F124	S125	K130	L134	K137	L138	M141	A142	L143	E144	D145	V146	K166	K185	S201
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- [illegible]

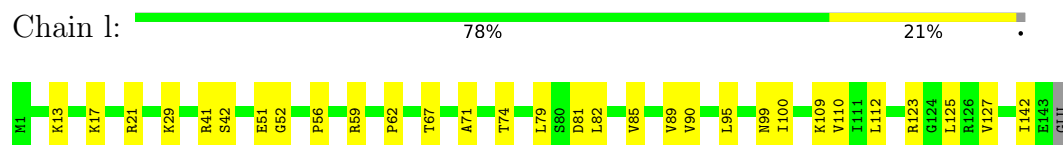
- | MET |
|------|
| S2 |
| A7 |
| K18 |
| I19 |
| N20 |
| V23 |
| T24 |
| T25 |
| G28 |
| T34 |
| R35 |
| T36 |
| L37 |
| V43 |
| K44 |
| H45 |
| A46 |
| T49 |
| A68 |
| R69 |
| V76 |
| I77 |
| G78 |
| V79 |
| K86 |
| T127 |
| E130 |
| I131 |
| V132 |
| D137 |
| V140 |
| E155 |
| P156 |
| V157 |
| K160 |
| K176 |

- [illegible]

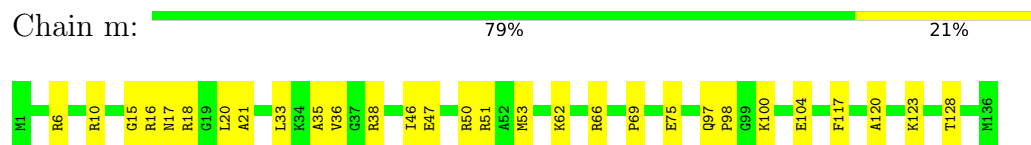
- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| M1 | K2 | T3 | V11 | D19 | K23 | L32 | L36 | R37 | T45 | T50 | T54 | M92 | R95 | R96 | R99 | E102 | V105 | M118 | F119 | R120 | K121 | L122 | Y125 | H132 | T142 |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| M1 | I2 | T6 | M7 | L8 | N9 | R18 | K23 | Y32 | K40 | T43 | K44 | D56 | V57 | V63 | R64 | T65 | K66 | K67 | R70 | R71 | V76 | N89 | P102 | R105 | E106 | L107 | E110 | M113 | E121 | V122 |
|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

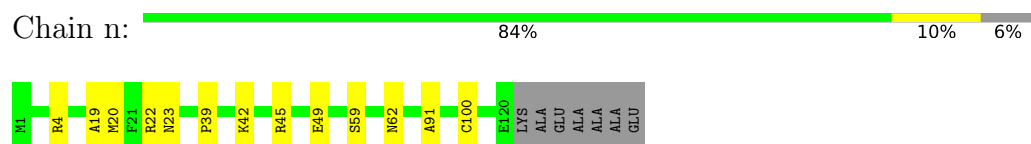
- WORLDWIDE
PDB
PROTEIN DATA BANK



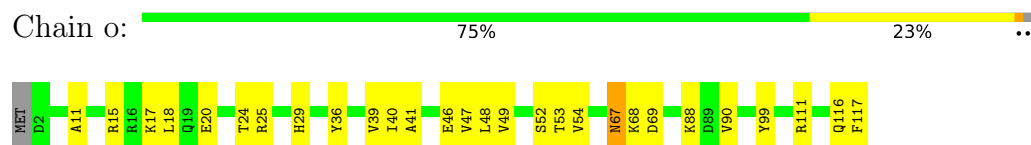
- Molecule 20: 50S ribosomal protein L16



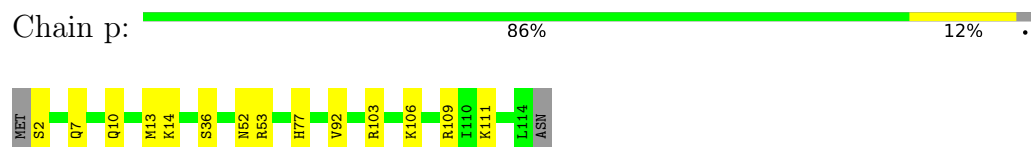
- Molecule 21: 50S ribosomal protein L17



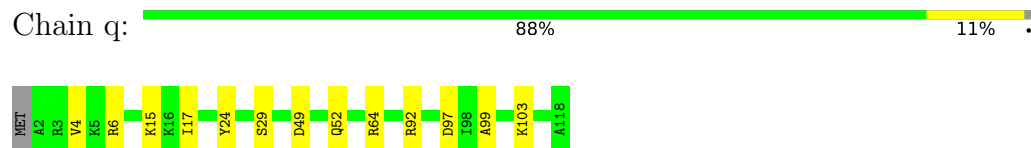
- Molecule 22: 50S ribosomal protein L18



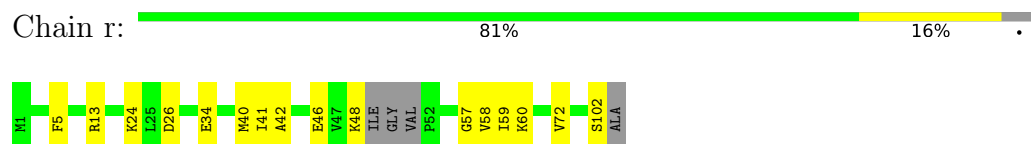
- Molecule 23: 50S ribosomal protein L19



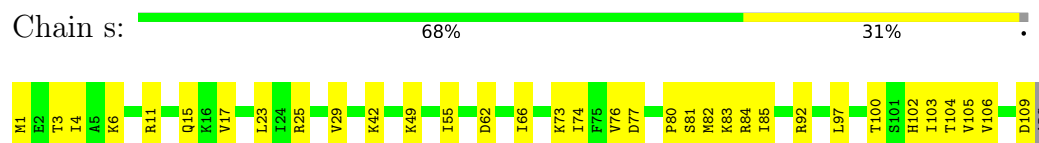
- Molecule 24: 50S ribosomal protein L20



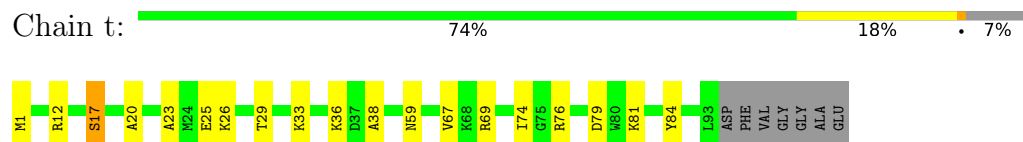
- Molecule 25: 50S ribosomal protein L21



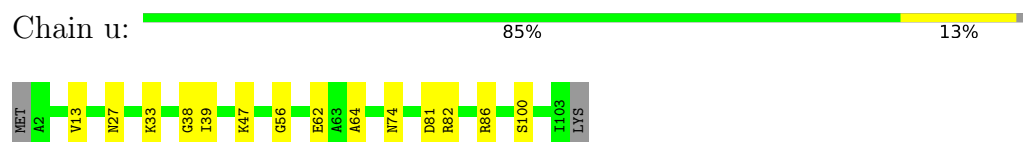
- Molecule 26: 50S ribosomal protein L22



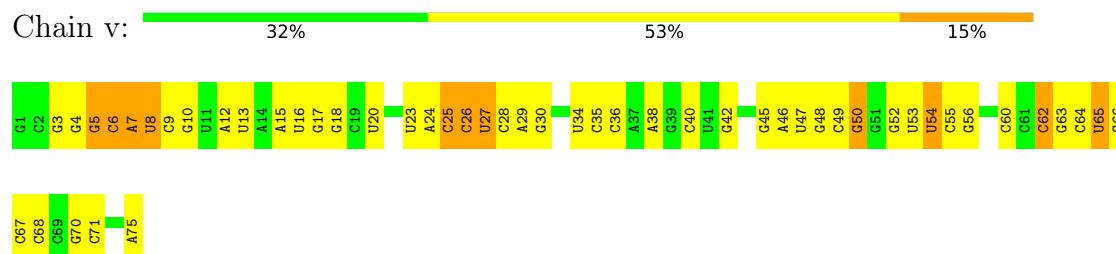
- Molecule 27: 50S ribosomal protein L23



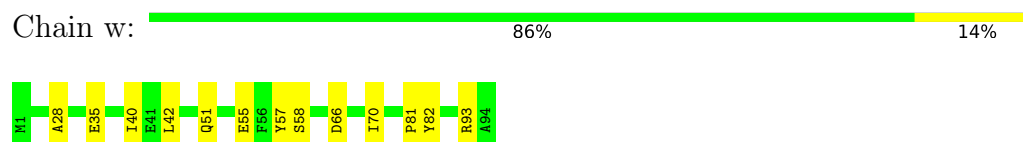
- Molecule 28: 50S ribosomal protein L24



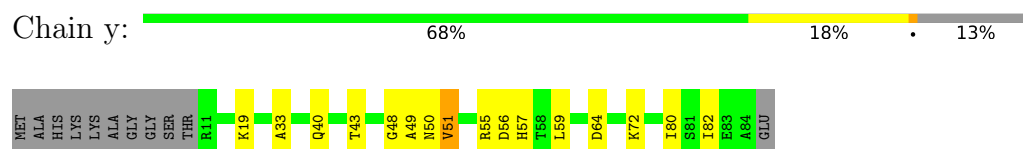
- Molecule 29: glycine-tRNA glyT



- Molecule 30: 50S ribosomal protein L25

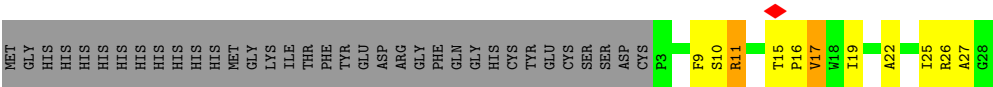


- Molecule 31: 50S ribosomal protein L27



- Molecule 32: Gamma-crystallin B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0	0.60	0/635	0.62	0/848
2	1	0.45	0/496	0.56	0/660
3	2	0.56	0/443	0.73	1/593 (0.2%)
4	3	0.67	0/440	0.62	0/588
5	4	0.42	0/416	0.65	1/554 (0.2%)
6	6	0.73	0/380	0.60	0/498
7	7	0.65	0/513	0.60	0/676
8	8	0.66	0/303	0.71	0/397
9	a	0.50	0/2824	0.53	0/4402
10	b	0.67	0/69444	0.53	6/108322 (0.0%)
11	c	0.63	0/2121	0.62	0/2852
12	d	0.63	0/1586	0.65	0/2134
13	e	0.58	0/1571	0.66	0/2113
14	f	0.38	0/1434	0.72	0/1926
15	g	0.41	0/1343	0.64	1/1816 (0.1%)
16	h	0.40	0/290	0.74	0/392
17	j	0.59	0/1152	0.55	0/1551
18	k	0.58	0/947	0.62	0/1268
19	l	0.60	0/1051	0.66	2/1400 (0.1%)
20	m	0.59	0/1093	0.58	0/1460
21	n	0.65	0/973	0.69	0/1301
22	o	0.42	0/902	0.69	0/1209
23	p	0.54	0/920	0.55	0/1231
24	q	0.70	0/960	0.61	0/1278
25	r	0.57	0/803	0.59	0/1070
26	s	0.61	0/852	0.57	0/1142
27	t	0.50	0/744	0.62	2/994 (0.2%)
28	u	0.45	0/787	0.75	0/1051
29	v	0.33	0/1764	0.56	0/2744
30	w	0.47	0/766	0.59	0/1025
31	y	0.63	0/566	0.70	0/750
32	z	0.22	0/426	0.52	0/578
All	All	0.64	0/98945	0.56	13/148823 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	5	ILE	N-CA-C	-7.47	105.08	112.17
15	g	77	ILE	N-CA-C	-7.09	105.62	112.29
10	b	1301	G	C2'-C3'-O3'	6.89	124.03	113.70
3	2	44	ILE	N-CA-C	-6.51	106.45	112.96
27	t	17	SER	CA-C-N	6.42	133.80	121.54
27	t	17	SER	C-N-CA	6.42	133.80	121.54
19	l	52	GLY	CA-C-N	-5.63	112.69	122.83
19	l	52	GLY	C-N-CA	-5.63	112.69	122.83
10	b	705	U	C2'-C3'-O3'	5.35	121.73	113.70
10	b	2462	G	O4'-C1'-N9	5.28	116.12	108.20
10	b	2539	G	C2'-C3'-O3'	5.15	121.43	113.70
10	b	1597	C	C2'-C3'-O3'	5.05	121.28	113.70
10	b	2868	G	C2'-C3'-O3'	5.04	121.26	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	5	0
2	1	495	0	526	7	0
3	2	439	0	482	3	0
4	3	434	0	445	10	0
5	4	409	0	440	6	0
6	6	377	0	418	9	0
7	7	504	0	572	10	0
8	8	302	0	341	3	0
9	a	2528	0	1283	49	0
10	b	62008	0	31189	464	0
11	c	2082	0	2154	34	0
12	d	1565	0	1616	16	0
13	e	1552	0	1619	22	0
14	f	1410	0	1444	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	g	1323	0	1371	15	0
16	h	287	0	307	6	0
17	j	1129	0	1162	16	0
18	k	938	0	1012	15	0
19	l	1042	0	1121	21	0
20	m	1074	0	1157	20	0
21	n	960	0	1000	10	0
22	o	892	0	923	21	0
23	p	908	0	956	11	0
24	q	947	0	1019	10	0
25	r	791	0	811	12	0
26	s	845	0	909	24	0
27	t	738	0	807	12	0
28	u	779	0	831	9	0
29	v	1583	0	807	35	0
30	w	753	0	780	9	0
31	y	559	0	575	13	0
32	z	412	0	398	12	0
All	All	90690	0	59127	854	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 6.

