



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 12:02 pm BST

PDB ID : 5LZE / pdb_00005lze
EMDB ID : EMD-4125
Title : Structure of the 70S ribosome with Sec-tRNA^{Sec} in the classical pre-translocation state (C)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

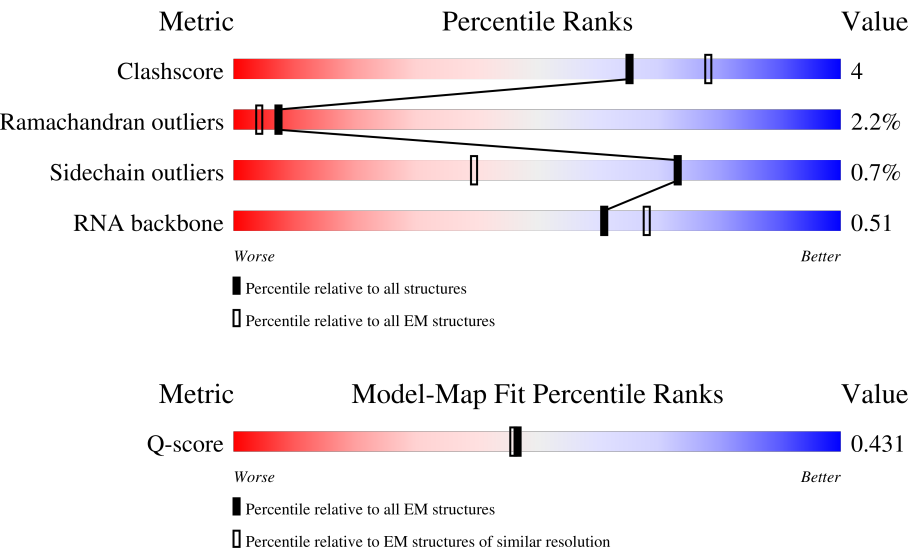
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	

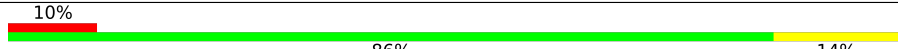
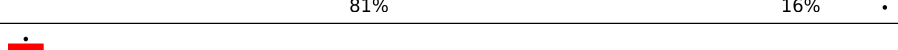
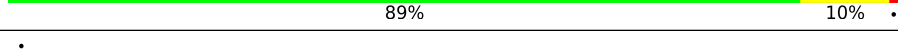
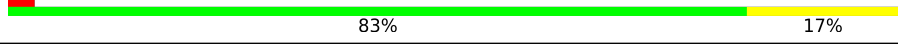
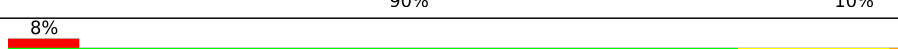
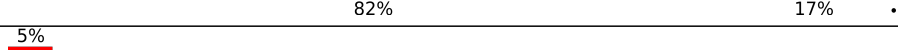
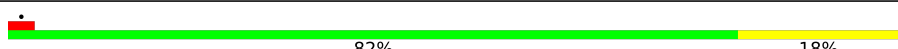
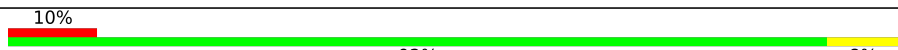
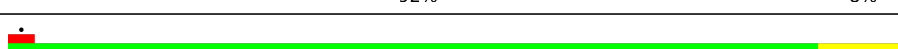
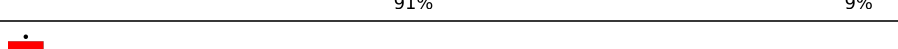
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Mol	Chain	Length	Quality of chain
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	100	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	77	
23	x	48	
24	y	95	
25	A	2903	
26	B	120	
27	C	271	
28	D	209	

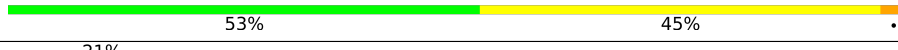
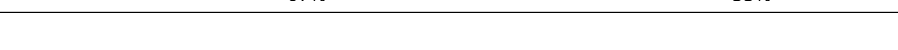
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Mol	Chain	Length	Quality of chain
29	E	201	
30	F	177	
31	G	176	
32	I	141	
33	H	149	
34	J	142	
35	K	122	
36	L	143	
37	M	136	
38	N	120	
39	O	116	
40	P	114	
41	Q	117	
42	R	103	
43	S	110	
44	T	93	
45	U	102	
46	V	94	
47	W	75	
48	X	77	
49	Y	63	
50	Z	58	
51	0	56	
52	1	50	
53	2	46	

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Mol	Chain	Length	Quality of chain
54	3	64	
55	4	38	
56	6	66	
57	w	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
25	G7M	A	2069	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called fMetSec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62274	27787	11459	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 57 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

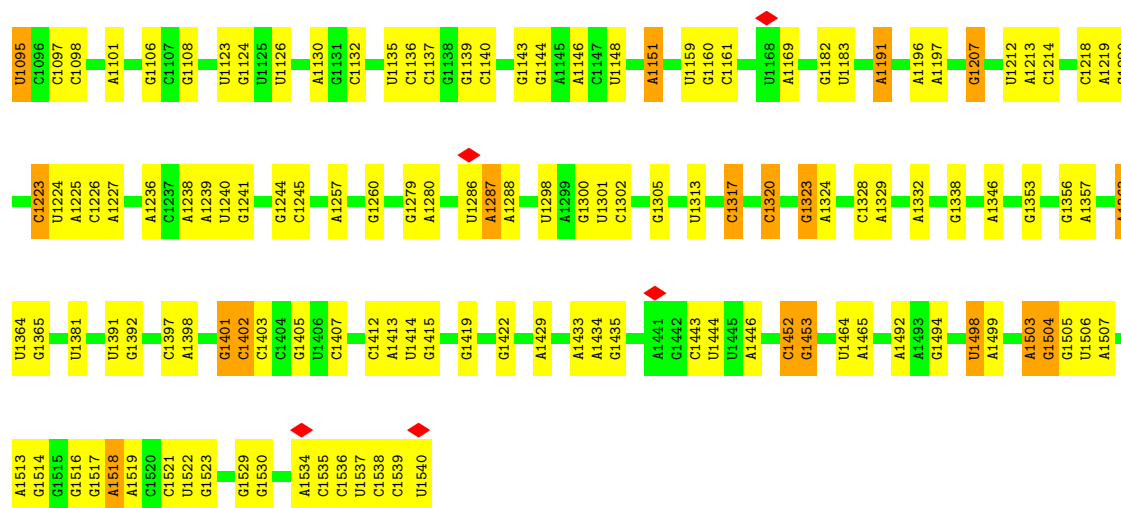
Mol	Chain	Residues	Atoms		AltConf
58	4	1	Total	Zn	0
			1	1	
58	6	1	Total	Zn	0
			1	1	

3 Residue-property plots

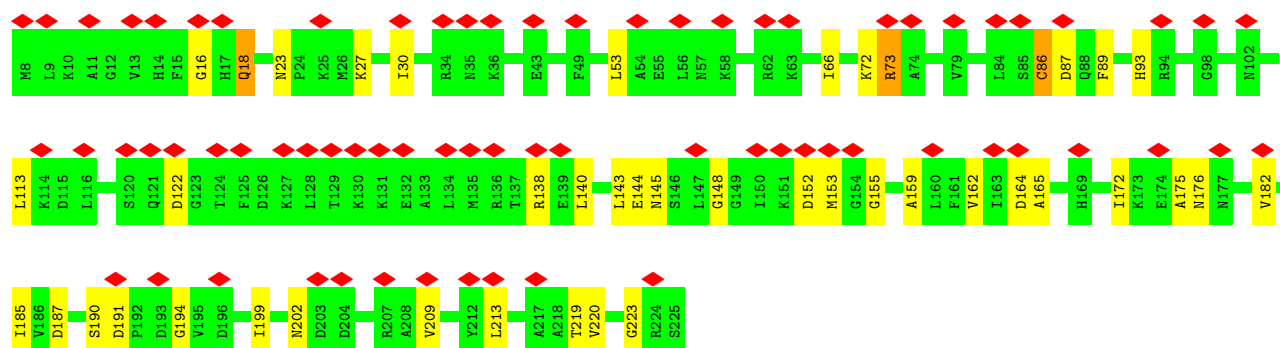
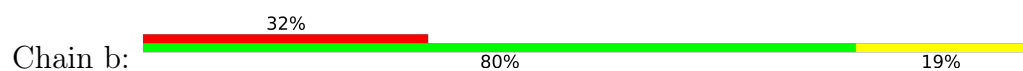
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

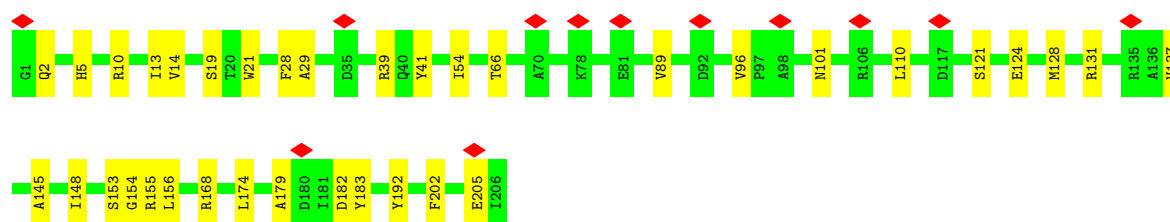
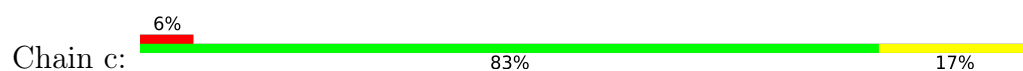




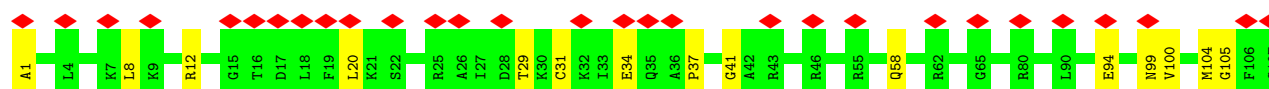
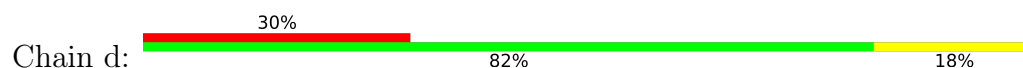
• Molecule 2: 30S ribosomal protein S2

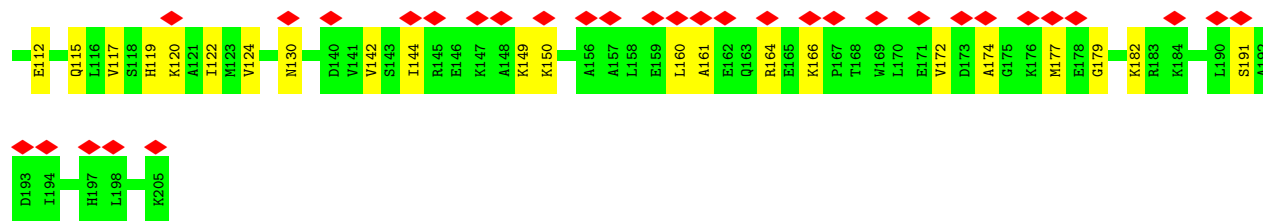


• Molecule 3: 30S ribosomal protein S3

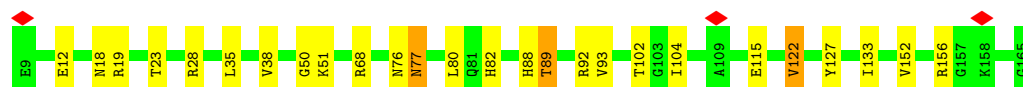
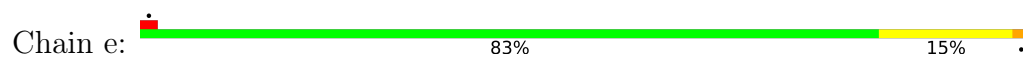


• Molecule 4: 30S ribosomal protein S4

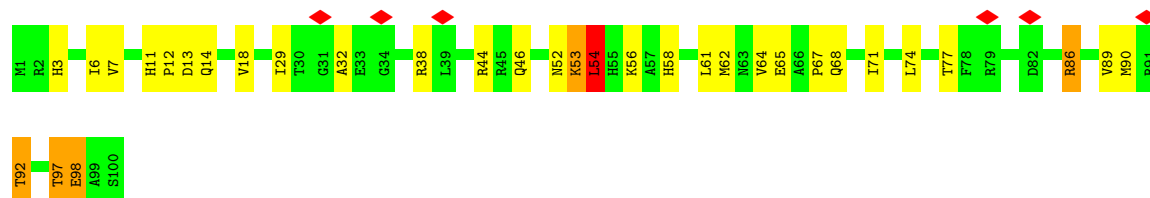




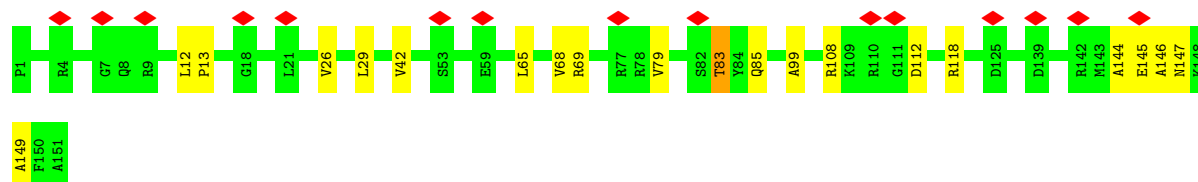
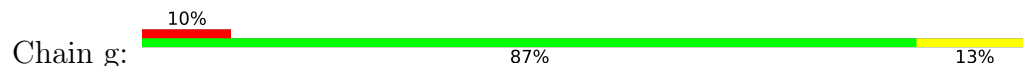
• Molecule 5: 30S ribosomal protein S5



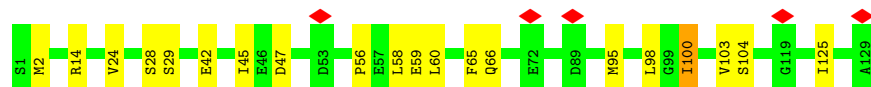
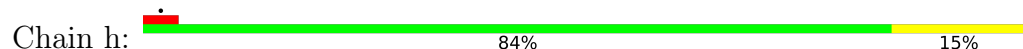
• Molecule 6: 30S ribosomal protein S6



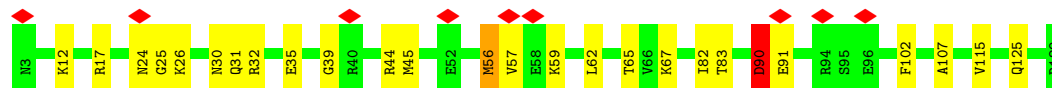
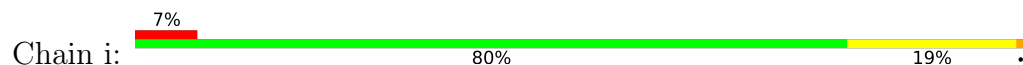
• Molecule 7: 30S ribosomal protein S7



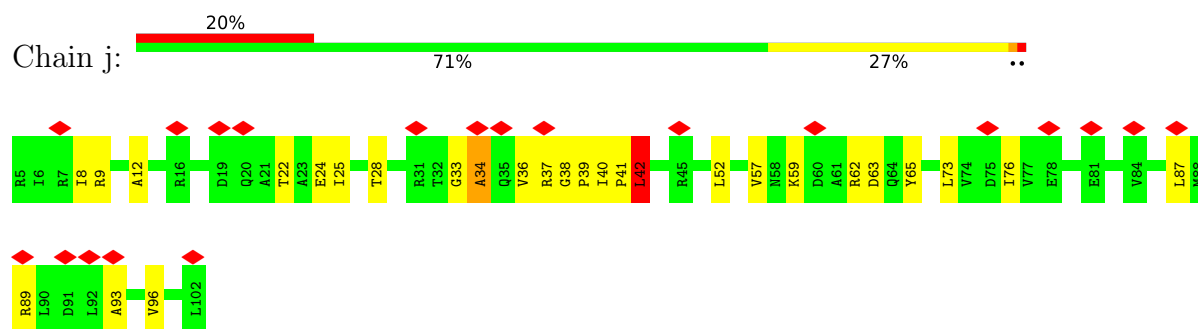
• Molecule 8: 30S ribosomal protein S8



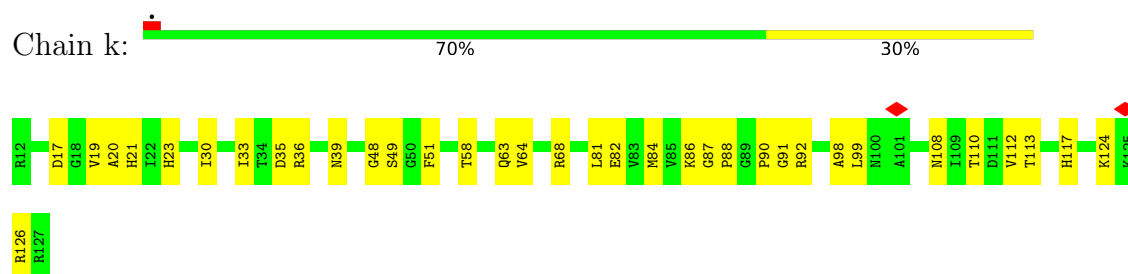
• Molecule 9: 30S ribosomal protein S9



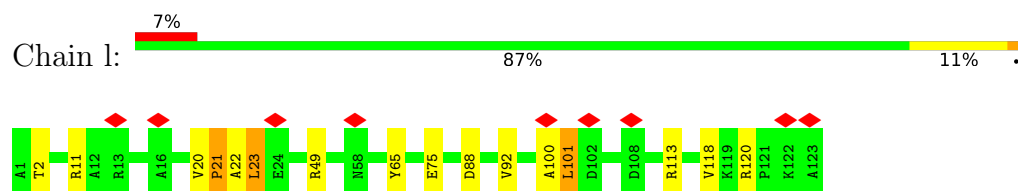
- Molecule 10: 30S ribosomal protein S10



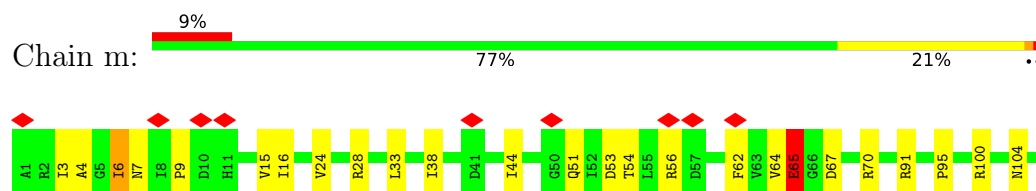
- Molecule 11: 30S ribosomal protein S11



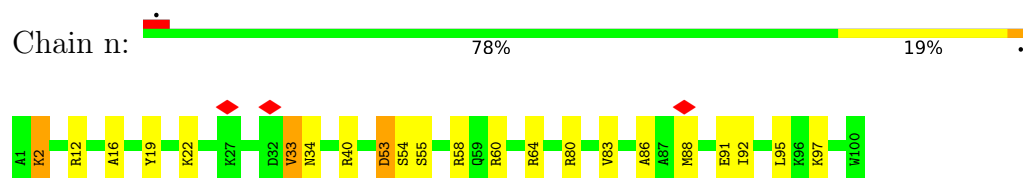
- Molecule 12: 30S ribosomal protein S12



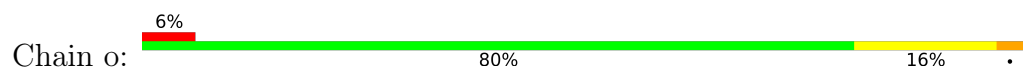
- Molecule 13: 30S ribosomal protein S13

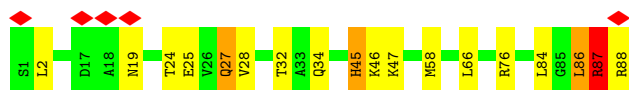


- Molecule 14: 30S ribosomal protein S14

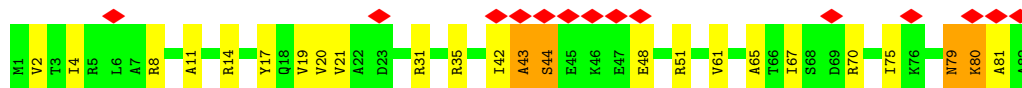


- Molecule 15: 30S ribosomal protein S15

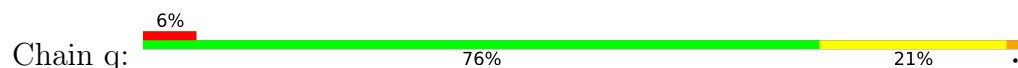




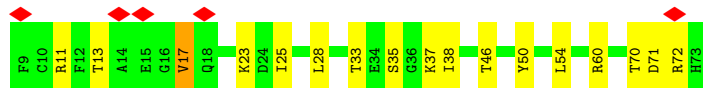
- Molecule 16: 30S ribosomal protein S16



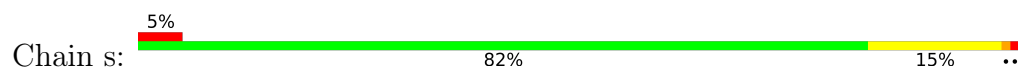
- Molecule 17: 30S ribosomal protein S17



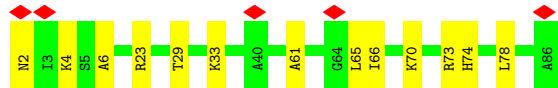
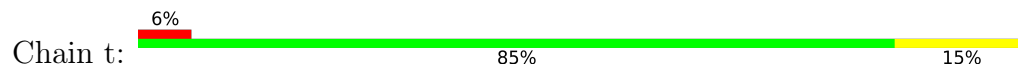
- Molecule 18: 30S ribosomal protein S18



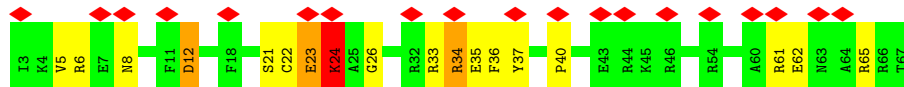
- Molecule 19: 30S ribosomal protein S19



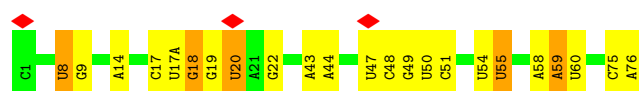
- Molecule 20: 30S ribosomal protein S20



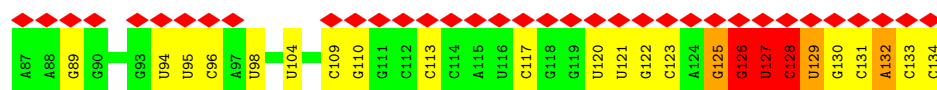
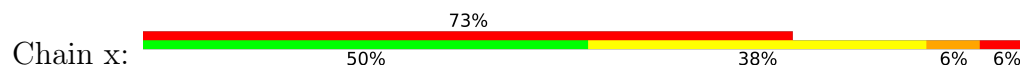
- Molecule 21: 30S ribosomal protein S21