All (854) 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)
10:b:511:U:C3'	10:b:512:G:H5'	1.67	1.22
13:e:137:LYS:O	13:e:138:LEU:CG	1.90	1.19
29:v:53:U:H2'	29:v:54:U:H5'	1.25	1.15
13:e:137:LYS:O	13:e:138:LEU:HG	0.97	1.14
10:b:511:U:O3'	10:b:512:G:H5'	1.49	1.11
29:v:26:C:H2'	29:v:27:U:C5	1.88	1.08
10:b:52:A:N7	10:b:119:A:N6	2.03	1.06
14:f:170:LEU:CD1	14:f:175:PHE:HB3	1.86	1.05
10:b:2271:A:N6	10:b:2276:U:H3	1.55	1.04
29:v:53:U:C2'	29:v:54:U:H5'	1.91	0.99
14:f:170:LEU:HD12	14:f:175:PHE:HB3	1.45	0.98
14:f:170:LEU:CD1	14:f:175:PHE:CB	2.41	0.97
14:f:170:LEU:HD12	14:f:175:PHE:CB	1.95	0.97
10:b:511:U:O3'	10:b:512:G:C5'	2.13	0.96
10:b:588:A:N1	10:b:811:G:O2'	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2271:A:H62	10:b:2276:U:H3	0.98	0.94
10:b:512:G:O3'	10:b:513:A:P	2.26	0.94
10:b:1668:G:N2	10:b:1998:C:O2	2.01	0.94
10:b:463:G:N2	10:b:466:A:OP2	2.03	0.91
10:b:976:G:H8	10:b:992:A:H62	1.11	0.91
14:f:158:THR:OG1	14:f:169:LEU:HD21	1.72	0.90
10:b:2271:A:N6	10:b:2276:U:O2	2.03	0.90
14:f:29:PRO:HB2	14:f:169:LEU:HD22	1.51	0.90
10:b:2271:A:N6	10:b:2276:U:N3	2.21	0.87
10:b:2664:A:O2'	10:b:2665:G:O4'	1.91	0.87
10:b:2073:G:N2	10:b:2446:C:O2	2.07	0.87
29:v:53:U:H2'	29:v:54:U:C5'	2.05	0.86
10:b:1412:G:N2	10:b:1594:C:O2	2.09	0.85
10:b:2271:A:N6	10:b:2276:U:C2	2.45	0.85
10:b:511:U:C3'	10:b:512:G:C5'	2.55	0.84
14:f:8:TYR:OH	14:f:28:VAL:HG13	1.79	0.83
9:a:9:G:C6	9:a:112:G:O6	2.32	0.83
10:b:511:U:H3'	10:b:512:G:H5'	1.61	0.82
29:v:26:C:H2'	29:v:27:U:C6	2.15	0.82
10:b:2382:A:C4	10:b:2383:G:C8	2.69	0.81
13:e:134:LEU:HD12	13:e:137:LYS:HB3	1.62	0.81
13:e:137:LYS:C	13:e:138:LEU:HG	2.03	0.79
10:b:1021:U:HO2'	10:b:1023:A:H2	1.30	0.79
14:f:170:LEU:HD11	14:f:175:PHE:HB3	1.64	0.79
10:b:949:A:HO2'	10:b:986:A:H2	1.31	0.78
14:f:169:LEU:HD12	14:f:169:LEU:O	1.83	0.78
31:y:51:VAL:HG21	31:y:80:ILE:O	1.84	0.78
10:b:511:U:O3'	10:b:512:G:P	2.42	0.78
10:b:2835:G:OP2	12:d:59:ARG:NH1	2.16	0.77
10:b:829:U:O2'	10:b:2072:U:N3	2.19	0.76
10:b:949:A:C2'	10:b:986:A:H2	1.98	0.75
1:0:12:PRO:HB3	1:0:30:LEU:HD23	1.68	0.74
9:a:33:G:N3	9:a:50:A:C2	2.55	0.74
10:b:275:C:H1'	10:b:363:G:H22	1.51	0.74
10:b:1799:G:HO2'	11:c:257:THR:HG1	1.33	0.74
10:b:511:U:C2'	10:b:512:G:H5'	2.17	0.73
9:a:113:C:H6	22:o:46:GLU:OE2	1.71	0.73
29:v:23:U:O4	29:v:24:A:N6	2.21	0.73
29:v:26:C:C2'	29:v:27:U:C5	2.71	0.71
10:b:1488:U:H3	10:b:1505:A:H61	1.38	0.71
14:f:158:THR:HG21	14:f:169:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1781:U:H5	10:b:1786:A:N7	1.86	0.71
9:a:42:C:O2	14:f:90:THR:HG22	1.90	0.71
10:b:1171:A:H2'	10:b:1172:C:O4'	1.91	0.71
10:b:2382:A:C4	10:b:2383:G:H8	2.07	0.70
10:b:839:C:N4	10:b:943:A:N6	2.39	0.70
10:b:2379:G:C6	10:b:2383:G:O6	2.45	0.70
32:z:9[B]:PHE:HB2	32:z:11[B]:ARG:HH21	1.56	0.70
10:b:247:G:OP2	10:b:249:C:N4	2.23	0.70
29:v:10:G:H1	29:v:23:U:H3	1.40	0.70
7:7:12:LYS:NZ	10:b:247:G:O6	2.22	0.69
13:e:124:PHE:CZ	13:e:137:LYS:HG2	2.26	0.69
10:b:949:A:H2'	10:b:986:A:H2	1.56	0.69
10:b:1021:U:H3	10:b:1144:A:H62	1.41	0.69
10:b:964:G:H21	10:b:2254:G:H1	1.41	0.68
14:f:170:LEU:CD1	14:f:175:PHE:CG	2.75	0.68
16:h:4:ILE:HG13	16:h:18:GLN:HB3	1.75	0.68
10:b:1441:A:H62	10:b:1554:A:H8	1.41	0.68
29:v:53:U:C3'	29:v:54:U:H5'	2.22	0.68
14:f:8:TYR:OH	14:f:30:ARG:HG3	1.94	0.68
9:a:43:C:H5''	9:a:43:C:H6	1.58	0.67
10:b:2662:C:H2'	10:b:2663:G:H5'	1.76	0.67
10:b:2662:C:C2'	10:b:2663:G:H5'	2.24	0.67
14:f:8:TYR:CZ	14:f:30:ARG:HG3	2.30	0.67
10:b:715:G:H21	10:b:720:A:H2	1.43	0.67
9:a:113:C:C6	22:o:46:GLU:OE2	2.47	0.67
10:b:1722:U:H2'	10:b:1723:G:O4'	1.94	0.66
10:b:2383:G:N3	10:b:2383:G:H2'	2.10	0.66
10:b:1040:G:H1	10:b:1118:G:H22	1.41	0.66
10:b:1801:G:N2	10:b:1820:U:O2'	2.29	0.66
13:e:58:LYS:HG3	13:e:71:GLY:HA2	1.78	0.66
10:b:1791:A:OP2	11:c:221:ARG:NH1	2.29	0.65
10:b:2382:A:C8	10:b:2383:G:N7	2.64	0.65
10:b:2462:G:H8	10:b:2463:A:H62	1.45	0.65
10:b:2686:A:H61	10:b:2732:U:H1'	1.61	0.65
10:b:2460:C:C2'	10:b:2461:U:H5'	2.26	0.65
10:b:1584:C:O2'	10:b:1587:C:N3	2.28	0.65
11:c:232:HIS:HA	11:c:242:LYS:HE3	1.78	0.65
14:f:170:LEU:HG	14:f:171:ALA:N	2.10	0.65
10:b:2382:A:C5	10:b:2383:G:C8	2.85	0.65
10:b:136:G:C5	10:b:137:U:C4	2.84	0.64
10:b:949:A:O2'	10:b:986:A:C2	2.48	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2104:G:C6	10:b:2105:A:C5	2.85	0.64
13:e:125:SER:O	13:e:137:LYS:HE2	1.98	0.64
10:b:10:A:H2'	10:b:11:C:H5'	1.78	0.64
10:b:1584:C:O2'	10:b:1587:C:N4	2.29	0.64
10:b:1021:U:O2'	10:b:1023:A:H2	1.79	0.64
10:b:528:A:C2	10:b:2047:C:H4'	2.33	0.64
27:t:25:GLU:HG3	27:t:26:LYS:HG2	1.80	0.64
10:b:976:G:C8	10:b:992:A:N6	2.57	0.63
10:b:511:U:H3'	10:b:512:G:C5'	2.24	0.63
10:b:623:A:OP2	19:l:99:ASN:ND2	2.31	0.63
10:b:807:G:O6	10:b:2072:U:H5	1.81	0.63
20:m:17:ASN:O	20:m:38:ARG:NH1	2.31	0.63
10:b:2066:A:N6	32:z:22[A]:ALA:O	2.31	0.63
9:a:51:G:O2'	9:a:52:A:O5'	2.17	0.62
10:b:1530:A:N6	10:b:1545:G:O2'	2.32	0.62
10:b:1173:G:H21	10:b:1174:C:H41	1.46	0.62
10:b:839:C:N4	10:b:943:A:H62	1.97	0.62
10:b:1800:U:OP2	11:c:271:ARG:NH2	2.33	0.62
17:j:125:TYR:HH	17:j:132:HIS:HE2	1.47	0.62
10:b:527:C:N4	10:b:2783:U:OP2	2.33	0.62
18:k:43:ILE:HD12	18:k:56:ASP:HB2	1.82	0.62
10:b:2316:U:OP1	14:f:70:ALA:O	2.18	0.62
9:a:9:G:C6	9:a:112:G:C6	2.88	0.61
10:b:2106:G:C2	10:b:2192:U:N3	2.68	0.61
25:r:40:MET:HG3	25:r:48:LYS:HG2	1.81	0.61
10:b:1723:G:O2'	10:b:1741:A:N6	2.34	0.61
14:f:170:LEU:HD12	14:f:175:PHE:HB2	1.77	0.61
10:b:579:G:OP1	10:b:2506:G:O2'	2.19	0.61
10:b:2769:A:H2'	10:b:2769:A:N3	2.14	0.61
29:v:50:G:H1	29:v:62:C:H42	1.46	0.61
3:2:19:LYS:NZ	10:b:922:A:OP1	2.33	0.61
14:f:158:THR:HG21	14:f:169:LEU:CD2	2.30	0.61
4:3:16:ARG:NE	10:b:1268:G:OP1	2.33	0.61
29:v:8:U:O2'	29:v:10:G:N7	2.33	0.61
10:b:2108:C:N3	10:b:2188:A:N6	2.47	0.61
14:f:158:THR:OG1	14:f:169:LEU:CD2	2.47	0.61
10:b:2585:G:OP2	10:b:2585:G:N2	2.31	0.61
29:v:23:U:H2'	29:v:24:A:C8	2.35	0.60
7:7:19:LYS:HG2	10:b:653:G:H5'	1.84	0.60
29:v:28:C:N3	29:v:29:A:C2	2.69	0.60
10:b:2014:G:H5''	26:s:42:LYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1411:U:O2	10:b:1595:A:N1	2.33	0.60
10:b:2117:U:OP1	10:b:2149:C:N4	2.35	0.60
10:b:1044:G:H1	10:b:1114:G:H1	1.49	0.60
15:g:18:LYS:HE2	15:g:20:ASN:HD21	1.67	0.60
25:r:34:GLU:HG3	25:r:60:LYS:HG2	1.84	0.60
10:b:2105:A:C2	10:b:2193:U:C2	2.89	0.60
10:b:2843:G:N2	21:n:91:ALA:O	2.30	0.60
22:o:69:ASP:OD1	22:o:69:ASP:N	2.33	0.60
26:s:6:LYS:HG2	26:s:104:THR:HG23	1.82	0.60
10:b:2138:A:H3'	10:b:2139:A:H8	1.67	0.59
14:f:158:THR:CB	14:f:169:LEU:HD21	2.31	0.59
24:q:49:ASP:OD1	24:q:52:GLN:NE2	2.35	0.59
10:b:949:A:O2'	10:b:986:A:H2	1.81	0.59
9:a:113:C:C6	9:a:113:C:C5'	2.86	0.59
10:b:301:G:OP2	28:u:82:ARG:NH1	2.35	0.59
10:b:2378:C:N4	10:b:2379:G:O6	2.35	0.59
20:m:38:ARG:HB2	20:m:98:PRO:HD3	1.84	0.59
1:0:72:ARG:NH1	1:0:78:TYR:OH	2.33	0.59
14:f:117:LEU:HB2	14:f:177:PHE:HA	1.85	0.59
10:b:2462:G:O2'	10:b:2464:U:O4	2.21	0.59
14:f:135:GLN:HE21	14:f:149:VAL:HA	1.66	0.59
10:b:491:G:O6	26:s:49:LYS:NZ	2.33	0.59
10:b:2382:A:C8	10:b:2383:G:C8	2.91	0.59
14:f:34:ILE:HG12	14:f:96:MET:HE3	1.85	0.59
14:f:63:GLN:NE2	14:f:90:THR:O	2.36	0.59
10:b:807:G:O6	10:b:2072:U:C5	2.56	0.58
10:b:2460:C:H2'	10:b:2461:U:H5'	1.83	0.58
14:f:165:GLU:O	14:f:169:LEU:CB	2.51	0.58
9:a:112:G:C8	9:a:112:G:C5'	2.87	0.58
10:b:275:C:H1'	10:b:363:G:N2	2.18	0.58
10:b:1096:U:N3	10:b:1098:A:OP2	2.36	0.58
14:f:170:LEU:HG	14:f:171:ALA:H	1.67	0.58
26:s:4:ILE:HG12	26:s:106:VAL:HG22	1.84	0.58
10:b:506:G:H4'	10:b:507:A:H5'	1.86	0.58
29:v:30:G:N2	29:v:40:C:O2	2.36	0.58
29:v:53:U:C2'	29:v:54:U:C5'	2.72	0.58
10:b:263:G:O2'	10:b:429:A:N3	2.34	0.58
10:b:1085:U:H2'	10:b:1086:A:H2'	1.85	0.58
14:f:170:LEU:HD11	14:f:175:PHE:CD1	2.38	0.58
2:1:7:ARG:HG3	2:1:56:LEU:HD11	1.86	0.58
12:d:46:ARG:NH2	12:d:88:GLU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:46:ILE:HD12	20:m:69:PRO:HG3	1.85	0.58
3:2:6:LYS:NZ	3:2:37:GLU:OE1	2.37	0.58
10:b:117:G:OP2	10:b:119:A:O2'	2.20	0.58
10:b:488:G:O2'	26:s:49:LYS:NZ	2.31	0.58
10:b:954:G:H21	10:b:2271:A:H2	1.51	0.58
10:b:1412:G:C5'	10:b:1412:G:C8	2.87	0.58
10:b:2382:A:N9	10:b:2383:G:C8	2.71	0.58
11:c:107:PRO:HD2	11:c:110:LEU:HD22	1.86	0.57
10:b:12:U:H2'	10:b:12:U:O2	2.04	0.57
15:g:155:GLU:HG3	15:g:157:TYR:H	1.69	0.57
10:b:2552:U:O2	18:k:23:LYS:NZ	2.37	0.57
10:b:483:A:O2'	28:u:56:GLY:O	2.22	0.56
9:a:33:G:C2	9:a:50:A:C2	2.93	0.56
24:q:97:ASP:OD1	25:r:13:ARG:NH1	2.34	0.56
10:b:2487:C:O2'	20:m:51:ARG:NH1	2.38	0.56
10:b:712:U:H3	10:b:723:A:H61	1.53	0.56
15:g:45:HIS:O	15:g:46:ALA:HB3	2.06	0.56
10:b:265:A:N6	10:b:427:U:O2'	2.31	0.56
10:b:1056:A:H1'	10:b:1108:G:H22	1.70	0.56
10:b:631:G:N3	10:b:641:U:O2'	2.39	0.56
14:f:29:PRO:O	14:f:169:LEU:HD13	2.05	0.56
26:s:92:ARG:HG3	32:z:16[B]:PRO:HG3	1.87	0.56
3:2:12:SER:HB3	3:2:32:ILE:HD11	1.88	0.56
10:b:1412:G:O5'	10:b:1412:G:H8	1.88	0.56
11:c:260:ASN:ND2	11:c:263:THR:OG1	2.39	0.56
14:f:116:GLY:HA3	14:f:178:ARG:HD3	1.87	0.56
22:o:29:HIS:HB3	22:o:36:TYR:HB2	1.87	0.56
10:b:1633:G:N1	10:b:1636:A:OP2	2.32	0.55
17:j:96:ARG:HH21	17:j:99:ARG:HG2	1.71	0.55
20:m:66:ARG:NH1	20:m:104:GLU:OE1	2.37	0.55
10:b:2055:A:C2	10:b:2056:A:N6	2.74	0.55
9:a:9:G:N1	9:a:112:G:C6	2.74	0.55
21:n:19:ALA:O	21:n:23:ASN:ND2	2.40	0.55
10:b:2802:U:O2'	10:b:2803:G:N2	2.34	0.55
14:f:135:GLN:NE2	14:f:148:ARG:O	2.40	0.55
10:b:835:A:H2'	10:b:836:G:C8	2.41	0.55
10:b:966:C:O2'	10:b:2277:A:N3	2.38	0.55
10:b:1023:A:H61	10:b:1144:A:H61	1.54	0.55
10:b:1856:A:H62	10:b:1892:G:H8	1.54	0.55
10:b:2379:G:C5	10:b:2383:G:O6	2.59	0.55
10:b:1301:G:O2'	10:b:1302:G:OP2	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1267:A:OP1	10:b:1267:A:H8	1.90	0.55
10:b:2639:A:O2'	12:d:49:GLN:NE2	2.40	0.55
14:f:34:ILE:HG22	14:f:156:ILE:HA	1.88	0.55
9:a:113:C:H2'	9:a:113:C:O2	2.07	0.55
6:6:1:MET:SD	6:6:1:MET:N	2.74	0.55
10:b:2772:U:O3'	17:j:95:ARG:NH2	2.39	0.55
14:f:165:GLU:O	14:f:169:LEU:HB3	2.06	0.55
31:y:49:ALA:O	31:y:51:VAL:HG22	2.07	0.55
26:s:73:LYS:HB2	26:s:106:VAL:HB	1.88	0.55
4:3:6:ASN:ND2	10:b:2024:A:H62	2.05	0.54
14:f:106:ILE:HG21	14:f:139:PRO:HG3	1.89	0.54
21:n:42:LYS:HA	21:n:45:ARG:HE	1.73	0.54
13:e:46:GLN:O	13:e:88:ARG:NH1	2.39	0.54
9:a:32:U:H3	9:a:50:A:H61	1.53	0.54
10:b:2067:C:H1'	32:z:27[A]:ALA:HB3	1.88	0.54
22:o:88:LYS:HB2	22:o:116:GLN:HG2	1.90	0.54
10:b:1165:G:OP1	25:r:24:LYS:NZ	2.41	0.54
14:f:164:GLU:HA	14:f:167:ARG:HB2	1.90	0.54
10:b:950:C:H1'	10:b:986:A:N3	2.21	0.54
28:u:33:LYS:HB3	28:u:64:ALA:HB1	1.88	0.54
10:b:1723:G:N2	10:b:1740:G:O2'	2.40	0.54
10:b:1268:G:H5''	26:s:15:GLN:HE22	1.72	0.54
10:b:1423:G:O2'	10:b:1496:A:N6	2.40	0.54
10:b:1660:C:H2'	10:b:1660:C:O2	2.08	0.54
11:c:3:VAL:HG12	11:c:19:VAL:HG12	1.90	0.54
13:e:125:SER:O	13:e:137:LYS:CE	2.56	0.53
5:4:5:ILE:O	5:4:28:ARG:NH1	2.41	0.53
10:b:871:G:O3'	20:m:6:ARG:NH1	2.41	0.53
22:o:17:LYS:HA	22:o:20:GLU:HG2	1.88	0.53
10:b:2343:C:H2'	10:b:2344:A:C8	2.43	0.53
18:k:65:THR:HG22	18:k:67:LYS:H	1.74	0.53
22:o:52:SER:OG	22:o:53:THR:N	2.41	0.53
26:s:74:ILE:HD13	26:s:105:VAL:HG22	1.90	0.53
1:0:29:PHE:HB3	10:b:396:G:H1'	1.90	0.53
9:a:33:G:C4	9:a:50:A:N1	2.77	0.53
9:a:113:C:C6	9:a:113:C:H5''	2.44	0.53
10:b:2664:A:C6	10:b:2665:G:C2	2.96	0.53
14:f:22:TYR:CG	14:f:27:GLN:HG3	2.43	0.53
18:k:7:MET:HE1	18:k:44:LYS:HG3	1.91	0.53
26:s:80:PRO:O	26:s:100:THR:OG1	2.26	0.53
6:6:39:ARG:NH2	10:b:468:G:N7	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:170:LEU:HD11	14:f:175:PHE:CG	2.43	0.53
25:r:58:VAL:H	25:r:102:SER:HB3	1.74	0.53
10:b:674:C:OP2	19:l:42:SER:OG	2.23	0.53
11:c:66:ASP:OD1	11:c:102:ARG:NH1	2.41	0.53
10:b:2449:G:OP1	13:e:69:ARG:NH1	2.34	0.53
10:b:1250:G:OP2	13:e:44:ARG:NH1	2.41	0.53
10:b:287:G:O6	10:b:352:A:N6	2.41	0.52
10:b:1549:C:H5''	10:b:1549:C:H6	1.73	0.52
29:v:26:C:N3	29:v:27:U:O4	2.42	0.52
10:b:1453:C:H5	10:b:1461:G:H1	1.57	0.52
29:v:26:C:C4	29:v:27:U:O4	2.62	0.52
30:w:51:GLN:OE1	30:w:57:TYR:OH	2.26	0.52
9:a:32:U:H3	9:a:50:A:N6	2.08	0.52
10:b:1201:U:H1'	24:q:4:VAL:HG22	1.92	0.52
10:b:1301:G:C8	10:b:1301:G:H3'	2.45	0.52
10:b:2106:G:N3	10:b:2192:U:N3	2.58	0.52
14:f:22:TYR:CG	14:f:27:GLN:CG	2.92	0.52
14:f:58:ALA:HB2	14:f:65:PRO:HD3	1.91	0.52
25:r:46:GLU:OE1	25:r:48:LYS:NZ	2.43	0.52
10:b:1412:G:C5'	10:b:1412:G:H8	2.22	0.52
10:b:2105:A:C2	10:b:2193:U:O2	2.62	0.52
20:m:36:VAL:HG12	30:w:82:TYR:HB2	1.90	0.52
23:p:7:GLN:OE1	23:p:10:GLN:NE2	2.42	0.52
10:b:116:C:O2'	10:b:126:A:C8	2.63	0.52
10:b:572:G:H2'	10:b:2034:A:N7	2.25	0.52
10:b:839:C:C4	10:b:943:A:N6	2.77	0.52
13:e:52:VAL:HG21	13:e:82:GLY:H	1.74	0.52
27:t:67:VAL:O	27:t:69:ARG:NH1	2.42	0.52
2:1:9:LYS:HE3	2:1:13:GLU:HG2	1.91	0.52
27:t:23:ALA:HB1	27:t:29:THR:HB	1.91	0.52
10:b:2812:G:O2'	10:b:2894:G:O6	2.24	0.52
22:o:67:ASN:OD1	22:o:67:ASN:N	2.42	0.52
29:v:7:A:N7	29:v:12:A:N6	2.57	0.52
22:o:24:THR:HG22	22:o:90:VAL:HG13	1.91	0.52
25:r:5:PHE:HB3	25:r:59:ILE:HD12	1.92	0.52
31:y:59:LEU:HD12	31:y:80:ILE:HD12	1.92	0.52
10:b:2066:A:N6	32:z:22[B]:ALA:O	2.44	0.51
10:b:2640:C:O2'	12:d:45:TYR:OH	2.26	0.51
13:e:143:LEU:HD13	13:e:146:VAL:HG21	1.92	0.51
10:b:2724:U:OP1	23:p:53:ARG:NH2	2.43	0.51
10:b:1443:G:H2'	10:b:1444:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:59:SER:OG	21:n:62:ASN:OD1	2.25	0.51
10:b:250:G:H4'	19:l:59:ARG:HD2	1.91	0.51
10:b:883:G:N2	10:b:899:C:O2'	2.42	0.51
10:b:2104:G:O6	10:b:2105:A:C6	2.63	0.51
10:b:2305:C:O2'	10:b:2306:U:H5'	2.11	0.51
9:a:112:G:C8	9:a:112:G:H5''	2.46	0.51
10:b:1530:A:OP2	10:b:1545:G:N2	2.39	0.51
10:b:2879:C:OP1	21:n:4:ARG:NH2	2.41	0.51
18:k:9:ASN:OD1	18:k:18:ARG:NH1	2.43	0.51
29:v:25:C:H2'	29:v:26:C:O4'	2.11	0.51
10:b:2131:G:N2	10:b:2165:C:N3	2.57	0.51
10:b:2473:A:N6	10:b:2485:G:O2'	2.44	0.51
10:b:2661:A:H62	10:b:2668:G:H21	1.57	0.51
7:7:8:ARG:NH2	10:b:244:A:OP2	2.42	0.51
10:b:1247:G:OP1	19:l:13:LYS:NZ	2.44	0.51
29:v:5:G:H2'	29:v:6:C:H4'	1.92	0.51
6:6:4:THR:HG22	10:b:689:C:H1'	1.93	0.51
10:b:240:C:OP2	10:b:241:A:O2'	2.26	0.51
10:b:587:G:N7	24:q:6:ARG:NH1	2.49	0.51
10:b:2802:U:O2	10:b:2803:G:N2	2.44	0.51
2:1:41:HIS:ND1	10:b:95:A:O2'	2.44	0.51
2:1:49:ASP:OD1	2:1:52:ARG:NH2	2.44	0.51
10:b:1330:A:H2'	10:b:1332:C:C5	2.46	0.51
10:b:1444:U:H2'	10:b:1445:U:C6	2.46	0.51
18:k:63:VAL:HG12	18:k:107:LEU:HD21	1.93	0.51
29:v:53:U:C3'	29:v:54:U:C5'	2.89	0.51
10:b:839:C:H42	10:b:943:A:N6	2.10	0.50
10:b:2067:C:H1'	32:z:27[B]:ALA:HB3	1.93	0.50
20:m:15:GLY:O	20:m:16:ARG:NH1	2.36	0.50
26:s:1:MET:N	26:s:109:ASP:OD1	2.44	0.50
10:b:1428:G:O2'	10:b:1574:A:N6	2.45	0.50
10:b:950:C:O4'	10:b:986:A:C2	2.65	0.50
10:b:2792:C:H2'	10:b:2793:C:C6	2.46	0.50
10:b:404:A:N6	10:b:421:C:O2'	2.44	0.50
10:b:2131:G:O2'	10:b:2133:C:N4	2.41	0.50
14:f:29:PRO:HB2	14:f:169:LEU:CD2	2.32	0.50
2:1:21:LEU:HB3	2:1:50:VAL:HG12	1.94	0.50
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.92	0.50
8:8:4:ARG:NH2	10:b:2481:U:O2	2.44	0.50
10:b:488:G:O2'	10:b:491:G:N7	2.36	0.50
10:b:1366:G:N2	10:b:1369:A:OP2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2055:A:H2	10:b:2056:A:N6	2.10	0.50
10:b:2172:G:H1	10:b:2174:A:H3'	1.76	0.50
15:g:28:GLY:HA3	15:g:79:VAL:HB	1.94	0.50
31:y:40:GLN:NE2	31:y:57:HIS:O	2.45	0.50
10:b:244:A:H5''	19:l:67:THR:HG21	1.93	0.50
10:b:1471:A:H2'	10:b:1472:A:C8	2.47	0.50
10:b:1584:C:O2'	10:b:1587:C:C4	2.64	0.50
10:b:2106:G:N2	10:b:2107:C:C2	2.80	0.50
10:b:2316:U:H2'	10:b:2317:C:H6	1.76	0.50
10:b:2316:U:H2'	10:b:2317:C:C6	2.46	0.50
20:m:17:ASN:OD1	20:m:97:GLN:NE2	2.45	0.50
22:o:40:ILE:HG12	22:o:47:VAL:HG12	1.92	0.50
5:4:37:LYS:HG2	5:4:48:ILE:HG13	1.93	0.50
10:b:2641:U:C4	10:b:2642:G:C6	3.00	0.50
28:u:27:ASN:N	28:u:27:ASN:OD1	2.45	0.50
10:b:997:C:O2	17:j:3:THR:OG1	2.26	0.50
10:b:1660:C:OP1	12:d:140:HIS:NE2	2.45	0.50
10:b:638:G:OP2	19:l:109:LYS:NZ	2.43	0.49
10:b:2115:U:O2	10:b:2147:C:O2'	2.29	0.49
10:b:2451:G:N2	10:b:2454:A:OP2	2.39	0.49
19:l:85:VAL:HG11	19:l:90:VAL:HG22	1.94	0.49
7:7:25:LYS:HB3	19:l:62:PRO:HG2	1.95	0.49
9:a:113:C:O4'	22:o:46:GLU:OE1	2.30	0.49
10:b:116:C:HO2'	10:b:126:A:H8	1.57	0.49
10:b:160:A:N3	10:b:2212:C:O2'	2.44	0.49
10:b:813:U:H2'	19:l:21:ARG:HA	1.94	0.49
10:b:1030:A:N3	10:b:2490:C:O2'	2.43	0.49
10:b:1324:A:H5''	26:s:82:MET:HE1	1.94	0.49
10:b:1452:G:N2	10:b:1454:G:O6	2.44	0.49
10:b:2661:A:O3'	15:g:160:LYS:NZ	2.45	0.49
10:b:1771:U:O2'	10:b:1962:C:OP1	2.30	0.49
10:b:2107:C:N4	10:b:2108:C:N3	2.61	0.49
5:4:14:SER:OG	5:4:50:LYS:NZ	2.45	0.49
17:j:102:GLU:HB3	17:j:119:PHE:HZ	1.77	0.49
19:l:79:LEU:HD11	19:l:112:LEU:HD12	1.94	0.49
10:b:1412:G:C8	10:b:1412:G:H5''	2.47	0.49
10:b:2104:G:C6	10:b:2105:A:C6	3.01	0.49
29:v:26:C:C2	29:v:27:U:O4	2.65	0.49
10:b:783:A:OP1	11:c:217:ARG:NH2	2.43	0.49
10:b:1021:U:H3	10:b:1144:A:N6	2.08	0.49
10:b:2305:C:H2'	10:b:2306:U:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2642:G:O2'	10:b:2779:G:N2	2.36	0.49
10:b:2798:U:H3	10:b:2806:A:H61	1.59	0.49
10:b:645:A:N6	10:b:2373:A:O2'	2.46	0.49
10:b:1793:A:N6	10:b:1830:G:O2'	2.40	0.49
10:b:2237:U:H2'	10:b:2238:G:C8	2.48	0.49
10:b:2065:G:H1	32:z:26[A]:ARG:HB3	1.78	0.49
10:b:2306:U:O2'	14:f:123:ASP:O	2.31	0.49
10:b:1047:C:H4'	10:b:1048:A:H5''	1.95	0.49
12:d:60:VAL:HG23	12:d:64:GLU:HG3	1.95	0.49
10:b:989:C:O2'	10:b:1002:A:N3	2.45	0.49
10:b:1984:G:O2'	10:b:1986:U:OP2	2.31	0.49
13:e:21:ARG:O	13:e:114:ARG:NH2	2.39	0.49
13:e:138:LEU:HA	13:e:141:MET:HB2	1.95	0.49
10:b:239:C:O2'	10:b:624:G:O2'	2.27	0.48
11:c:144:VAL:HB	11:c:154:LEU:HB2	1.95	0.48
11:c:161:TYR:HB3	11:c:194:GLU:HB2	1.95	0.48
23:p:10:GLN:HA	23:p:13:MET:HG3	1.94	0.48
30:w:40:ILE:HD12	30:w:42:LEU:HD21	1.95	0.48
9:a:24:G:C8	9:a:56:G:C8	3.02	0.48
4:3:24:ALA:HB2	26:s:23:LEU:HD22	1.94	0.48
10:b:579:G:O2'	10:b:1256:A:OP1	2.31	0.48
10:b:686:G:C2	10:b:796:A:C2	3.02	0.48
10:b:2664:A:C6	10:b:2665:G:N2	2.81	0.48
12:d:37:VAL:HG12	12:d:48:ILE:HG22	1.94	0.48
24:q:99:ALA:O	24:q:103:LYS:NZ	2.46	0.48
26:s:77:ASP:HB2	26:s:102:HIS:HB2	1.95	0.48
10:b:1334:G:N7	10:b:1611:A:O2'	2.38	0.48
11:c:115:GLN:O	11:c:125:LYS:NZ	2.46	0.48
20:m:20:LEU:HD13	30:w:81:PRO:HG2	1.94	0.48
28:u:74:ASN:ND2	28:u:81:ASP:OD2	2.44	0.48
2:1:14:LEU:HD11	2:1:56:LEU:HD23	1.95	0.48
9:a:42:C:C2	14:f:90:THR:HG22	2.49	0.48
10:b:766:A:H5''	11:c:209:GLY:HA3	1.95	0.48
10:b:1000:C:OP1	24:q:92:ARG:NH2	2.44	0.48
10:b:1042:A:H61	10:b:1116:C:H42	1.61	0.48
17:j:118:MET:HA	17:j:121:LYS:HE2	1.96	0.48
10:b:263:G:H2'	10:b:264:C:O4'	2.14	0.48
10:b:364:C:O2'	10:b:365:U:H5'	2.14	0.48
10:b:888:A:O2'	10:b:890:C:OP2	2.31	0.48
10:b:1317:C:O2'	10:b:1394:A:N3	2.46	0.48
13:e:134:LEU:HA	13:e:137:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:l:82:LEU:HD22	19:l:90:VAL:HG21	1.95	0.48
27:t:76:ARG:NH2	27:t:79:ASP:OD1	2.46	0.48
9:a:112:G:O5'	9:a:112:G:H8	1.96	0.48
10:b:1653:G:H4'	21:n:39:PRO:HG2	1.96	0.48
10:b:2664:A:C8	10:b:2664:A:H5'	2.48	0.48
10:b:2880:G:OP1	23:p:2:SER:N	2.46	0.48
15:g:23:VAL:HG13	15:g:36:THR:HB	1.94	0.48