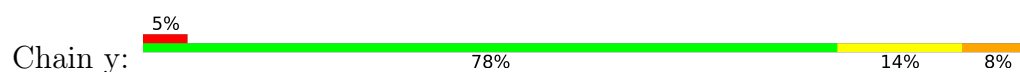
- Molecule 22: tRNA^{fMet}



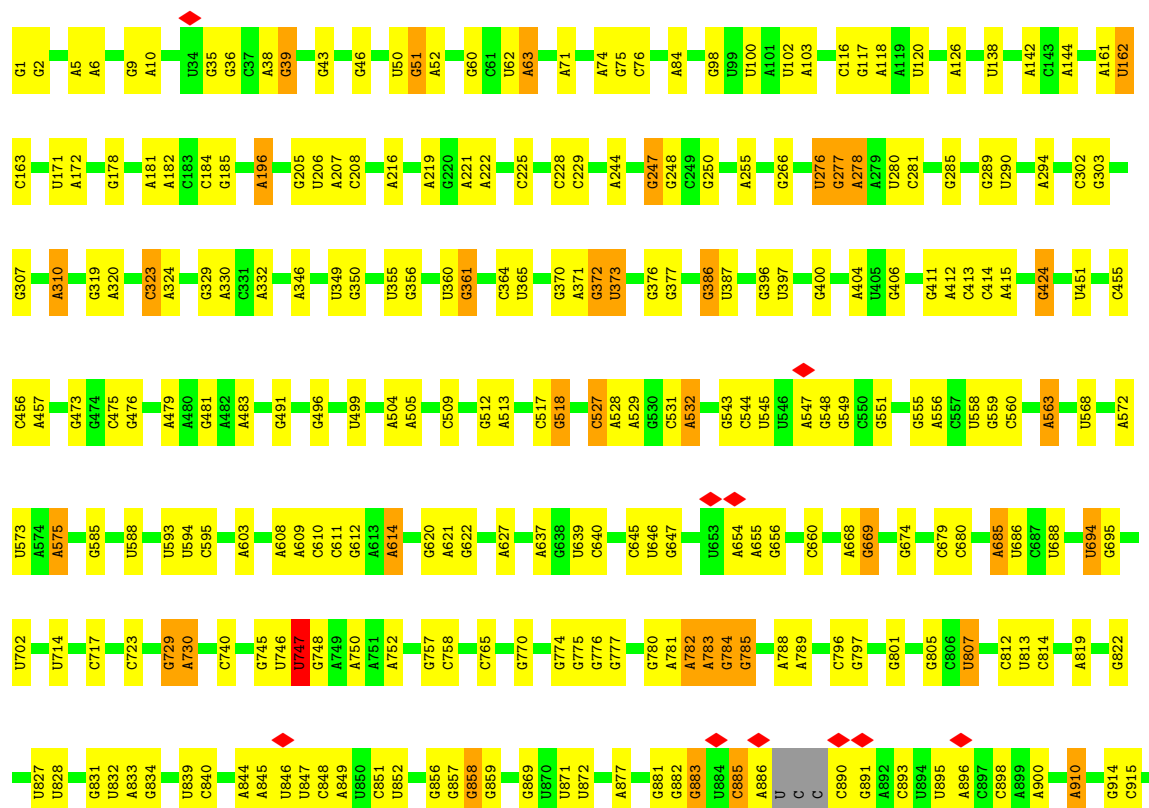
• Molecule 23: SECIS mRNA



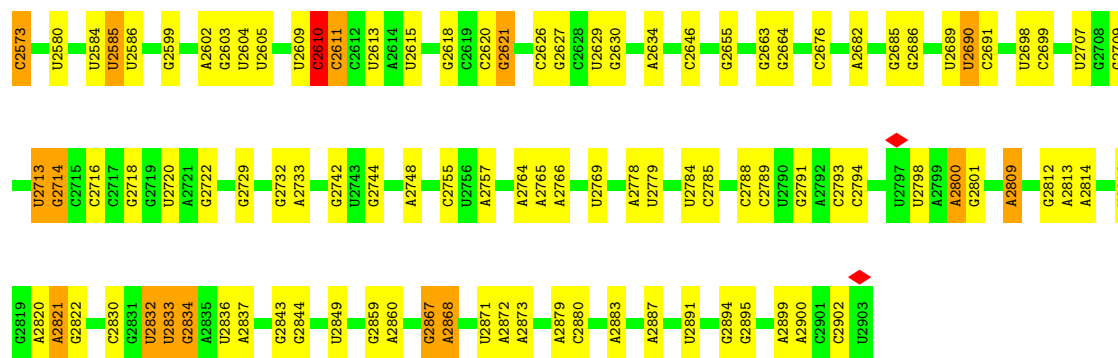
• Molecule 24: fMetSec-tRNA^{Sec}



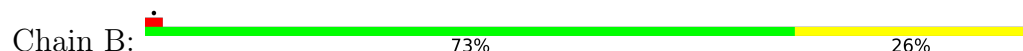
• Molecule 25: 23S ribosomal RNA



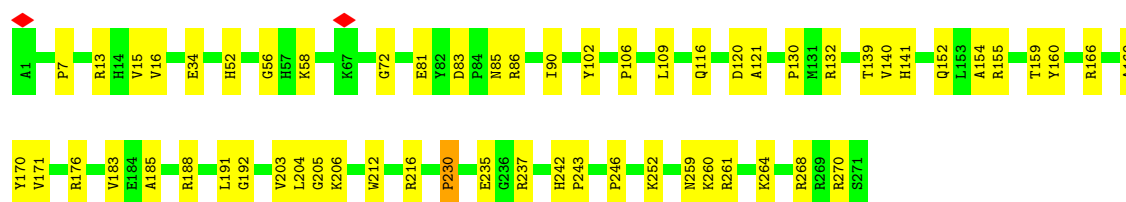
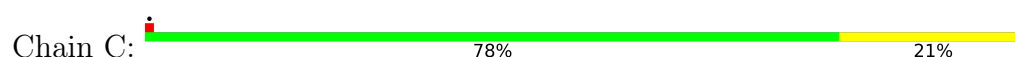
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G2445	A2184	A2185	U2034	C1764	A1583	U1438	G1271	A1165	C1064	A941
G2447	G2035	G2186	C2036	A1773	U1584	A1453	U1273	C1170	U1066	G942
U2449	G2040	U2126	G2040	U1779	A1597	C1454	C1278	C1171	U1067	A945
U2457	U2041	G2127	U2041	A1780	A1598	U1458	G1279	C1172	A968	C946
U2464	A2042	G2128	A2042	U1781	G1601	G1459	A1287	U1173	A1069	U955
C2467	C2129	U2130	C2044	U1782	C1607	A1469	G1300	U1174	A1070	U958
A2468	U2131	U2132	G2049	A1783	A1608	A1470	A1301	A1175	G1071	A959
A2469	U2133	U2134	C2050	A1784	A1614	G1475	C1306	U1176	G1072	A960
G2470	A1917	G2135	A1916	A1791	C1615	G1478	C1314	C1177	A1073	C961
A2476	A1918	A2136	A1918	A1794	A1616	U1487	U1325	C1178	G1074	A973
G2481	U2137	G2137	G1929	U1795	C1617	G1482	U1352	U1181	C1075	G974
A2482	A2138	U2138	U2060	G1796	A1618	U1488	U1354	U1182	C1076	A983
C2483	G2224	U2139	G2061	G1797	G1622	C1488	U1326	U1183	A1077	A984
G2484	A2062	U2140	A2062	U1798	G1627	C1498	G1332	G1186	U1078	C985
A2498	C2065	U2141	C2065	G1799	G1646	C1498	U1340	G1190	C1079	G989
G2502	G2069	G2142	A1936	U1800	U1647	A1504	C1345	A1194	A1084	A990
A2503	A2070	A2143	A1937	C1804	U1648	A1509	U1352	G1197	G1087	C985
U2504	A2071	G2144	A1938	A1805	G1649	U1510	A1353	U1198	A1088	A996
G2505	C2072	C2145	U1939	A1808	A1665	G1513	A1354	A1204	A1089	U1012
U2506	U2086	G2146	C1941	A1809	A1669	G1514	A1365	A1205	C1092	C1013
C2507	C2087	A2147	C1942	U1812	G1674	A1515	G1386	G1223	U1093	U1019
G2512	U2092	U2148	U1965	C1816	G1682	G1524	U1379	G1210	U1094	A1020
A2513	G2093	U2149	A1966	U1817	G1685	C1533	A1387	C1211	A1095	A1021
U2514	C2096	G2150	C1967	U1818	G1695	U1534	G1388	A1213	U1096	G1022
C2515	A2097	U2151	U1970	A1829	A1698	A1535	C1386	G1227	U1097	U1023
U2518	U2098	G2152	U1971	C1833	U1715	G1537	A1387	C1104	C1104	G1025
U2519	G2100	C2153	G1972	G1835	U1716	U1539	G1388	U1105	G1026	G1026
C2520	C2103	A2154	U1991	C1838	G1723	A1548	A1395	G1236	U1033	U1033
G2535	C2104	U2155	G1992	G1839	G1724	A1549	G1410	A1237	A1040	A1040
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U2547	G2107	A2158	C1997	C1857	G1730	G1557	G1416	G1239	C1044	C1044
U2552	A2108	U2160	U1997	A1858	G1731	C1558	C1417	A1247	C1045	C1045
G2553	G2110	G2161	G2012	C1868	U1732	U1559	G1421	G1248	A1046	A1046
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C2566	G2112	U2166	U2022	C1870	U1736	C1565	C1429	G1250	C1053	C1053
G2567	U2113	U2167	G2023	A1871	G1737	A1566	G1429	C1251	A1054	A1054
U2568	A2114	G2168	G2024	G1873	G1738	G1567	G1432	A1252	A1057	A1057
G2569	G2115	U2169	C2024	U1744	A1745	A1569	A1433	U1253	U1058	U1058
A2572	G2116	A2170	A2030	A1746	U1747	U1578	A1434	A1256	G1059	G1059
	A2117	A2171	G2032	U1880	U1747	G1581	G1435	A1266	U1060	U1060
	U2118	G2120		G1884			G1436	A1141	U1061	U1061
	A2119	G2121						A1142	G1062	G1062
	G2121							U1148		
								A1155		
								C1158		



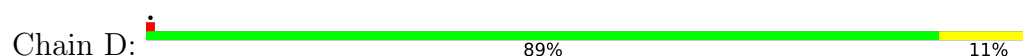
• Molecule 26: 5S ribosomal RNA



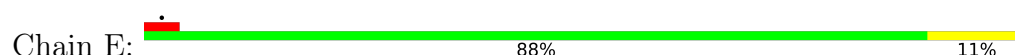
• Molecule 27: 50S ribosomal protein L2



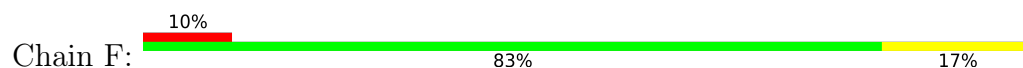
• Molecule 28: 50S ribosomal protein L3

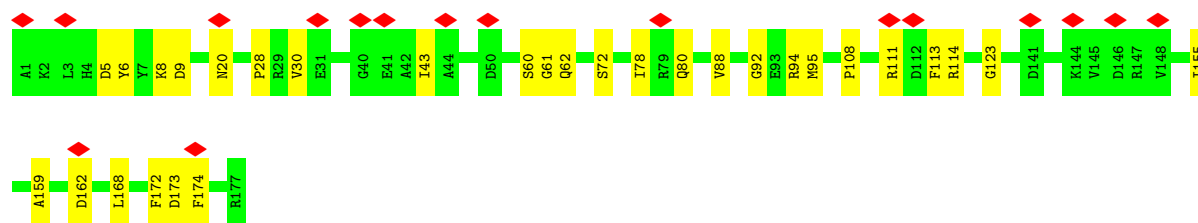


• Molecule 29: 50S ribosomal protein L4

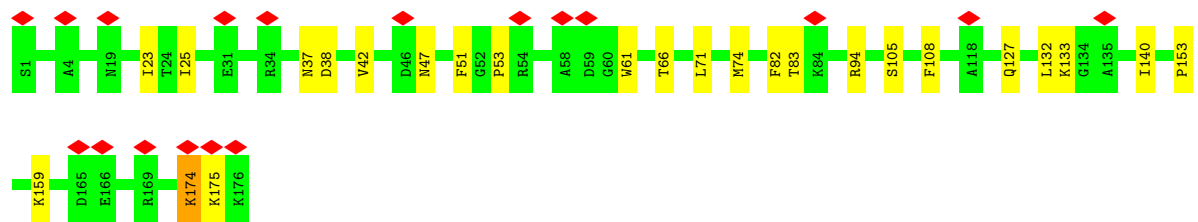
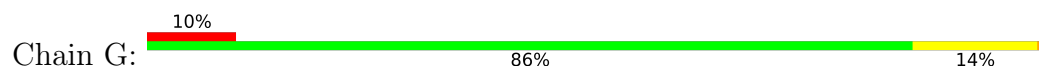


• Molecule 30: 50S ribosomal protein L5

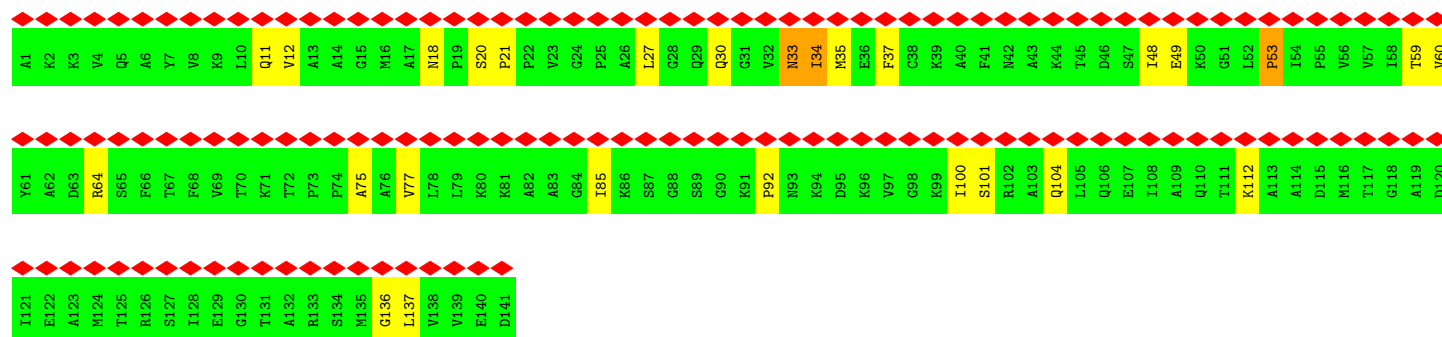
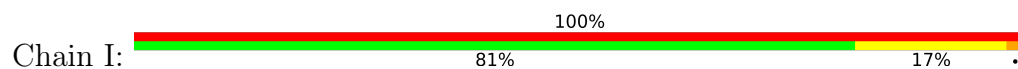




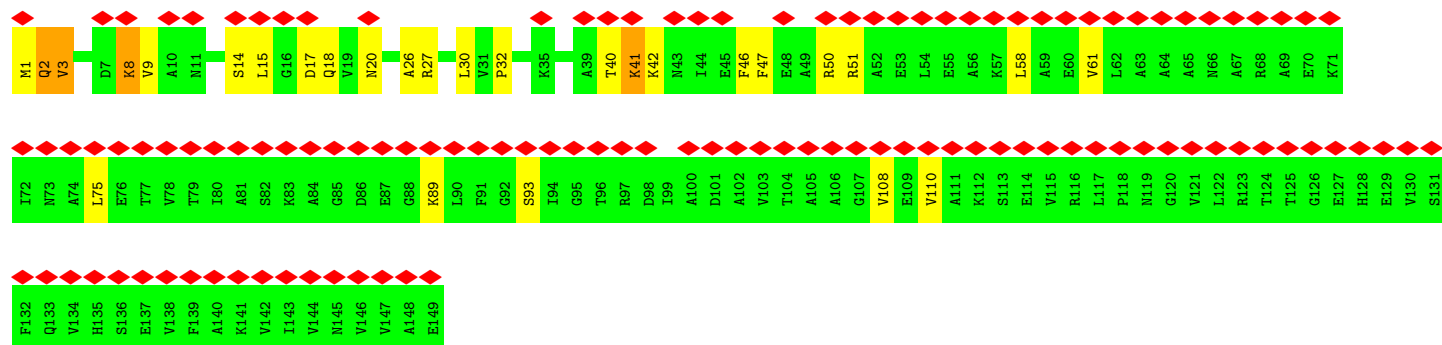
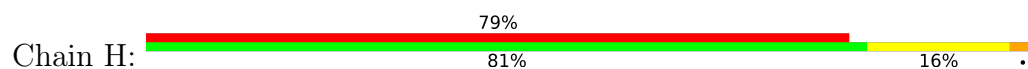
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L11

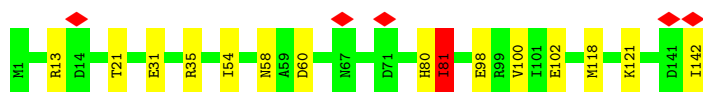


• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13

Chain J:  89% 10%



- Molecule 35: 50S ribosomal protein L14

Chain K:  82% 16%

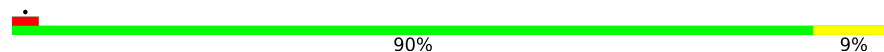


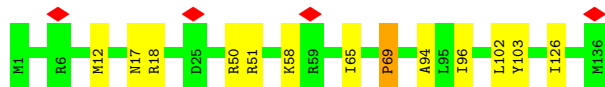
- Molecule 36: 50S ribosomal protein L15

Chain L:  83% 17%



- Molecule 37: 50S ribosomal protein L16

Chain M:  90% 9%

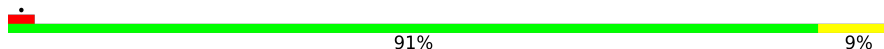


- Molecule 38: 50S ribosomal protein L17

Chain N:  87% 13%



- Molecule 39: 50S ribosomal protein L18

Chain O:  91% 9%



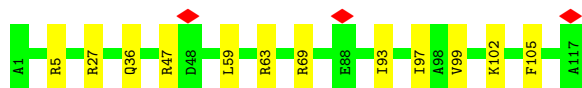
- Molecule 40: 50S ribosomal protein L19

Chain P:  7% 82% 18%



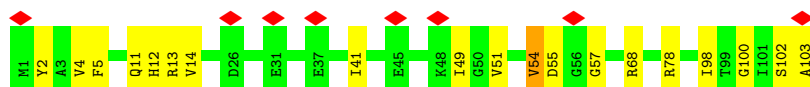
- Molecule 41: 50S ribosomal protein L20

Chain Q:  90% 10%



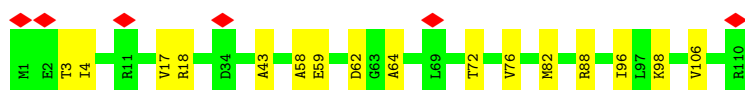
- Molecule 42: 50S ribosomal protein L21

Chain R:  8% 82% 17%



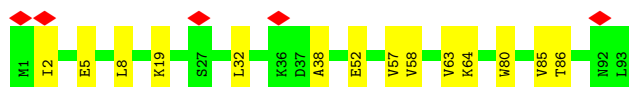
- Molecule 43: 50S ribosomal protein L22

Chain S:  5% 85% 15%



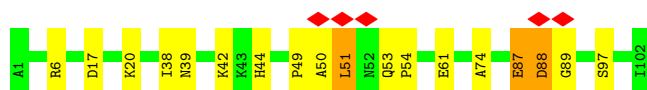
- Molecule 44: 50S ribosomal protein L23

Chain T:  5% 85% 15%



- Molecule 45: 50S ribosomal protein L24

Chain U:  5% 82% 15%



- Molecule 46: 50S ribosomal protein L25

Chain V:  5% 83% 17%

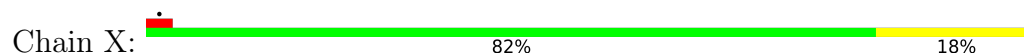


- Molecule 47: 50S ribosomal protein L27

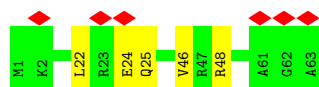
Chain W:  85% 13%



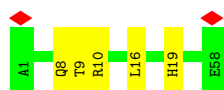
- Molecule 48: 50S ribosomal protein L28



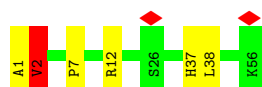
- Molecule 49: 50S ribosomal protein L29



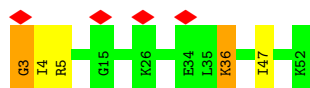
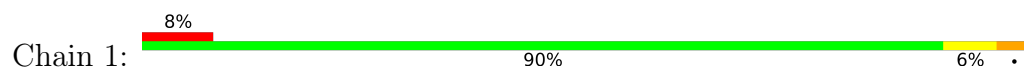
- Molecule 50: 50S ribosomal protein L30



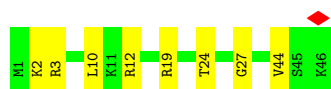
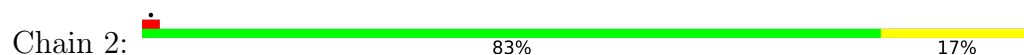
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

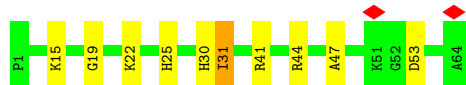


- Molecule 53: 50S ribosomal protein L34



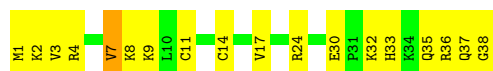
- Molecule 54: 50S ribosomal protein L35

Chain 3:  84% 14%



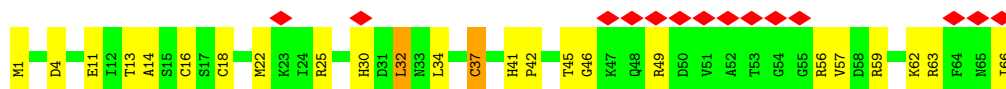
- Molecule 55: 50S ribosomal protein L36

Chain 4:  53% 45%



- Molecule 56: 50S ribosomal protein L31

Chain 6:  21% 64% 33%



- Molecule 57: CCA 3' end of E-site tRNA^{Sec} (low occupancy)

Chain w:  67% 67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	4.297	Depositor
Minimum map value	-2.327	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.273	Depositor
Recommended contour level	0.54	Depositor
Map size ($\text{\AA}$)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, OMC, H2U, 2MA, PSU, 5MU, 4SU, ZN, UR3, 2MG, 3TD, G7M, 4OC, OMG, 6IA, MA6, 1MG, 5MC, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.43	1/36701 (0.0%)	0.51	4/57246 (0.0%)
2	b	0.44	0/1736	0.91	1/2338 (0.0%)
3	c	0.43	0/1652	0.83	0/2225
4	d	0.40	0/1665	0.89	1/2227 (0.0%)
5	e	0.47	0/1170	0.98	2/1573 (0.1%)
6	f	0.51	0/836	1.05	5/1128 (0.4%)
7	g	0.39	0/1196	0.84	0/1602
8	h	0.42	0/989	0.86	0/1326
9	i	0.50	0/1034	0.97	2/1375 (0.1%)
10	j	0.46	0/797	0.91	1/1077 (0.1%)
11	k	0.45	0/886	0.93	3/1195 (0.3%)
12	l	0.43	0/969	1.00	4/1300 (0.3%)
13	m	0.47	0/893	1.00	1/1193 (0.1%)
14	n	0.54	0/806	0.98	0/1074
15	o	0.51	0/722	0.96	4/964 (0.4%)
16	p	0.52	0/659	1.01	3/884 (0.3%)
17	q	0.47	0/658	0.97	3/881 (0.3%)
18	r	0.47	0/512	1.00	0/689
19	s	0.48	0/653	1.03	5/877 (0.6%)
20	t	0.52	0/671	0.92	0/888
21	u	0.58	0/501	1.32	8/668 (1.2%)
22	v	0.40	0/1747	0.50	0/2721
23	x	0.55	0/1145	1.00	14/1781 (0.8%)
24	y	0.33	0/2162	0.49	0/3351
25	A	0.48	1/69171 (0.0%)	0.53	11/107904 (0.0%)
26	B	0.40	0/2873	0.52	0/4478
27	C	0.52	0/2122	0.88	0/2852
28	D	0.48	0/1586	0.86	0/2134
29	E	0.46	0/1571	0.82	2/2113 (0.1%)
30	F	0.48	0/1435	0.89	2/1926 (0.1%)
31	G	0.41	0/1343	0.78	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	I	0.46	0/1046	0.92	4/1410 (0.3%)
33	H	0.42	0/1122	0.90	1/1515 (0.1%)
34	J	0.47	0/1152	0.85	1/1551 (0.1%)
35	K	0.52	0/948	0.92	0/1268
36	L	0.49	0/1054	1.00	0/1403
37	M	0.46	0/1093	0.83	0/1460
38	N	0.52	0/974	0.87	0/1301
39	O	0.45	0/902	0.81	0/1209
40	P	0.47	0/929	0.84	0/1242
41	Q	0.57	0/960	0.89	0/1278
42	R	0.44	0/829	0.88	0/1107
43	S	0.46	0/864	0.90	2/1156 (0.2%)
44	T	0.43	0/745	0.79	0/994
45	U	0.47	0/788	1.08	6/1051 (0.6%)
46	V	0.40	0/766	0.76	0/1025
47	W	0.44	0/582	0.79	0/769
48	X	0.46	0/635	0.76	0/848
49	Y	0.47	0/510	0.84	1/677 (0.1%)
50	Z	0.42	0/453	0.80	0/605
51	0	0.48	0/450	0.93	1/599 (0.2%)
52	1	0.42	0/417	0.96	0/554
53	2	0.51	0/380	0.85	0/498
54	3	0.51	0/513	0.89	1/676 (0.1%)
55	4	0.68	0/303	1.22	1/397 (0.3%)
56	6	0.61	0/532	1.23	3/709 (0.4%)
57	w	0.16	0/68	0.33	0/103
All	All	0.46	2/159876 (0.0%)	0.65	97/239211 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
2	b	0	1
5	e	0	3
6	f	0	2
9	i	0	2
10	j	0	3
12	l	0	2
13	m	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	o	0	1
16	p	0	1
17	q	0	1
19	s	0	1
21	u	0	2
25	A	2	0
27	C	0	1
28	D	0	1
29	E	0	1
30	F	0	1
33	H	0	3
35	K	0	1
36	L	0	1
45	U	0	2
51	0	0	1
52	1	0	1
54	3	0	1
All	All	4	35

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	G7M	O3'-P	6.79	1.63	1.56
25	A	2069	G7M	O3'-P	6.69	1.62	1.56