29:v:10:G:C2	29:v:24:A:C2	3.02	0.48
9:a:6:G:H2'	9:a:7:G:C8	2.49	0.48
10:b:83:A:N6	10:b:102:U:OP1	2.34	0.48
29:v:24:A:C2'	29:v:25:C:H5'	2.44	0.48
6:6:37:LYS:NZ	10:b:469:G:N7	2.62	0.48
9:a:90:C:H5''	20:m:18:ARG:HG2	1.94	0.48
10:b:831:A:N7	10:b:2251:A:O2'	2.44	0.48
10:b:1756:A:HO2'	23:p:103:ARG:HH12	1.62	0.48
11:c:104:ILE:HD13	11:c:116:ILE:HD13	1.94	0.48
10:b:511:U:C3'	10:b:512:G:P	3.02	0.47
10:b:1443:G:O2'	10:b:1444:U:H5'	2.14	0.47
10:b:1724:A:H2'	10:b:1725:G:C8	2.49	0.47
10:b:2835:G:OP1	12:d:56:LYS:NZ	2.44	0.47
17:j:45:THR:HB	24:q:64:ARG:HH21	1.79	0.47
10:b:607:G:N3	10:b:659:U:O2'	2.47	0.47
10:b:2391:U:OP1	31:y:55:ARG:NH2	2.47	0.47
10:b:2769:A:N3	10:b:2769:A:C2'	2.77	0.47
29:v:55:C:N4	29:v:56:G:O6	2.47	0.47
32:z:10[B]:SER:O	32:z:10[B]:SER:OG	2.32	0.47
9:a:41:G:N2	10:b:2343:C:O2'	2.41	0.47
10:b:665:G:H5''	19:l:17:LYS:HD2	1.96	0.47
10:b:884:G:H2'	10:b:885:G:C8	2.50	0.47
10:b:1173:G:C5'	10:b:1174:C:H5'	2.44	0.47
10:b:1792:C:H2'	10:b:1793:A:C5	2.49	0.47
11:c:132:MET:HE3	11:c:190:ALA:HB2	1.96	0.47
14:f:29:PRO:HB2	14:f:169:LEU:HD13	1.96	0.47
9:a:115:A:H2'	9:a:116:G:H8	1.78	0.47
10:b:1323:A:O2'	26:s:11:ARG:NH2	2.47	0.47
11:c:37:ASN:HB2	11:c:62:TYR:HB2	1.96	0.47
28:u:13:VAL:HG21	28:u:39:ILE:HG21	1.96	0.47
10:b:62:U:H2'	10:b:63:A:H2	1.78	0.47
10:b:1647:G:H5''	10:b:1648:C:H5'	1.97	0.47
10:b:1755:G:N2	10:b:1758:G:OP2	2.40	0.47
10:b:2853:U:N3	10:b:2871:G:O4'	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:43:ILE:HG12	21:n:100:CYS:HA	1.96	0.47
9:a:24:G:C8	9:a:56:G:N7	2.83	0.47
10:b:1173:G:H4'	10:b:1174:C:H5'	1.97	0.47
10:b:1669:G:O2'	10:b:1995:U:O4	2.23	0.47
10:b:2754:A:O2'	10:b:2756:C:N4	2.44	0.47
32:z:17[A]:VAL:HG12	32:z:19[A]:ILE:HD12	1.97	0.47
8:8:32:LYS:HE2	10:b:2482:A:H5'	1.96	0.47
9:a:22:U:H2'	9:a:23:G:C8	2.50	0.47
10:b:33:C:O2	10:b:447:A:N6	2.46	0.47
10:b:1865:G:HO2'	10:b:2415:A:HO2'	1.60	0.47
19:l:51:GLU:HG3	19:l:56:PRO:HA	1.97	0.47
10:b:1411:U:O2	10:b:1595:A:C2	2.68	0.47
10:b:2262:C:O2'	10:b:2431:C:OP2	2.31	0.47
10:b:2277:A:H2'	10:b:2278:A:C8	2.49	0.47
15:g:137:ASP:HB3	15:g:140:VAL:HB	1.97	0.47
18:k:110:GLU:HA	18:k:113:MET:HG2	1.96	0.47
18:k:121:GLU:HG2	18:k:122:VAL:HG23	1.97	0.47
6:6:29:GLN:NE2	10:b:210:C:OP1	2.47	0.47
9:a:112:G:H2'	22:o:46:GLU:OE2	2.14	0.47
10:b:355:U:H2'	10:b:356:G:C8	2.50	0.47
10:b:1023:A:C8	10:b:1023:A:H3'	2.50	0.47
10:b:494:G:H4'	26:s:6:LYS:HB2	1.97	0.46
10:b:2119:G:N3	10:b:2121:A:N6	2.63	0.46
10:b:2166:G:O2'	10:b:2176:U:O4	2.33	0.46
27:t:59:ASN:O	27:t:84:TYR:N	2.44	0.46
4:3:52:ARG:HH11	4:3:54:VAL:HA	1.80	0.46
10:b:807:G:H22	10:b:830:U:H5''	1.80	0.46
10:b:2383:G:N3	10:b:2383:G:C2'	2.78	0.46
10:b:572:G:OP1	10:b:974:A:O2'	2.24	0.46
10:b:1436:A:H62	10:b:1560:C:H42	1.62	0.46
10:b:345:A:H1'	10:b:346:A:H2	1.81	0.46
16:h:12:LEU:H	16:h:12:LEU:HG	1.57	0.46
16:h:30:LEU:HB3	16:h:36:ALA:HB3	1.98	0.46
19:l:81:ASP:HB3	19:l:100:ILE:HD13	1.96	0.46
5:4:23:THR:OG1	10:b:2290:G:O6	2.26	0.46
10:b:459:U:H2'	10:b:460:A:H8	1.80	0.46
10:b:2659:G:O2'	10:b:2668:G:N1	2.46	0.46
12:d:77:ARG:NH2	12:d:200:ASP:OD1	2.49	0.46
14:f:30:ARG:HE	14:f:30:ARG:HB2	1.35	0.46
25:r:41:ILE:HD11	25:r:57:GLY:HA3	1.97	0.46
26:s:85:ILE:HD11	32:z:11[A]:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1533:C:H42	10:b:1542:G:H1	1.64	0.46
10:b:2488:G:O2'	20:m:123:LYS:O	2.31	0.46
10:b:2631:G:O2'	10:b:2785:A:N1	2.38	0.46
29:v:27:U:OP2	29:v:27:U:H6	1.98	0.46
7:7:32:ILE:HG22	7:7:32:ILE:O	2.16	0.46
10:b:463:G:N2	10:b:465:G:H3'	2.31	0.46
14:f:44:ILE:HG21	14:f:79:ILE:HG22	1.97	0.46
9:a:89:U:O2'	10:b:960:U:O2	2.28	0.46
10:b:588:A:C2	10:b:811:G:O2'	2.59	0.46
10:b:1066:C:H42	10:b:1075:A:H62	1.63	0.46
10:b:1175:U:O2'	10:b:1179:G:O6	2.23	0.46
19:l:127:VAL:HG21	19:l:142:ILE:HD13	1.98	0.46
29:v:7:A:H61	29:v:13:U:H5''	1.81	0.46
29:v:23:U:C4	29:v:24:A:N6	2.84	0.46
9:a:14:U:OP2	9:a:70:C:O2'	2.31	0.46
9:a:50:A:H2'	9:a:51:G:H5'	1.97	0.46
10:b:976:G:H8	10:b:992:A:N6	1.95	0.46
10:b:2382:A:H4'	22:o:117:PHE:HB2	1.98	0.46
29:v:28:C:C4	29:v:29:A:C6	3.03	0.46
9:a:33:G:C4	9:a:50:A:C2	3.04	0.45
10:b:10:A:H2	10:b:2633:U:H3	1.64	0.45
10:b:948:C:H2'	10:b:949:A:H8	1.81	0.45
10:b:1781:U:C5	10:b:1786:A:N7	2.76	0.45
20:m:47:GLU:OE2	20:m:50:ARG:NH1	2.38	0.45
22:o:99:TYR:HH	22:o:111:ARG:HH12	1.58	0.45
23:p:14:LYS:HG3	23:p:77:HIS:HA	1.98	0.45
10:b:63:A:N6	10:b:91:A:H62	2.14	0.45
10:b:481:G:H2'	10:b:507:A:N1	2.31	0.45
10:b:1496:A:H2'	10:b:1497:A:C8	2.51	0.45
10:b:1654:A:C2	10:b:2009:A:N6	2.84	0.45
10:b:2382:A:N9	10:b:2383:G:H8	2.10	0.45
10:b:2585:G:H2'	10:b:2585:G:N3	2.30	0.45
14:f:49:LEU:HA	14:f:52:ASN:HB2	1.98	0.45
15:g:25:THR:HG23	15:g:34:THR:HB	1.98	0.45
10:b:1412:G:N2	10:b:1594:C:C2	2.66	0.45
10:b:1724:A:N6	10:b:1740:G:H1'	2.31	0.45
10:b:1818:C:H41	11:c:35:GLU:CD	2.25	0.45
14:f:33:LYS:HG3	14:f:157:THR:HB	1.99	0.45
25:r:24:LYS:HE2	25:r:24:LYS:HB3	1.83	0.45
6:6:25:LYS:HB3	6:6:25:LYS:HE3	1.82	0.45
9:a:3:C:H42	9:a:117:G:H1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1940:A:H61	10:b:1967:U:H3	1.64	0.45
10:b:2576:A:OP1	10:b:2578:G:H4'	2.17	0.45
11:c:16:VAL:HG22	11:c:206:GLY:HA3	1.99	0.45
14:f:22:TYR:CD2	14:f:27:GLN:HG3	2.52	0.45
19:l:89:VAL:HG13	19:l:123:ARG:HD3	1.98	0.45
10:b:2568:A:OP1	10:b:2652:G:O2'	2.29	0.45
11:c:34:LEU:HD23	11:c:34:LEU:HA	1.84	0.45
13:e:18:THR:HG23	13:e:106:LYS:HG2	1.99	0.45
14:f:8:TYR:HH	14:f:28:VAL:HG13	1.76	0.45
19:l:110:VAL:HB	19:l:127:VAL:HG12	1.97	0.45
22:o:41:ALA:HB2	22:o:48:LEU:HD21	1.99	0.45
10:b:948:C:H2'	10:b:949:A:C8	2.52	0.45
10:b:2073:G:N1	10:b:2446:C:N3	2.47	0.45
10:b:2843:G:O2'	21:n:49:GLU:OE1	2.29	0.45
14:f:29:PRO:CB	14:f:169:LEU:HD22	2.36	0.45
29:v:26:C:C2	29:v:27:U:C4	3.05	0.45
7:7:18:GLY:N	10:b:631:G:OP1	2.50	0.45
8:8:4:ARG:O	8:8:38:GLY:N	2.49	0.45
10:b:219:A:N3	10:b:234:U:O2'	2.39	0.45
10:b:1570:G:OP1	11:c:63:ARG:NH2	2.39	0.45
10:b:2544:C:O2'	10:b:2744:A:N3	2.47	0.45
14:f:22:TYR:CG	14:f:27:GLN:HG2	2.51	0.45
10:b:1175:U:N3	10:b:1178:U:C4	2.84	0.45
10:b:1869:G:H1	10:b:1878:C:H42	1.64	0.45
13:e:141:MET:HE3	13:e:141:MET:HB3	1.78	0.45
14:f:29:PRO:O	14:f:169:LEU:CD1	2.65	0.45
10:b:2106:G:C2	10:b:2192:U:C4	3.05	0.45
16:h:12:LEU:HB2	16:h:19:VAL:HG21	1.98	0.45
10:b:785:A:O2'	10:b:787:G:OP1	2.35	0.45
10:b:989:C:H2'	10:b:990:A:O4'	2.17	0.45
10:b:1063:U:H3	10:b:1070:G:H1'	1.82	0.45
10:b:1565:U:H2'	10:b:1566:C:C6	2.52	0.45
10:b:2245:A:H2'	10:b:2246:G:C8	2.52	0.45
10:b:500:G:N1	10:b:503:A:OP2	2.45	0.44
10:b:581:G:O2'	10:b:2023:A:OP1	2.34	0.44
10:b:1028:G:H2'	10:b:1029:A:H8	1.81	0.44
10:b:2186:U:H2'	10:b:2187:A:C8	2.52	0.44
10:b:2664:A:H5'	10:b:2664:A:H8	1.81	0.44
15:g:86:LYS:HG2	15:g:132:VAL:HG12	1.98	0.44
10:b:481:G:O2'	10:b:506:G:N2	2.51	0.44
10:b:1173:G:H5''	10:b:1174:C:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2305:C:H2'	10:b:2306:U:C6	2.52	0.44
10:b:2390:A:H4'	31:y:56:ASP:HA	1.99	0.44
18:k:71:ARG:HH22	18:k:105:ARG:HG2	1.82	0.44
4:3:38:HIS:ND1	4:3:39:LEU:O	2.37	0.44
7:7:31:HIS:H	7:7:31:HIS:CD2	2.36	0.44
10:b:695:A:O2'	10:b:1355:A:N3	2.47	0.44
10:b:731:G:C6	11:c:207:LYS:HB2	2.53	0.44
10:b:943:A:H2'	10:b:944:G:O4'	2.17	0.44
10:b:1353:C:H2'	10:b:1354:U:O4'	2.17	0.44
10:b:2576:A:N7	12:d:150:GLN:HB2	2.32	0.44
10:b:2855:A:H2'	10:b:2856:G:O4'	2.17	0.44
9:a:43:C:H6	9:a:43:C:C5'	2.26	0.44
10:b:136:G:C6	10:b:137:U:C4	3.06	0.44
10:b:835:A:H2'	10:b:836:G:H8	1.81	0.44
10:b:1040:G:H22	10:b:1118:G:N2	2.15	0.44
10:b:1301:G:C8	10:b:1301:G:C3'	3.01	0.44
10:b:2043:U:H2'	10:b:2044:G:H8	1.81	0.44
10:b:2104:G:N1	10:b:2105:A:C4	2.86	0.44
10:b:2282:A:OP1	20:m:10:ARG:NH2	2.50	0.44
14:f:169:LEU:HD12	14:f:169:LEU:C	2.42	0.44
10:b:84:A:N1	10:b:98:G:O2'	2.47	0.44
10:b:2106:G:C8	10:b:2106:G:OP2	2.70	0.44
20:m:21:ALA:HB1	20:m:100:LYS:HD3	1.99	0.44
26:s:17:VAL:HB	26:s:76:VAL:HG11	2.00	0.44
9:a:41:G:H3'	9:a:42:C:H5''	1.99	0.44
10:b:69:C:O2	10:b:73:A:O2'	2.28	0.44
10:b:1301:G:O5'	10:b:1301:G:H8	2.00	0.44
10:b:2208:G:OP2	11:c:150:LYS:NZ	2.36	0.44
17:j:121:LYS:HB2	17:j:121:LYS:HE3	1.82	0.44
19:l:71:ALA:HA	19:l:74:THR:HG22	1.99	0.44
9:a:112:G:C8	9:a:112:G:O5'	2.70	0.44
10:b:2189:U:H2'	10:b:2190:G:H8	1.81	0.44
10:b:2641:U:O4	10:b:2642:G:C6	2.71	0.44
11:c:154:LEU:HD22	11:c:176:LEU:HD22	1.99	0.44
12:d:13:ARG:HD2	12:d:21:SER:HB2	1.99	0.44
18:k:102:PRO:HB3	18:k:121:GLU:HB3	2.00	0.44
30:w:55:GLU:HA	30:w:58:SER:HB3	2.00	0.44
30:w:70:ILE:HG21	30:w:93:ARG:HE	1.82	0.44
9:a:113:C:C6	9:a:113:C:O5'	2.70	0.44
10:b:2335:G:H4'	31:y:43:THR:H	1.83	0.44
22:o:39:VAL:HB	22:o:49:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:3:THR:OG1	26:s:62:ASP:OD2	2.32	0.44
10:b:155:A:H2'	10:b:156:A:C8	2.53	0.43
10:b:1396:U:H4'	10:b:1605:A:H4'	2.00	0.43
11:c:259:SER:O	11:c:259:SER:OG	2.31	0.43
17:j:36:LEU:HD11	17:j:122:LEU:HD13	1.99	0.43
21:n:22:ARG:HE	21:n:22:ARG:HB2	1.66	0.43
10:b:483:A:OP1	28:u:47:LYS:NZ	2.51	0.43
10:b:655:U:O2'	10:b:657:A:OP1	2.36	0.43
10:b:657:A:H4'	10:b:658:G:H5'	2.01	0.43
10:b:2896:G:H5''	10:b:2897:A:H5'	2.00	0.43
17:j:92:MET:HE3	17:j:92:MET:HB3	1.85	0.43
29:v:27:U:C6	29:v:27:U:OP2	2.70	0.43
29:v:65:U:H2'	29:v:66:G:C8	2.53	0.43
9:a:50:A:OP1	22:o:68:LYS:N	2.43	0.43
10:b:143:C:H2'	10:b:144:A:C8	2.53	0.43
10:b:568:U:H5''	19:l:29:LYS:HE3	2.00	0.43
10:b:1187:G:H5''	10:b:1187:G:H8	1.83	0.43
10:b:1672:C:O2	12:d:134:HIS:NE2	2.36	0.43
10:b:2319:G:H2'	10:b:2320:G:H8	1.83	0.43
9:a:40:U:C2	9:a:43:C:H5'	2.54	0.43
10:b:184:C:H2'	10:b:185:G:C8	2.53	0.43
10:b:1431:G:H2'	10:b:1432:G:H8	1.83	0.43
10:b:2100:C:H2'	10:b:2101:A:C8	2.54	0.43
10:b:2335:G:H21	10:b:2340:A:H8	1.67	0.43
15:g:127:THR:OG1	15:g:130:GLU:OE1	2.32	0.43
20:m:35:ALA:HA	20:m:128:THR:HG22	2.00	0.43
20:m:53:MET:HG3	20:m:120:ALA:HB2	2.01	0.43
26:s:55:ILE:HG23	26:s:66:ILE:HD12	2.00	0.43
29:v:25:C:C6	29:v:25:C:OP2	2.70	0.43
9:a:24:G:C5	9:a:56:G:C4	3.07	0.43
10:b:364:C:H2'	10:b:365:U:H6	1.83	0.43
10:b:729:A:OP1	10:b:1433:A:O2'	2.28	0.43
10:b:1330:A:H4'	10:b:1331:U:H5	1.83	0.43
10:b:1443:G:C2'	10:b:1444:U:H5'	2.48	0.43
17:j:23:LYS:HE2	17:j:142:ILE:HB	2.00	0.43
28:u:38:GLY:N	28:u:62:GLU:OE1	2.41	0.43
10:b:2382:A:H3'	10:b:2383:G:C8	2.53	0.43
9:a:24:G:N7	9:a:56:G:C4	2.86	0.43
10:b:1023:A:H3'	10:b:1023:A:H8	1.82	0.43
10:b:1479:A:N1	10:b:1559:C:O2'	2.51	0.43
14:f:64:LYS:HA	14:f:65:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1143:U:H4'	10:b:1144:A:O4'	2.18	0.43
10:b:2471:C:O2	20:m:123:LYS:NZ	2.51	0.43
13:e:145:ASP:HA	13:e:166:LYS:HB3	2.00	0.43
14:f:22:TYR:CD1	14:f:27:GLN:HG2	2.54	0.43
14:f:158:THR:CG2	14:f:169:LEU:CD2	2.97	0.43
10:b:700:C:O2'	10:b:736:A:N6	2.50	0.43
24:q:15:LYS:HE2	24:q:15:LYS:HB3	1.75	0.43
27:t:38:ALA:O	27:t:81:LYS:NZ	2.46	0.43
1:0:56:MET:HB3	1:0:56:MET:HE2	1.89	0.43
10:b:1009:C:OP1	17:j:37:ARG:NH2	2.51	0.43
10:b:1434:G:H2'	10:b:1435:A:C8	2.53	0.43
10:b:1915:U:H3'	10:b:1922:A:H61	1.83	0.43
10:b:2072:U:H5''	10:b:2072:U:H6	1.83	0.43
11:c:53:HIS:HA	11:c:217:ARG:HB2	2.01	0.43
10:b:340:A:H2'	10:b:341:C:O4'	2.19	0.42
10:b:1602:C:OP1	27:t:81:LYS:NZ	2.41	0.42
10:b:2381:A:O2'	22:o:111:ARG:NH2	2.52	0.42
12:d:33:ARG:NH1	12:d:75:ALA:O	2.52	0.42
16:h:3:VAL:HG12	16:h:38:PRO:HA	2.00	0.42
25:r:26:ASP:OD1	25:r:26:ASP:N	2.51	0.42
9:a:24:G:N7	9:a:56:G:C8	2.87	0.42
14:f:51:ASP:O	14:f:55:ALA:N	2.52	0.42
15:g:7:ALA:O	15:g:69:ARG:NE	2.52	0.42
5:4:23:THR:OG1	5:4:24:THR:N	2.52	0.42
10:b:1794:G:H5'	11:c:204:VAL:HG13	2.00	0.42
11:c:155:ALA:HB2	11:c:162:VAL:HG13	2.01	0.42
17:j:11:VAL:HG21	17:j:50:THR:HA	2.01	0.42
29:v:25:C:OP2	29:v:25:C:C5	2.71	0.42
10:b:527:C:C5	10:b:2783:U:H2'	2.54	0.42
10:b:735:G:O6	10:b:763:A:C8	2.73	0.42
10:b:2780:A:H4'	10:b:2781:G:H5''	2.00	0.42
23:p:106:LYS:HA	23:p:109:ARG:HG3	2.01	0.42
9:a:4:C:H42	9:a:115:A:H61	1.66	0.42
9:a:4:C:N4	9:a:115:A:H61	2.16	0.42
10:b:391:A:H1'	10:b:411:G:O4'	2.20	0.42
10:b:514:A:N3	10:b:583:C:O2'	2.50	0.42
10:b:1569:G:H3'	11:c:85:PRO:HG3	2.02	0.42
17:j:105:VAL:HG11	17:j:122:LEU:HD22	2.01	0.42
4:3:37:LYS:HB2	4:3:37:LYS:HE3	1.84	0.42
9:a:6:G:H2'	9:a:7:G:H8	1.82	0.42
10:b:1023:A:C8	10:b:1023:A:C3'	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1591:U:H2'	10:b:1592:A:C8	2.55	0.42
10:b:1756:A:O2'	23:p:103:ARG:NH1	2.50	0.42
18:k:2:ILE:HD12	18:k:6:THR:HG21	2.01	0.42
10:b:964:G:N2	10:b:2254:G:H1	2.14	0.42
10:b:1049:G:O2'	10:b:1112:G:N1	2.30	0.42
10:b:2051:C:O2'	10:b:2827:A:N1	2.44	0.42
12:d:25:THR:HG21	12:d:193:VAL:HG22	2.02	0.42
14:f:127:ASN:ND2	14:f:158:THR:H	2.16	0.42
16:h:8:LYS:O	16:h:8:LYS:NZ	2.42	0.42
27:t:17:SER:HB3	27:t:20:ALA:H	1.85	0.42
31:y:50:ASN:HB2	31:y:82:ILE:HB	2.01	0.42
6:6:2:LYS:HE2	10:b:689:C:H5''	2.02	0.42
10:b:912:A:N3	10:b:2268:C:O2'	2.46	0.42
10:b:2036:G:N2	12:d:151:THR:OG1	2.45	0.42
10:b:2319:G:H2'	10:b:2320:G:C8	2.54	0.42
10:b:2792:C:O2'	10:b:2813:A:N3	2.52	0.42
10:b:2849:U:H5''	23:p:52:ASN:O	2.19	0.42
14:f:22:TYR:CD1	14:f:27:GLN:CG	3.03	0.42
14:f:125:ARG:HD3	14:f:125:ARG:HA	1.86	0.42
14:f:129:SER:HB2	14:f:155:THR:HG23	2.02	0.42
10:b:364:C:H2'	10:b:365:U:C6	2.54	0.42
10:b:414:C:H2'	10:b:415:A:C8	2.54	0.42
10:b:1127:G:OP2	10:b:1128:A:O2'	2.29	0.42
10:b:1342:U:OP1	27:t:84:TYR:OH	2.30	0.42
10:b:1552:C:OP1	10:b:1722:U:O2'	2.33	0.42
12:d:121:THR:HB	12:d:127:PHE:CD2	2.55	0.42
14:f:34:ILE:HG13	14:f:91:LEU:HB2	2.02	0.42
10:b:27:G:H1'	10:b:513:A:N6	2.34	0.42
10:b:2664:A:O2'	10:b:2665:G:C5'	2.68	0.42
13:e:146:VAL:HG23	13:e:185:LYS:HB2	2.02	0.42
14:f:170:LEU:CG	14:f:171:ALA:N	2.81	0.42
10:b:2801:U:H6	10:b:2801:U:H2'	1.67	0.41
11:c:210:ALA:HA	11:c:213:TRP:CE2	2.55	0.41
14:f:170:LEU:O	14:f:172:ALA:N	2.53	0.41
15:g:37:LEU:HD13	15:g:68:ALA:HB1	2.02	0.41
7:7:30:ARG:HD2	7:7:30:ARG:HA	1.75	0.41
10:b:980:G:O2'	10:b:1004:G:O2'	2.34	0.41
10:b:1330:A:H4'	10:b:1331:U:C5	2.55	0.41
10:b:2640:C:H2'	10:b:2641:U:C6	2.55	0.41
10:b:2696:G:N3	10:b:2851:U:O2'	2.52	0.41
11:c:71:LYS:NZ	11:c:100:GLU:OE1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:96:TYR:HE1	11:c:102:ARG:HG3	1.85	0.41
10:b:320:A:O2'	10:b:322:A:OP2	2.34	0.41
10:b:1587:C:H3'	10:b:1588:A:H8	1.86	0.41
26:s:17:VAL:HG11	26:s:103:ILE:HG12	2.01	0.41
27:t:36:LYS:HA	27:t:36:LYS:HD2	1.86	0.41
7:7:51:SER:OG	7:7:52:LYS:N	2.54	0.41
10:b:1367:A:H8	10:b:1810:A:H61	1.66	0.41
10:b:2510:U:O4'	32:z:26[A]:ARG:NH1	2.37	0.41
11:c:111:LYS:HE3	11:c:111:LYS:HB3	1.88	0.41
19:l:95:LEU:HD11	19:l:125:LEU:HD21	2.02	0.41
26:s:81:SER:HB3	26:s:97:LEU:HD22	2.02	0.41
10:b:670:A:H2'	10:b:672:A:H62	1.85	0.41
10:b:2265:C:OP1	31:y:19:LYS:NZ	2.37	0.41
11:c:78:VAL:HG21	11:c:110:LEU:HD11	2.01	0.41
14:f:37:ASN:HB3	14:f:153:ASP:HB2	2.02	0.41
17:j:32:LEU:HD22	17:j:54:ILE:HG21	2.01	0.41
25:r:60:LYS:HB2	25:r:60:LYS:HE3	1.89	0.41
10:b:1024:G:N2	10:b:1025:U:O4	2.45	0.41
10:b:1431:G:H2'	10:b:1432:G:C8	2.56	0.41
10:b:2389:C:H2'	10:b:2390:A:C8	2.56	0.41
10:b:2519:C:H2'	10:b:2520:A:H8	1.85	0.41
11:c:13:ARG:HD2	11:c:13:ARG:HA	1.86	0.41
14:f:26:MET:SD	14:f:30:ARG:NH1	2.94	0.41
17:j:19:ASP:O	17:j:23:LYS:NZ	2.34	0.41
22:o:18:LEU:HD13	22:o:25:ARG:HG2	2.02	0.41
31:y:19:LYS:HA	31:y:19:LYS:HD3	1.79	0.41
9:a:45:A:O4'	14:f:92:ARG:NE	2.53	0.41
10:b:477:A:H2'	10:b:478:A:C8	2.55	0.41
10:b:604:A:O2'	10:b:606:G:O2'	2.25	0.41
20:m:33:LEU:HD13	20:m:117:PHE:HB3	2.02	0.41
24:q:24:TYR:O	24:q:29:SER:OG	2.33	0.41
10:b:583:C:H2'	10:b:584:A:C8	2.56	0.41
10:b:808:C:OP2	19:l:41:ARG:NH1	2.45	0.41
10:b:2303:U:OP2	14:f:71:ARG:NH1	2.52	0.41
10:b:2454:A:OP1	10:b:2501:A:O2'	2.33	0.41
30:w:35:GLU:OE1	30:w:93:ARG:NH2	2.54	0.41
5:4:9:ILE:HA	5:4:53:LYS:HB2	2.02	0.41
6:6:3:ARG:HA	6:6:3:ARG:HD3	1.85	0.41
6:6:40:ALA:N	10:b:459:U:OP1	2.43	0.41
10:b:332:A:O2'	10:b:334:C:OP2	2.33	0.41
10:b:778:G:N7	10:b:795:A:O2'	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1921:U:H2'	10:b:1922:A:O4'	2.21	0.41
14:f:170:LEU:C	14:f:172:ALA:N	2.78	0.41
15:g:76:VAL:HA	15:g:79:VAL:HG22	2.02	0.41
18:k:1:MET:HA	18:k:32:TYR:HB3	2.02	0.41
21:n:20:MET:HE2	21:n:20:MET:HB3	1.80	0.41
22:o:52:SER:HB3	22:o:54:VAL:HG12	2.02	0.41
24:q:17:ILE:HD13	24:q:17:ILE:HA	1.95	0.41
29:v:4:G:H1	29:v:66:G:H1	1.69	0.41
30:w:55:GLU:N	30:w:55:GLU:OE2	2.54	0.41
31:y:72:LYS:HE3	31:y:72:LYS:HB3	1.94	0.41
10:b:893:G:H4'	10:b:894:A:C4	2.55	0.41
10:b:1784:U:H1'	10:b:2613:U:H5''	2.03	0.41
18:k:70:ARG:HD2	18:k:76:VAL:HG22	2.02	0.41
26:s:83:LYS:O	26:s:84:ARG:NH2	2.49	0.41
7:7:31:HIS:H	7:7:31:HIS:HD2	1.69	0.40
10:b:2:G:N2	10:b:2905:C:O2	2.53	0.40
10:b:10:A:C2'	10:b:11:C:H5'	2.50	0.40
10:b:507:A:O4'	10:b:509:C:C2	2.74	0.40
10:b:538:A:H3'	10:b:539:G:H8	1.86	0.40
10:b:1175:U:C2	10:b:1178:U:C4	3.09	0.40
10:b:2034:A:C2	10:b:2503:C:H5''	2.56	0.40
15:g:46:ALA:HB3	15:g:49:THR:O	2.21	0.40
10:b:588:A:H2	10:b:811:G:N3	2.19	0.40
10:b:1173:G:H5'	10:b:1174:C:H6	1.86	0.40
10:b:1752:G:O2'	10:b:2864:A:N1	2.46	0.40
10:b:2034:A:N3	10:b:2503:C:H5''	2.36	0.40
10:b:2519:C:H2'	10:b:2520:A:C8	2.56	0.40
13:e:130:LYS:HB3	13:e:130:LYS:HE3	1.88	0.40
26:s:25:ARG:NH2	26:s:74:ILE:O	2.46	0.40
27:t:12:ARG:HB2	27:t:33:LYS:HG2	2.02	0.40
31:y:33:ALA:N	31:y:64:ASP:OD1	2.54	0.40
32:z:15[A]:THR:HA	32:z:16[A]:PRO:HD2	1.93	0.40
1:0:61:LYS:HD2	10:b:372:G:C8	2.57	0.40
2:1:40:SER:O	2:1:40:SER:OG	2.34	0.40
4:3:13:ARG:NH1	10:b:517:C:OP1	2.49	0.40
10:b:20:C:H2'	10:b:21:A:C8	2.55	0.40
10:b:809:U:O2'	10:b:2064:A:N1	2.49	0.40
10:b:1175:U:C4	10:b:1178:U:C5	3.09	0.40
10:b:2295:U:H2'	10:b:2296:U:C6	2.57	0.40
10:b:2892:C:H2'	10:b:2893:C:C6	2.56	0.40
18:k:40:LYS:NZ	18:k:89:ASN:OD1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:11:ALA:O	22:o:15:ARG:N	2.45	0.40
23:p:36:SER:O	23:p:36:SER:OG	2.38	0.40
23:p:111:LYS:HE2	23:p:111:LYS:HB3	1.79	0.40
30:w:28:ALA:HB3	30:w:40:ILE:HG13	2.03	0.40
9:a:40:U:N3	9:a:44:G:OP2	2.43	0.40
10:b:360:U:H3'	10:b:361:G:C8	2.56	0.40
13:e:138:LEU:HB3	13:e:143:LEU:HB2	2.03	0.40
14:f:40:VAL:HB	14:f:50:LEU:HD12	2.04	0.40
15:g:176:LYS:HA	15:g:176:LYS:HD2	1.82	0.40
18:k:40:LYS:HE3	18:k:57:VAL:HG12	2.03	0.40
28:u:86:ARG:NH1	28:u:100:SER:O	2.55	0.40
4:3:4:GLN:HA	10:b:2619:U:C2	2.57	0.40
9:a:42:C:H3'	9:a:43:C:H5''	2.04	0.40
10:b:107:G:H2'	10:b:108:G:H8	1.86	0.40
10:b:141:G:H8	27:t:1:MET:HE2	1.87	0.40
10:b:876:G:OP1	20:m:62:LYS:NZ	2.42	0.40
10:b:1999:U:H3'	10:b:2000:C:H2'	2.04	0.40
25:r:40:MET:HE3	25:r:42:ALA:HB2	2.04	0.40
31:y:48:GLY:O	31:y:51:VAL:HG23	2.21	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	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	24	43
14	f	175/179 (98%)	154 (88%)	20 (11%)	1 (1%)	21	39
15	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	21	39
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	11	23
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	48/61 (79%)	38 (79%)	10 (21%)	0	100	100
All	All	3091/3328 (93%)	2867 (93%)	220 (7%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	e	138	LEU
14	f	171	ALA
30	w	66	ASP
15	g	46	ALA