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	65	GLU	N-CA-CB	-8.82	95.58	110.49
23	x	125	G	C4'-C3'-O3'	8.58	125.87	113.00
2	b	73	ARG	N-CA-CB	-8.54	96.07	110.49
16	p	44	SER	N-CA-CB	-8.36	96.37	110.49
9	i	90	ASP	N-CA-CB	-8.26	96.53	110.49
19	s	5	LYS	CB-CA-C	-8.01	94.48	110.42
45	U	88	ASP	N-CA-C	-7.77	94.24	110.80
43	S	62	ASP	CA-C-N	7.65	138.25	121.19
43	S	62	ASP	C-N-CA	7.65	138.25	121.19
6	f	53	LYS	N-CA-CB	7.65	123.42	110.49
29	E	82	GLY	CA-C-O	-7.55	107.43	120.57
45	U	89	GLY	N-CA-C	-7.48	103.99	115.66
25	A	2069	G7M	P-O3'-C3'	7.46	128.65	119.70
30	F	172	PHE	CA-C-N	7.45	135.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	172	PHE	C-N-CA	7.45	135.76	121.54
19	s	5	LYS	CB-CG-CD	7.44	128.42	111.30
23	x	125	G	N9-C1'-C2'	-7.42	100.87	112.00
21	u	24	LYS	N-CA-CB	-7.42	97.96	110.49
17	q	69	THR	N-CA-CB	7.40	122.99	110.49
45	U	88	ASP	N-CA-CB	7.39	122.97	110.49
1	a	527	G7M	P-O3'-C3'	7.18	128.32	119.70
15	o	87	ARG	CA-C-O	-7.09	110.38	120.51
56	6	32	LEU	CA-CB-CG	6.99	140.78	116.30
5	e	89	THR	N-CA-CB	-6.86	98.90	110.49
6	f	98	GLU	N-CA-CB	6.86	122.08	110.49
6	f	53	LYS	N-CA-C	-6.83	96.25	110.80
56	6	18	CYS	CA-CB-SG	-6.68	99.04	114.40
21	u	26	GLY	N-CA-C	6.54	120.58	112.73
5	e	77	ASN	N-CA-CB	-6.52	99.47	110.49
21	u	35	GLU	CA-C-N	6.44	133.84	121.54
21	u	35	GLU	C-N-CA	6.44	133.84	121.54
54	3	31	ILE	N-CA-CB	-6.43	100.62	111.23
19	s	4	LEU	CA-C-N	6.33	133.63	121.54
19	s	4	LEU	C-N-CA	6.33	133.63	121.54
11	k	90	PRO	CA-C-N	6.28	127.99	120.14
11	k	90	PRO	C-N-CA	6.28	127.99	120.14
23	x	129	U	C5'-C4'-C3'	6.24	125.35	116.00
17	q	68	LYS	CA-C-O	-6.17	114.89	122.36
45	U	51	LEU	N-CA-CB	-6.17	100.07	110.49
23	x	133	C	N1-C1'-C2'	-6.08	102.88	112.00
17	q	69	THR	N-CA-C	-6.07	97.87	110.80
15	o	86	LEU	CA-C-N	6.02	133.04	121.54
15	o	86	LEU	C-N-CA	6.02	133.04	121.54
25	A	2610	C	C4'-C3'-O3'	5.97	118.36	109.40
10	j	42	LEU	N-CA-C	5.96	122.99	109.81
11	k	91	GLY	N-CA-C	5.94	121.02	113.24
9	i	90	ASP	N-CA-C	5.94	123.45	110.80
21	u	61	ARG	CA-C-N	5.93	132.86	121.54
21	u	61	ARG	C-N-CA	5.93	132.86	121.54
33	H	3	VAL	N-CA-CB	-5.85	101.58	111.23
21	u	24	LYS	N-CA-C	5.82	123.19	110.80
23	x	126	G	P-O3'-C3'	5.81	128.91	120.20
12	l	21	PRO	CA-C-N	5.77	132.60	121.18
12	l	21	PRO	C-N-CA	5.77	132.60	121.18
16	p	80	LYS	CA-C-N	5.76	130.48	120.68
16	p	80	LYS	C-N-CA	5.76	130.48	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y	25	GLN	N-CA-C	-5.76	106.29	113.55
23	x	126	G	C2'-C3'-O3'	-5.75	100.88	109.50
23	x	132	A	P-O5'-C5'	5.74	129.50	120.90
15	o	88	ARG	N-CA-CB	5.72	120.22	110.50
29	E	82	GLY	N-CA-C	5.63	126.52	113.18
21	u	24	LYS	CA-CB-CG	5.58	125.27	114.10
23	x	125	G	O3'-P-O5'	5.54	112.31	104.00
55	4	7	VAL	N-CA-C	5.54	117.53	111.77
12	l	100	ALA	CA-C-N	5.53	132.11	121.54
12	l	100	ALA	C-N-CA	5.53	132.11	121.54
4	d	34	GLU	N-CA-C	5.52	122.55	110.80
23	x	126	G	O5'-C5'-C4'	5.51	119.96	111.70
23	x	127	U	P-O3'-C3'	5.46	128.39	120.20
19	s	4	LEU	CA-C-O	-5.41	112.77	120.51
1	a	1301	U	C2'-C3'-O3'	5.39	117.59	109.50
1	a	1498	UR3	OP1-P-O3'	5.39	117.06	105.20
56	6	37	CYS	CA-CB-SG	5.37	126.75	114.40
25	A	1900	A	C4'-C3'-O3'	5.37	117.45	109.40
25	A	51	G	C4'-C3'-O3'	5.34	117.42	109.40
34	J	81	ILE	N-CA-C	5.34	120.45	109.34
45	U	74	ALA	N-CA-C	-5.34	106.77	113.28
25	A	2069	G7M	OP2-P-O3'	5.32	116.90	105.20
25	A	1567	G	P-O3'-C3'	5.25	128.07	120.20
25	A	2610	C	P-O3'-C3'	5.25	128.07	120.20
32	I	33	ASN	CA-C-N	5.20	127.86	120.53
32	I	33	ASN	C-N-CA	5.20	127.86	120.53
23	x	128	C	C3'-C2'-C1'	5.19	106.49	101.30
1	a	960	U	P-O3'-C3'	5.18	127.97	120.20
25	A	2061	G	P-O3'-C3'	5.17	127.95	120.20
25	A	1111	A	P-O3'-C3'	5.16	127.93	120.20
32	I	20	SER	N-CA-C	5.13	121.15	109.81
6	f	54	LEU	N-CA-C	5.12	121.72	110.80
25	A	1070	A	P-O3'-C3'	5.12	127.87	120.20
45	U	87	GLU	CA-C-O	-5.11	115.59	122.44
32	I	21	PRO	N-CA-C	5.10	116.92	110.70
25	A	1900	A	P-O3'-C3'	5.09	127.83	120.20
23	x	125	G	C3'-C2'-C1'	5.08	106.38	101.30
51	0	2	VAL	N-CA-CB	-5.06	102.88	111.23
23	x	129	U	P-O5'-C5'	5.03	128.45	120.90
6	f	98	GLU	N-CA-C	-5.03	100.09	110.80
23	x	127	U	C3'-C2'-O2'	5.02	122.13	114.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
25	A	2069	G7M	C4',C3'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	0	1	ALA	Mainchain
52	1	3	GLY	Mainchain
54	3	30	HIS	Peptide
27	C	120	ASP	Peptide
28	D	166	GLY	Peptide
29	E	82	GLY	Mainchain
30	F	173	ASP	Mainchain
33	H	2	GLN	Peptide
33	H	41	LYS	Mainchain
33	H	8	LYS	Peptide
35	K	89	ASN	Mainchain
36	L	29	LYS	Mainchain
45	U	50	ALA	Peptide
45	U	87	GLU	Mainchain
2	b	72	LYS	Peptide
5	e	76	ASN	Peptide,Mainchain
5	e	88	HIS	Peptide
6	f	52	ASN	Mainchain
6	f	97	THR	Mainchain
9	i	56	MET	Peptide,Mainchain
10	j	33	GLY	Peptide,Mainchain
10	j	34	ALA	Mainchain
12	l	101	LEU	Mainchain
12	l	23	LEU	Mainchain
13	m	3	ILE	Peptide
13	m	64	VAL	Peptide
15	o	87	ARG	Mainchain
16	p	43	ALA	Peptide
17	q	68	LYS	Mainchain
19	s	4	LEU	Mainchain
21	u	23	GLU	Mainchain
21	u	24	LYS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16644	192	0
2	b	1705	0	1732	23	0
3	c	1625	0	1699	19	0
4	d	1643	0	1710	24	0
5	e	1157	0	1199	13	0
6	f	818	0	808	19	0
7	g	1182	0	1240	11	0
8	h	979	0	1034	12	0
9	i	1022	0	1070	13	0
10	j	787	0	828	19	0
11	k	870	0	878	23	0
12	l	955	0	1019	6	0
13	m	884	0	944	14	0
14	n	794	0	836	15	0
15	o	714	0	737	8	0
16	p	649	0	666	12	0
17	q	649	0	691	10	0
18	r	505	0	502	11	0
19	s	638	0	665	10	0
20	t	665	0	714	13	0
21	u	496	0	486	7	0
22	v	1644	0	840	5	0
23	x	1025	0	518	2	0
24	y	2031	0	1046	8	0
25	A	62274	0	31342	275	0
26	B	2570	0	1301	7	0
27	C	2083	0	2157	35	0
28	D	1565	0	1616	14	0
29	E	1552	0	1619	17	0
30	F	1411	0	1447	18	0
31	G	1323	0	1374	14	0
32	I	1032	0	1088	11	0
33	H	1111	0	1148	14	0
34	J	1129	0	1162	10	0
35	K	939	0	1012	11	0
36	L	1045	0	1117	18	0
37	M	1074	0	1157	10	0
38	N	961	0	1000	9	0
39	O	892	0	923	6	0
40	P	917	0	965	13	0
41	Q	947	0	1022	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	R	816	0	839	11	0
43	S	857	0	922	9	0
44	T	739	0	807	7	0
45	U	780	0	834	5	0
46	V	753	0	780	8	0
47	W	575	0	592	8	0
48	X	625	0	655	10	0
49	Y	509	0	543	2	0
50	Z	449	0	491	3	0
51	0	444	0	461	3	0
52	1	410	0	440	3	0
53	2	377	0	418	6	0
54	3	504	0	574	6	0
55	4	302	0	340	12	0
56	6	523	0	521	12	0
57	w	62	0	34	1	0
58	4	1	0	0	0	0
58	6	1	0	0	0	0
All	All	148018	0	99207	936	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 4.