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	
1	0	67/68 (98%)	66 (98%)	1 (2%)	57	77
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	46 (98%)	1 (2%)	47	70
4	3	46/48 (96%)	46 (100%)	0	100	100
5	4	45/49 (92%)	44 (98%)	1 (2%)	45	69
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	49 (96%)	2 (4%)	28	53
8	8	34/34 (100%)	34 (100%)	0	100	100
11	c	216/218 (99%)	215 (100%)	1 (0%)	81	90
12	d	164/164 (100%)	162 (99%)	2 (1%)	63	80
13	e	165/165 (100%)	163 (99%)	2 (1%)	63	80
14	f	148/150 (99%)	144 (97%)	4 (3%)	39	63
15	g	137/138 (99%)	136 (99%)	1 (1%)	76	88
16	h	30/114 (26%)	29 (97%)	1 (3%)	33	58
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	102 (100%)	0	100	100
20	m	109/109 (100%)	108 (99%)	1 (1%)	70	84
21	n	100/103 (97%)	100 (100%)	0	100	100
22	o	86/87 (99%)	85 (99%)	1 (1%)	63	80
23	p	98/100 (98%)	97 (99%)	1 (1%)	68	83
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	82/84 (98%)	81 (99%)	1 (1%)	63	80
26	s	92/93 (99%)	91 (99%)	1 (1%)	65	81
27	t	80/84 (95%)	79 (99%)	1 (1%)	61	79
28	u	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	w	78/78 (100%)	78 (100%)	0	100	100
31	y	55/63 (87%)	54 (98%)	1 (2%)	51	74
32	z	44/53 (83%)	38 (86%)	6 (14%)	3	7
All	All	2559/2694 (95%)	2530 (99%)	29 (1%)	65	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
3	2	36	VAL
5	4	23	THR
7	7	6	THR
7	7	30	ARG
11	c	184	VAL
12	d	121	THR
12	d	151	THR
13	e	121	VAL
13	e	137	LYS
14	f	30	ARG
14	f	146	VAL
14	f	169	LEU
14	f	170	LEU
15	g	43	VAL
16	h	12	LEU
20	m	75	GLU
22	o	67	ASN
23	p	92	VAL
25	r	72	VAL
26	s	29	VAL
27	t	74	ILE
31	y	51	VAL
32	z	11[A]	ARG
32	z	11[B]	ARG
32	z	17[A]	VAL
32	z	17[B]	VAL
32	z	25[A]	ILE
32	z	25[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	6	GLN
1	0	17	ASN
1	0	20	HIS
2	1	25	GLN
2	1	36	GLN
4	3	6	ASN
7	7	28	ASN
11	c	142	HIS
11	c	163	GLN
11	c	260	ASN
12	d	32	ASN
12	d	150	GLN
13	e	9	GLN
13	e	90	GLN
14	f	5	HIS
14	f	27	GLN
14	f	127	ASN
14	f	135	GLN
15	g	20	ASN
15	g	73	ASN
15	g	115	HIS
16	h	28	ASN
17	j	80	HIS
18	k	90	ASN
19	l	99	ASN
20	m	13	HIS
20	m	97	GLN
21	n	73	ASN
22	o	98	GLN
23	p	56	HIS
23	p	66	ASN
24	q	52	GLN
24	q	71	GLN
24	q	81	ASN
25	r	12	HIS
26	s	7	HIS
26	s	15	GLN
26	s	40	ASN
27	t	15	HIS
27	t	59	ASN
28	u	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2882/2906 (99%)	767 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3072/3101 (99%)	837 (27%)	0

All (837) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G
9	a	24	G
9	a	25	U
9	a	26	C
9	a	29	A
9	a	30	C
9	a	35	C
9	a	39	A
9	a	42	C
9	a	43	C
9	a	44	G
9	a	52	A
9	a	53	A
9	a	56	G
9	a	66	A
9	a	67	G
9	a	87	U
9	a	88	C
9	a	89	U
9	a	90	C
9	a	91	C
9	a	93	C
9	a	99	A
9	a	109	A
9	a	112	G
9	a	113	C
9	a	114	C
9	a	117	G
9	a	118	C
10	b	4	U
10	b	10	A

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Mol	Chain	Res	Type
10	b	12	U
10	b	15	G
10	b	28	A
10	b	34	U
10	b	35	G
10	b	46	G
10	b	51	G
10	b	62	U
10	b	63	A
10	b	71	A
10	b	74	A
10	b	75	G
10	b	84	A
10	b	91	A
10	b	92	U
10	b	93	G
10	b	100	U
10	b	101	A
10	b	102	U
10	b	103	A
10	b	118	A
10	b	119	A
10	b	120	U
10	b	121	G
10	b	122	G
10	b	125	A
10	b	136	G
10	b	137	U
10	b	142	A
10	b	144	A
10	b	159	G
10	b	160	A
10	b	163	C
10	b	174	U
10	b	175	G
10	b	177	G
10	b	196	A
10	b	199	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A

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Mol	Chain	Res	Type
10	b	223	A
10	b	224	U
10	b	229	C
10	b	230	G
10	b	233	A
10	b	245	G
10	b	248	G
10	b	252	G
10	b	255	A
10	b	264	C
10	b	265	A
10	b	266	G
10	b	271	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	294	A
10	b	298	G
10	b	300	A
10	b	302	C
10	b	317	G
10	b	318	C
10	b	322	A
10	b	329	G
10	b	330	A
10	b	331	C
10	b	332	A
10	b	343	C
10	b	345	A
10	b	346	A
10	b	347	A
10	b	352	A
10	b	353	C
10	b	355	U
10	b	358	U
10	b	359	G
10	b	362	A
10	b	363	G
10	b	366	C
10	b	367	G
10	b	371	A

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Mol	Chain	Res	Type
10	b	372	G
10	b	373	U
10	b	386	G
10	b	387	U
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G
10	b	405	U
10	b	406	G
10	b	417	C
10	b	418	C
10	b	439	A
10	b	442	G
10	b	446	G
10	b	451	U
10	b	457	A
10	b	464	U
10	b	467	G
10	b	471	A
10	b	472	A
10	b	474	G
10	b	481	G
10	b	487	C
10	b	491	G
10	b	501	A
10	b	503	A
10	b	505	A
10	b	507	A
10	b	508	A
10	b	509	C
10	b	510	C
10	b	512	G
10	b	527	C
10	b	529	A
10	b	531	C
10	b	532	A
10	b	538	A
10	b	558	A
10	b	559	C
10	b	565	A
10	b	570	U

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Mol	Chain	Res	Type
10	b	575	U
10	b	577	A
10	b	579	G
10	b	590	U
10	b	604	A
10	b	605	A
10	b	606	G
10	b	608	U
10	b	615	A
10	b	616	A
10	b	617	U
10	b	624	G
10	b	629	A
10	b	636	C
10	b	639	A
10	b	642	C
10	b	644	U
10	b	648	U
10	b	649	G
10	b	655	U
10	b	656	A
10	b	657	A
10	b	661	G
10	b	670	A
10	b	671	G
10	b	672	A
10	b	688	U
10	b	704	U
10	b	706	G
10	b	719	C
10	b	720	A
10	b	725	C
10	b	729	A
10	b	732	A
10	b	740	G
10	b	749	U
10	b	750	G
10	b	754	A
10	b	759	G
10	b	764	U
10	b	766	A
10	b	767	C

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Mol	Chain	Res	Type
10	b	777	G
10	b	778	G
10	b	784	A
10	b	786	G
10	b	787	G
10	b	791	A
10	b	793	C
10	b	807	G
10	b	808	C
10	b	811	G
10	b	813	U
10	b	814	C
10	b	821	A
10	b	829	U
10	b	832	G
10	b	848	U
10	b	849	U
10	b	858	G
10	b	860	G
10	b	861	G
10	b	868	A
10	b	871	G
10	b	874	U
10	b	875	C
10	b	878	C
10	b	879	A
10	b	880	A
10	b	882	G
10	b	883	G
10	b	884	G
10	b	885	G
10	b	886	U
10	b	889	U
10	b	890	C
10	b	896	U
10	b	897	U
10	b	898	A
10	b	899	C
10	b	902	A
10	b	909	G
10	b	912	A
10	b	913	A