All (936) 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)
25:A:2164:C:H41	25:A:2171:A:H61	1.23	0.85
25:A:1171:G:H1	25:A:1177:G:H1	1.26	0.82
1:a:664:G:H22	1:a:741:G:H1	1.30	0.78
25:A:1171:G:N2	25:A:1178:C:O2	2.18	0.77
55:4:2:LYS:HD2	55:4:4:ARG:HH12	1.50	0.76
25:A:585:G:N7	41:Q:5:ARG:NH1	2.32	0.76
13:m:9:PRO:HG2	13:m:44:ILE:HG21	1.68	0.76
4:d:105:GLY:HA3	4:d:161:ALA:HB2	1.69	0.74
25:A:1270:C:H5''	25:A:1271:G:H5'	1.68	0.74
53:2:24:THR:HG23	53:2:27:GLY:H	1.53	0.73
25:A:1053:C:H42	25:A:1106:G:H1	1.37	0.73
25:A:1798:U:OP2	27:C:270:ARG:NH2	2.23	0.72
30:F:62:GLN:OE1	30:F:94:ARG:NH2	2.23	0.71
25:A:2691:C:HO2'	25:A:2871:U:HO2'	1.38	0.70
1:a:1081:A:OP2	5:e:51:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:621:A:OP2	36:L:99:ASN:ND2	2.25	0.69
43:S:4:ILE:HG22	43:S:106:VAL:HG22	1.74	0.69
11:k:19:VAL:HG13	11:k:82:GLU:HB2	1.75	0.68
25:A:910:A:H62	37:M:12:MET:HA	1.57	0.68
25:A:1601:G:OP1	44:T:64:LYS:NZ	2.27	0.67
34:J:21:THR:OG1	34:J:58:ASN:ND2	2.27	0.67
1:a:1106:G:O2'	3:c:168:ARG:NH1	2.28	0.67
27:C:141:HIS:ND1	27:C:192:GLY:O	2.26	0.67
47:W:33:ILE:HG22	47:W:34:VAL:HG23	1.77	0.67
5:e:156:ARG:NH2	8:h:98:LEU:O	2.28	0.66
31:G:83:THR:HA	31:G:132:LEU:O	1.95	0.66
6:f:90:MET:SD	18:r:60:ARG:NH2	2.63	0.66
5:e:35:LEU:HD11	5:e:133:ILE:HG12	1.77	0.66
25:A:2483:C:O2'	37:M:51:ARG:NH2	2.29	0.66
36:L:100:ILE:HG13	36:L:101:ILE:HG23	1.77	0.66
40:P:88:ARG:HE	40:P:112:ARG:HH21	1.44	0.66
56:6:14:ALA:HB3	56:6:22:MET:HB2	1.78	0.66
1:a:375:U:OP1	16:p:70:ARG:NH1	2.28	0.65
25:A:881:G:H21	25:A:896:A:H62	1.42	0.65
21:u:33:ARG:HG3	21:u:34:ARG:HG2	1.77	0.65
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.79	0.65
21:u:22:CYS:SG	21:u:23:GLU:N	2.69	0.65
1:a:677:U:H3	1:a:713:G:H22	1.45	0.65
1:a:212:G:H2'	1:a:213:G:H8	1.61	0.65
1:a:1151:A:H1'	10:j:41:PRO:HB2	1.78	0.65
7:g:26:VAL:HG22	7:g:42:VAL:HG21	1.77	0.65
1:a:1223:C:H5''	1:a:1224:U:H5''	1.78	0.64
30:F:94:ARG:HH22	56:6:1:MET:HE1	1.62	0.64
19:s:5:LYS:HG3	19:s:6:LYS:HG2	1.78	0.64
55:4:2:LYS:NZ	55:4:32:LYS:O	2.31	0.64
5:e:152:VAL:HG21	8:h:98:LEU:HD13	1.78	0.64
25:A:307:G:N2	25:A:310:A:OP2	2.29	0.64
1:a:1077:G:N2	1:a:1080:A:OP2	2.28	0.64
17:q:29:LYS:HA	17:q:36:PHE:HA	1.80	0.64
40:P:59:THR:HG22	40:P:72:VAL:HG12	1.80	0.64
1:a:407:U:O2'	4:d:112:GLU:OE1	2.16	0.63
42:R:14:VAL:HG21	42:R:98:ILE:HG13	1.80	0.63
46:V:45:ASP:O	46:V:49:ASN:ND2	2.32	0.63
1:a:405:U:O4	4:d:1:ALA:N	2.29	0.63
6:f:7:VAL:HG22	6:f:61:LEU:HG	1.79	0.63
8:h:24:VAL:O	8:h:59:GLU:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:132:LEU:HB3	31:G:140:ILE:HD11	1.81	0.63
25:A:885:C:O2'	25:A:891:G:N2	2.28	0.63
29:E:146:VAL:HG12	29:E:185:LYS:HB2	1.80	0.63
15:o:34:GLN:HB3	15:o:58:MET:HE1	1.81	0.63
25:A:1019:U:H3	25:A:1142:A:H62	1.47	0.62
15:o:25:GLU:OE2	15:o:76:ARG:NH1	2.31	0.62
27:C:169:ALA:O	27:C:185:ALA:N	2.29	0.62
1:a:210:C:O2'	1:a:211:G:N2	2.33	0.62
25:A:2514:U:H4'	34:J:81:ILE:HD11	1.81	0.62
35:K:121:GLU:HG2	35:K:122:VAL:HG23	1.82	0.61
52:1:36:LYS:HD2	52:1:47:ILE:HG13	1.82	0.61
1:a:951:G:OP2	13:m:100:ARG:NH2	2.33	0.61
5:e:92:ARG:HB2	5:e:127:TYR:HB2	1.82	0.61
53:2:12:ARG:HE	53:2:44:VAL:HG21	1.65	0.61
25:A:1040:A:H61	25:A:1115:G:H1	1.46	0.61
3:c:13:ILE:HG22	3:c:14:VAL:HG13	1.81	0.61
1:a:718:A:OP1	1:a:720:C:N4	2.34	0.61
48:X:5:GLN:O	48:X:73:ARG:NH2	2.33	0.61
1:a:61:G:OP2	20:t:4:LYS:NZ	2.34	0.60
20:t:65:LEU:HG	20:t:66:ILE:HG12	1.81	0.60
1:a:875:U:O2'	8:h:14:ARG:NH1	2.33	0.60
17:q:19:SER:OG	17:q:20:ILE:N	2.34	0.60
34:J:98:GLU:O	34:J:102:GLU:HB2	2.01	0.60
1:a:311:C:OP1	16:p:31:ARG:NH1	2.35	0.60
1:a:143:A:H5''	1:a:144:G:H5'	1.83	0.59
21:u:12:ASP:OD1	21:u:12:ASP:N	2.35	0.59
30:F:43:ILE:HG21	30:F:78:ILE:HG22	1.84	0.59
25:A:196:A:OP2	36:L:47:ARG:NH1	2.36	0.59
25:A:1386:C:H2'	25:A:1387:A:C8	2.37	0.59
25:A:2199:A:OP1	48:X:36:ARG:NH2	2.35	0.59
25:A:1478:G:H1	25:A:1513:U:H3	1.50	0.59
43:S:3:THR:HG21	43:S:58:ALA:HB2	1.83	0.59
1:a:261:U:OP2	20:t:73:ARG:NH2	2.36	0.59
2:b:23:ASN:ND2	2:b:191:ASP:OD1	2.36	0.59
25:A:320:A:N3	29:E:163:ASN:ND2	2.51	0.59
27:C:106:PRO:HD2	27:C:109:LEU:HD22	1.84	0.59
29:E:119:ILE:O	29:E:187:VAL:HA	2.03	0.59
35:K:24:VAL:HG13	35:K:33:ALA:HB2	1.84	0.59
25:A:750:A:OP1	25:A:1615:C:N4	2.36	0.59
25:A:1264:A:H5'	51:0:7:PRO:HG2	1.85	0.59
1:a:414:A:OP2	1:a:428:G:N2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:680:C:O2'	27:C:268:ARG:NH2	2.34	0.59
10:j:40:ILE:HB	10:j:73:LEU:HB2	1.85	0.59
7:g:144:ALA:O	7:g:146:ALA:N	2.35	0.58
13:m:91:ARG:NH1	25:A:890:C:O2'	2.36	0.58
27:C:7:PRO:HB3	27:C:13:ARG:HG3	1.85	0.58
28:D:123:LYS:HG2	28:D:165:MET:HE1	1.85	0.58
42:R:4:VAL:HA	42:R:12:HIS:O	2.03	0.58
1:a:412:A:H62	1:a:431:A:H61	1.51	0.58
10:j:42:LEU:HD11	10:j:73:LEU:HG	1.85	0.58
21:u:36:PHE:HB3	21:u:40:PRO:HD3	1.85	0.58
25:A:2394:C:H5''	36:L:63:LYS:HE3	1.85	0.58
41:Q:99:VAL:O	41:Q:102:LYS:NZ	2.36	0.58
1:a:749:A:O2'	15:o:19:ASN:OD1	2.20	0.58
1:a:1391:U:H2'	1:a:1392:G:C8	2.39	0.58
25:A:848:C:H2'	25:A:849:A:C8	2.38	0.58
34:J:21:THR:HG1	34:J:58:ASN:ND2	2.00	0.58
54:3:41:ARG:HG2	54:3:44:ARG:HH21	1.67	0.58
1:a:345:C:OP1	40:P:38:ARG:NH2	2.37	0.58
20:t:66:ILE:HG23	20:t:70:LYS:HD3	1.85	0.58
46:V:64:VAL:HA	46:V:68:LYS:O	2.03	0.58
1:a:1363:A:O2'	1:a:1365:G:N7	2.35	0.58
44:T:5:GLU:HA	44:T:8:LEU:HD12	1.86	0.58
25:A:1515:A:HO2'	25:A:1556:C:HO2'	1.52	0.58
14:n:12:ARG:O	14:n:16:ALA:HB2	2.04	0.57
25:A:2676:C:OP1	35:K:31:ARG:NH2	2.37	0.57
11:k:87:GLY:H	11:k:113:THR:HG22	1.68	0.57
18:r:25:ILE:HA	18:r:28:LEU:HB3	1.86	0.57
47:W:17:LEU:O	47:W:20:LYS:NZ	2.36	0.57
1:a:422:C:O2'	1:a:423:G:N2	2.37	0.57
1:a:1097:C:O2'	1:a:1169:A:O2'	2.17	0.57
16:p:2:VAL:HG23	16:p:65:ALA:HA	1.86	0.57
25:A:1173:U:O2'	25:A:1177:G:N2	2.36	0.57
27:C:16:VAL:HB	27:C:203:VAL:HG22	1.87	0.57
33:H:14:SER:OG	33:H:17:ASP:OD2	2.22	0.57
2:b:18:GLN:NE2	2:b:187:ASP:OD2	2.37	0.57
30:F:28:PRO:HB3	30:F:159:ALA:HB2	1.86	0.57
35:K:109:SER:O	35:K:111:LYS:N	2.38	0.57
52:1:3:GLY:O	52:1:5:ARG:N	2.38	0.57
25:A:126:A:H5'	53:2:19:ARG:HG3	1.86	0.57
24:y:76:A:OP1	25:A:2573:C:N4	2.37	0.57
17:q:59:GLU:HB2	17:q:76:ARG:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:172:VAL:HG12	4:d:174:ALA:H	1.70	0.56
9:i:35:GLU:HA	9:i:39:GLY:HA3	1.86	0.56
34:J:60:ASP:OD1	34:J:60:ASP:N	2.39	0.56
27:C:170:TYR:HA	27:C:183:VAL:O	2.06	0.56
55:4:3:VAL:HG12	55:4:36:ARG:HD3	1.87	0.56
2:b:86:CYS:SG	2:b:87:ASP:N	2.79	0.56
3:c:110:LEU:HD22	3:c:145:ALA:HB2	1.88	0.56
56:6:11:GLU:OE1	56:6:25:ARG:NH1	2.36	0.56
1:a:946:A:H2'	1:a:947:G:C8	2.41	0.56
1:a:1218:C:H2'	1:a:1219:A:C8	2.41	0.56
1:a:1405:G:H21	1:a:1518:MA6:H8	1.71	0.56
10:j:65:TYR:HB3	14:n:95:LEU:HD11	1.87	0.56
25:A:2377:A:O2'	39:O:117:PHE:O	2.23	0.56
1:a:958:A:OP1	19:s:54:ARG:NH2	2.39	0.56
36:L:95:LEU:HD22	36:L:100:ILE:HD11	1.88	0.56
49:Y:24:GLU:HB3	49:Y:46:VAL:HG21	1.86	0.56
1:a:331:G:O2'	20:t:2:ASN:ND2	2.40	0.55
2:b:53:LEU:HB3	2:b:219:THR:HG21	1.87	0.55
10:j:59:LYS:HE2	10:j:62:ARG:HH21	1.71	0.55
32:I:75:ALA:HB2	32:I:112:LYS:HE3	1.87	0.55
1:a:1148:U:O2'	9:i:67:LYS:NZ	2.39	0.55
6:f:3:HIS:HB2	6:f:92:THR:HA	1.89	0.55
11:k:35:ASP:OD1	11:k:39:ASN:N	2.39	0.55
25:A:2375:G:N2	25:A:2378:A:OP2	2.37	0.55
1:a:944:G:N1	1:a:1338:G:OP2	2.37	0.55
6:f:74:LEU:O	6:f:77:THR:OG1	2.20	0.55
25:A:1326:U:O2'	25:A:2010:G:O2'	2.23	0.55
27:C:72:GLY:HA2	27:C:116:GLN:HE21	1.70	0.55
30:F:28:PRO:HB2	30:F:168:LEU:HD22	1.88	0.55
39:O:66:GLY:O	39:O:102:ARG:NH2	2.38	0.55
42:R:57:GLY:HA2	42:R:102:SER:O	2.06	0.55
1:a:1191:A:OP1	3:c:2:GLN:NE2	2.40	0.55
14:n:12:ARG:O	14:n:16:ALA:CB	2.55	0.55
39:O:30:ARG:HA	39:O:35:ILE:HD12	1.89	0.55
4:d:172:VAL:HA	4:d:179:GLY:HA2	1.88	0.55
18:r:35:SER:OG	21:u:23:GLU:OE2	2.20	0.55
1:a:1279:G:OP1	10:j:9:ARG:NH2	2.39	0.55
25:A:2271:G:H5'	47:W:16:ARG:HG2	1.89	0.55
1:a:202:G:H21	1:a:466:A:H61	1.54	0.55
13:m:15:VAL:HG23	13:m:16:ILE:HD12	1.89	0.55
25:A:1094:U:N3	25:A:1097:U:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:15:VAL:HG22	27:C:205:GLY:HA3	1.89	0.55
45:U:49:PRO:O	45:U:53:GLN:NE2	2.40	0.55
25:A:413:C:HO2'	25:A:1880:U:HO2'	1.54	0.54
25:A:2133:G:H21	25:A:2158:A:H61	1.55	0.54
31:G:51:PHE:HZ	31:G:71:LEU:HD22	1.71	0.54
4:d:100:VAL:HG12	4:d:104:MET:HE2	1.90	0.54
1:a:447:G:H1	1:a:486:U:P	2.30	0.54
4:d:117:VAL:HG22	4:d:122:ILE:HG13	1.89	0.54
32:I:53:PRO:HD2	32:I:77:VAL:HG21	1.88	0.54
1:a:235:C:H2'	1:a:236:A:C8	2.42	0.54
25:A:1012:U:OP2	41:Q:69:ARG:NH1	2.39	0.54
47:W:61:GLY:HA3	47:W:79:GLU:O	2.07	0.54
16:p:61:VAL:HG22	16:p:67:ILE:HD11	1.89	0.54
25:A:376:G:H2'	25:A:377:G:H8	1.73	0.54
27:C:86:ARG:HH12	27:C:155:ARG:HH21	1.54	0.54
35:K:35:VAL:HG22	35:K:69:VAL:HG12	1.90	0.54
16:p:79:ASN:C	16:p:81:ALA:H	2.16	0.54
24:y:74:C:N4	25:A:2507:C:O2'	2.40	0.54
25:A:747:5MU:H5''	25:A:748:G:H5''	1.90	0.54
25:A:2127:G:N2	25:A:2161:C:O2'	2.40	0.54
25:A:2506:U:H3	25:A:2585:U:H3	1.54	0.54
25:A:563:A:N3	41:Q:36:GLN:NE2	2.56	0.53
25:A:1223:G:OP1	42:R:68:ARG:NH2	2.42	0.53
25:A:290:U:O2	25:A:350:G:O6	2.27	0.53
31:G:82:PHE:O	31:G:133:LYS:HA	2.08	0.53
33:H:40:THR:O	33:H:42:LYS:N	2.42	0.53
12:l:65:TYR:HB2	12:l:92:VAL:HG11	1.89	0.53
25:A:848:C:H2'	25:A:849:A:H8	1.74	0.53
46:V:58:SER:OG	46:V:59:GLU:OE1	2.25	0.53
25:A:610:C:H2'	25:A:611:C:H6	1.74	0.53
25:A:2327:A:H2'	25:A:2328:A:C8	2.44	0.53
25:A:2690:U:OP1	38:N:14:SER:OG	2.26	0.53
25:A:2469:A:N6	25:A:2481:G:O2'	2.42	0.53
29:E:49:ARG:HE	29:E:75:SER:HA	1.74	0.53
33:H:26:ALA:HA	33:H:30:LEU:HB2	1.91	0.53
1:a:160:A:H2'	1:a:161:A:O4'	2.09	0.53
25:A:414:C:H2'	25:A:415:A:C8	2.43	0.53
1:a:269:C:H2'	1:a:270:A:C8	2.44	0.53
13:m:28:ARG:HH21	13:m:62:PHE:HB2	1.73	0.53
25:A:518:G:OP1	43:S:18:ARG:NH1	2.42	0.53
30:F:9:ASP:OD1	30:F:9:ASP:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:276:U:O2'	25:A:278:A:N6	2.42	0.52
25:A:2130:U:H4'	25:A:2159:G:H22	1.73	0.52
26:B:90:C:OP2	37:M:18:ARG:NH2	2.42	0.52
31:G:23:ILE:HD11	31:G:42:VAL:HG11	1.91	0.52
37:M:50:ARG:HD3	37:M:65:ILE:HD11	1.92	0.52
42:R:49:ILE:HG22	42:R:54:VAL:HA	1.90	0.52
17:q:22:VAL:HG11	17:q:60:ILE:HD11	1.91	0.52
27:C:140:VAL:HG12	27:C:191:LEU:HD23	1.91	0.52
25:A:1386:C:H2'	25:A:1387:A:H8	1.74	0.52
8:h:28:SER:OG	8:h:29:SER:N	2.40	0.52
25:A:2359:C:O2'	54:3:53:ASP:OD2	2.27	0.52
30:F:72:SER:OG	30:F:80:GLN:N	2.43	0.52
38:N:45:ARG:HG2	38:N:95:THR:HG21	1.90	0.52
9:i:115:VAL:HG21	10:j:62:ARG:HB2	1.92	0.52
25:A:1340:U:OP1	44:T:19:LYS:NZ	2.33	0.52
25:A:1868:C:H2'	25:A:1869:G:O4'	2.09	0.52
25:A:2330:G:H21	47:W:38:GLY:HA2	1.75	0.52
23:x:127:U:O2'	23:x:128:C:OP2	2.28	0.52
1:a:981:U:H4'	14:n:60:ARG:HG2	1.90	0.52
7:g:12:LEU:HD12	7:g:13:PRO:HD2	1.92	0.52
40:P:91:VAL:HG21	40:P:96:LEU:HD21	1.92	0.52
50:Z:8:GLN:NE2	50:Z:10:ARG:O	2.39	0.52
24:y:34:U:O2'	24:y:35:C:O5'	2.27	0.52
25:A:1972:G:OP2	27:C:237:ARG:NH1	2.43	0.52
2:b:140:LEU:O	2:b:144:GLU:HB2	2.11	0.51
25:A:9:G:O2'	25:A:2800:A:N6	2.43	0.51
25:A:1794:A:H2'	25:A:1795:C:C6	2.45	0.51
9:i:83:THR:HG21	9:i:102:PHE:HB3	1.92	0.51
40:P:26:GLU:HG2	40:P:43:GLU:HB2	1.91	0.51
1:a:401:C:O2'	1:a:621:A:N3	2.38	0.51
25:A:560:C:O2'	41:Q:47:ARG:NH2	2.44	0.51
25:A:2830:C:H5''	28:D:56:LYS:HZ1	1.75	0.51
29:E:94:GLN:N	29:E:94:GLN:OE1	2.43	0.51
39:O:71:ALA:HB2	39:O:102:ARG:HG3	1.93	0.51
44:T:57:VAL:O	44:T:86:THR:OG1	2.29	0.51
1:a:1513:A:H2'	1:a:1514:G:C8	2.45	0.51
2:b:172:ILE:O	2:b:176:ASN:HB2	2.11	0.51
28:D:121:THR:HG21	28:D:143:PRO:HB3	1.93	0.51
44:T:58:VAL:HG22	44:T:85:VAL:HG13	1.93	0.51
1:a:522:C:H41	12:l:49:ARG:HH22	1.58	0.51
16:p:20:VAL:HG23	16:p:35:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:558:U:H2'	25:A:559:G:C8	2.46	0.51
1:a:500:G:H5'	12:l:120:ARG:NH2	2.25	0.51
1:a:545:C:OP2	4:d:58:GLN:NE2	2.43	0.51
1:a:1124:G:H5''	10:j:37:ARG:HG3	1.93	0.51
20:t:4:LYS:HG3	20:t:6:ALA:H	1.75	0.51
32:I:100:ILE:HG22	32:I:101:SER:H	1.76	0.51
19:s:64:GLU:O	56:6:56:ARG:NH2	2.44	0.51
33:H:2:GLN:HB3	33:H:18:GLN:HB3	1.93	0.51
4:d:94:GLU:OE1	4:d:99:ASN:ND2	2.44	0.51
13:m:51:GLN:O	13:m:54:THR:OG1	2.26	0.51
1:a:419:C:OP1	1:a:513:C:O2'	2.26	0.50
25:A:780:G:H21	25:A:783:A:H62	1.58	0.50
5:e:80:LEU:HG	5:e:122:VAL:HG21	1.94	0.50
13:m:6:ILE:HG13	13:m:7:ASN:H	1.77	0.50
25:A:881:G:N2	25:A:896:A:H62	2.10	0.50
25:A:1779:U:H5	25:A:1784:A:N7	2.10	0.50
25:A:2267:A:H5''	25:A:2268:A:H5''	1.92	0.50
36:L:93:ASN:O	36:L:95:LEU:N	2.45	0.50
42:R:2:TYR:HA	42:R:14:VAL:O	2.11	0.50
25:A:796:C:H2'	25:A:797:G:C8	2.47	0.50
25:A:1040:A:N6	25:A:1115:G:H1	2.09	0.50
27:C:203:VAL:O	27:C:205:GLY:N	2.43	0.50
1:a:207:C:H1'	1:a:213:G:C2	2.47	0.50
3:c:29:ALA:HB1	14:n:64:ARG:HH22	1.77	0.50
3:c:137:VAL:HA	3:c:148:ILE:HD13	1.92	0.50
25:A:2512:C:O2'	28:D:159:LYS:NZ	2.36	0.50
41:Q:93:ILE:HD12	42:R:13:ARG:HB2	1.92	0.50
47:W:19:VAL:HG22	47:W:34:VAL:HG22	1.93	0.50
1:a:1323:G:H2'	1:a:1324:A:C8	2.46	0.50
25:A:1194:A:OP2	36:L:14:LYS:NZ	2.45	0.50
37:M:69:PRO:HA	37:M:94:ALA:HB2	1.94	0.50
1:a:59:A:H3'	1:a:331:G:H22	1.77	0.50
25:A:1918:A:O2'	25:A:1919:A:N7	2.43	0.50
25:A:2618:G:O2'	28:D:155:VAL:O	2.29	0.50
38:N:44:LEU:HD23	38:N:113:ILE:HD13	1.93	0.50
25:A:247:G:O2'	25:A:386:G:N1	2.44	0.49
1:a:842:U:OP2	1:a:846:G:N1	2.45	0.49
25:A:277:G:H1'	25:A:361:G:H1	1.78	0.49
42:R:49:ILE:HB	42:R:51:VAL:O	2.13	0.49
43:S:82:MET:HB2	43:S:98:LYS:HB2	1.93	0.49
25:A:1469:A:H2'	25:A:1470:A:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:501:C:H2'	1:a:502:A:C8	2.48	0.49
1:a:1144:G:H21	1:a:1146:A:H62	1.60	0.49
14:n:33:VAL:HA	14:n:40:ARG:HH22	1.78	0.49
14:n:80:ARG:HA	14:n:83:VAL:HG12	1.94	0.49
25:A:355:U:H2'	25:A:356:G:H8	1.78	0.49
25:A:2291:U:H2'	25:A:2292:U:C6	2.47	0.49
40:P:29:VAL:HG12	40:P:80:VAL:HG12	1.94	0.49
55:4:11:CYS:SG	55:4:14:CYS:N	2.86	0.49
45:U:17:ASP:HB3	45:U:20:LYS:HD2	1.94	0.49
1:a:188:C:H2'	1:a:189:A:O4'	2.12	0.49
1:a:1401:G:O6	1:a:1504:G:N2	2.46	0.49
2:b:165:ALA:HB3	2:b:190:SER:HB3	1.94	0.49
6:f:18:VAL:HG21	6:f:58:HIS:HD2	1.78	0.49
25:A:84:A:N1	25:A:98:G:O2'	2.36	0.49
25:A:1816:C:N4	27:C:34:GLU:OE2	2.44	0.49
34:J:35:ARG:HB2	34:J:54:ILE:HD11	1.94	0.49
1:a:1244:G:H2'	1:a:1245:C:C6	2.48	0.49
1:a:1414:U:H2'	1:a:1415:G:H8	1.78	0.49
2:b:220:VAL:O	2:b:223:GLY:N	2.46	0.49
27:C:130:PRO:HD3	27:C:188:ARG:NH1	2.28	0.49
46:V:20:LEU:HD21	46:V:41:GLU:HG3	1.95	0.49
36:L:19:LEU:HA	36:L:27:LEU:HD13	1.95	0.49
1:a:269:C:H2'	1:a:270:A:H8	1.77	0.48
1:a:505:G:H5'	1:a:534:U:H2'	1.95	0.48
9:i:62:LEU:HD21	9:i:82:ILE:HG12	1.95	0.48
9:i:90:ASP:OD1	9:i:91:GLU:N	2.43	0.48
25:A:1858:A:N6	25:A:1884:G:O2'	2.45	0.48
42:R:5:PHE:O	42:R:11:GLN:HA	2.13	0.48
1:a:979:C:H1'	1:a:1317:C:H41	1.78	0.48
1:a:1320:C:C2	19:s:71:GLY:HA3	2.48	0.48
7:g:112:ASP:H	7:g:118:ARG:HD3	1.79	0.48
25:A:639:U:H2'	25:A:640:C:C6	2.49	0.48
25:A:770:G:H5''	53:2:10:LEU:HD23	1.94	0.48
28:D:37:VAL:HG22	28:D:48:ILE:HG22	1.94	0.48
33:H:108:VAL:HG12	33:H:110:VAL:H	1.78	0.48
40:P:20:ARG:HH12	40:P:112:ARG:HD3	1.78	0.48
6:f:61:LEU:HD21	18:r:23:LYS:HZ1	1.78	0.48
1:a:148:G:H1	1:a:174:A:H61	1.62	0.48
1:a:1123:U:O2'	10:j:39:PRO:O	2.30	0.48
22:v:58:A:O2'	22:v:59:A:O5'	2.29	0.48
29:E:106:LYS:HG3	29:E:200:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:57:LEU:HD22	54:3:53:ASP:HB3	1.96	0.48
1:a:1026:G:H2'	1:a:1027:C:C6	2.48	0.48
1:a:1098:C:OP1	2:b:138:ARG:NH2	2.46	0.48
25:A:856:G:H2'	25:A:857:G:C8	2.48	0.48
25:A:1278:C:H2'	25:A:1279:G:H8	1.78	0.48
25:A:2391:G:H2'	25:A:2424:C:N4	2.29	0.48
25:A:2832:U:H4'	25:A:2833:U:H5'	1.95	0.48
1:a:1010:U:H2'	1:a:1011:C:C6	2.48	0.48
2:b:176:ASN:ND2	2:b:194:GLY:O	2.45	0.48
24:y:29:G:H2'	24:y:30:G:H8	1.79	0.48
54:3:22:LYS:HA	54:3:47:ALA:O	2.14	0.48
1:a:176:C:H5''	20:t:23:ARG:HH12	1.78	0.48
1:a:1356:G:H2'	1:a:1357:A:C8	2.47	0.48
1:a:1402:4OC:HM22	1:a:1403:C:H5'	1.95	0.48
6:f:32:ALA:HB1	6:f:67:PRO:HD2	1.96	0.48
25:A:414:C:H2'	25:A:415:A:H8	1.78	0.48
25:A:558:U:H2'	25:A:559:G:H8	1.79	0.48
25:A:1073:A:H2'	25:A:1074:G:O4'	2.14	0.48
25:A:2514:U:H2'	25:A:2515:C:C6	2.49	0.48
25:A:2813:A:H2'	25:A:2814:A:C8	2.49	0.48
1:a:1240:U:O4	7:g:108:ARG:NE	2.47	0.48
25:A:181:A:H2'	25:A:182:A:C8	2.48	0.48
25:A:2065:C:H4'	25:A:2251:OMG:HM23	1.94	0.48
31:G:94:ARG:HB2	31:G:105:SER:HB3	1.96	0.48
34:J:80:HIS:CE1	34:J:81:ILE:HG22	2.49	0.48
38:N:96:ARG:HH22	38:N:116:VAL:HG13	1.78	0.48
8:h:28:SER:HB2	8:h:58:LEU:HD23	1.95	0.48
11:k:17:ASP:OD2	11:k:36:ARG:NH2	2.40	0.48
35:K:76:VAL:H	40:P:72:VAL:HG22	1.79	0.48
1:a:113:G:H1'	1:a:354:G:H5'	1.95	0.48
1:a:1004:A:H2'	1:a:1005:A:O4'	2.14	0.48
6:f:6:ILE:HB	6:f:62:MET:HB2	1.95	0.48
13:m:67:ASP:OD2	56:6:49:ARG:NH1	2.47	0.48
17:q:59:GLU:HB3	17:q:75:VAL:HB	1.96	0.48
34:J:31:GLU:HG2	34:J:142:ILE:HG12	1.95	0.48
1:a:140:U:O2'	1:a:183:C:N4	2.47	0.47
1:a:1049:U:H2'	14:n:2:LYS:HD2	1.96	0.47
25:A:5:A:H2'	25:A:6:A:C8	2.49	0.47
28:D:25:THR:HG21	28:D:193:VAL:HG22	1.96	0.47
11:k:51:PHE:CE2	11:k:64:VAL:HG11	2.49	0.47
25:A:694:U:OP1	27:C:58:LYS:NZ	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2394:C:H42	57:w:76:A:H1'	1.79	0.47
25:A:184:C:H2'	25:A:185:G:H8	1.79	0.47
1:a:360:G:H2'	1:a:361:G:C8	2.50	0.47
1:a:624:C:H2'	1:a:625:U:C6	2.49	0.47
9:i:24:ASN:OD1	9:i:25:GLY:N	2.47	0.47
25:A:2040:G:H2'	25:A:2041:U:O4'	2.14	0.47
25:A:2333:A:OP2	47:W:73:ARG:NH2	2.43	0.47
20:t:74:HIS:O	20:t:78:LEU:HB2	2.14	0.47
22:v:43:A:H2'	22:v:44:A:C8	2.49	0.47
25:A:1723:G:H2'	25:A:1724:G:O4'	2.15	0.47
29:E:15:SER:HB2	29:E:18:THR:HB	1.97	0.47
1:a:384:G:H2'	1:a:385:C:C6	2.49	0.47
1:a:977:A:N6	1:a:1224:U:O4'	2.47	0.47
2:b:23:ASN:ND2	2:b:190:SER:O	2.47	0.47
25:A:2087:G:H2'	25:A:2088:A:C8	2.50	0.47
35:K:43:ILE:HD13	35:K:56:ASP:HB2	1.95	0.47
1:a:70:U:O2	1:a:71:A:N6	2.47	0.47
1:a:222:C:H2'	1:a:223:A:H8	1.78	0.47
2:b:153:MET:HG2	2:b:155:GLY:H	1.79	0.47
5:e:35:LEU:HD21	5:e:133:ILE:HA	1.96	0.47
11:k:49:SER:HA	11:k:68:ARG:HH11	1.80	0.47
25:A:1054:A:H61	25:A:1105:U:H3	1.60	0.47
25:A:2013:A:H4'	43:S:96:ILE:HG22	1.97	0.47
25:A:2813:A:H2'	25:A:2814:A:H8	1.80	0.47
33:H:47:PHE:HA	33:H:51:ARG:HB2	1.95	0.47
45:U:61:GLU:N	45:U:61:GLU:OE1	2.47	0.47
55:4:9:LYS:HG3	55:4:14:CYS:HB2	1.96	0.47
3:c:155:ARG:NH1	3:c:192:TYR:O	2.48	0.47
13:m:65:GLU:OE2	30:F:111:ARG:NH1	2.48	0.47
23:x:126:G:H8	23:x:126:G:OP2	1.96	0.47
25:A:277:G:H8	25:A:360:U:O4	1.97	0.47
25:A:1109:C:N3	25:A:1110:G:N2	2.62	0.47
47:W:37:ARG:HA	47:W:37:ARG:HD3	1.58	0.47
1:a:719:C:O2	18:r:38:ILE:N	2.46	0.47
4:d:122:ILE:HD13	4:d:144:ILE:HG12	1.96	0.47
10:j:12:ALA:HB2	10:j:96:VAL:HG22	1.96	0.47
25:A:373:U:OP2	25:A:400:G:N1	2.47	0.47
9:i:24:ASN:HD21	9:i:26:LYS:HE3	1.80	0.47
25:A:612:G:N2	25:A:614:A:O2'	2.48	0.47
25:A:839:U:H2'	25:A:840:C:C6	2.50	0.47
25:A:877:A:O2'	25:A:900:A:N6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2626:C:H2'	25:A:2627:G:C8	2.50	0.47
1:a:675:A:H1'	11:k:117:HIS:CD2	2.51	0.46
1:a:690:G:H2'	1:a:691:G:O4'	2.15	0.46
5:e:104:ILE:HD12	5:e:115:GLU:HG3	1.96	0.46
9:i:90:ASP:CG	9:i:91:GLU:H	2.23	0.46
11:k:48:GLY:O	11:k:68:ARG:NH1	2.48	0.46
25:A:370:G:O2'	25:A:424:G:OP1	2.32	0.46
25:A:1071:G:N2	25:A:1089:A:O2'	2.44	0.46
55:4:17:VAL:HG23	55:4:24:ARG:HB2	1.97	0.46
1:a:429:U:H5'	4:d:8:LEU:HD12	1.96	0.46
18:r:70:THR:OG1	18:r:71:ASP:N	2.48	0.46
25:A:2092:U:OP2	33:H:27:ARG:NH2	2.31	0.46
32:I:85:ILE:HD11	32:I:137:LEU:HD21	1.96	0.46
48:X:37:PHE:O	48:X:45:PHE:HA	2.16	0.46
1:a:88:U:H2'	1:a:89:U:C6	2.50	0.46
1:a:178:C:H2'	1:a:179:A:H8	1.80	0.46
1:a:1071:C:H2'	1:a:1072:G:H8	1.80	0.46
1:a:1412:C:H2'	1:a:1413:A:C8	2.50	0.46
11:k:81:LEU:HD11	11:k:99:LEU:HD23	1.96	0.46
25:A:1251:C:O2'	25:A:1253:A:OP2	2.34	0.46
25:A:1387:A:H2'	25:A:1388:G:H8	1.80	0.46
54:3:25:HIS:CE1	54:3:47:ALA:HB2	2.50	0.46
1:a:999:C:N3	1:a:1042:A:N6	2.63	0.46
1:a:1536:C:H2'	1:a:1537:U:C6	2.50	0.46
25:A:910:A:N3	25:A:2264:C:O2'	2.41	0.46
25:A:1548:A:H2'	25:A:1549:A:C8	2.51	0.46
25:A:2183:A:H2'	25:A:2184:A:C8	2.50	0.46
25:A:280:U:H2'	25:A:281:C:C6	2.51	0.46
25:A:688:U:P	53:2:2:LYS:HZ1	2.37	0.46
25:A:2626:C:H2'	25:A:2627:G:H8	1.81	0.46
25:A:2709:G:OP1	38:N:18:GLN:NE2	2.48	0.46
25:A:2713:U:H3'	25:A:2714:G:H5''	1.97	0.46
27:C:56:GLY:HA2	27:C:212:TRP:HA	1.98	0.46
1:a:337:G:H2'	1:a:338:A:C8	2.51	0.46
1:a:1523:G:H5''	11:k:124:LYS:HE2	1.96	0.46
31:G:174:LYS:HG2	31:G:175:LYS:H	1.81	0.46
6:f:11:HIS:CE1	6:f:54:LEU:HD22	2.50	0.46
14:n:53:ASP:HA	14:n:58:ARG:HD3	1.96	0.46
15:o:45:HIS:C	15:o:47:LYS:H	2.24	0.46
25:A:76:C:OP1	49:Y:48:ARG:NH1	2.49	0.46
25:A:532:A:H5'	41:Q:27:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:230:PRO:HD2	27:C:246:PRO:HA	1.97	0.46
30:F:62:GLN:HE21	30:F:88:VAL:HG13	1.80	0.46
1:a:331:G:HO2'	20:t:2:ASN:ND2	2.14	0.46
1:a:595:A:N6	1:a:641:U:O2'	2.48	0.46
2:b:113:LEU:HD22	2:b:143:LEU:HB3	1.97	0.46
19:s:30:LEU:HD22	19:s:48:ILE:HG22	1.97	0.46
1:a:189:A:H2'	1:a:190:A:O4'	2.16	0.46
1:a:517:G:N1	1:a:533:A:OP2	2.41	0.46
16:p:14:ARG:HE	16:p:42:ILE:HD12	1.81	0.46
32:I:18:ASN:HD21	32:I:34:ILE:HG22	1.81	0.46
33:H:46:PHE:HB3	33:H:50:ARG:HD2	1.97	0.46
33:H:75:LEU:HD23	33:H:75:LEU:HA	1.57	0.46
39:O:40:ILE:HG12	39:O:47:VAL:HG12	1.98	0.46
1:a:635:A:H2'	1:a:636:U:C6	2.52	0.46
1:a:1144:G:N2	1:a:1146:A:H62	2.14	0.46
1:a:922:G:H2'	1:a:923:A:C8	2.51	0.45
2:b:185:ILE:HA	2:b:199:ILE:O	2.16	0.45
25:A:1746:A:H2'	25:A:1747:U:C6	2.52	0.45
25:A:2415:G:H2'	25:A:2416:C:C6	2.52	0.45
46:V:58:SER:O	46:V:73:LYS:NZ	2.49	0.45
1:a:501:C:H2'	1:a:502:A:H8	1.82	0.45
1:a:927:G:O2'	1:a:1503:A:N7	2.48	0.45
1:a:1464:U:H2'	1:a:1465:A:H8	1.82	0.45
3:c:128:MET:H	3:c:131:ARG:NH2	2.14	0.45
4:d:115:GLN:OE1	4:d:119:HIS:NE2	2.49	0.45
9:i:56:MET:O	9:i:59:LYS:N	2.31	0.45
25:A:729:G:H5''	25:A:730:A:O5'	2.16	0.45
25:A:882:G:O2'	25:A:883:G:H8	1.99	0.45
25:A:1434:A:H2'	25:A:1435:G:C8	2.51	0.45
25:A:1736:U:H2'	25:A:1737:G:O4'	2.16	0.45
27:C:132:ARG:NH1	33:H:93:SER:OG	2.49	0.45
33:H:58:LEU:HA	33:H:61:VAL:HG22	1.98	0.45
35:K:58:LEU:HD11	35:K:86:LEU:HD13	1.98	0.45
53:2:3:ARG:HD3	53:2:3:ARG:HA	1.63	0.45
8:h:45:ILE:HD12	8:h:60:LEU:HD22	1.98	0.45
25:A:1432:G:H2'	25:A:1433:A:C8	2.50	0.45
25:A:2584:U:H2'	25:A:2585:U:H5''	1.99	0.45
1:a:539:A:H2'	1:a:540:G:C8	2.51	0.45
1:a:707:U:H4'	11:k:21:HIS:ND1	2.32	0.45
1:a:1031:C:P	1:a:1032:G:H21	2.40	0.45
2:b:175:ALA:HB3	2:b:182:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:71:ASP:N	18:r:71:ASP:OD1	2.39	0.45
25:A:729:G:C5	27:C:206:LYS:HB2	2.51	0.45
25:A:1597:A:H5''	25:A:1598:A:H5'	1.98	0.45
25:A:2467:C:OP1	55:4:8:LYS:NZ	2.39	0.45
30:F:5:ASP:OD1	30:F:6:TYR:N	2.49	0.45
55:4:11:CYS:HB3	55:4:33:HIS:CE1	2.52	0.45
1:a:1023:U:H2'	1:a:1024:G:C8	2.52	0.45
25:A:171:U:H2'	25:A:172:A:H8	1.81	0.45
25:A:851:C:H2'	25:A:852:U:C6	2.52	0.45
27:C:166:ARG:HG3	27:C:171:VAL:HG22	1.99	0.45
1:a:201:G:O2'	1:a:469:C:O2'	2.34	0.45
3:c:182:ASP:OD1	3:c:183:TYR:N	2.50	0.45
6:f:38:ARG:HD3	6:f:97:THR:HA	1.99	0.45
16:p:11:ALA:HB3	16:p:14:ARG:HB2	1.99	0.45
25:A:1817:G:OP1	27:C:86:ARG:NH2	2.49	0.45
25:A:2285:C:OP2	52:1:5:ARG:NH1	2.50	0.45
32:I:30:GLN:HB3	32:I:60:VAL:HG11	1.99	0.45
1:a:560:A:H5'	1:a:566:G:N2	2.31	0.45
1:a:1521:C:H2'	1:a:1522:U:C6	2.52	0.45
15:o:86:LEU:HD12	15:o:87:ARG:HB2	1.99	0.45
19:s:76:THR:OG1	19:s:77:ARG:N	2.50	0.45
38:N:103:ARG:HB2	38:N:110:MET:HE3	1.98	0.45
55:4:7:VAL:HG13	55:4:38:GLY:HA3	1.99	0.45
1:a:17:U:H2'	1:a:18:C:C6	2.52	0.45
1:a:180:U:O2	1:a:195:A:N7	2.50	0.45
1:a:1513:A:H2'	1:a:1514:G:H8	1.81	0.45
10:j:52:LEU:HD21	10:j:59:LYS:HD2	1.98	0.45
25:A:1:G:H2'	25:A:2:G:C8	2.52	0.45
25:A:1365:A:OP1	48:X:2:ARG:NH1	2.47	0.45
25:A:1744:A:H3'	25:A:1745:A:H8	1.82	0.45
25:A:1796:U:H2'	25:A:1797:G:H8	1.81	0.45
25:A:2830:C:H5''	28:D:56:LYS:NZ	2.32	0.45
27:C:259:ASN:O	27:C:261:ARG:N	2.44	0.45
37:M:96:ILE:HG21	37:M:126:ILE:HD13	1.98	0.45
1:a:224:U:H2'	1:a:225:C:C6	2.52	0.45
4:d:172:VAL:HG22	4:d:179:GLY:HA3	1.99	0.45
5:e:12:GLU:HG3	5:e:38:VAL:HG12	1.98	0.45
29:E:7:ASP:OD1	29:E:7:ASP:N	2.48	0.45
44:T:63:VAL:HB	44:T:80:TRP:O	2.17	0.45
3:c:66:THR:HA	3:c:101:ASN:O	2.17	0.44
7:g:65:LEU:O	7:g:69:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:108:ASN:HB2	21:u:5:VAL:O	2.17	0.44
13:m:53:ASP:OD1	13:m:56:ARG:NH1	2.50	0.44
25:A:1:G:H2'	25:A:2:G:H8	1.81	0.44
25:A:499:U:H5''	45:U:42:LYS:HE2	1.99	0.44
25:A:871:U:H2'	25:A:872:U:C6	2.53	0.44
25:A:1023:U:OP2	25:A:1025:G:O2'	2.35	0.44
30:F:113:PHE:HD2	56:6:41:HIS:HE1	1.64	0.44
3:c:10:ARG:NH2	3:c:174:LEU:O	2.50	0.44
4:d:120:LYS:HG2	4:d:130:ASN:HB3	1.98	0.44
9:i:44:ARG:HG3	9:i:45:MET:HG3	1.99	0.44
22:v:18:G:H1	22:v:55:PSU:H6	1.63	0.44
25:A:289:G:H2'	25:A:290:U:O4'	2.17	0.44
25:A:674:G:H1'	29:E:69:ARG:HH12	1.81	0.44
25:A:781:A:OP1	27:C:216:ARG:NH2	2.47	0.44
25:A:832:U:H5'	36:L:38:GLN:HB3	1.99	0.44
25:A:942:G:OP2	36:L:39:LYS:NZ	2.45	0.44
1:a:299:G:H2'	1:a:300:A:C8	2.53	0.44
1:a:1391:U:H2'	1:a:1392:G:H8	1.80	0.44
25:A:278:A:N1	25:A:361:G:C6	2.85	0.44
1:a:1038:C:H2'	1:a:1039:G:C8	2.52	0.44
1:a:1287:A:H2'	1:a:1288:A:C8	2.52	0.44
11:k:20:ALA:HA	11:k:33:ILE:HA	1.98	0.44
36:L:29:LYS:C	36:L:31:GLY:H	2.26	0.44
1:a:1538:C:H2'	1:a:1539:C:C6	2.53	0.44
25:A:483:A:O4'	45:U:44:HIS:HB3	2.17	0.44
27:C:83:ASP:HB2	27:C:90:ILE:HG12	2.00	0.44
31:G:53:PRO:HG3	31:G:61:TRP:CE2	2.52	0.44
51:0:37:HIS:ND1	51:0:38:LEU:O	2.35	0.44
1:a:102:G:H2'	1:a:103:U:H6	1.82	0.44
1:a:335:C:H2'	1:a:336:A:H8	1.81	0.44
1:a:842:U:H3'	1:a:843:U:H4'	2.00	0.44
2:b:89:PHE:HE1	2:b:152:ASP:HB2	1.82	0.44
2:b:93:HIS:CE1	2:b:145:ASN:HB2	2.52	0.44
9:i:30:ASN:C	9:i:32:ARG:H	2.26	0.44
10:j:52:LEU:HD23	10:j:62:ARG:HG2	2.00	0.44
11:k:63:GLN:HG3	11:k:98:ALA:HB2	2.00	0.44
14:n:19:TYR:O	14:n:22:LYS:HB3	2.16	0.44
17:q:56:ASP:HB3	17:q:81:ALA:H	1.82	0.44
25:A:1278:C:H2'	25:A:1279:G:C8	2.52	0.44
25:A:1838:C:H4'	25:A:1839:G:H5''	2.00	0.44
30:F:108:PRO:HB3	56:6:41:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:53:PRO:HG3	31:G:61:TRP:CD2	2.53	0.44
39:O:25:ARG:HA	39:O:91:SER:O	2.18	0.44
1:a:264:C:H2'	1:a:265:G:O4'	2.18	0.44
1:a:1434:A:H2'	1:a:1435:G:O4'	2.17	0.44
6:f:13:ASP:OD1	6:f:14:GLN:N	2.51	0.44
27:C:252:LYS:HB2	27:C:252:LYS:HE2	1.84	0.44
1:a:102:G:H2'	1:a:103:U:C6	2.52	0.44
1:a:1095:U:P	1:a:1108:G:H1	2.41	0.44
2:b:162:VAL:HG12	2:b:164:ASP:H	1.83	0.44
3:c:121:SER:HA	3:c:124:GLU:HG2	2.00	0.44
3:c:153:SER:OG	3:c:154:GLY:N	2.47	0.44
4:d:124:VAL:HG22	4:d:142:VAL:HG13	1.99	0.44
25:A:568:U:H1'	25:A:2030:6MZ:H9C1	1.98	0.44
25:A:610:C:H2'	25:A:611:C:C6	2.52	0.44
25:A:2098:U:H2'	25:A:2099:U:O4'	2.18	0.44
25:A:2788:C:H2'	25:A:2789:C:C6	2.52	0.44
30:F:92:GLY:O	30:F:95:MET:HG2	2.17	0.44
35:K:65:THR:HG23	35:K:68:GLY:H	1.82	0.44
38:N:83:LEU:HD22	38:N:87:PHE:HE2	1.83	0.44
1:a:202:G:H21	1:a:466:A:N6	2.16	0.44
1:a:1452:C:H4'	1:a:1453:G:C4	2.52	0.44
2:b:113:LEU:HB2	2:b:143:LEU:HD23	2.00	0.44
6:f:29:ILE:HG21	6:f:64:VAL:HG21	1.99	0.44
16:p:48:GLU:OE2	16:p:51:ARG:HB2	2.18	0.44
25:A:2328:A:H2'	25:A:2329:U:C6	2.53	0.44
30:F:30:VAL:HG23	30:F:155:ILE:HG23	2.00	0.44
37:M:102:LEU:HD11	37:M:126:ILE:HD11	2.00	0.44
40:P:21:PRO:HD3	40:P:49:ILE:HD12	1.99	0.44
1:a:728:A:H2'	1:a:729:A:C8	2.53	0.43
4:d:12:ARG:HD3	4:d:31:CYS:O	2.18	0.43
25:A:1646:C:H5''	25:A:1647:U:H5''	2.00	0.43
35:K:41:ILE:HG13	35:K:58:LEU:O	2.18	0.43
1:a:142:G:H2'	1:a:143:A:O4'	2.18	0.43
1:a:985:C:H2'	1:a:986:U:C6	2.53	0.43
24:y:47(F):C:H2'	24:y:47(H):A:H62	1.83	0.43
25:A:528:A:N1	25:A:2042:A:H2'	2.33	0.43
25:A:1607:C:N4	25:A:1622:G:OP2	2.41	0.43
25:A:2834:G:H2'	25:A:2879:A:H61	1.83	0.43
54:3:15:LYS:HE2	54:3:19:GLY:HA2	2.00	0.43
1:a:1313:U:P	19:s:5:LYS:HB3	2.59	0.43
12:l:20:VAL:C	12:l:22:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:62:U:O2'	25:A:63:A:N7	2.49	0.43
25:A:679:C:H2'	25:A:680:C:C6	2.53	0.43
25:A:1804:C:H2'	25:A:1805:A:H8	1.82	0.43
25:A:1869:G:N2	25:A:1872:A:OP2	2.49	0.43
25:A:2243:U:H2'	25:A:2244:U:C6	2.54	0.43
25:A:2788:C:O2'	25:A:2809:A:N3	2.46	0.43
27:C:86:ARG:NH1	27:C:155:ARG:HH21	2.16	0.43
32:I:104:GLN:N	32:I:104:GLN:OE1	2.49	0.43
46:V:77:VAL:HG23	46:V:89:ILE:HG12	2.00	0.43
1:a:36:C:H2'	1:a:37:U:O4'	2.18	0.43
1:a:131:A:H2'	1:a:132:C:H6	1.84	0.43
1:a:376:G:H2'	1:a:377:G:H8	1.83	0.43
1:a:446:G:C2	1:a:489:C:C2	3.07	0.43
3:c:19:SER:HB3	3:c:21:TRP:HE1	1.84	0.43
4:d:94:GLU:HA	4:d:99:ASN:HD22	1.83	0.43
7:g:79:VAL:HG12	7:g:83:THR:HA	2.00	0.43
25:A:161:A:H3'	25:A:162:U:H5''	1.99	0.43
25:A:2812:G:H2'	25:A:2813:A:C8	2.54	0.43
25:A:2867:G:O2'	25:A:2868:A:H8	2.01	0.43
33:H:1:MET:O	33:H:20:ASN:ND2	2.51	0.43
1:a:321:A:H2'	1:a:322:C:C6	2.53	0.43
1:a:1023:U:H2'	1:a:1024:G:H8	1.83	0.43
1:a:1443:C:H2'	1:a:1444:U:O4'	2.18	0.43
18:r:50:TYR:O	18:r:54:LEU:HB2	2.17	0.43
25:A:319:G:H1	25:A:323:C:H5	1.67	0.43
25:A:1509:A:H2'	25:A:1510:G:C8	2.52	0.43
25:A:2036:C:H6	25:A:2036:C:H5'	1.83	0.43
25:A:2899:A:H2'	25:A:2900:A:C8	2.53	0.43
40:P:24:THR:O	40:P:86:LYS:HB2	2.18	0.43
55:4:30:GLU:O	55:4:33:HIS:HB2	2.19	0.43
1:a:673:A:O3'	6:f:86:ARG:NH2	2.51	0.43
10:j:22:THR:HA	10:j:25:ILE:HG22	1.99	0.43
11:k:108:ASN:HD22	21:u:6:ARG:HG2	1.83	0.43
16:p:8:ARG:HD3	16:p:17:TYR:HE1	1.83	0.43
25:A:302:C:H2'	25:A:303:G:H8	1.83	0.43
25:A:1932:A:H2'	25:A:1933:G:O4'	2.18	0.43
28:D:116:LYS:HG3	28:D:165:MET:HE3	2.01	0.43
1:a:131:A:H2'	1:a:132:C:C6	2.53	0.43
1:a:268:U:H2'	1:a:269:C:C6	2.53	0.43
6:f:68:GLN:HA	6:f:71:ILE:HG22	2.01	0.43
7:g:149:ALA:HB1	11:k:58:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:65:PHE:CD2	8:h:66:GLN:HG3	2.54	0.43
25:A:2024:G:O3'	28:D:154:LYS:NZ	2.48	0.43
1:a:151:A:H2'	1:a:152:A:O4'	2.18	0.43
1:a:487:A:H3'	1:a:488:C:H6	1.83	0.43
1:a:635:A:H2'	1:a:636:U:H6	1.83	0.43
4:d:8:LEU:HD13	4:d:31:CYS:HB3	2.00	0.43
18:r:72:ARG:HA	18:r:72:ARG:HD3	1.78	0.43
25:A:1437:C:H2'	25:A:1438:U:C6	2.54	0.43
25:A:2258:C:O2'	25:A:2427:C:OP2	2.37	0.43
55:4:36:ARG:HG2	55:4:37:GLN:HB3	2.00	0.43
56:6:42:PRO:O	56:6:46:GLY:N	2.48	0.43
15:o:28:VAL:HG11	15:o:66:LEU:HD21	2.01	0.43
24:y:36:A:H2'	24:y:37:6IA:H8	2.01	0.43
25:A:476:G:N1	25:A:479:A:OP2	2.48	0.43
25:A:883:G:H1	25:A:893:C:H42	1.67	0.43
25:A:2104:C:H2'	25:A:2105:U:H6	1.84	0.43
31:G:37:ASN:OD1	31:G:38:ASP:N	2.52	0.43
48:X:39:VAL:HG12	48:X:42:GLU:H	1.84	0.43
1:a:176:C:H4'	20:t:23:ARG:HH22	1.83	0.43
25:A:882:G:H22	25:A:895:U:H1'	1.84	0.43
25:A:1487:U:H2'	25:A:1488:C:C6	2.54	0.43
25:A:1614:A:H61	43:S:88:ARG:H	1.66	0.43
32:I:30:GLN:HG2	32:I:60:VAL:HB	2.00	0.43
33:H:32:PRO:HA	48:X:38:TRP:CD1	2.54	0.43
41:Q:59:LEU:HD21	41:Q:63:ARG:HH12	1.84	0.43
42:R:41:ILE:HD13	42:R:103:ALA:HA	2.01	0.43
1:a:222:C:H2'	1:a:223:A:C8	2.53	0.42
6:f:46:GLN:HA	6:f:56:LYS:HA	2.01	0.42
12:l:113:ARG:HB2	12:l:118:VAL:HB	1.99	0.42
25:A:2140:G:H2'	25:A:2141:G:C8	2.53	0.42
25:A:2141:G:H2'	25:A:2142:A:H8	1.83	0.42
1:a:715:A:H2'	1:a:716:A:C8	2.54	0.42
25:A:38:A:H2'	25:A:39:G:O4'	2.18	0.42
25:A:2599:G:C8	27:C:235:GLU:HG2	2.54	0.42
1:a:155:A:H2'	1:a:156:C:O4'	2.19	0.42
1:a:680:C:H2'	1:a:681:A:C8	2.54	0.42
1:a:960:U:H4'	1:a:961:U:O5'	2.19	0.42
25:A:1126:A:H4'	25:A:1127:A:H5''	2.01	0.42
25:A:1469:A:H2'	25:A:1470:A:H8	1.84	0.42
25:A:2655:G:O2'	25:A:2664:G:O6	2.34	0.42
26:B:30:C:H2'	26:B:31:C:H5'	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:93:C:H2'	26:B:94:A:C8	2.55	0.42
29:E:154:ASP:OD1	29:E:154:ASP:N	2.49	0.42
34:J:13:ARG:HE	34:J:121:LYS:HZ1	1.67	0.42
40:P:12:MET:O	40:P:14:GLN:NE2	2.52	0.42
1:a:884:U:H4'	1:a:885:G:H5''	2.02	0.42
1:a:1239:A:H4'	1:a:1240:U:H5'	2.01	0.42
1:a:1397:C:P	5:e:28:ARG:HH22	2.43	0.42
2:b:144:GLU:O	2:b:148:GLY:HA3	2.19	0.42
10:j:24:GLU:O	10:j:28:THR:OG1	2.31	0.42
13:m:24:VAL:HG23	13:m:28:ARG:HB3	2.00	0.42
18:r:13:THR:O	18:r:17:VAL:HA	2.20	0.42
20:t:61:ALA:HA	20:t:66:ILE:O	2.20	0.42
25:A:608:A:H2'	25:A:609:A:C8	2.54	0.42
25:A:1197:G:H2'	25:A:1198:U:H6	1.84	0.42
28:D:184:ARG:HH12	40:P:6:GLN:HG2	1.84	0.42
56:6:62:LYS:HG2	56:6:63:ARG:NH1	2.34	0.42
25:A:2843:G:H2'	25:A:2844:G:O4'	2.20	0.42
1:a:373:A:H61	1:a:391:G:H1'	1.84	0.42
1:a:470:C:H2'	1:a:471:U:C6	2.55	0.42
1:a:1143:G:H2'	1:a:1144:G:H8	1.84	0.42
1:a:1405:G:N2	1:a:1518:MA6:H8	2.35	0.42
11:k:23:HIS:HB3	11:k:30:ILE:HG23	2.01	0.42
16:p:79:ASN:C	16:p:81:ALA:N	2.77	0.42
25:A:116:C:H2'	25:A:117:G:O4'	2.18	0.42
25:A:990:A:N1	42:R:78:ARG:NH1	2.67	0.42
26:B:28:C:H2'	26:B:29:A:C8	2.55	0.42
43:S:17:VAL:HB	43:S:76:VAL:HG11	2.01	0.42
56:6:56:ARG:O	56:6:59:ARG:HG2	2.20	0.42
1:a:769:G:H4'	1:a:1513:A:H4'	2.01	0.42
1:a:1328:C:H2'	1:a:1329:A:O4'	2.19	0.42
3:c:5:HIS:HB3	14:n:88:MET:HE3	2.02	0.42
4:d:149:LYS:HE2	4:d:177:MET:SD	2.60	0.42
17:q:11:VAL:HG12	17:q:55:GLY:H	1.84	0.42
19:s:10:ILE:HG21	19:s:40:PHE:CE2	2.54	0.42
25:A:685:A:H5''	25:A:788:A:H62	1.84	0.42
25:A:1387:A:H2'	25:A:1388:G:C8	2.54	0.42
25:A:1818:U:O2'	27:C:152:GLN:O	2.30	0.42
34:J:118:MET:HA	34:J:121:LYS:HG2	2.02	0.42
41:Q:97:ILE:HG22	41:Q:105:PHE:HB2	2.02	0.42
2:b:66:ILE:HD12	2:b:159:ALA:HB3	2.02	0.42
3:c:28:PHE:HZ	14:n:92:ILE:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:76:ILE:HD12	10:j:87:LEU:HD11	2.01	0.42
11:k:84:MET:SD	11:k:110:THR:OG1	2.67	0.42
25:A:144:A:H4'	44:T:2:ILE:HD11	2.02	0.42
25:A:1353:A:H2'	25:A:1354:A:C8	2.54	0.42
31:G:94:ARG:HD2	31:G:127:GLN:HE21	1.85	0.42
1:a:262:A:H2'	1:a:263:A:C8	2.54	0.42
1:a:1074:G:OP1	5:e:68:ARG:NH1	2.53	0.42
14:n:53:ASP:C	14:n:55:SER:H	2.27	0.42
25:A:2086:U:H2'	25:A:2087:G:C8	2.55	0.42
25:A:2301:C:H2'	25:A:2302:U:C6	2.55	0.42
35:K:25:LEU:HD12	35:K:38:ILE:HG22	2.02	0.42
4:d:160:LEU:O	4:d:164:ARG:HG2	2.20	0.42
7:g:85:GLN:HB2	7:g:147:ASN:HD21	1.85	0.42
8:h:28:SER:HB3	8:h:56:PRO:HB2	2.01	0.42
10:j:8:ILE:HD11	10:j:87:LEU:HD13	2.02	0.42
19:s:41:PRO:HG3	56:6:57:VAL:HG23	2.01	0.42
20:t:23:ARG:HD3	20:t:23:ARG:HA	1.81	0.42
25:A:2391:G:O2'	25:A:2392:A:O5'	2.36	0.42
25:A:2742:G:H5''	55:4:1:MET:HE3	2.01	0.42
25:A:2821:A:H2'	25:A:2822:G:O4'	2.20	0.42
26:B:95:U:H2'	26:B:96:G:H8	1.85	0.42
38:N:28:LEU:HD23	38:N:48:VAL:HG21	2.02	0.42
48:X:36:ARG:HA	48:X:47:THR:HA	2.01	0.42
1:a:335:C:H2'	1:a:336:A:C8	2.54	0.41
5:e:18:ASN:OD1	5:e:19:ARG:N	2.53	0.41
24:y:47(E):G:N2	24:y:47(K):G:O2'	2.53	0.41
25:A:207:A:H2'	25:A:208:C:O4'	2.20	0.41
25:A:2087:G:H2'	25:A:2088:A:H8	1.83	0.41
50:Z:9:THR:OG1	50:Z:10:ARG:N	2.53	0.41
56:6:37:CYS:O	56:6:41:HIS:HB2	2.20	0.41
1:a:562:U:H5''	1:a:563:A:C5	2.55	0.41
1:a:1244:G:H2'	1:a:1245:C:H6	1.84	0.41
2:b:16:GLY:HA2	2:b:202:ASN:HA	2.03	0.41
4:d:37:PRO:HD2	4:d:41:GLY:HA3	2.03	0.41
9:i:17:ARG:NH1	9:i:65:THR:OG1	2.54	0.41
11:k:126:ARG:HA	11:k:126:ARG:HD3	1.94	0.41
14:n:86:ALA:HB1	14:n:91:GLU:HB2	2.02	0.41
19:s:36:ARG:H	19:s:36:ARG:HG2	1.63	0.41
25:A:660:C:H5''	29:E:94:GLN:HG3	2.01	0.41
25:A:782:A:H4'	25:A:783:A:H5'	2.01	0.41
25:A:2376:A:H2'	25:A:2377:A:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:49:C:H2'	26:B:50:A:C8	2.56	0.41
29:E:52:VAL:HG21	29:E:82:GLY:H	1.85	0.41
29:E:117:ARG:NH1	36:L:2:ARG:HG2	2.35	0.41
30:F:5:ASP:O	30:F:8:LYS:HB2	2.19	0.41
31:G:153:PRO:HA	31:G:159:LYS:O	2.20	0.41
1:a:45:G:H2'	1:a:46:G:C8	2.55	0.41
1:a:673:A:H2'	1:a:674:G:C8	2.55	0.41
4:d:149:LYS:HG2	4:d:150:LYS:HG3	2.02	0.41
8:h:104:SER:HB2	8:h:125:ILE:HD11	2.02	0.41
10:j:36:VAL:HG22	10:j:38:GLY:H	1.85	0.41
10:j:37:ARG:HD3	10:j:37:ARG:HA	1.90	0.41
25:A:5:A:H2'	25:A:6:A:H8	1.84	0.41
25:A:527:C:C4	25:A:2779:U:H2'	2.55	0.41
25:A:1213:A:H1'	25:A:1237:A:C2	2.55	0.41
25:A:1266:G:O2'	25:A:2012:G:O6	2.39	0.41
25:A:2572:A:N7	28:D:150:GLN:HG2	2.35	0.41
1:a:130:A:C8	17:q:64:ARG:HG3	2.55	0.41
2:b:209:VAL:O	2:b:213:LEU:HB2	2.21	0.41
3:c:179:ALA:HB1	3:c:202:PHE:HE1	1.85	0.41
6:f:86:ARG:HH11	6:f:86:ARG:HD2	1.61	0.41
15:o:32:THR:HG21	15:o:84:LEU:HD11	2.02	0.41
25:A:397:U:OP2	48:X:9:LYS:NZ	2.36	0.41
25:A:801:G:O4'	29:E:49:ARG:NH2	2.54	0.41
25:A:833:A:H2'	25:A:834:G:C8	2.55	0.41
25:A:2757:A:N1	31:G:66:THR:OG1	2.47	0.41
27:C:242:HIS:HA	27:C:243:PRO:HD3	1.90	0.41
7:g:85:GLN:HB2	7:g:147:ASN:ND2	2.36	0.41
22:v:48:C:C2	22:v:59:A:H1'	2.56	0.41
25:A:364:C:H2'	25:A:365:U:C6	2.55	0.41
28:D:35:THR:OG1	28:D:49:GLN:HG3	2.20	0.41
40:P:46:VAL:HG22	40:P:60:VAL:HG22	2.01	0.41
43:S:17:VAL:HA	43:S:43:ALA:HB1	2.03	0.41
1:a:946:A:H2'	1:a:947:G:H8	1.85	0.41
3:c:39:ARG:NH1	3:c:54:ILE:O	2.53	0.41
4:d:182:LYS:HE3	4:d:182:LYS:HB2	1.81	0.41
5:e:82:HIS:CE1	8:h:95:MET:HE3	2.56	0.41
25:A:517:C:OP1	51:0:12:ARG:NH2	2.54	0.41
25:A:669:G:N3	25:A:669:G:H2'	2.35	0.41
25:A:2800:A:C2	25:A:2895:G:H1'	2.56	0.41
36:L:110:VAL:HG21	36:L:127:VAL:HG22	2.01	0.41
37:M:65:ILE:HG12	37:M:103:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:298:A:H2'	1:a:299:G:O4'	2.21	0.41
10:j:63:ASP:OD1	14:n:97:LYS:NZ	2.54	0.41
17:q:76:ARG:HG3	17:q:78:VAL:HG13	2.02	0.41
24:y:37:6IA:O2'	25:A:1913:A:N1	2.54	0.41
25:A:171:U:H2'	25:A:172:A:C8	2.56	0.41
25:A:620:G:H4'	25:A:621:A:O5'	2.21	0.41
25:A:2141:G:H2'	25:A:2142:A:C8	2.56	0.41
25:A:2784:U:H2'	25:A:2785:C:C6	2.55	0.41
32:I:92:PRO:HG3	32:I:136:GLY:HA2	2.03	0.41
1:a:447:G:O2'	1:a:487:A:N6	2.53	0.41
1:a:693:G:OP1	11:k:126:ARG:NH1	2.54	0.41
6:f:6:ILE:HG13	6:f:89:VAL:HG22	2.02	0.41
25:A:475:C:O2	25:A:479:A:N6	2.53	0.41
25:A:593:U:H2'	25:A:594:U:C6	2.56	0.41
33:H:8:LYS:HE3	33:H:8:LYS:HB3	1.90	0.41
1:a:280:C:N4	17:q:40:THR:OG1	2.54	0.41
1:a:632:U:H3'	1:a:633:G:H5'	2.02	0.41
1:a:680:C:H2'	1:a:681:A:H8	1.85	0.41
1:a:996:A:H2'	1:a:997:U:H6	1.86	0.41
6:f:12:PRO:O	6:f:44:ARG:NH2	2.54	0.41
11:k:86:LYS:HB2	11:k:112:VAL:HG23	2.02	0.41
13:m:95:PRO:HA	13:m:108:ARG:HG2	2.03	0.41
25:A:1538:G:H2'	25:A:1539:U:C6	2.56	0.41
25:A:2247:A:H2'	25:A:2248:C:H6	1.86	0.41
25:A:2698:U:H2'	25:A:2699:C:C6	2.56	0.41
28:D:2:ILE:HG21	28:D:84:LEU:HD23	2.03	0.41
29:E:49:ARG:HH21	29:E:49:ARG:HD3	1.74	0.41
31:G:25:ILE:HD12	31:G:74:MET:HE2	2.03	0.41
32:I:11:GLN:HE21	32:I:53:PRO:C	2.28	0.41
32:I:48:ILE:HG13	32:I:49:GLU:H	1.86	0.41
37:M:96:ILE:HD12	37:M:96:ILE:HA	1.93	0.41
43:S:59:GLU:HA	43:S:64:ALA:HB2	2.03	0.41
1:a:652:U:O4	1:a:752:G:O2'	2.33	0.41
1:a:692:U:H5''	11:k:126:ARG:HH22	1.85	0.41
25:A:244:A:H5''	36:L:67:THR:HG21	2.03	0.41
25:A:594:U:H2'	25:A:595:C:C6	2.55	0.41
27:C:159:THR:HG23	27:C:176:ARG:HG2	2.03	0.41
30:F:60:SER:OG	30:F:61:GLY:N	2.54	0.41
1:a:328:C:H4'	1:a:329:A:H5'	2.03	0.40
1:a:562:U:H1'	12:l:11:ARG:HG2	2.01	0.40
1:a:1219:A:H2'	1:a:1220:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:42:GLU:HG2	8:h:100:ILE:HG12	2.02	0.40
22:v:50:U:H2'	22:v:51:C:C6	2.55	0.40
25:A:575:A:OP2	25:A:2055:C:N4	2.51	0.40
25:A:807:U:H1'	25:A:2445:2MG:H5'	2.02	0.40
25:A:857:G:H2'	25:A:858:G:O4'	2.21	0.40
25:A:2297:A:N1	25:A:2321:U:H5	2.18	0.40
25:A:2610:C:H4'	25:A:2611:C:H5'	2.02	0.40
36:L:29:LYS:O	36:L:31:GLY:N	2.54	0.40
36:L:55:MET:HA	36:L:56:PRO:HD3	1.97	0.40
1:a:714:G:H2'	1:a:715:A:C8	2.56	0.40
1:a:725:G:H2'	1:a:726:C:C6	2.56	0.40
6:f:3:HIS:ND1	6:f:65:GLU:OE1	2.54	0.40
18:r:33:THR:HG22	18:r:37:LYS:H	1.86	0.40
20:t:29:THR:O	20:t:33:LYS:HB2	2.21	0.40
25:A:1170:C:H2'	25:A:1171:G:C8	2.56	0.40
37:M:17:ASN:O	37:M:17:ASN:ND2	2.55	0.40
38:N:59:SER:O	38:N:63:ARG:HG2	2.21	0.40
48:X:3:VAL:HG22	48:X:10:ARG:HB3	2.03	0.40
1:a:79:G:H2'	1:a:80:A:O4'	2.21	0.40
1:a:721:G:H4'	1:a:722:G:O4'	2.21	0.40
15:o:24:THR:O	15:o:27:GLN:HB2	2.21	0.40
25:A:1141:U:H4'	25:A:1142:A:O4'	2.20	0.40
25:A:1158:C:H2'	25:A:1159:U:H6	1.86	0.40
25:A:1178:C:H2'	25:A:1179:G:C8	2.56	0.40
25:A:1565:C:O2'	25:A:1566:A:H2'	2.20	0.40
25:A:2353:G:H2'	25:A:2354:C:O4'	2.21	0.40
25:A:2620:C:H2'	25:A:2621:G:O4'	2.22	0.40
27:C:81:GLU:HG3	27:C:102:TYR:HE1	1.87	0.40
27:C:264:LYS:HE3	27:C:264:LYS:HB2	1.87	0.40
29:E:26:ALA:HB2	36:L:9:ALA:HB2	2.03	0.40
30:F:123:GLY:HA2	30:F:162:ASP:HB3	2.03	0.40
46:V:56:PHE:CE1	46:V:61:LEU:HD21	2.57	0.40
1:a:182:A:N6	1:a:194:C:O2	2.53	0.40
1:a:1464:U:H2'	1:a:1465:A:C8	2.57	0.40
7:g:68:VAL:HG23	7:g:99:ALA:HB1	2.04	0.40
11:k:87:GLY:N	11:k:113:THR:HG22	2.35	0.40
25:A:679:C:H2'	25:A:680:C:H6	1.86	0.40
25:A:1410:G:H2'	25:A:1411:U:H6	1.87	0.40
25:A:1779:U:H5''	25:A:1780:A:H5''	2.03	0.40
25:A:2326:C:O2'	25:A:2327:A:OP1	2.36	0.40
25:A:2685:G:H2'	25:A:2686:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2836:U:H2'	25:A:2837:A:C8	2.56	0.40
25:A:2859:G:H2'	25:A:2860:A:C8	2.57	0.40
26:B:54:G:H2'	26:B:55:U:H6	1.86	0.40
46:V:72:VAL:HG12	46:V:93:ARG:HA	2.02	0.40
50:Z:16:LEU:HB2	50:Z:19:HIS:ND1	2.37	0.40
1:a:954:G:H2'	1:a:955:U:C6	2.57	0.40
1:a:1012:A:H2'	1:a:1013:G:O4'	2.21	0.40
1:a:1015:G:H2'	1:a:1016:A:C8	2.57	0.40
3:c:41:TYR:CZ	3:c:89:VAL:HG11	2.56	0.40
4:d:20:LEU:HD23	4:d:20:LEU:HA	1.96	0.40
13:m:33:LEU:HG	13:m:38:ILE:HB	2.03	0.40
13:m:70:ARG:NH1	30:F:114:ARG:HH11	2.19	0.40
25:A:372:G:H5''	48:X:60:LYS:NZ	2.36	0.40
25:A:784:G:H5'	25:A:785:G:OP1	2.21	0.40
25:A:813:U:H2'	25:A:814:C:C6	2.57	0.40
25:A:2185:U:H2'	25:A:2186:G:C8	2.57	0.40
25:A:2834:G:H2'	25:A:2879:A:N6	2.36	0.40
27:C:139:THR:HG23	27:C:160:TYR:HB2	2.03	0.40
29:E:149:ILE:HD11	29:E:172:ALA:HA	2.04	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	
2	b	216/218 (99%)	190 (88%)	23 (11%)	3 (1%)	9	38
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	8	37
4	d	203/205 (99%)	181 (89%)	19 (9%)	3 (2%)	8	37
5	e	155/157 (99%)	139 (90%)	9 (6%)	7 (4%)	2	17
6	f	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	6	32
8	h	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	7	36
9	i	125/127 (98%)	105 (84%)	14 (11%)	6 (5%)	2	16
10	j	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	1	14
11	k	114/116 (98%)	102 (90%)	10 (9%)	2 (2%)	6	34
12	l	121/123 (98%)	101 (84%)	14 (12%)	6 (5%)	1	15
13	m	112/114 (98%)	100 (89%)	8 (7%)	4 (4%)	2	22
14	n	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	2	19
15	o	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	2	17
16	p	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	1	15
17	q	78/80 (98%)	65 (83%)	11 (14%)	2 (3%)	4	27
18	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	16
19	s	77/79 (98%)	71 (92%)	5 (6%)	1 (1%)	9	39
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	8
27	C	269/271 (99%)	245 (91%)	19 (7%)	5 (2%)	6	33
28	D	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	9	38
29	E	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	8	37
30	F	175/177 (99%)	160 (91%)	13 (7%)	2 (1%)	11	43
31	G	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	7	35
32	I	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	3	26
33	H	147/149 (99%)	125 (85%)	17 (12%)	5 (3%)	3	23
34	J	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	9	38
35	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	23
36	L	141/143 (99%)	127 (90%)	10 (7%)	4 (3%)	4	26
37	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	8	37
38	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
39	O	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	14	47
40	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
41	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
42	R	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
44	T	91/93 (98%)	78 (86%)	11 (12%)	2 (2%)	5	30
45	U	100/102 (98%)	87 (87%)	7 (7%)	6 (6%)	1	12
46	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
47	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	9	38
48	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	Y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	36
50	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
51	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	6	33
52	1	48/50 (96%)	47 (98%)	0	1 (2%)	5	31
53	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
54	3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	36
55	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
56	6	64/66 (97%)	58 (91%)	5 (8%)	1 (2%)	7	36
All	All	5717/5817 (98%)	5151 (90%)	439 (8%)	127 (2%)	7	30