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Mol	Chain	Res	Type
10	b	914	C
10	b	921	U
10	b	933	U
10	b	943	A
10	b	947	A
10	b	948	C
10	b	963	C
10	b	975	A
10	b	976	G
10	b	985	A
10	b	991	G
10	b	992	A
10	b	998	A
10	b	1005	G
10	b	1007	C
10	b	1012	A
10	b	1014	U
10	b	1015	C
10	b	1021	U
10	b	1024	G
10	b	1028	G
10	b	1035	U
10	b	1037	U
10	b	1040	G
10	b	1049	G
10	b	1055	C
10	b	1056	A
10	b	1058	G
10	b	1059	A
10	b	1060	U
10	b	1061	G
10	b	1062	U
10	b	1063	U
10	b	1064	G
10	b	1066	C
10	b	1068	U
10	b	1069	A
10	b	1070	G
10	b	1071	A
10	b	1072	A
10	b	1073	G
10	b	1075	A

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Mol	Chain	Res	Type
10	b	1076	G
10	b	1077	C
10	b	1078	C
10	b	1079	A
10	b	1080	U
10	b	1081	C
10	b	1082	A
10	b	1083	U
10	b	1086	A
10	b	1087	A
10	b	1088	A
10	b	1089	G
10	b	1090	A
10	b	1091	A
10	b	1092	A
10	b	1097	A
10	b	1099	U
10	b	1100	A
10	b	1101	G
10	b	1102	C
10	b	1103	U
10	b	1104	C
10	b	1106	C
10	b	1107	U
10	b	1108	G
10	b	1111	C
10	b	1113	A
10	b	1114	G
10	b	1119	C
10	b	1121	U
10	b	1132	U
10	b	1134	U
10	b	1135	A
10	b	1136	A
10	b	1137	C
10	b	1138	G
10	b	1144	A
10	b	1170	G
10	b	1171	A
10	b	1172	C
10	b	1173	G
10	b	1174	C

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Mol	Chain	Res	Type
10	b	1175	U
10	b	1177	A
10	b	1178	U
10	b	1179	G
10	b	1187	G
10	b	1189	G
10	b	1190	U
10	b	1197	G
10	b	1206	A
10	b	1207	A
10	b	1208	G
10	b	1209	C
10	b	1212	G
10	b	1214	G
10	b	1226	U
10	b	1229	G
10	b	1234	G
10	b	1238	G
10	b	1239	A
10	b	1240	G
10	b	1242	U
10	b	1243	A
10	b	1244	U
10	b	1246	A
10	b	1249	A
10	b	1251	U
10	b	1252	G
10	b	1255	A
10	b	1257	U
10	b	1258	G
10	b	1268	G
10	b	1273	G
10	b	1274	A
10	b	1275	U
10	b	1277	A
10	b	1278	A
10	b	1281	G
10	b	1286	A
10	b	1289	A
10	b	1291	C
10	b	1302	G
10	b	1303	A

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Mol	Chain	Res	Type
10	b	1304	A
10	b	1313	G
10	b	1321	C
10	b	1323	A
10	b	1328	U
10	b	1331	U
10	b	1336	G
10	b	1342	U
10	b	1346	U
10	b	1354	U
10	b	1361	A
10	b	1367	A
10	b	1370	G
10	b	1380	A
10	b	1381	U
10	b	1382	G
10	b	1385	A
10	b	1388	C
10	b	1397	A
10	b	1398	U
10	b	1402	U
10	b	1412	G
10	b	1413	U
10	b	1417	U
10	b	1418	G
10	b	1421	A
10	b	1422	A
10	b	1423	G
10	b	1429	A
10	b	1430	C
10	b	1444	U
10	b	1453	C
10	b	1454	G
10	b	1455	A
10	b	1456	C
10	b	1457	G
10	b	1461	G
10	b	1462	U
10	b	1463	C
10	b	1469	U
10	b	1471	A
10	b	1473	G

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Mol	Chain	Res	Type
10	b	1477	G
10	b	1478	U
10	b	1479	A
10	b	1480	G
10	b	1484	G
10	b	1495	C
10	b	1497	A
10	b	1498	A
10	b	1499	U
10	b	1500	C
10	b	1505	A
10	b	1507	A
10	b	1510	A
10	b	1511	A
10	b	1525	U
10	b	1526	G
10	b	1531	G
10	b	1534	A
10	b	1535	C
10	b	1538	C
10	b	1539	G
10	b	1540	G
10	b	1541	U
10	b	1542	G
10	b	1544	U
10	b	1545	G
10	b	1549	C
10	b	1554	A
10	b	1556	U
10	b	1558	C
10	b	1561	U
10	b	1567	C
10	b	1568	A
10	b	1570	G
10	b	1571	A
10	b	1580	U
10	b	1583	G
10	b	1585	A
10	b	1586	U
10	b	1587	C
10	b	1598	A
10	b	1601	U

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Mol	Chain	Res	Type
10	b	1609	C
10	b	1610	A
10	b	1612	A
10	b	1620	A
10	b	1621	G
10	b	1649	U
10	b	1650	U
10	b	1651	G
10	b	1662	G
10	b	1670	A
10	b	1676	G
10	b	1677	C
10	b	1680	A
10	b	1697	G
10	b	1705	G
10	b	1707	A
10	b	1708	C
10	b	1709	G
10	b	1717	G
10	b	1720	G
10	b	1723	G
10	b	1724	A
10	b	1732	C
10	b	1733	G
10	b	1735	G
10	b	1736	G
10	b	1740	G
10	b	1750	C
10	b	1758	G
10	b	1759	A
10	b	1760	U
10	b	1765	G
10	b	1766	C
10	b	1775	A
10	b	1778	G
10	b	1783	U
10	b	1784	U
10	b	1786	A
10	b	1788	A
10	b	1793	A
10	b	1802	C
10	b	1803	A

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Mol	Chain	Res	Type
10	b	1810	A
10	b	1813	G
10	b	1818	C
10	b	1831	A
10	b	1835	C
10	b	1844	G
10	b	1851	G
10	b	1859	G
10	b	1864	G
10	b	1870	C
10	b	1886	U
10	b	1888	G
10	b	1899	C
10	b	1910	G
10	b	1911	G
10	b	1912	C
10	b	1914	G
10	b	1917	A
10	b	1918	C
10	b	1922	A
10	b	1924	C
10	b	1931	A
10	b	1933	G
10	b	1934	G
10	b	1935	U
10	b	1941	A
10	b	1942	A
10	b	1944	U
10	b	1959	U
10	b	1971	C
10	b	1974	A
10	b	1975	U
10	b	1976	G
10	b	1978	C
10	b	1979	G
10	b	1985	A
10	b	1986	U
10	b	1995	U
10	b	1996	G
10	b	1997	U
10	b	2001	C
10	b	2024	A

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Mol	Chain	Res	Type
10	b	2027	C
10	b	2034	A
10	b	2035	A
10	b	2036	G
10	b	2037	A
10	b	2039	G
10	b	2040	C
10	b	2047	C
10	b	2053	G
10	b	2059	C
10	b	2060	G
10	b	2064	A
10	b	2065	G
10	b	2066	A
10	b	2067	C
10	b	2071	G
10	b	2073	G
10	b	2081	A
10	b	2084	A
10	b	2097	G
10	b	2102	U
10	b	2103	U
10	b	2105	A
10	b	2106	G
10	b	2107	C
10	b	2109	U
10	b	2111	G
10	b	2112	A
10	b	2113	U
10	b	2115	U
10	b	2116	G
10	b	2119	G
10	b	2120	G
10	b	2121	A
10	b	2122	U
10	b	2124	G
10	b	2125	G
10	b	2126	U
10	b	2127	G
10	b	2128	G
10	b	2129	G
10	b	2131	G

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Mol	Chain	Res	Type
10	b	2132	G
10	b	2134	U
10	b	2136	U
10	b	2139	A
10	b	2140	G
10	b	2142	G
10	b	2146	A
10	b	2149	C
10	b	2150	C
10	b	2151	A
10	b	2152	G
10	b	2153	U
10	b	2155	U
10	b	2156	G
10	b	2159	U
10	b	2160	G
10	b	2162	A
10	b	2163	G
10	b	2164	C
10	b	2166	G
10	b	2167	G
10	b	2168	C
10	b	2169	C
10	b	2170	U
10	b	2172	G
10	b	2173	A
10	b	2174	A
10	b	2176	U
10	b	2177	A
10	b	2179	C
10	b	2180	A
10	b	2181	C
10	b	2183	C
10	b	2185	U
10	b	2186	U
10	b	2189	U
10	b	2191	U
10	b	2192	U
10	b	2196	U
10	b	2202	A
10	b	2203	A
10	b	2207	U

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Mol	Chain	Res	Type
10	b	2208	G
10	b	2215	G
10	b	2216	A
10	b	2217	U
10	b	2218	C
10	b	2229	A
10	b	2233	U
10	b	2242	G
10	b	2243	G
10	b	2247	U
10	b	2272	A
10	b	2275	G
10	b	2283	G
10	b	2284	G
10	b	2287	C
10	b	2291	A
10	b	2292	A
10	b	2300	U
10	b	2309	U
10	b	2310	C
10	b	2312	G
10	b	2313	A
10	b	2315	A
10	b	2316	U
10	b	2326	A
10	b	2329	G
10	b	2334	G
10	b	2335	G
10	b	2337	A
10	b	2338	U
10	b	2339	A
10	b	2340	A
10	b	2349	G
10	b	2351	C
10	b	2352	U
10	b	2354	C
10	b	2358	C
10	b	2361	G
10	b	2365	G
10	b	2379	G
10	b	2380	A
10	b	2381	A

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Mol	Chain	Res	Type
10	b	2383	G
10	b	2384	C
10	b	2385	A
10	b	2387	G
10	b	2388	U
10	b	2389	C
10	b	2393	G
10	b	2395	G
10	b	2406	U
10	b	2408	U
10	b	2409	G
10	b	2410	A
10	b	2411	A
10	b	2417	G
10	b	2426	C
10	b	2427	U
10	b	2429	A
10	b	2430	A
10	b	2433	G
10	b	2434	A
10	b	2438	A
10	b	2445	U
10	b	2451	G
10	b	2452	A
10	b	2461	U
10	b	2463	A
10	b	2478	U
10	b	2480	A
10	b	2482	A
10	b	2488	G
10	b	2490	C
10	b	2494	G
10	b	2498	G
10	b	2501	A
10	b	2506	G
10	b	2508	U
10	b	2509	G
10	b	2510	U
10	b	2521	C
10	b	2522	A
10	b	2533	G
10	b	2539	G

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Mol	Chain	Res	Type
10	b	2540	G
10	b	2551	A
10	b	2558	U
10	b	2560	C
10	b	2566	U
10	b	2570	A
10	b	2571	G
10	b	2572	U
10	b	2576	A
10	b	2577	C
10	b	2585	G
10	b	2586	G
10	b	2590	U
10	b	2599	G
10	b	2606	A
10	b	2607	G
10	b	2613	U
10	b	2617	U
10	b	2618	A
10	b	2619	U
10	b	2627	G
10	b	2633	U
10	b	2645	G
10	b	2650	C
10	b	2653	C
10	b	2654	U
10	b	2659	G
10	b	2663	G
10	b	2664	A
10	b	2665	G
10	b	2667	G
10	b	2673	G
10	b	2677	G
10	b	2686	A
10	b	2688	U
10	b	2689	G
10	b	2693	U
10	b	2703	C
10	b	2711	U
10	b	2718	G
10	b	2720	C
10	b	2730	A

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Mol	Chain	Res	Type
10	b	2732	U
10	b	2736	G
10	b	2737	A
10	b	2740	A
10	b	2742	A
10	b	2748	G
10	b	2752	A
10	b	2755	G
10	b	2756	C
10	b	2757	A
10	b	2762	A
10	b	2765	A
10	b	2766	C
10	b	2769	A
10	b	2781	G
10	b	2782	A
10	b	2783	U
10	b	2786	G
10	b	2795	G
10	b	2797	C
10	b	2800	C
10	b	2801	U
10	b	2802	U
10	b	2803	G
10	b	2804	A
10	b	2812	G
10	b	2813	A
10	b	2815	G
10	b	2822	U
10	b	2824	A
10	b	2825	A
10	b	2837	U
10	b	2839	A
10	b	2852	G
10	b	2854	A
10	b	2865	U
10	b	2869	U
10	b	2870	U
10	b	2871	G
10	b	2877	A
10	b	2881	G
10	b	2883	A

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Mol	Chain	Res	Type
10	b	2884	C
10	b	2887	A
10	b	2888	U
10	b	2889	G
10	b	2890	A
10	b	2897	A
10	b	2898	G
10	b	2899	G
10	b	2905	C
29	v	3	G
29	v	5	G
29	v	6	C
29	v	7	A
29	v	8	U
29	v	9	C
29	v	15	A
29	v	16	U
29	v	17	G
29	v	18	G
29	v	20	U
29	v	25	C
29	v	26	C
29	v	27	U
29	v	34	U
29	v	35	C
29	v	36	C
29	v	38	A
29	v	42	G
29	v	45	G
29	v	46	A
29	v	47	U
29	v	48	G
29	v	49	C
29	v	50	G
29	v	52	G
29	v	54	U
29	v	60	C
29	v	62	C
29	v	63	G
29	v	64	C
29	v	65	U
29	v	67	C

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Mol	Chain	Res	Type
29	v	68	C
29	v	70	G
29	v	71	C
29	v	75	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
10	b	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	511:U	O3'	512:G	P	2.42
1	b	512:G	O3'	513:A	P	2.26

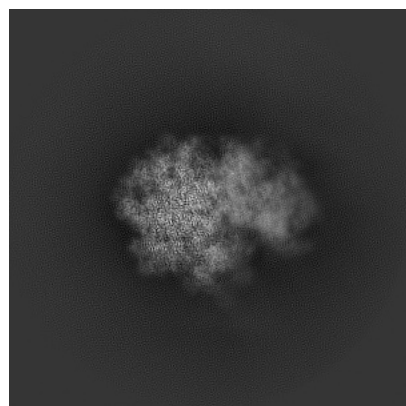
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4531. These allow visual inspection of the internal detail of the map and identification of artifacts.

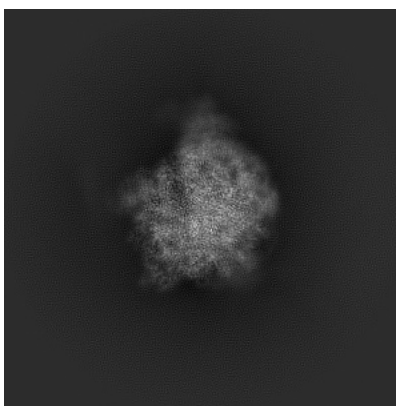
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

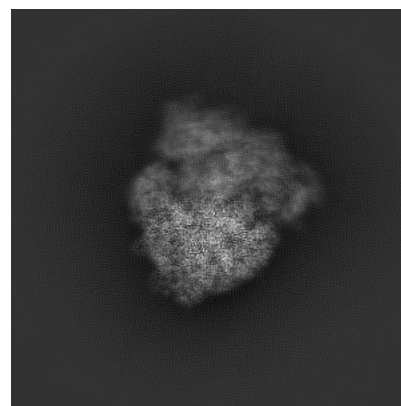
6.1.1 Primary map



X

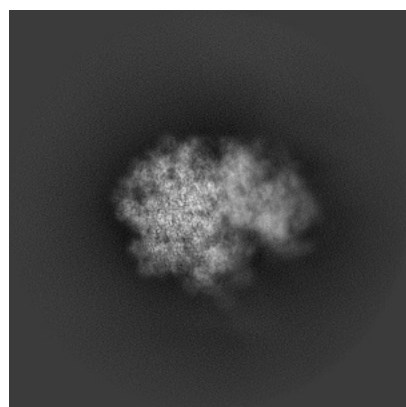


Y

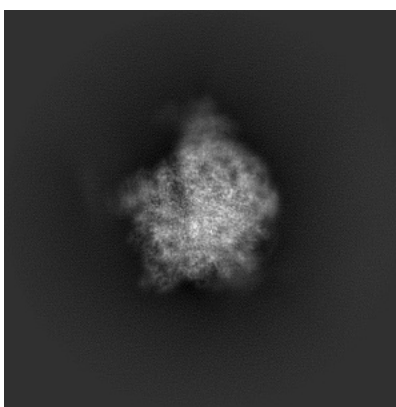


Z

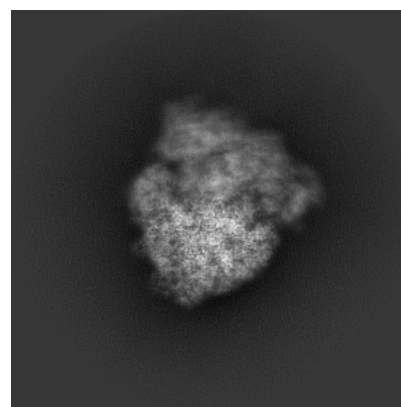
6.1.2 Raw map



X



Y

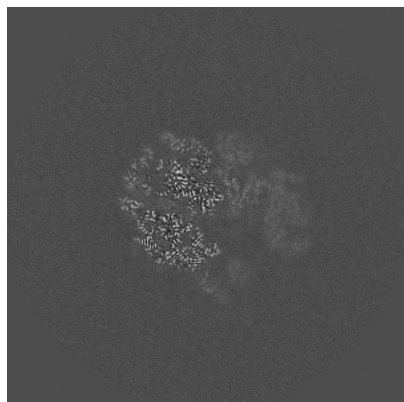


Z

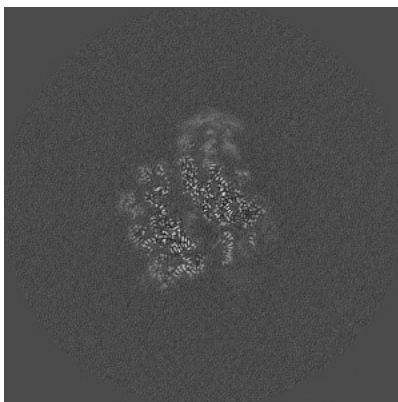
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