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	73	ARG
5	e	77	ASN
5	e	89	THR
5	e	93	VAL
6	f	53	LYS
6	f	54	LEU
6	f	98	GLU
9	i	57	VAL
9	i	90	ASP
10	j	34	ALA
11	k	88	PRO
12	l	23	LEU
12	l	75	GLU
13	m	4	ALA
13	m	65	GLU
16	p	44	SER
16	p	79	ASN
16	p	80	LYS

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Mol	Chain	Res	Type
17	q	69	THR
18	r	11	ARG
19	s	4	LEU
21	u	24	LYS
27	C	121	ALA
28	D	167	ASN
29	E	83	VAL
30	F	174	PHE
31	G	108	PHE
33	H	3	VAL
33	H	9	VAL
33	H	41	LYS
35	K	35	VAL
35	K	110	GLU
36	L	36	LYS
45	U	6	ARG
45	U	38	ILE
45	U	51	LEU
45	U	88	ASP
51	0	2	VAL
52	1	4	ILE
54	3	31	ILE
2	b	18	GLN
3	c	156	LEU
6	f	92	THR
7	g	145	GLU
10	j	57	VAL
13	m	6	ILE
14	n	34	ASN
15	o	46	LYS
18	r	17	VAL
18	r	46	THR
21	u	62	GLU
27	C	204	LEU
28	D	153	GLY
30	F	20	ASN
31	G	174	LYS
36	L	29	LYS
36	L	111	ILE
39	O	63	LYS
42	R	100	GLY
49	Y	22	LEU

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Mol	Chain	Res	Type
56	6	4	ASP
4	d	191	SER
5	e	23	THR
5	e	50	GLY
5	e	102	THR
5	e	122	VAL
6	f	86	ARG
7	g	29	LEU
7	g	83	THR
8	h	47	ASP
9	i	12	LYS
9	i	107	ALA
9	i	125	GLN
10	j	42	LEU
10	j	93	ALA
11	k	92	ARG
13	m	104	ASN
14	n	2	LYS
14	n	53	ASP
15	o	2	LEU
16	p	43	ALA
21	u	8	ASN
29	E	80	SER
29	E	122	GLU
32	I	53	PRO
32	I	59	THR
42	R	55	ASP
45	U	54	PRO
45	U	97	SER
3	c	96	VAL
3	c	205	GLU
4	d	29	THR
9	i	31	GLN
10	j	89	ARG
17	q	17	GLU
27	C	52	HIS
28	D	139	SER
31	G	47	ASN
32	I	64	ARG
33	H	15	LEU
35	K	89	ASN
44	T	38	ALA

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Mol	Chain	Res	Type
8	h	2	MET
12	l	2	THR
12	l	21	PRO
12	l	88	ASP
12	l	101	LEU
15	o	27	GLN
15	o	45	HIS
27	C	154	ALA
33	H	89	LYS
36	L	94	THR
37	M	58	LYS
44	T	52	GLU
47	W	17	LEU
4	d	166	LYS
14	n	54	SER
21	u	34	ARG
21	u	65	ARG
27	C	260	LYS
35	K	93	GLN
37	M	69	PRO
2	b	27	LYS
42	R	54	VAL
32	I	12	VAL
34	J	81	ILE
34	J	100	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	177 (98%)	3 (2%)	53	70
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	102 (98%)	2 (2%)	50	68
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	78 (99%)	1 (1%)	61	72
15	o	76/76 (100%)	75 (99%)	1 (1%)	61	72
16	p	65/65 (100%)	63 (97%)	2 (3%)	35	59
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	41 (93%)	3 (7%)	14	40
27	C	216/216 (100%)	214 (99%)	2 (1%)	70	76
28	D	164/164 (100%)	163 (99%)	1 (1%)	78	79
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/148 (100%)	148 (100%)	0	100	100
31	G	137/137 (100%)	137 (100%)	0	100	100
32	I	109/109 (100%)	104 (95%)	5 (5%)	24	50
33	H	114/114 (100%)	114 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/103 (100%)	103 (100%)	0	100	100
36	L	102/102 (100%)	102 (100%)	0	100	100
37	M	109/109 (100%)	109 (100%)	0	100	100
38	N	100/100 (100%)	100 (100%)	0	100	100
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	99/99 (100%)	99 (100%)	0	100	100
41	Q	89/89 (100%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	S	93/93 (100%)	92 (99%)	1 (1%)	65	74
44	T	80/80 (100%)	79 (99%)	1 (1%)	61	72
45	U	83/83 (100%)	82 (99%)	1 (1%)	63	73
46	V	78/78 (100%)	77 (99%)	1 (1%)	61	72
47	W	57/57 (100%)	57 (100%)	0	100	100
48	X	67/67 (100%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/48 (100%)	48 (100%)	0	100	100
51	0	47/47 (100%)	46 (98%)	1 (2%)	47	66
52	1	45/45 (100%)	44 (98%)	1 (2%)	45	65
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/51 (100%)	51 (100%)	0	100	100
55	4	34/34 (100%)	33 (97%)	1 (3%)	37	60
56	6	59/59 (100%)	52 (88%)	7 (12%)	5	23
All	All	4728/4751 (100%)	4694 (99%)	34 (1%)	73	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	30	ILE
2	b	86	CYS
2	b	122	ASP
8	h	100	ILE
8	h	103	VAL
14	n	33	VAL
15	o	87	ARG
16	p	19	VAL
16	p	75	ILE
21	u	12	ASP
21	u	21	SER
21	u	37	TYR
27	C	85	ASN
27	C	230	PRO
28	D	48	ILE
32	I	27	LEU
32	I	33	ASN
32	I	34	ILE

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Mol	Chain	Res	Type
32	I	35	MET
32	I	37	PHE
43	S	72	THR
44	T	32	LEU
45	U	39	ASN
46	V	42	LEU
51	0	2	VAL
52	1	36	LYS
55	4	35	GLN
56	6	13	THR
56	6	16	CYS
56	6	30	HIS
56	6	32	LEU
56	6	34	LEU
56	6	45	THR
56	6	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	119	GLN
2	b	177	ASN
3	c	122	GLN
5	e	147	ASN
6	f	58	HIS
7	g	147	ASN
8	h	20	ASN
11	k	14	GLN
11	k	80	ASN
11	k	108	ASN
12	l	5	GLN
14	n	3	GLN
14	n	65	GLN
15	o	34	GLN
15	o	41	HIS
16	p	79	ASN
17	q	49	ASN
20	t	47	GLN
20	t	69	ASN
27	C	44	ASN
27	C	45	ASN
27	C	52	HIS

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Mol	Chain	Res	Type
27	C	89	ASN
27	C	116	GLN
28	D	32	ASN
29	E	41	GLN
29	E	90	GLN
30	F	126	ASN
31	G	127	GLN
33	H	20	ASN
34	J	58	ASN
34	J	128	ASN
35	K	93	GLN
38	N	18	GLN
38	N	31	HIS
39	O	98	GLN
40	P	14	GLN
40	P	76	HIS
44	T	48	GLN
45	U	39	ASN
46	V	78	GLN
48	X	15	ASN
48	X	19	HIS
52	1	44	GLN
54	3	27	ASN
56	6	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	248 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	23 (48%)	0
24	y	94/95 (98%)	13 (13%)	0
25	A	2898/2903 (99%)	518 (17%)	34 (1%)
26	B	119/120 (99%)	19 (15%)	3 (2%)
57	w	2/3 (66%)	0	0
All	All	4774/4785 (99%)	836 (17%)	37 (0%)

All (836) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G

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Mol	Chain	Res	Type
1	a	7	A
1	a	8	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	41	G
1	a	42	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	61	G
1	a	65	A
1	a	71	A
1	a	79	G
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	88	U
1	a	94	G
1	a	95	C
1	a	96	U
1	a	116	A
1	a	118	U
1	a	121	U
1	a	126	G
1	a	127	G
1	a	131	A
1	a	168	G
1	a	174	A
1	a	178	C
1	a	181	A
1	a	183	C
1	a	195	A
1	a	197	A
1	a	208	U
1	a	210	C
1	a	211	G
1	a	226	G

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Mol	Chain	Res	Type
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	264	C
1	a	266	G
1	a	267	C
1	a	281	G
1	a	289	G
1	a	319	G
1	a	328	C
1	a	330	C
1	a	340	U
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	369	G
1	a	372	C
1	a	373	A
1	a	384	G
1	a	397	A
1	a	398	U
1	a	406	G
1	a	410	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	423	G
1	a	429	U
1	a	441	A
1	a	446	G
1	a	466	A
1	a	467	U
1	a	481	G
1	a	482	A
1	a	486	U
1	a	496	A

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Mol	Chain	Res	Type
1	a	497	G
1	a	499	A
1	a	506	G
1	a	509	A
1	a	511	C
1	a	512	U
1	a	518	C
1	a	527	G7M
1	a	528	C
1	a	532	A
1	a	546	A
1	a	547	A
1	a	550	G
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	615	G
1	a	617	G
1	a	633	G
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	701	U
1	a	702	A
1	a	713	G
1	a	718	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	733	G
1	a	734	G
1	a	759	A
1	a	777	A
1	a	793	U
1	a	794	A

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Mol	Chain	Res	Type
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	829	G
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	845	A
1	a	846	G
1	a	849	G
1	a	872	A
1	a	873	A
1	a	885	G
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	967	5MC
1	a	968	A
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	991	U
1	a	992	U
1	a	993	G
1	a	996	A
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1028	C
1	a	1031	C
1	a	1032	G

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Mol	Chain	Res	Type
1	a	1033	G
1	a	1034	G
1	a	1053	G
1	a	1066	C
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1126	U
1	a	1130	A
1	a	1132	C
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1151	A
1	a	1159	U
1	a	1160	G
1	a	1161	C
1	a	1182	G
1	a	1183	U
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1223	C
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1241	G
1	a	1257	A
1	a	1260	G
1	a	1280	A
1	a	1286	U
1	a	1287	A

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Mol	Chain	Res	Type
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1332	A
1	a	1346	A
1	a	1353	G
1	a	1363	A
1	a	1364	U
1	a	1381	U
1	a	1398	A
1	a	1401	G
1	a	1419	G
1	a	1422	G
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1453	G
1	a	1492	A
1	a	1494	G
1	a	1498	UR3
1	a	1499	A
1	a	1503	A
1	a	1504	G
1	a	1505	G
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1540	U
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	17	C
22	v	17(A)	U

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Mol	Chain	Res	Type
22	v	18	G
22	v	19	G
22	v	20	H2U
22	v	22	G
22	v	47	U
22	v	49	G
22	v	59	A
22	v	60	U
22	v	75	C
22	v	76	A
23	x	89	G
23	x	94	U
23	x	95	U
23	x	96	C
23	x	98	U
23	x	104	U
23	x	109	C
23	x	110	G
23	x	113	C
23	x	117	C
23	x	120	U
23	x	121	U
23	x	122	G
23	x	123	C
23	x	125	G
23	x	126	G
23	x	127	U
23	x	128	C
23	x	129	U
23	x	130	G
23	x	131	C
23	x	132	A
23	x	134	C
24	y	10	C
24	y	17	G
24	y	19	H2U
24	y	20	G
24	y	35	C
24	y	47(F)	C
24	y	47(G)	C
24	y	47(K)	G
24	y	51	A

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Mol	Chain	Res	Type
24	y	55	PSU
24	y	68	C
24	y	74	C
24	y	76	A
25	A	10	A
25	A	35	G
25	A	36	G
25	A	39	G
25	A	43	G
25	A	46	G
25	A	50	U
25	A	51	G
25	A	52	A
25	A	60	G
25	A	63	A
25	A	71	A
25	A	74	A
25	A	75	G
25	A	100	U
25	A	102	U
25	A	103	A
25	A	118	A
25	A	120	U
25	A	138	U
25	A	142	A
25	A	162	U
25	A	163	C
25	A	178	G
25	A	196	A
25	A	205	G
25	A	206	U
25	A	216	A
25	A	219	A
25	A	221	A
25	A	222	A
25	A	225	C
25	A	228	C
25	A	229	C
25	A	247	G
25	A	248	G
25	A	250	G
25	A	255	A

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Mol	Chain	Res	Type
25	A	266	G
25	A	276	U
25	A	277	G
25	A	278	A
25	A	285	G
25	A	294	A
25	A	310	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	332	A
25	A	346	A
25	A	349	U
25	A	361	G
25	A	371	A
25	A	372	G
25	A	373	U
25	A	386	G
25	A	387	U
25	A	396	G
25	A	404	A
25	A	406	G
25	A	411	G
25	A	412	A
25	A	424	G
25	A	451	U
25	A	455	C
25	A	456	C
25	A	457	A
25	A	473	G
25	A	481	G
25	A	491	G
25	A	496	G
25	A	504	A
25	A	505	A
25	A	509	C
25	A	513	A
25	A	518	G
25	A	527	C
25	A	529	A
25	A	531	C

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Mol	Chain	Res	Type
25	A	532	A
25	A	543	G
25	A	544	C
25	A	545	U
25	A	547	A
25	A	548	G
25	A	549	G
25	A	551	G
25	A	556	A
25	A	563	A
25	A	572	A
25	A	573	U
25	A	575	A
25	A	588	U
25	A	603	A
25	A	614	A
25	A	622	G
25	A	627	A
25	A	637	A
25	A	645	C
25	A	646	U
25	A	647	G
25	A	654	A
25	A	655	A
25	A	656	G
25	A	668	A
25	A	669	G
25	A	685	A
25	A	686	U
25	A	694	U
25	A	695	G
25	A	702	U
25	A	714	U
25	A	717	C
25	A	723	C
25	A	729	G
25	A	730	A
25	A	740	C
25	A	747	5MU
25	A	752	A
25	A	757	G
25	A	765	C

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Mol	Chain	Res	Type
25	A	775	G
25	A	776	G
25	A	777	G
25	A	782	A
25	A	783	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	805	G
25	A	807	U
25	A	812	C
25	A	819	A
25	A	822	G
25	A	827	U
25	A	828	U
25	A	831	G
25	A	844	A
25	A	845	A
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	869	G
25	A	883	G
25	A	885	C
25	A	886	A
25	A	898	C
25	A	910	A
25	A	914	G
25	A	915	C
25	A	932	U
25	A	941	A
25	A	945	A
25	A	946	C
25	A	958	U
25	A	959	A
25	A	961	C
25	A	973	A
25	A	974	G
25	A	983	A
25	A	985	C
25	A	990	A

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Mol	Chain	Res	Type
25	A	995	C
25	A	996	A
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1033	U
25	A	1034	G
25	A	1040	A
25	A	1043	C
25	A	1045	C
25	A	1046	A
25	A	1047	G
25	A	1053	C
25	A	1054	A
25	A	1057	A
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1065	U
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1072	C
25	A	1076	C
25	A	1079	C
25	A	1084	A
25	A	1088	A
25	A	1097	U
25	A	1104	C
25	A	1106	G
25	A	1112	G
25	A	1116	G
25	A	1132	U
25	A	1135	C
25	A	1136	G
25	A	1137	G
25	A	1142	A

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Mol	Chain	Res	Type
25	A	1148	U
25	A	1155	A
25	A	1165	A
25	A	1172	C
25	A	1174	U
25	A	1175	A
25	A	1178	C
25	A	1179	G
25	A	1180	U
25	A	1183	U
25	A	1186	G
25	A	1204	A
25	A	1205	A
25	A	1210	G
25	A	1211	C
25	A	1212	G
25	A	1213	A
25	A	1227	G
25	A	1237	A
25	A	1238	G
25	A	1247	A
25	A	1248	G
25	A	1250	G
25	A	1251	C
25	A	1253	A
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1287	A
25	A	1300	G
25	A	1301	A
25	A	1306	C
25	A	1314	C
25	A	1325	U
25	A	1326	U
25	A	1332	G
25	A	1345	C
25	A	1352	U
25	A	1365	A
25	A	1368	G
25	A	1379	U

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Mol	Chain	Res	Type
25	A	1383	A
25	A	1386	C
25	A	1395	A
25	A	1416	G
25	A	1417	C
25	A	1421	G
25	A	1428	C
25	A	1429	G
25	A	1453	A
25	A	1454	C
25	A	1458	U
25	A	1459	G
25	A	1475	G
25	A	1482	G
25	A	1498	C
25	A	1504	A
25	A	1515	A
25	A	1524	G
25	A	1533	C
25	A	1536	C
25	A	1558	C
25	A	1559	U
25	A	1560	G
25	A	1567	G
25	A	1568	G
25	A	1569	A
25	A	1578	U
25	A	1581	G
25	A	1583	A
25	A	1584	U
25	A	1608	A
25	A	1617	C
25	A	1618	6MZ
25	A	1627	G
25	A	1646	C
25	A	1647	U
25	A	1648	U
25	A	1649	G
25	A	1665	A
25	A	1669	A
25	A	1674	G
25	A	1682	G

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Mol	Chain	Res	Type
25	A	1695	G
25	A	1698	A
25	A	1715	G
25	A	1716	U
25	A	1729	U
25	A	1730	C
25	A	1732	C
25	A	1733	G
25	A	1738	G
25	A	1758	U
25	A	1764	C
25	A	1773	A
25	A	1781	U
25	A	1782	U
25	A	1784	A
25	A	1791	A
25	A	1800	C
25	A	1801	A
25	A	1808	A
25	A	1809	A
25	A	1812	U
25	A	1816	C
25	A	1829	A
25	A	1833	C
25	A	1847	A
25	A	1857	G
25	A	1870	C
25	A	1873	G
25	A	1884	G
25	A	1899	A
25	A	1901	A
25	A	1906	G
25	A	1913	A
25	A	1919	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1936	A
25	A	1937	A
25	A	1938	A
25	A	1941	C
25	A	1942	C

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Mol	Chain	Res	Type
25	A	1955	U
25	A	1966	A
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1991	U
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2030	6MZ
25	A	2031	A
25	A	2032	G
25	A	2034	U
25	A	2036	C
25	A	2043	C
25	A	2044	C
25	A	2049	G
25	A	2050	C
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	G7M
25	A	2070	A
25	A	2072	C
25	A	2093	G
25	A	2096	C
25	A	2100	G
25	A	2108	A
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2116	G
25	A	2118	U
25	A	2119	A
25	A	2120	G
25	A	2121	G
25	A	2122	U
25	A	2125	G

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Mol	Chain	Res	Type
25	A	2127	G
25	A	2129	C
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2137	U
25	A	2145	C
25	A	2147	A
25	A	2152	G
25	A	2153	C
25	A	2159	G
25	A	2160	C
25	A	2166	U
25	A	2169	A
25	A	2170	A
25	A	2172	U
25	A	2173	A
25	A	2178	C
25	A	2182	U
25	A	2183	A
25	A	2189	U
25	A	2192	U
25	A	2198	A
25	A	2199	A
25	A	2204	G
25	A	2211	A
25	A	2213	U
25	A	2223	G
25	A	2225	A
25	A	2238	G
25	A	2239	G
25	A	2250	G
25	A	2268	A
25	A	2279	G
25	A	2283	C
25	A	2287	A
25	A	2294	G
25	A	2305	U
25	A	2309	A
25	A	2312	U
25	A	2321	U
25	A	2322	A

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Mol	Chain	Res	Type
25	A	2325	G
25	A	2327	A
25	A	2331	G
25	A	2333	A
25	A	2347	C
25	A	2350	C
25	A	2354	C
25	A	2383	G
25	A	2385	C
25	A	2392	A
25	A	2402	U
25	A	2403	C
25	A	2406	A
25	A	2429	G
25	A	2430	A
25	A	2435	A
25	A	2441	U
25	A	2445	2MG
25	A	2447	G
25	A	2448	A
25	A	2464	G
25	A	2470	G
25	A	2476	A
25	A	2484	G
25	A	2494	G
25	A	2502	G
25	A	2503	2MA
25	A	2504	PSU
25	A	2505	G
25	A	2506	U
25	A	2513	A
25	A	2518	A
25	A	2519	U
25	A	2520	C
25	A	2535	G
25	A	2542	A
25	A	2547	A
25	A	2554	U
25	A	2567	G
25	A	2569	G
25	A	2572	A
25	A	2573	C

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Mol	Chain	Res	Type
25	A	2585	U
25	A	2586	U
25	A	2602	A
25	A	2603	G
25	A	2609	U
25	A	2610	C
25	A	2611	C
25	A	2613	U
25	A	2615	U
25	A	2621	G
25	A	2629	U
25	A	2630	G
25	A	2634	A
25	A	2646	C
25	A	2663	G
25	A	2682	A
25	A	2689	U
25	A	2690	U
25	A	2707	U
25	A	2713	U
25	A	2714	G
25	A	2716	C
25	A	2718	G
25	A	2720	U
25	A	2722	G
25	A	2729	G
25	A	2732	G
25	A	2733	A
25	A	2744	G
25	A	2748	A
25	A	2755	C
25	A	2764	A
25	A	2765	A
25	A	2766	A
25	A	2769	U
25	A	2778	A
25	A	2791	G
25	A	2793	C
25	A	2794	C
25	A	2798	U
25	A	2800	A
25	A	2801	G

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Mol	Chain	Res	Type
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2832	U
25	A	2833	U
25	A	2834	G
25	A	2849	U
25	A	2867	G
25	A	2868	A
25	A	2872	A
25	A	2873	A
25	A	2880	C
25	A	2883	A
25	A	2887	A
25	A	2891	U
25	A	2894	G
25	A	2902	C
26	B	4	C
26	B	9	G
26	B	12	C
26	B	13	G
26	B	24	G
26	B	25	U
26	B	26	C
26	B	35	C
26	B	40	U
26	B	41	G
26	B	44	G
26	B	67	G
26	B	68	C
26	B	87	U
26	B	88	C
26	B	89	U
26	B	90	C
26	B	97	C
26	B	109	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G

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Mol	Chain	Res	Type
25	A	205	G
25	A	228	C
25	A	372	G
25	A	512	G
25	A	555	G
25	A	758	C
25	A	774	G
25	A	989	G
25	A	1070	A
25	A	1111	A
25	A	1182	G
25	A	1190	G
25	A	1212	G
25	A	1236	G
25	A	1240	U
25	A	1432	G
25	A	1458	U
25	A	1567	G
25	A	1715	G
25	A	1900	A
25	A	1930	G
25	A	1940	U
25	A	2061	G
25	A	2128	G
25	A	2326	C
25	A	2391	G
25	A	2447	G
25	A	2566	A
25	A	2610	C
25	A	2800	A
25	A	2820	A
25	A	2832	U
25	A	2867	G
26	B	24	G
26	B	66	A
26	B	88	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	A	2580	25	18,21,22	1.56	5 (27%)	22,30,33	1.90	4 (18%)
25	PSU	A	746	25	18,21,22	1.45	4 (22%)	22,30,33	1.90	4 (18%)
1	G7M	a	527	1	23,26,27	1.71	4 (17%)	35,39,42	2.20	8 (22%)
1	5MC	a	967	1	18,22,23	0.99	2 (11%)	26,32,35	1.18	2 (7%)
24	PSU	y	55	24	18,21,22	1.42	3 (16%)	22,30,33	1.90	4 (18%)
24	H2U	y	19	24	18,21,22	1.02	2 (11%)	21,30,33	1.20	2 (9%)
24	5MU	y	54	24	19,22,23	1.41	5 (26%)	28,32,35	1.85	6 (21%)
25	PSU	A	955	25	18,21,22	1.54	4 (22%)	22,30,33	1.87	4 (18%)
25	G7M	A	2069	25	23,26,27	1.82	4 (17%)	35,39,42	2.02	6 (17%)
25	PSU	A	2605	25	18,21,22	1.45	5 (27%)	22,30,33	2.03	4 (18%)
1	2MG	a	1516	1	23,26,27	1.30	3 (13%)	32,38,41	2.25	6 (18%)
1	5MC	a	1407	1	18,22,23	0.88	1 (5%)	26,32,35	1.30	3 (11%)
25	5MC	A	1962	25	18,22,23	0.98	2 (11%)	26,32,35	1.28	2 (7%)
25	PSU	A	2604	25	18,21,22	1.46	4 (22%)	22,30,33	1.77	4 (18%)
25	2MA	A	2503	25	22,25,26	1.40	4 (18%)	33,37,40	2.27	9 (27%)
25	5MU	A	1939	25	19,22,23	1.48	4 (21%)	28,32,35	2.48	6 (21%)
1	2MG	a	966	1	23,26,27	1.25	3 (13%)	32,38,41	2.42	7 (21%)
25	1MG	A	745	25	22,26,27	1.18	2 (9%)	33,39,42	1.66	5 (15%)
1	4OC	a	1402	1	20,23,24	0.82	0	26,32,35	0.94	1 (3%)
25	OMU	A	2552	25	19,22,23	1.22	2 (10%)	26,31,34	1.93	7 (26%)
24	6IA	y	37	24	26,29,30	1.33	5 (19%)	37,41,44	1.95	11 (29%)
25	PSU	A	1917	25	18,21,22	1.44	5 (27%)	22,30,33	2.00	3 (13%)
1	MA6	a	1519	1	23,26,27	1.43	6 (26%)	34,38,41	2.46	15 (44%)
1	2MG	a	1207	1	23,26,27	1.38	4 (17%)	32,38,41	2.18	6 (18%)
25	PSU	A	2457	25	18,21,22	1.65	5 (27%)	22,30,33	2.26	5 (22%)
25	H2U	A	2449	25	18,21,22	1.29	3 (16%)	21,30,33	1.55	4 (19%)
1	MA6	a	1518	1	23,26,27	1.54	5 (21%)	34,38,41	2.30	13 (38%)
25	OMG	A	2251	25,22	23,26,27	1.28	3 (13%)	33,38,41	1.96	5 (15%)
22	H2U	v	20	22	18,21,22	0.99	2 (11%)	21,30,33	1.25	3 (14%)
25	2MG	A	2445	25	23,26,27	1.33	3 (13%)	32,38,41	2.30	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	A	2504	25	18,21,22	1.47	3 (16%)	22,30,33	1.97	4 (18%)
25	3TD	A	1915	25	18,22,23	3.90	7 (38%)	22,32,35	1.83	3 (13%)
1	PSU	a	516	1	18,21,22	1.42	4 (22%)	22,30,33	1.80	4 (18%)
25	5MU	A	747	25	19,22,23	1.41	4 (21%)	28,32,35	1.95	5 (17%)
25	2MG	A	1835	25	23,26,27	1.36	5 (21%)	32,38,41	2.29	7 (21%)
25	6MZ	A	2030	25	22,25,26	1.56	4 (18%)	30,36,39	2.78	10 (33%)
22	5MU	v	54	22	19,22,23	1.33	5 (26%)	28,32,35	1.93	8 (28%)
22	4SU	v	8	22	18,21,22	1.85	4 (22%)	26,30,33	2.50	6 (23%)
1	UR3	a	1498	1	19,22,23	1.01	1 (5%)	26,32,35	1.80	6 (23%)
25	OMC	A	2498	25	19,22,23	1.00	2 (10%)	26,31,34	1.38	3 (11%)
25	PSU	A	1911	25	18,21,22	1.41	5 (27%)	22,30,33	1.95	3 (13%)
25	6MZ	A	1618	25	22,25,26	1.55	4 (18%)	30,36,39	2.46	10 (33%)
22	PSU	v	55	22	18,21,22	1.45	3 (16%)	22,30,33	1.90	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	746	25	-	2/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	1/7/25/26	0/3/3/3
1	5MC	a	967	1	-	2/7/25/26	0/2/2/2
24	PSU	y	55	24	-	2/7/25/26	0/2/2/2
24	H2U	y	19	24	-	6/7/38/39	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
25	G7M	A	2069	25	2/2/5/5	2/7/25/26	0/3/3/3
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
25	5MC	A	1962	25	-	4/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	2/7/25/26	0/2/2/2
25	2MA	A	2503	25	-	4/7/25/26	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
1	4OC	a	1402	1	-	2/9/29/30	0/2/2/2
25	OMU	A	2552	25	-	2/9/27/28	0/2/2/2
24	6IA	y	37	24	-	1/13/31/32	0/3/3/3
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	1/11/29/30	0/3/3/3
1	2MG	a	1207	1	-	1/9/27/28	0/3/3/3
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
1	MA6	a	1518	1	-	3/11/29/30	0/3/3/3
25	OMG	A	2251	25,22	-	0/9/27/28	0/3/3/3
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
25	2MG	A	2445	25	-	2/9/27/28	0/3/3/3
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	2/7/25/26	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
25	5MU	A	747	25	-	0/7/25/26	0/2/2/2
25	2MG	A	1835	25	-	1/9/27/28	0/3/3/3
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	4/7/25/26	0/2/2/2
25	OMC	A	2498	25	-	1/9/27/28	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	2/9/27/28	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	11.51	1.48	1.35
25	A	1915	3TD	C2-N1	8.66	1.48	1.37
25	A	2069	G7M	C5-N7	-5.69	1.32	1.39
25	A	1915	3TD	C6-N1	5.42	1.45	1.36
1	a	527	G7M	C5-N7	-5.30	1.33	1.39
25	A	1618	6MZ	C5-C4	5.19	1.48	1.39
25	A	2030	6MZ	C5-C4	5.11	1.48	1.39
22	v	8	4SU	C4-S4	-4.80	1.59	1.68
1	a	1518	MA6	C5-C4	4.30	1.47	1.39
24	y	37	6IA	C5-C4	4.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2503	2MA	C5-C4	4.01	1.46	1.39
1	a	1519	MA6	C5-C4	3.78	1.46	1.39
25	A	2457	PSU	C4-N3	-3.73	1.31	1.38
25	A	745	1MG	C5-C4	3.57	1.48	1.38
25	A	1939	5MU	C4-N3	-3.55	1.32	1.38
25	A	1835	2MG	C6-N1	-3.36	1.32	1.38
22	v	8	4SU	C5-C4	-3.33	1.38	1.42
25	A	747	5MU	C4-N3	-3.33	1.32	1.38
25	A	2580	PSU	C4-N3	-3.24	1.32	1.38
1	a	527	G7M	C5-C4	3.23	1.46	1.38
25	A	1915	3TD	C2-N3	3.22	1.45	1.38
25	A	2069	G7M	C5-C4	3.21	1.46	1.38
25	A	955	PSU	C4-N3	-3.20	1.32	1.38
25	A	2504	PSU	C4-N3	-3.20	1.32	1.38
22	v	55	PSU	C4-N3	-3.18	1.32	1.38
25	A	2251	OMG	C6-N1	-3.18	1.32	1.38
22	v	8	4SU	C4-N3	-3.17	1.34	1.37
24	y	55	PSU	C6-C5	3.14	1.39	1.35
25	A	1939	5MU	C2-N3	-3.11	1.32	1.38
25	A	2069	G7M	C6-N1	-3.11	1.33	1.38
25	A	2605	PSU	C4-N3	-3.09	1.33	1.38
25	A	2449	H2U	C4-N3	-3.07	1.32	1.37
25	A	2445	2MG	C6-N1	-3.06	1.33	1.38
24	y	54	5MU	C6-C5	3.05	1.39	1.34
22	v	55	PSU	C6-C5	3.05	1.38	1.35
1	a	1207	2MG	C5-C4	3.05	1.47	1.38
25	A	1939	5MU	C6-N1	-3.03	1.32	1.38
1	a	1516	2MG	C6-N1	-3.03	1.33	1.38
25	A	746	PSU	C4-N3	-2.99	1.33	1.38
25	A	2604	PSU	C4-N3	-2.97	1.33	1.38
1	a	516	PSU	C4-N3	-2.97	1.33	1.38
1	a	1207	2MG	C6-N1	-2.96	1.33	1.38
25	A	2449	H2U	C2-N3	-2.93	1.32	1.38
25	A	1915	3TD	O4-C4	-2.92	1.16	1.23
25	A	2457	PSU	C2-N3	-2.91	1.32	1.37
1	a	527	G7M	C6-N1	-2.90	1.33	1.38
25	A	1917	PSU	C4-N3	-2.89	1.33	1.38
24	y	55	PSU	C4-N3	-2.88	1.33	1.38
22	v	54	5MU	C4-N3	-2.87	1.33	1.38
25	A	1911	PSU	C4-N3	-2.86	1.33	1.38
1	a	1516	2MG	C5-C4	2.84	1.46	1.38
25	A	955	PSU	C2-N1	-2.83	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	967	5MC	C6-N1	-2.82	1.33	1.38
25	A	1835	2MG	C5-N7	-2.79	1.33	1.39
25	A	1618	6MZ	C5-C6	2.78	1.49	1.41
1	a	1518	MA6	C4-N9	-2.78	1.31	1.37
25	A	2605	PSU	C6-C5	2.76	1.38	1.35
24	y	54	5MU	C4-N3	-2.76	1.33	1.38
25	A	1917	PSU	C6-C5	2.75	1.38	1.35
1	a	966	2MG	C5-C4	2.73	1.46	1.38
25	A	2580	PSU	C2-N1	-2.71	1.33	1.36
25	A	1962	5MC	C6-N1	-2.71	1.33	1.38
25	A	1911	PSU	C6-C5	2.71	1.38	1.35
22	v	55	PSU	C2-N3	-2.69	1.32	1.37
25	A	2030	6MZ	C5-C6	2.68	1.48	1.41
25	A	2251	OMG	C5-C4	2.65	1.46	1.38
25	A	1962	5MC	C6-C5	2.63	1.38	1.34
1	a	1207	2MG	C5-N7	-2.63	1.34	1.39
22	v	20	H2U	C2-N3	-2.63	1.33	1.38
25	A	2445	2MG	C5-N7	-2.62	1.34	1.39
25	A	1915	3TD	O2-C2	-2.62	1.18	1.23
1	a	516	PSU	C6-C5	2.61	1.38	1.35
25	A	2069	G7M	O2'-C2'	-2.60	1.36	1.43
24	y	19	H2U	C2-N3	-2.60	1.33	1.38
25	A	955	PSU	C2-N3	-2.59	1.33	1.37
25	A	2552	OMU	C4-N3	-2.58	1.33	1.38
25	A	2251	OMG	C5-N7	-2.58	1.34	1.39
25	A	2445	2MG	C5-C4	2.58	1.45	1.38
1	a	966	2MG	C6-N1	-2.57	1.34	1.38
25	A	2605	PSU	C2-N3	-2.57	1.33	1.37
25	A	2604	PSU	C6-C5	2.57	1.38	1.35
25	A	2449	H2U	C2-N1	-2.56	1.32	1.35
24	y	19	H2U	C4-N3	-2.53	1.33	1.37
25	A	747	5MU	C2-N3	-2.53	1.33	1.38
25	A	1835	2MG	C5-C4	2.51	1.45	1.38
25	A	747	5MU	C6-N1	-2.49	1.33	1.38
25	A	746	PSU	C6-C5	2.49	1.38	1.35
1	a	1407	5MC	C6-N1	-2.48	1.33	1.38
25	A	2503	2MA	C5-C6	2.46	1.47	1.41
1	a	1518	MA6	C5-C6	2.46	1.48	1.41
25	A	2503	2MA	C5-N7	-2.45	1.34	1.39
1	a	1519	MA6	C4-N9	-2.44	1.32	1.37
1	a	966	2MG	C5-N7	-2.42	1.34	1.39
1	a	527	G7M	O2'-C2'	-2.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2580	PSU	O4'-C1'	-2.41	1.40	1.43
25	A	2504	PSU	C6-C5	2.41	1.38	1.35
25	A	1917	PSU	C2-N1	-2.40	1.33	1.36
1	a	1518	MA6	C5-N7	-2.40	1.34	1.39
1	a	1519	MA6	C5-N7	-2.40	1.34	1.39
1	a	1519	MA6	C5-C6	2.40	1.47	1.41
1	a	967	5MC	C6-C5	2.39	1.38	1.34
25	A	2604	PSU	C2-N3	-2.38	1.33	1.37
25	A	2580	PSU	C2-N3	-2.38	1.33	1.37
24	y	37	6IA	C5-N7	-2.38	1.34	1.39
25	A	2504	PSU	C2-N3	-2.37	1.33	1.37
25	A	747	5MU	C6-C5	2.37	1.38	1.34
1	a	1518	MA6	C8-N9	-2.36	1.33	1.37
25	A	2580	PSU	C6-C5	2.33	1.38	1.35
25	A	2457	PSU	C6-C5	2.33	1.38	1.35
25	A	2457	PSU	C2-N1	-2.33	1.33	1.36
24	y	37	6IA	C4-N9	-2.32	1.32	1.37
24	y	37	6IA	C8-N7	2.29	1.35	1.31
25	A	2503	2MA	C8-N7	2.29	1.35	1.31
25	A	1915	3TD	C4-N3	2.28	1.45	1.40
24	y	37	6IA	C5-C6	2.28	1.47	1.41
22	v	54	5MU	C6-N1	-2.28	1.34	1.38
1	a	516	PSU	C2-N3	-2.26	1.33	1.37
25	A	746	PSU	O4'-C1'	-2.23	1.40	1.43
22	v	54	5MU	C2-N3	-2.23	1.34	1.38
25	A	2552	OMU	C2-N3	-2.22	1.34	1.38
1	a	1516	2MG	C5-N7	-2.22	1.34	1.39
22	v	54	5MU	C6-C5	2.22	1.38	1.34
25	A	2604	PSU	C2-N1	-2.22	1.33	1.36
1	a	1519	MA6	C8-N9	-2.21	1.33	1.37
24	y	54	5MU	C6-N1	-2.21	1.34	1.38
25	A	1917	PSU	C2-N3	-2.21	1.33	1.37
25	A	2498	OMC	C5-C4	-2.21	1.37	1.42
25	A	1911	PSU	C2-N3	-2.17	1.33	1.37
25	A	746	PSU	C2-N1	-2.17	1.33	1.36
25	A	1911	PSU	C2-N1	-2.17	1.33	1.36
25	A	1835	2MG	C2-N1	-2.16	1.33	1.36
22	v	54	5MU	C4-C5	2.16	1.48	1.44
25	A	2030	6MZ	C5-N7	-2.14	1.35	1.39
25	A	1835	2MG	C4-N9	-2.13	1.32	1.38
25	A	1618	6MZ	C8-N7	2.13	1.35	1.31
24	y	54	5MU	C4-C5	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1498	UR3	C5-C4	-2.12	1.38	1.43
24	y	55	PSU	C2-N3	-2.11	1.33	1.37
25	A	1917	PSU	O4'-C1'	-2.11	1.40	1.43
1	a	1207	2MG	C2-N3	2.10	1.35	1.31
25	A	2498	OMC	C6-N1	-2.10	1.32	1.38
25	A	1618	6MZ	C5-N7	-2.09	1.35	1.39
25	A	2457	PSU	O4'-C1'	-2.09	1.40	1.43
22	v	8	4SU	C2-N1	2.09	1.41	1.38
25	A	2030	6MZ	C8-N7	2.08	1.35	1.31
25	A	2605	PSU	C2-N1	-2.08	1.33	1.36
25	A	955	PSU	C6-C5	2.07	1.37	1.35
1	a	516	PSU	C2-N1	-2.07	1.33	1.36
25	A	745	1MG	C5-N7	-2.06	1.35	1.39
1	a	1519	MA6	C8-N7	2.06	1.35	1.31
25	A	1939	5MU	C6-C5	2.05	1.38	1.34
25	A	2605	PSU	O4'-C1'	-2.05	1.41	1.43
22	v	20	H2U	C4-N3	-2.05	1.34	1.37
25	A	1911	PSU	O4'-C1'	-2.04	1.41	1.43
24	y	54	5MU	C2-N3	-2.02	1.34	1.38

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	C2-N3-C4	8.58	122.67	112.04
25	A	2503	2MA	C5-C4-N3	-8.49	117.64	127.19
25	A	1835	2MG	C2-N3-C4	7.66	121.53	112.04
25	A	2457	PSU	N1-C2-N3	7.58	123.72	115.13
25	A	2445	2MG	C2-N3-C4	7.47	121.31	112.04
1	a	1516	2MG	C2-N3-C4	7.44	121.26	112.04
25	A	2030	6MZ	C9-N6-C6	-7.27	116.61	122.87
22	v	8	4SU	C4-N3-C2	-7.26	120.29	127.34
1	a	1207	2MG	C2-N3-C4	7.16	120.92	112.04
25	A	1618	6MZ	C5-C4-N3	-6.79	117.90	126.75
1	a	966	2MG	C5-C4-N3	-6.59	117.78	128.46
25	A	2445	2MG	C5-C4-N3	-6.45	118.00	128.46
25	A	2504	PSU	N1-C2-N3	6.40	122.38	115.13
25	A	2030	6MZ	C5-C4-N3	-6.36	118.45	126.75
1	a	1207	2MG	C5-C4-N3	-6.33	118.20	128.46
25	A	1939	5MU	C4-N3-C2	-6.31	119.19	127.35
25	A	2503	2MA	N3-C4-N9	6.29	135.71	126.99
1	a	1516	2MG	C5-C4-N3	-6.26	118.30	128.46
25	A	1835	2MG	C5-C4-N3	-6.24	118.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2251	OMG	C5-C4-N3	-6.18	118.43	128.46
25	A	1917	PSU	N1-C2-N3	6.14	122.09	115.13
24	y	55	PSU	N1-C2-N3	6.02	121.95	115.13
1	a	527	G7M	C5-C4-N3	-6.00	116.64	128.15
22	v	8	4SU	C5-C4-N3	5.97	120.23	114.69
1	a	527	G7M	N9-C4-N3	5.95	137.89	125.94
25	A	1911	PSU	N1-C2-N3	5.94	121.86	115.13
25	A	2580	PSU	N1-C2-N3	5.94	121.86	115.13
24	y	37	6IA	C5-C4-N3	-5.83	119.15	126.75
22	v	55	PSU	N1-C2-N3	5.82	121.72	115.13
25	A	1915	3TD	N1-C2-N3	5.81	120.72	116.14
25	A	2605	PSU	N1-C2-N3	5.80	121.70	115.13
22	v	8	4SU	C5-C4-S4	-5.77	117.03	124.47
1	a	516	PSU	N1-C2-N3	5.77	121.67	115.13
25	A	746	PSU	N1-C2-N3	5.75	121.64	115.13
25	A	1939	5MU	C5-C4-N3	5.75	120.22	115.31
1	a	1519	MA6	C5-C4-N3	-5.71	119.30	126.75
25	A	2069	G7M	N9-C4-N3	5.65	137.29	125.94
25	A	2604	PSU	N1-C2-N3	5.62	121.50	115.13
25	A	1939	5MU	C5-C6-N1	-5.44	117.75	123.34
25	A	2069	G7M	C5-C4-N3	-5.43	117.75	128.15
25	A	1939	5MU	N3-C2-N1	5.39	122.04	114.89
25	A	1618	6MZ	N3-C4-N9	5.33	135.87	127.08
25	A	955	PSU	N1-C2-N3	5.32	121.16	115.13
1	a	1518	MA6	C5-C4-N3	-5.22	119.94	126.75
24	y	54	5MU	N3-C2-N1	5.19	121.78	114.89
25	A	1835	2MG	N9-C4-N3	5.18	136.35	125.94
1	a	966	2MG	N9-C4-N3	5.17	136.32	125.94
25	A	2030	6MZ	C6-C5-N7	5.16	137.98	132.39
25	A	2030	6MZ	N3-C4-N9	5.10	135.49	127.08
25	A	745	1MG	C5-C4-N3	-5.07	120.24	128.46
1	a	527	G7M	C2-N3-C4	5.06	121.32	112.30
25	A	2445	2MG	N9-C4-N3	5.04	136.06	125.94
1	a	1518	MA6	C10-N6-C6	-4.93	107.61	120.40
25	A	747	5MU	N3-C2-N1	4.91	121.41	114.89
1	a	1207	2MG	N9-C4-N3	4.89	135.75	125.94
22	v	54	5MU	N3-C2-N1	4.88	121.37	114.89
1	a	1498	UR3	C4-N3-C2	-4.82	120.03	124.56
25	A	747	5MU	C4-N3-C2	-4.75	121.20	127.35
25	A	2251	OMG	C2-N3-C4	4.71	120.70	112.30
25	A	2449	H2U	C4-N3-C2	-4.67	121.92	125.79
25	A	2498	OMC	O2-C2-N3	-4.62	114.82	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2457	PSU	C4-N3-C2	-4.61	119.70	126.34
25	A	1618	6MZ	C6-C5-N7	4.58	137.34	132.39
22	v	54	5MU	C4-N3-C2	-4.57	121.44	127.35
25	A	2605	PSU	C4-N3-C2	-4.53	119.81	126.34
24	y	54	5MU	C4-N3-C2	-4.51	121.52	127.35
1	a	1518	MA6	C2-N1-C6	4.50	122.38	111.75
25	A	1618	6MZ	C2-N3-C4	4.48	122.32	111.75
25	A	2552	OMU	N3-C2-N1	4.47	120.82	114.89
25	A	2251	OMG	N9-C4-N3	4.46	134.90	125.94
25	A	2552	OMU	C4-N3-C2	-4.44	120.72	126.58
1	a	1519	MA6	C2-N1-C6	4.44	122.24	111.75
24	y	37	6IA	N3-C4-N9	4.42	134.36	127.08
1	a	1498	UR3	C1'-N1-C2	4.35	124.34	116.99
25	A	1939	5MU	O4-C4-C5	-4.33	119.89	124.90
25	A	2069	G7M	C2-N3-C4	4.30	119.97	112.30
25	A	1618	6MZ	C9-N6-C6	-4.30	119.17	122.87
25	A	747	5MU	C5-C4-N3	4.28	118.97	115.31
25	A	2030	6MZ	C4-C5-N7	-4.26	105.43	110.62
1	a	1516	2MG	N9-C4-N3	4.19	134.36	125.94
1	a	1519	MA6	N3-C4-N9	4.16	133.94	127.08
25	A	2504	PSU	C4-N3-C2	-4.13	120.38	126.34
25	A	1917	PSU	C4-N3-C2	-4.08	120.45	126.34
25	A	1915	3TD	C4-N3-C2	-4.08	120.19	124.61
25	A	745	1MG	C2-N3-C4	4.07	121.13	111.98
1	a	1498	UR3	O2-C2-N3	-4.05	115.64	121.34
22	v	8	4SU	N3-C2-N1	4.04	120.25	114.89
25	A	746	PSU	C4-N3-C2	-4.04	120.52	126.34
1	a	1519	MA6	C4-C5-N7	-4.03	105.71	110.62
25	A	1911	PSU	C4-N3-C2	-4.03	120.53	126.34
25	A	2552	OMU	C1'-N1-C2	4.02	124.85	117.57
25	A	2030	6MZ	C2-N3-C4	3.98	121.16	111.75
1	a	1518	MA6	N3-C4-N9	3.91	133.53	127.08
1	a	967	5MC	C5-C6-N1	-3.90	119.33	123.34
25	A	745	1MG	N9-C4-N3	3.86	133.69	125.94
1	a	1519	MA6	N1-C6-N6	3.82	121.27	117.08
1	a	1519	MA6	C2-N3-C4	3.81	120.76	111.75
25	A	747	5MU	O4-C4-C5	-3.80	120.50	124.90
25	A	746	PSU	O2-C2-N1	-3.79	118.61	122.79
22	v	55	PSU	C4-N3-C2	-3.79	120.88	126.34
24	y	55	PSU	C4-N3-C2	-3.79	120.88	126.34
25	A	1911	PSU	O2-C2-N1	-3.76	118.65	122.79
25	A	1917	PSU	O2-C2-N1	-3.74	118.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	v	20	H2U	C4-N3-C2	-3.69	122.73	125.79
25	A	2580	PSU	C4-N3-C2	-3.69	121.03	126.34
24	y	37	6IA	C2-N3-C4	3.67	120.43	111.75
25	A	2030	6MZ	C5-N7-C8	3.66	108.71	103.51
1	a	1516	2MG	C6-C5-N7	3.66	137.05	130.25
1	a	1518	MA6	C2-N3-C4	3.65	120.38	111.75
24	y	37	6IA	C6-C5-N7	3.65	136.34	132.39
25	A	1962	5MC	C5-C6-N1	-3.64	119.59	123.34
25	A	955	PSU	C4-N3-C2	-3.63	121.10	126.34
25	A	2552	OMU	C5-C4-N3	3.62	120.25	114.84
25	A	1939	5MU	O2-C2-N1	-3.61	117.99	122.79
25	A	1618	6MZ	C4-C5-N7	-3.59	106.24	110.62
1	a	1519	MA6	C9-N6-C6	-3.57	111.13	120.40
25	A	2580	PSU	O2-C2-N1	-3.57	118.86	122.79
1	a	527	G7M	O3'-C3'-C4'	3.55	121.30	111.05
1	a	1518	MA6	C10-N6-C9	-3.53	104.74	116.12
25	A	1618	6MZ	N1-C2-N3	-3.53	123.08	128.60
22	v	54	5MU	C5-C4-N3	3.52	118.32	115.31
25	A	2069	G7M	O3'-C3'-C4'	3.48	121.11	111.05
1	a	1518	MA6	C4-C5-N7	-3.47	106.39	110.62
1	a	516	PSU	C4-N3-C2	-3.45	121.37	126.34
25	A	2069	G7M	CN7-N7-C5	3.45	131.05	126.77
25	A	955	PSU	C6-C5-C4	-3.44	115.79	118.20
24	y	54	5MU	O4-C4-C5	-3.44	120.92	124.90
1	a	1519	MA6	N1-C2-N3	-3.41	123.27	128.60
1	a	1407	5MC	O2-C2-N3	-3.37	116.85	122.33
25	A	2030	6MZ	C4-N9-C8	3.33	109.34	105.73
22	v	54	5MU	O4-C4-C5	-3.31	121.06	124.90
25	A	747	5MU	C5-C6-N1	-3.29	119.95	123.34
1	a	1519	MA6	C5-N7-C8	3.28	108.18	103.51
1	a	1518	MA6	N1-C2-N3	-3.28	123.47	128.60
24	y	37	6IA	C4-C5-N7	-3.27	106.63	110.62
1	a	527	G7M	O3'-C3'-C2'	3.26	122.36	111.82
24	y	54	5MU	C5-C4-N3	3.25	118.08	115.31
25	A	2504	PSU	O2-C2-N1	-3.24	119.22	122.79
25	A	2503	2MA	C4-C5-N7	-3.23	106.68	110.62
24	y	55	PSU	O2-C2-N1	-3.21	119.26	122.79
25	A	955	PSU	O2-C2-N1	-3.20	119.26	122.79
25	A	2604	PSU	C4-N3-C2	-3.19	121.74	126.34
1	a	1519	MA6	C4-N9-C8	3.18	109.18	105.73
24	y	54	5MU	C5-C6-N1	-3.18	120.07	123.34
25	A	2605	PSU	O2-C2-N1	-3.15	119.33	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2251	OMG	C6-C5-N7	3.10	136.02	130.25
25	A	2498	OMC	O2-C2-N1	3.10	125.29	118.89
1	a	1519	MA6	C10-N6-C6	-3.09	112.39	120.40
25	A	2457	PSU	O2-C2-N1	-3.07	119.41	122.79
1	a	1518	MA6	C9-N6-C6	-3.06	112.46	120.40
22	v	54	5MU	C5-C6-N1	-3.06	120.19	123.34
1	a	1516	2MG	C4-C5-N7	-3.05	105.90	110.72
25	A	2605	PSU	C6-C5-C4	-3.03	116.08	118.20
1	a	966	2MG	C6-C5-N7	3.02	135.86	130.25
1	a	1519	MA6	C10-N6-C9	-3.01	106.43	116.12
1	a	516	PSU	O2-C2-N1	-2.99	119.50	122.79
24	y	37	6IA	N3-C2-N1	-2.98	123.95	128.60
25	A	2030	6MZ	N1-C2-N3	-2.98	123.95	128.60
25	A	745	1MG	C6-C5-N7	2.92	135.96	129.35
25	A	745	1MG	C4-C5-N7	-2.92	106.10	110.72
24	y	19	H2U	C4-N3-C2	-2.90	123.38	125.79
25	A	1962	5MC	C5-C4-N3	-2.90	118.54	121.67
25	A	2445	2MG	C6-C5-N7	2.88	135.61	130.25
22	v	54	5MU	O2-C2-N1	-2.87	118.97	122.79
25	A	2552	OMU	O4-C4-C5	-2.85	120.14	125.16
22	v	55	PSU	C6-C5-C4	-2.85	116.21	118.20
1	a	527	G7M	CN7-N7-C5	2.83	130.28	126.77
25	A	2251	OMG	C4-C5-N7	-2.77	106.33	110.72
25	A	1835	2MG	C6-C5-N7	2.76	135.38	130.25
22	v	54	5MU	C5M-C5-C4	2.74	121.79	118.77
1	a	1519	MA6	N9-C8-N7	-2.73	110.18	113.91
24	y	37	6IA	C4-N9-C8	2.72	108.68	105.73
1	a	1207	2MG	C6-C5-N7	2.68	135.24	130.25
25	A	2604	PSU	O2-C2-N1	-2.67	119.85	122.79
25	A	2449	H2U	C5-C6-N1	-2.67	102.83	111.61
1	a	1498	UR3	C6-N1-C2	-2.66	119.40	121.79
25	A	2457	PSU	O2-C2-N3	-2.66	116.80	121.82
25	A	2069	G7M	O3'-C3'-C2'	2.66	120.41	111.82
25	A	1618	6MZ	C5-N7-C8	2.65	107.28	103.51
25	A	2552	OMU	O2-C2-N3	-2.63	116.60	121.50
25	A	2503	2MA	C5-N7-C8	2.63	107.24	103.51
24	y	37	6IA	C5-N7-C8	2.61	107.21	103.51
22	v	8	4SU	S4-C4-N3	2.57	122.74	120.21
1	a	1407	5MC	C5-C6-N1	-2.56	120.70	123.34
24	y	19	H2U	N3-C2-N1	2.55	119.35	116.65
25	A	2030	6MZ	N9-C8-N7	-2.53	110.46	113.91
1	a	1498	UR3	C3U-N3-C4	2.51	121.48	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2457	PSU	C5-C6-N1	-2.51	118.35	122.11
25	A	1835	2MG	C5-C6-N1	2.49	119.51	113.19
1	a	1407	5MC	C5-C4-N3	-2.48	119.00	121.67
1	a	966	2MG	O6-C6-C5	-2.47	120.04	126.60
1	a	1402	4OC	O2-C2-N3	-2.46	118.34	122.33
25	A	2445	2MG	C2-N1-C6	-2.45	121.66	124.48
1	a	1518	MA6	C6-C5-N7	2.45	137.40	133.28
1	a	1518	MA6	C4-N9-C8	2.43	108.37	105.73
25	A	2498	OMC	C1'-N1-C2	2.43	123.84	118.42
1	a	967	5MC	C5-C4-N3	-2.43	119.05	121.67
1	a	527	G7M	C5-C6-N1	2.41	116.81	111.79
25	A	1835	2MG	C2-N1-C6	-2.39	121.73	124.48
1	a	1519	MA6	C6-C5-N7	2.39	137.30	133.28
25	A	2445	2MG	C4-C5-N7	-2.38	106.96	110.72
22	v	54	5MU	C5M-C5-C6	-2.35	119.71	122.85
25	A	2503	2MA	C2-N1-C6	2.34	121.73	118.08
1	a	1519	MA6	C5-C6-N6	-2.34	121.23	125.30
25	A	1915	3TD	O4-C4-N3	-2.33	116.03	120.30
22	v	20	H2U	C5-C4-N3	2.32	119.26	116.65
1	a	1516	2MG	C2-N1-C6	-2.30	121.83	124.48
24	y	37	6IA	C2'-C1'-N9	-2.30	107.48	113.30
22	v	8	4SU	C1'-N1-C2	2.30	121.73	117.57
22	v	55	PSU	O2-C2-N3	-2.29	117.49	121.82
25	A	2503	2MA	C6-C5-N7	2.29	136.29	132.02
25	A	2503	2MA	N6-C6-N1	2.25	120.21	117.03
25	A	2445	2MG	O6-C6-C5	-2.23	120.67	126.60
25	A	1618	6MZ	C4-N9-C8	2.23	108.14	105.73
25	A	1835	2MG	O6-C6-C5	-2.23	120.69	126.60
1	a	966	2MG	C5-C6-N1	2.22	118.82	113.19
25	A	2503	2MA	C2-N3-C4	2.21	122.42	116.99
1	a	1207	2MG	O6-C6-C5	-2.19	120.79	126.60
25	A	2445	2MG	CM2-N2-C2	-2.17	119.06	123.86
1	a	966	2MG	C4-C5-N7	-2.17	107.29	110.72
22	v	20	H2U	C5-C6-N1	-2.16	104.50	111.61
25	A	746	PSU	C5-C6-N1	-2.16	118.87	122.11
25	A	2503	2MA	C4-N9-C8	2.15	108.06	105.73
24	y	55	PSU	C5-C6-N1	-2.14	118.90	122.11
24	y	37	6IA	N9-C8-N7	-2.14	110.99	113.91
1	a	1207	2MG	C4-C5-N7	-2.13	107.34	110.72
1	a	1518	MA6	C5-N7-C8	2.13	106.53	103.51
1	a	1498	UR3	C1'-N1-C6	-2.11	116.25	120.84
1	a	1518	MA6	N1-C6-N6	2.10	119.38	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	37	6IA	C12-N6-C6	-2.10	119.39	122.95
24	y	54	5MU	O2-C2-N3	-2.10	117.59	121.50
25	A	2445	2MG	C5-C6-N1	2.04	118.38	113.19
25	A	2504	PSU	C5-C6-N1	-2.04	119.04	122.11
25	A	2449	H2U	O2-C2-N1	-2.04	120.54	123.11
1	a	516	PSU	O4'-C1'-C2'	2.04	108.01	105.14
22	v	55	PSU	O4'-C1'-C2'	2.03	108.01	105.14
25	A	2604	PSU	C6-C5-C4	-2.03	116.78	118.20
25	A	2580	PSU	C6-C5-C4	-2.02	116.78	118.20
25	A	2552	OMU	C1'-N1-C6	-2.01	116.46	120.84
1	a	527	G7M	O2'-C2'-C1'	2.01	116.74	110.02
25	A	2449	H2U	O4-C4-N3	2.00	123.46	120.28
25	A	1618	6MZ	C2-N1-C6	2.00	121.97	115.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
25	A	2069	G7M	C4'
25	A	2069	G7M	C3'