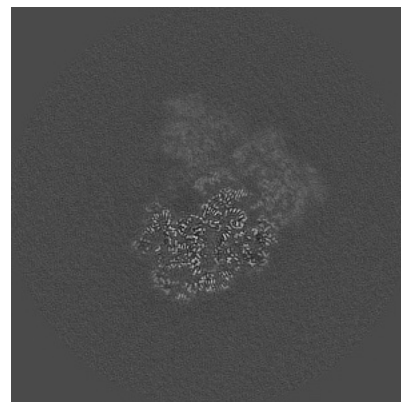
6.2.1 Primary map



X Index: 240

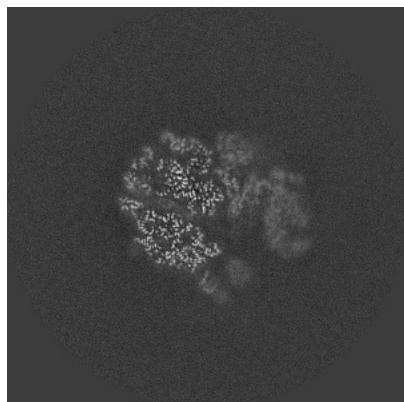


Y Index: 240

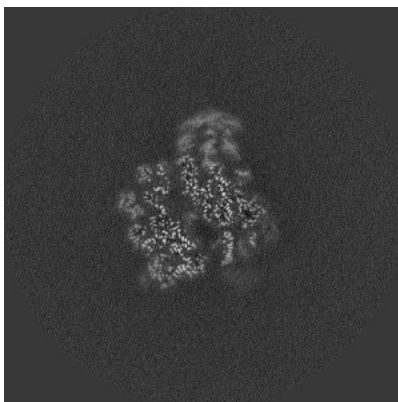


Z Index: 240

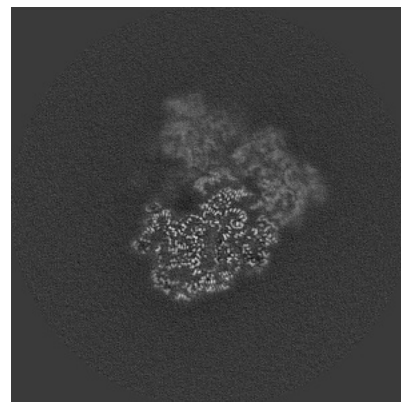
6.2.2 Raw map



X Index: 240



Y Index: 240

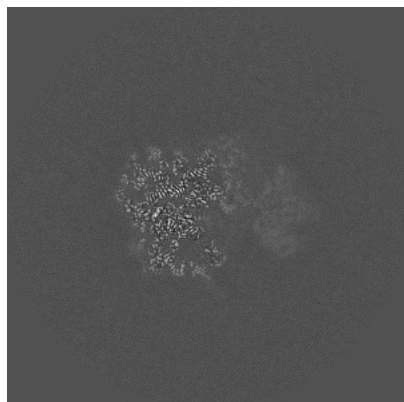


Z Index: 240

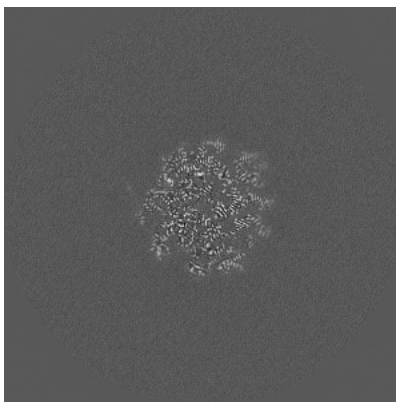
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

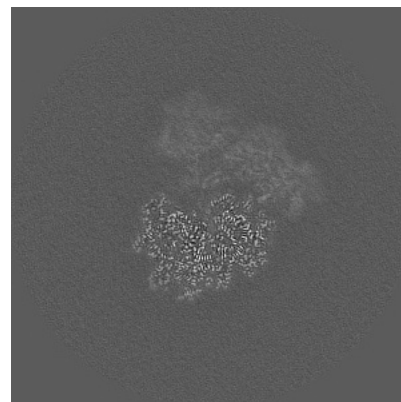
6.3.1 Primary map



X Index: 229

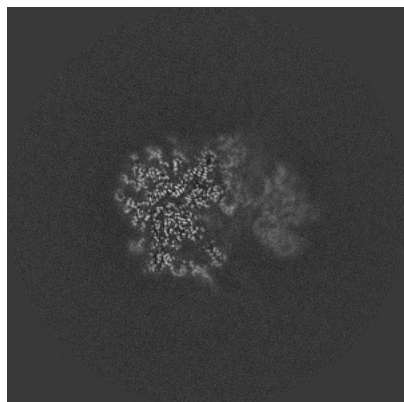


Y Index: 207

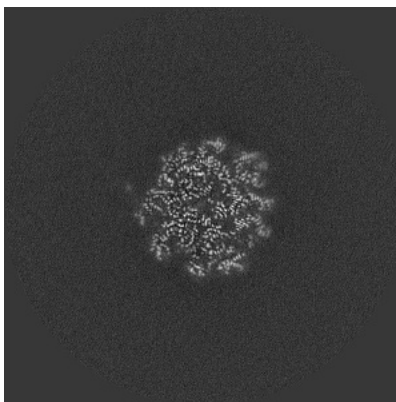


Z Index: 231

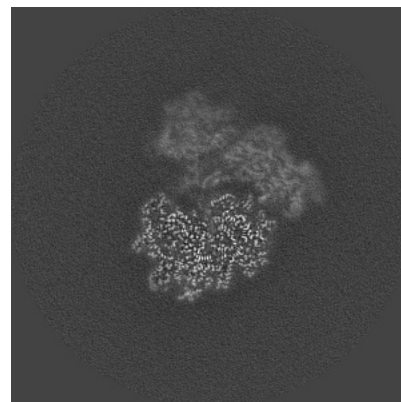
6.3.2 Raw map



X Index: 230



Y Index: 207

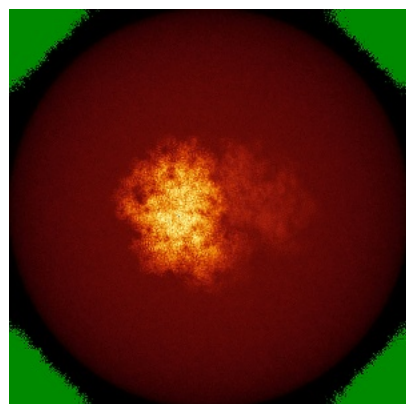


Z Index: 231

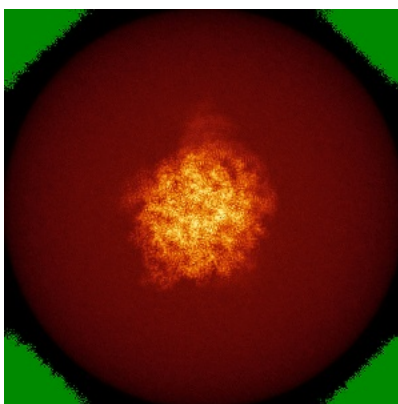
The images above show the largest variance slices of the map in three orthogonal directions.

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

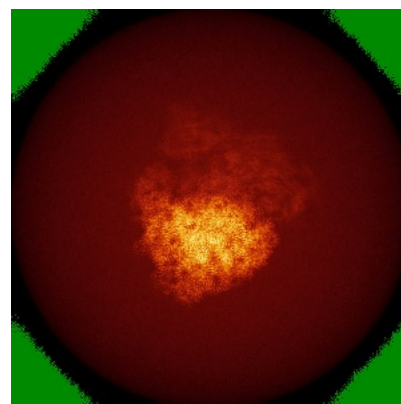
6.4.1 Primary map



X

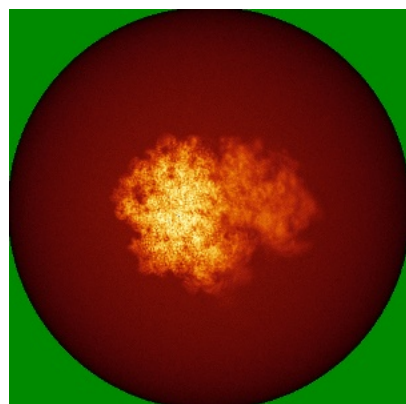


Y

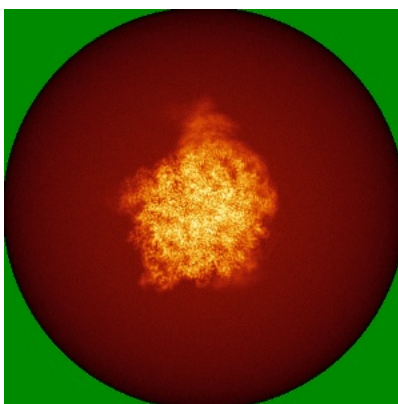


Z

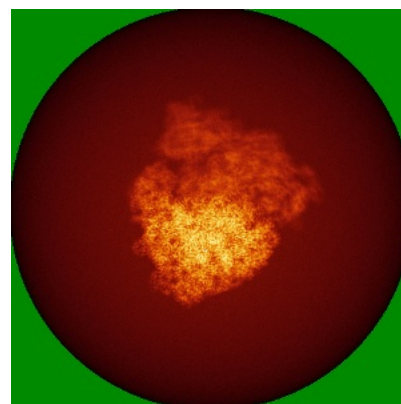
6.4.2 Raw map



X



Y

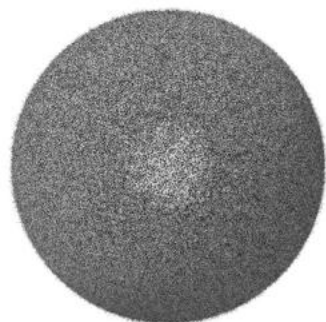


Z

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

6.5 Orthogonal surface views [i](#)

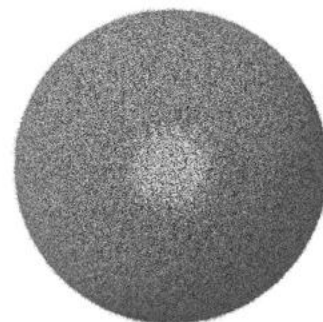
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

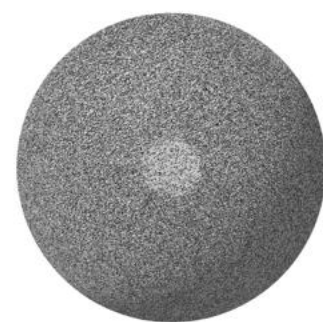
6.5.2 Raw map



X



Y



Z

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

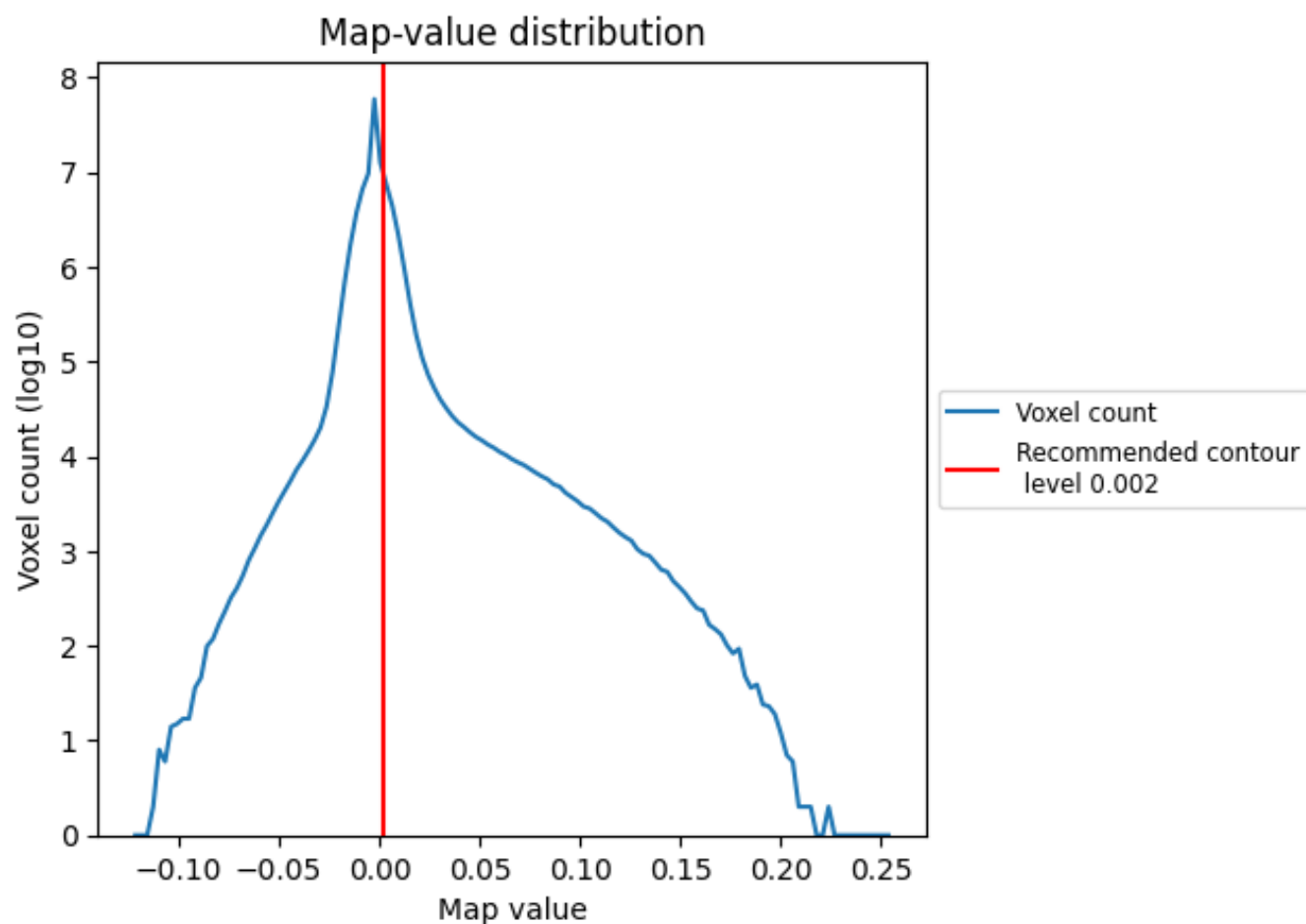
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

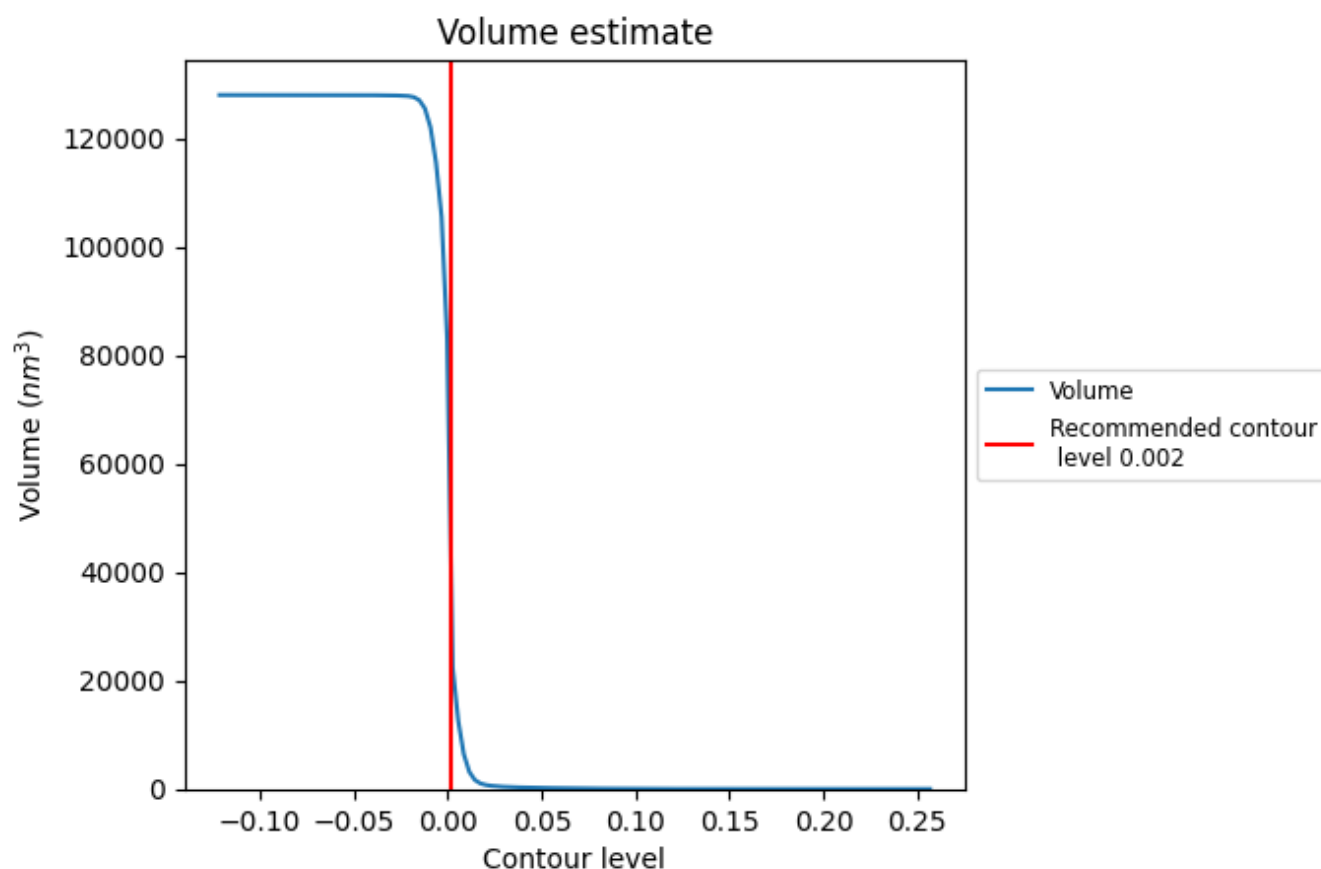
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

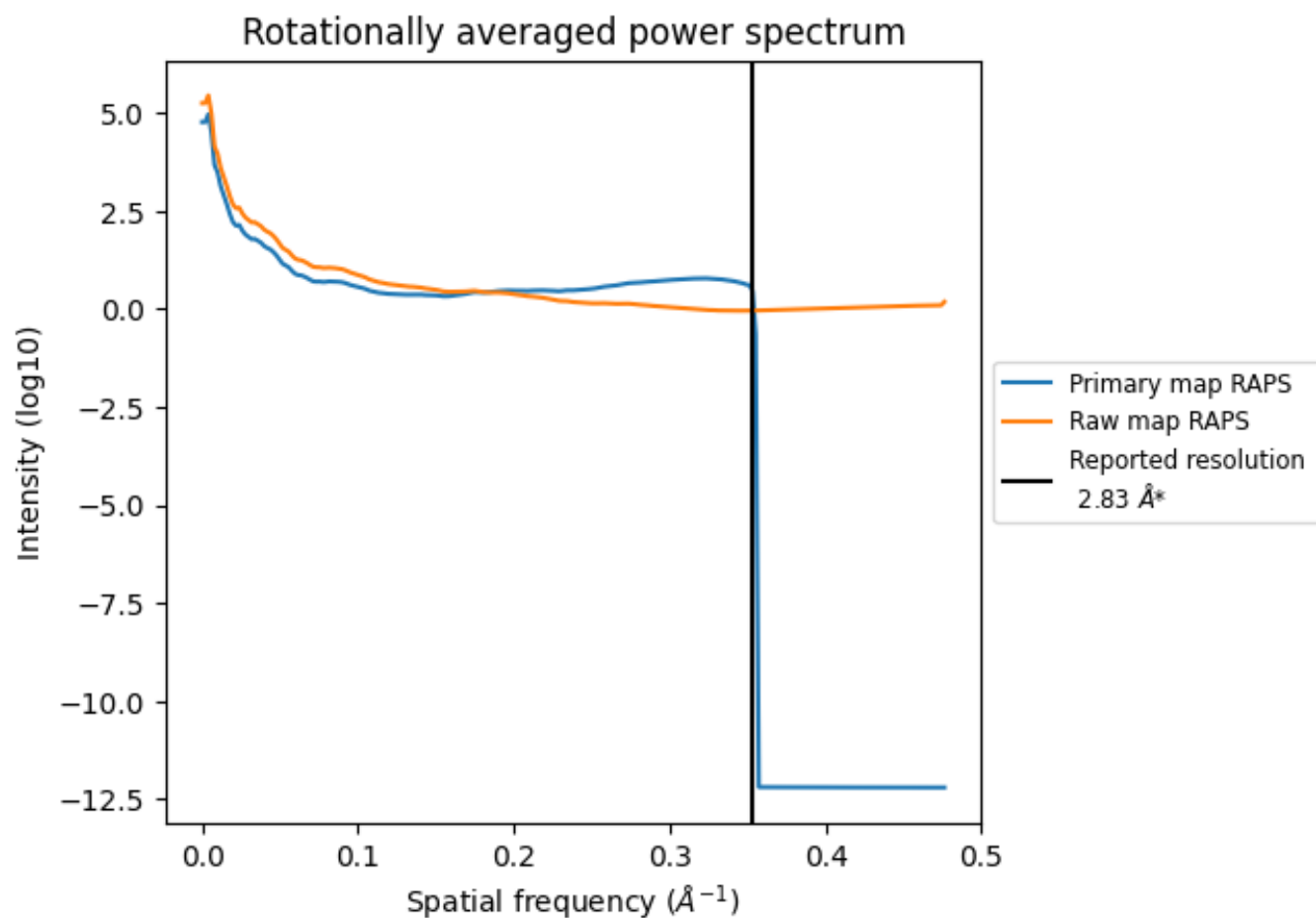
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35519 nm^3 ; this corresponds to an approximate mass of 32085 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 ⓘ

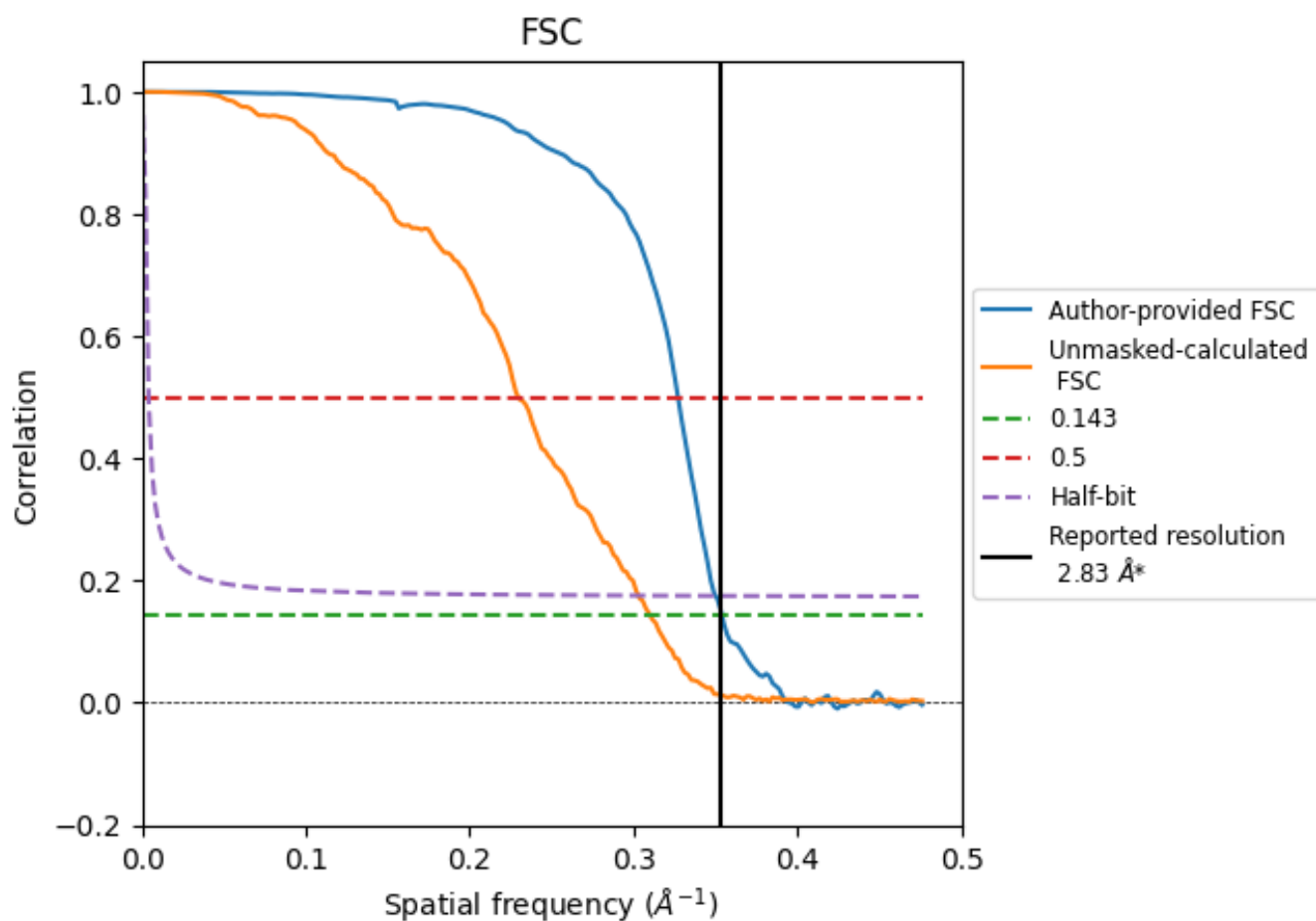


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

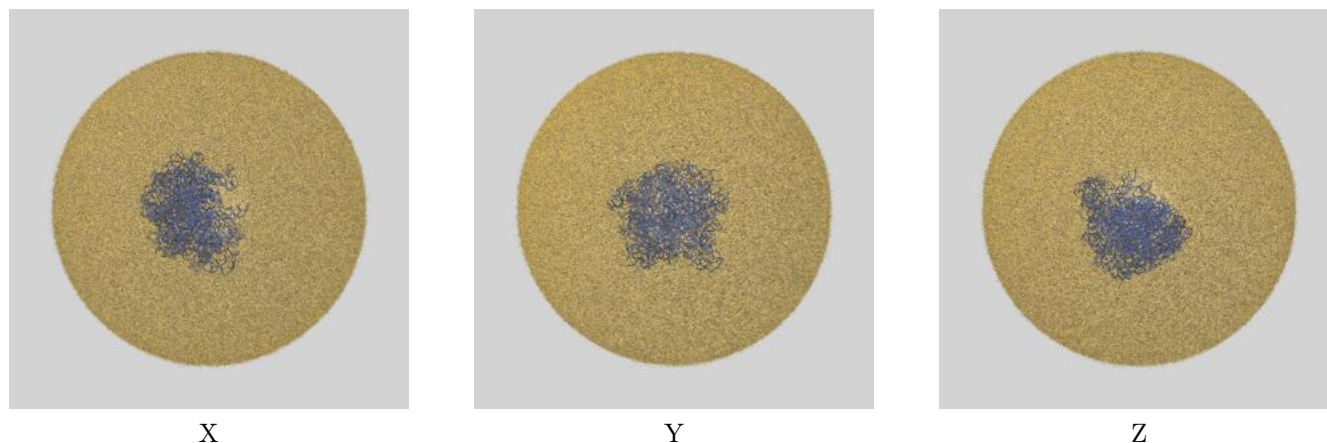
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.06	2.86
Unmasked-calculated*	3.22	4.36	3.30

*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 3.22 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

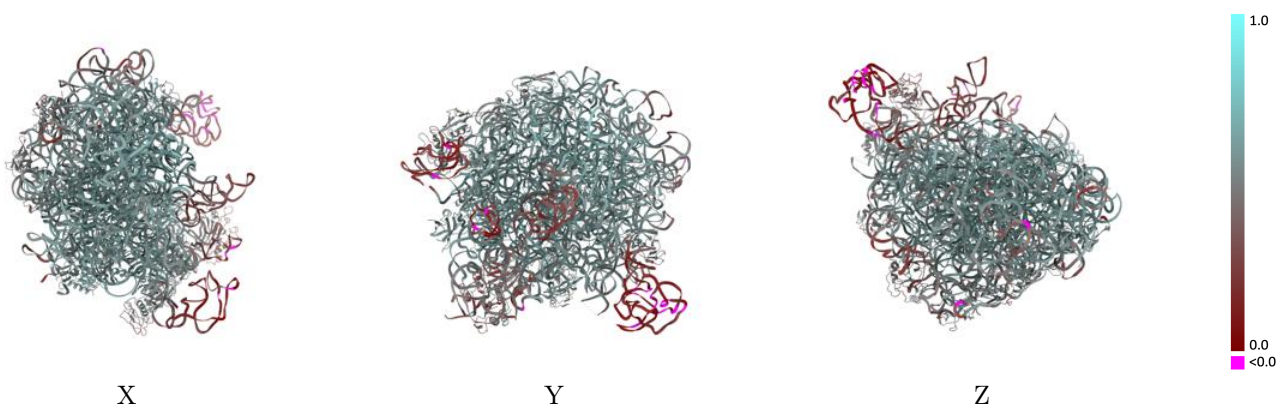
This section contains information regarding the fit between EMDB map EMD-4531 and PDB model 6QDW. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



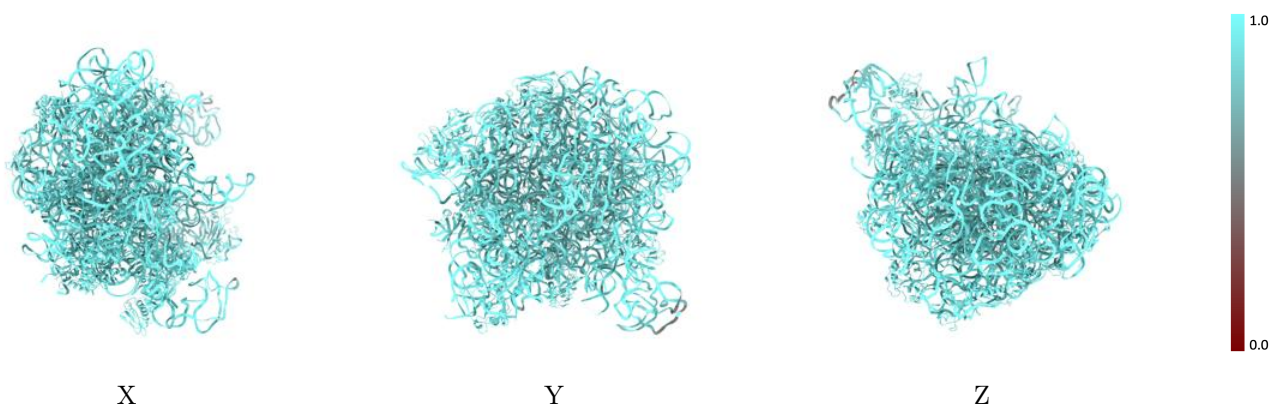
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



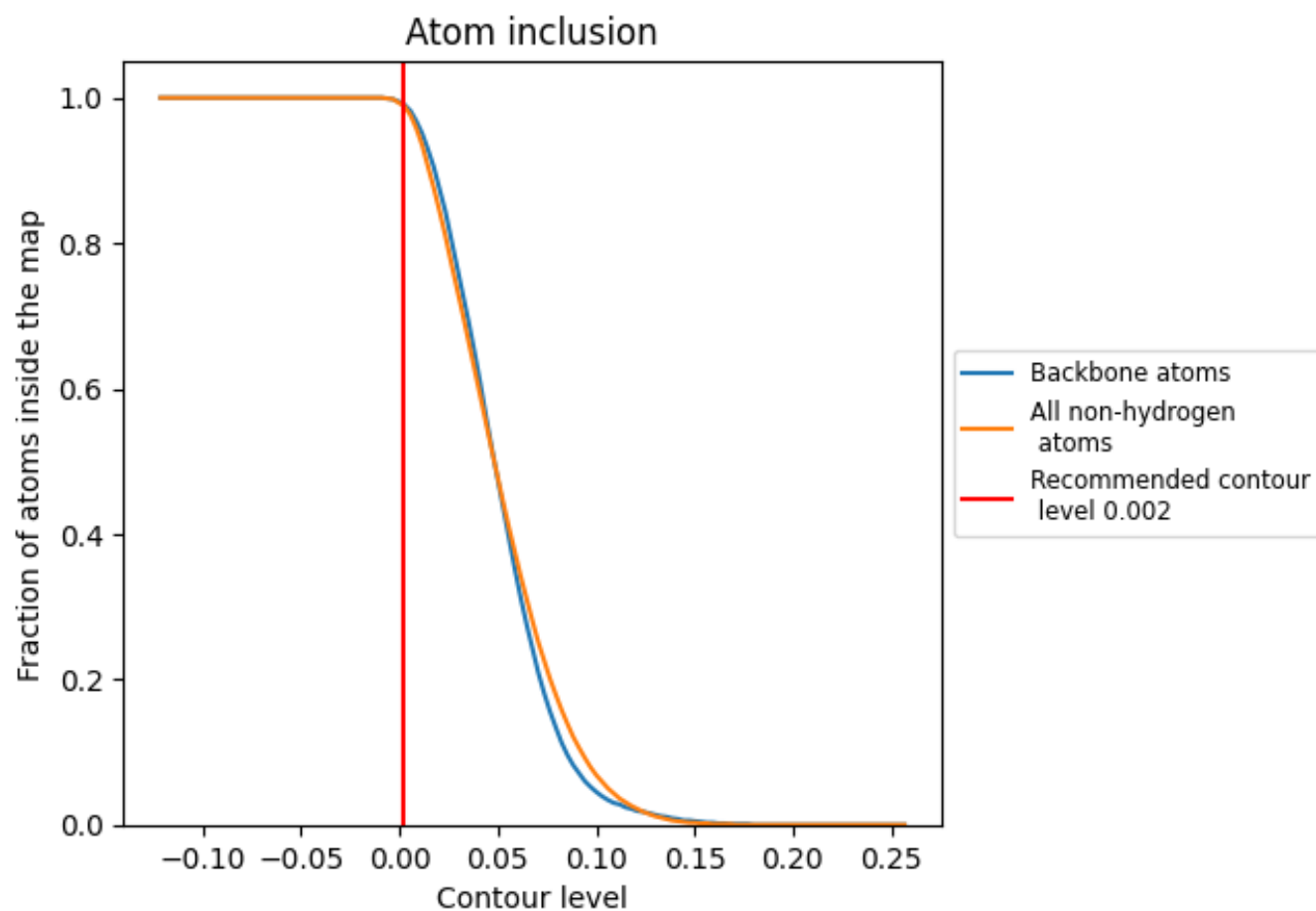
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.002).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.5410
0	 0.9880	 0.5580
1	 0.9770	 0.4710
2	 0.9980	 0.5990
3	 0.9950	 0.5550
4	 0.9680	 0.5120
6	 0.9920	 0.6080
7	 0.9960	 0.6150
8	 1.0000	 0.5820
a	 0.9930	 0.5000
b	 0.9910	 0.5510
c	 0.9930	 0.5910
d	 0.9890	 0.5650
e	 0.9850	 0.5240
f	 0.9830	 0.3410
g	 0.9870	 0.4600
h	 0.9790	 0.4550
j	 0.9950	 0.5910
k	 0.9920	 0.5730
l	 0.9850	 0.5590
m	 0.9940	 0.5920
n	 0.9940	 0.5660
o	 0.9880	 0.4670
p	 0.9840	 0.5340
q	 0.9970	 0.6130
r	 0.9900	 0.5800
s	 0.9930	 0.5770
t	 0.9890	 0.5100
u	 0.9840	 0.4570
v	 0.9260	 0.2810
w	 0.9930	 0.5560
y	 0.9910	 0.5980
z	 0.8500	 0.2500