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	967	5MC	O4'-C4'-C5'-O5'
1	a	967	5MC	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C4'-C5'-O5'
1	a	1498	UR3	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
22	v	55	PSU	O4'-C1'-C5-C4
22	v	55	PSU	O4'-C1'-C5-C6
24	y	19	H2U	O4'-C1'-N1-C6
24	y	19	H2U	C2'-C1'-N1-C2
24	y	19	H2U	C2'-C1'-N1-C6
24	y	37	6IA	N6-C12-C13-C14
25	A	746	PSU	C2'-C1'-C5-C4
25	A	1618	6MZ	O4'-C4'-C5'-O5'
25	A	1618	6MZ	C3'-C4'-C5'-O5'
25	A	1835	2MG	N3-C2-N2-CM2
25	A	1915	3TD	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
25	A	1915	3TD	O4'-C1'-C5-C6
25	A	1962	5MC	C2'-C1'-N1-C2
25	A	1962	5MC	C2'-C1'-N1-C6
25	A	2030	6MZ	O4'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
25	A	2445	2MG	O4'-C4'-C5'-O5'
25	A	2445	2MG	C3'-C4'-C5'-O5'
25	A	2552	OMU	O4'-C1'-N1-C2
1	a	1402	4OC	C3'-C4'-C5'-O5'
25	A	2069	G7M	O4'-C4'-C5'-O5'
25	A	2503	2MA	O4'-C1'-N9-C8
25	A	2552	OMU	O4'-C1'-N1-C6
25	A	2503	2MA	O4'-C1'-N9-C4
1	a	1402	4OC	O4'-C4'-C5'-O5'
24	y	19	H2U	O4'-C4'-C5'-O5'
25	A	2069	G7M	C3'-C4'-C5'-O5'
24	y	19	H2U	C3'-C4'-C5'-O5'
24	y	55	PSU	C3'-C4'-C5'-O5'
25	A	2604	PSU	O4'-C4'-C5'-O5'
24	y	55	PSU	O4'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C4
25	A	2503	2MA	C4'-C5'-O5'-P
1	a	1518	MA6	O4'-C1'-N9-C8
1	a	1518	MA6	C5-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C9
1	a	527	G7M	C4'-C5'-O5'-P
22	v	20	H2U	C4'-C5'-O5'-P
25	A	1962	5MC	O4'-C1'-N1-C6
25	A	746	PSU	O4'-C1'-C5-C4
25	A	2604	PSU	C3'-C4'-C5'-O5'
25	A	1962	5MC	O4'-C1'-N1-C2
25	A	2503	2MA	O4'-C4'-C5'-O5'
1	a	1207	2MG	C4'-C5'-O5'-P
24	y	19	H2U	O4'-C1'-N1-C2
25	A	2498	OMC	C2'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1402	4OC	1	0
24	y	37	6IA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1518	MA6	2	0
25	A	2251	OMG	1	0
25	A	2445	2MG	1	0
25	A	747	5MU	1	0
25	A	2030	6MZ	1	0
22	v	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	y	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	5(A):A	O3'	6:U	P	3.00
1	y	47(Q):G	O3'	48:G	P	3.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	67(A):U	O3'	68:C	P	3.00
1	y	5:G	O3'	5(A):A	P	2.99
1	y	67:A	O3'	67(A):U	P	2.99
1	y	47:G	O3'	47(A):G	P	2.97

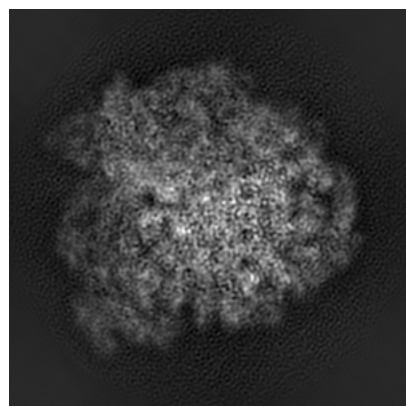
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4125. These allow visual inspection of the internal detail of the map and identification of artifacts.

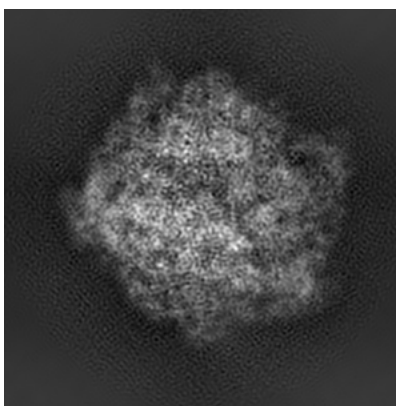
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

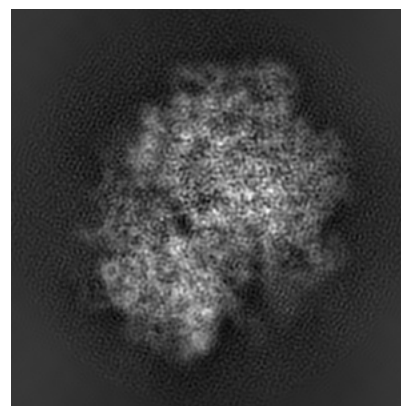
6.1.1 Primary map



X

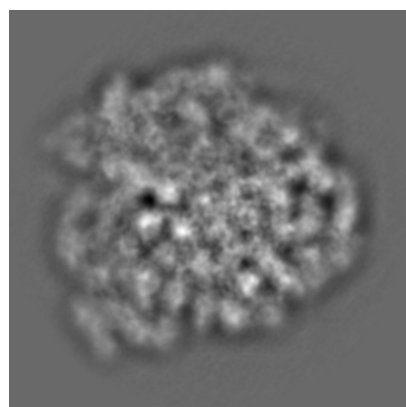


Y

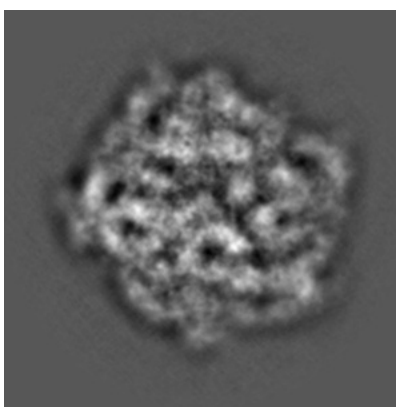


Z

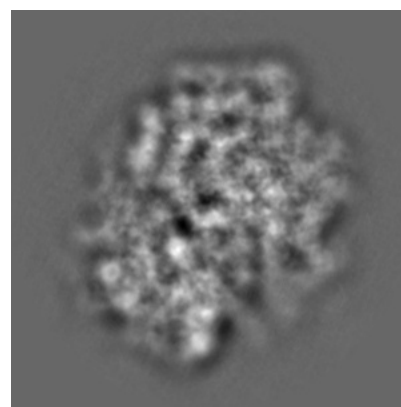
6.1.2 Raw map



X



Y

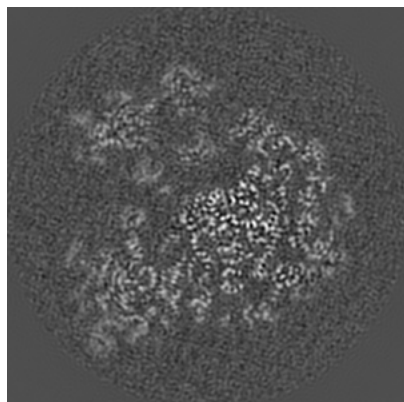


Z

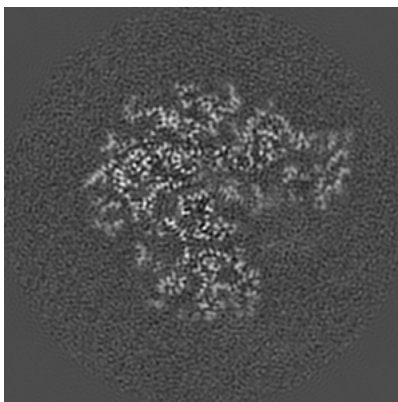
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

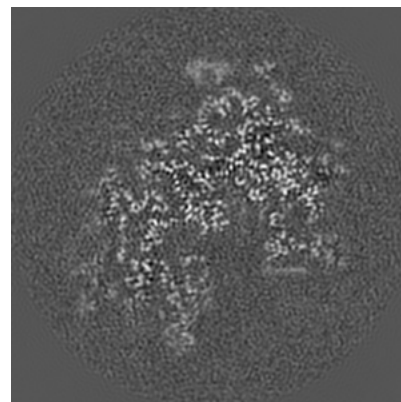
6.2.1 Primary map



X Index: 136

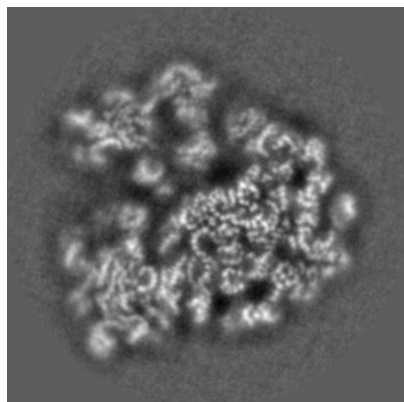


Y Index: 136

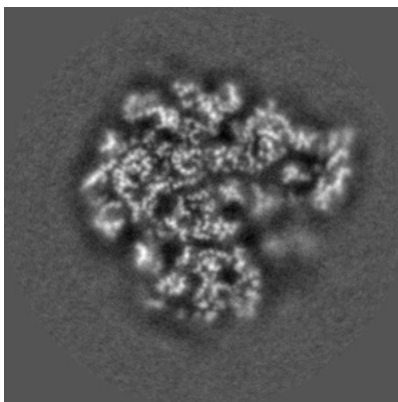


Z Index: 136

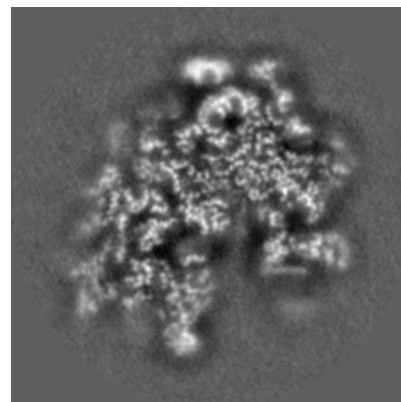
6.2.2 Raw map



X Index: 136



Y Index: 136

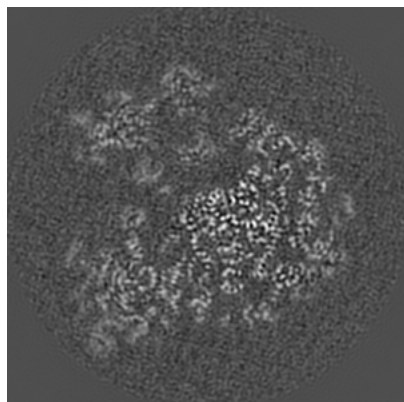


Z Index: 136

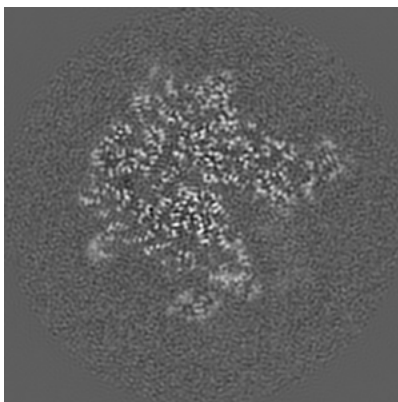
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

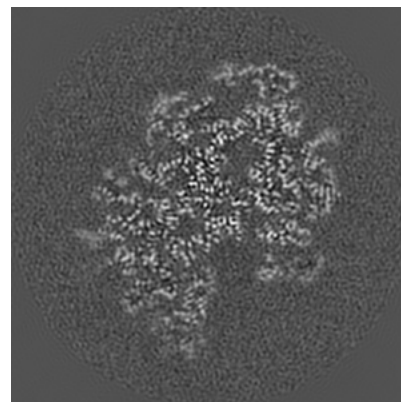
6.3.1 Primary map



X Index: 136

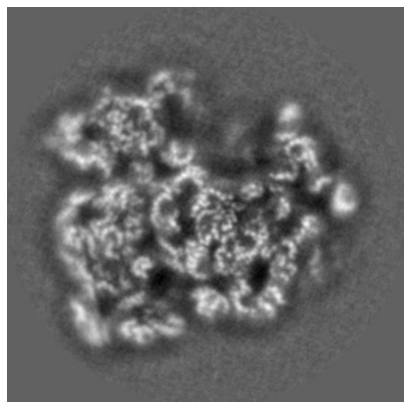


Y Index: 152

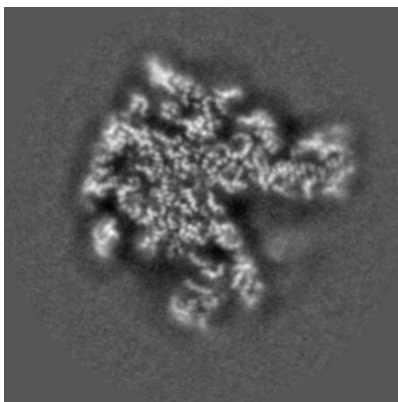


Z Index: 123

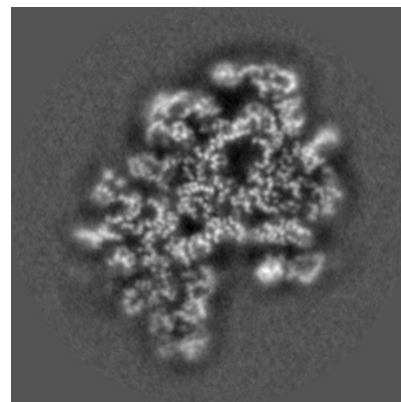
6.3.2 Raw map



X Index: 125



Y Index: 146

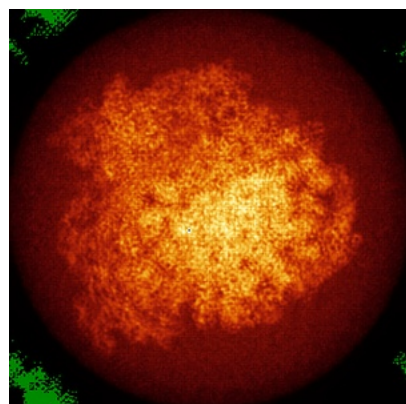


Z Index: 122

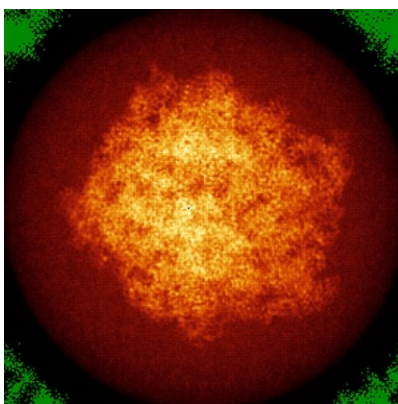
The images above show the largest variance slices of the map in three orthogonal directions.

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

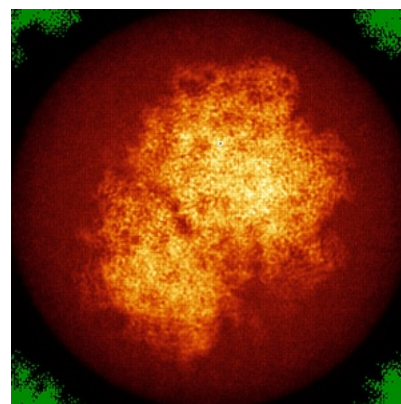
6.4.1 Primary map



X

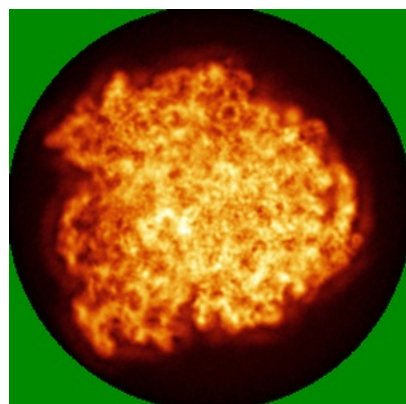


Y

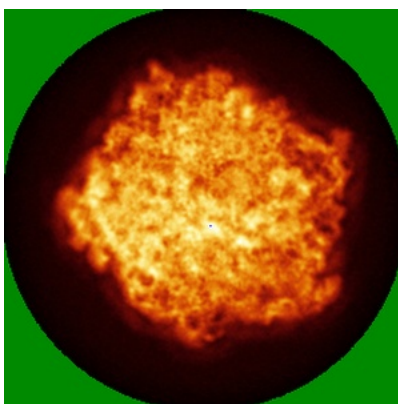


Z

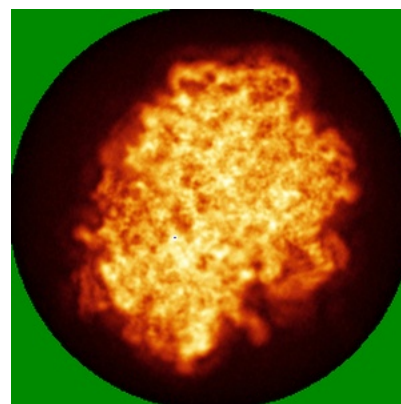
6.4.2 Raw map



X



Y

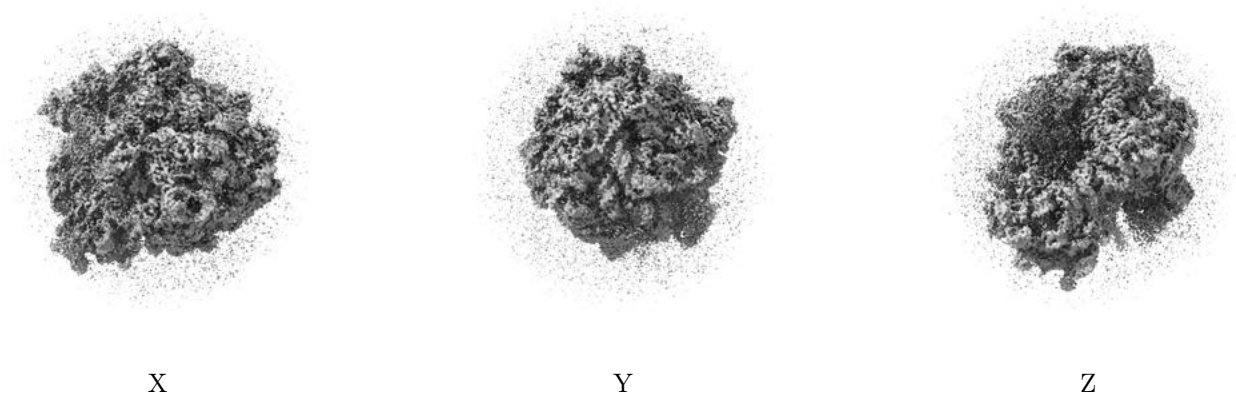


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.54. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

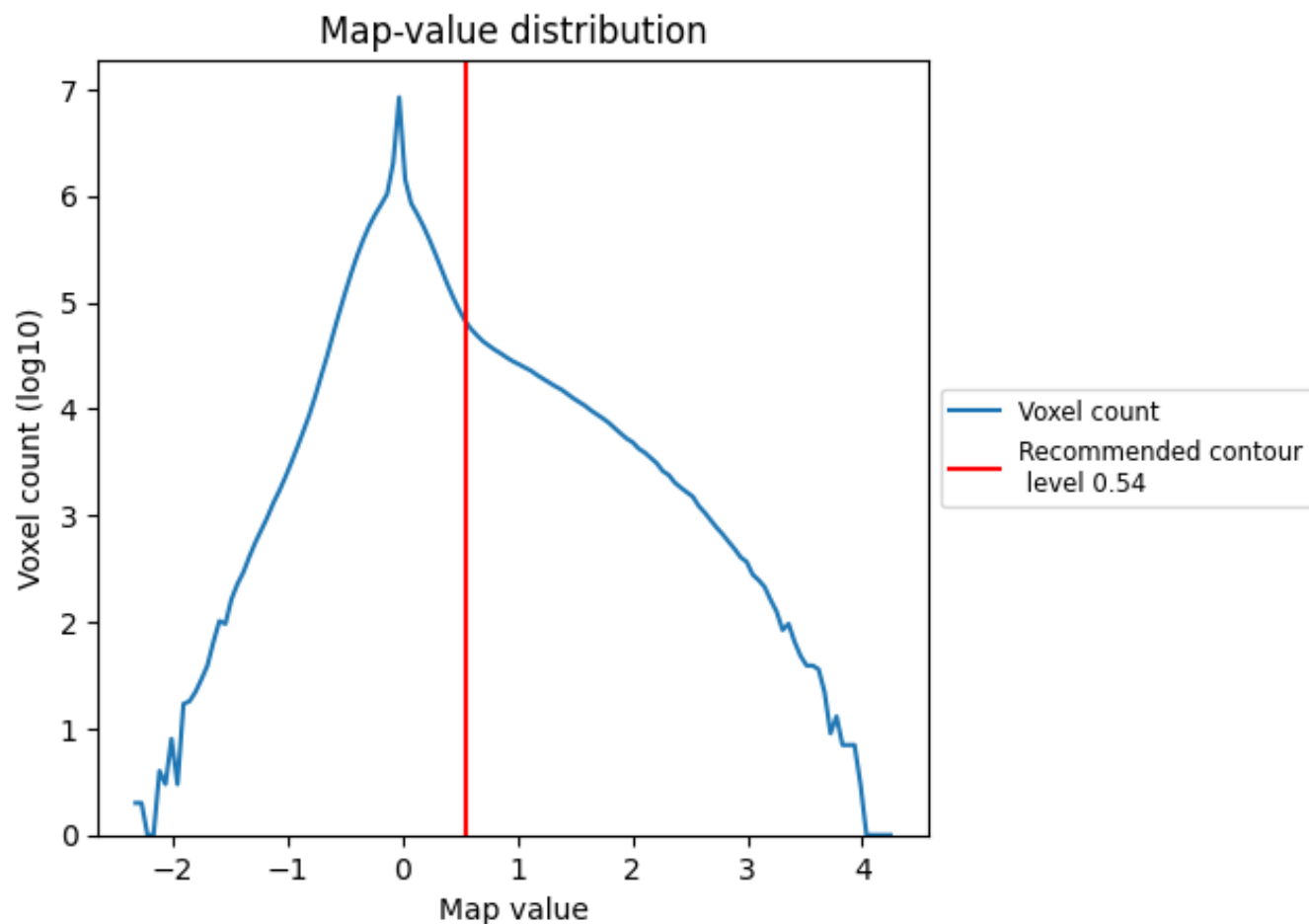
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

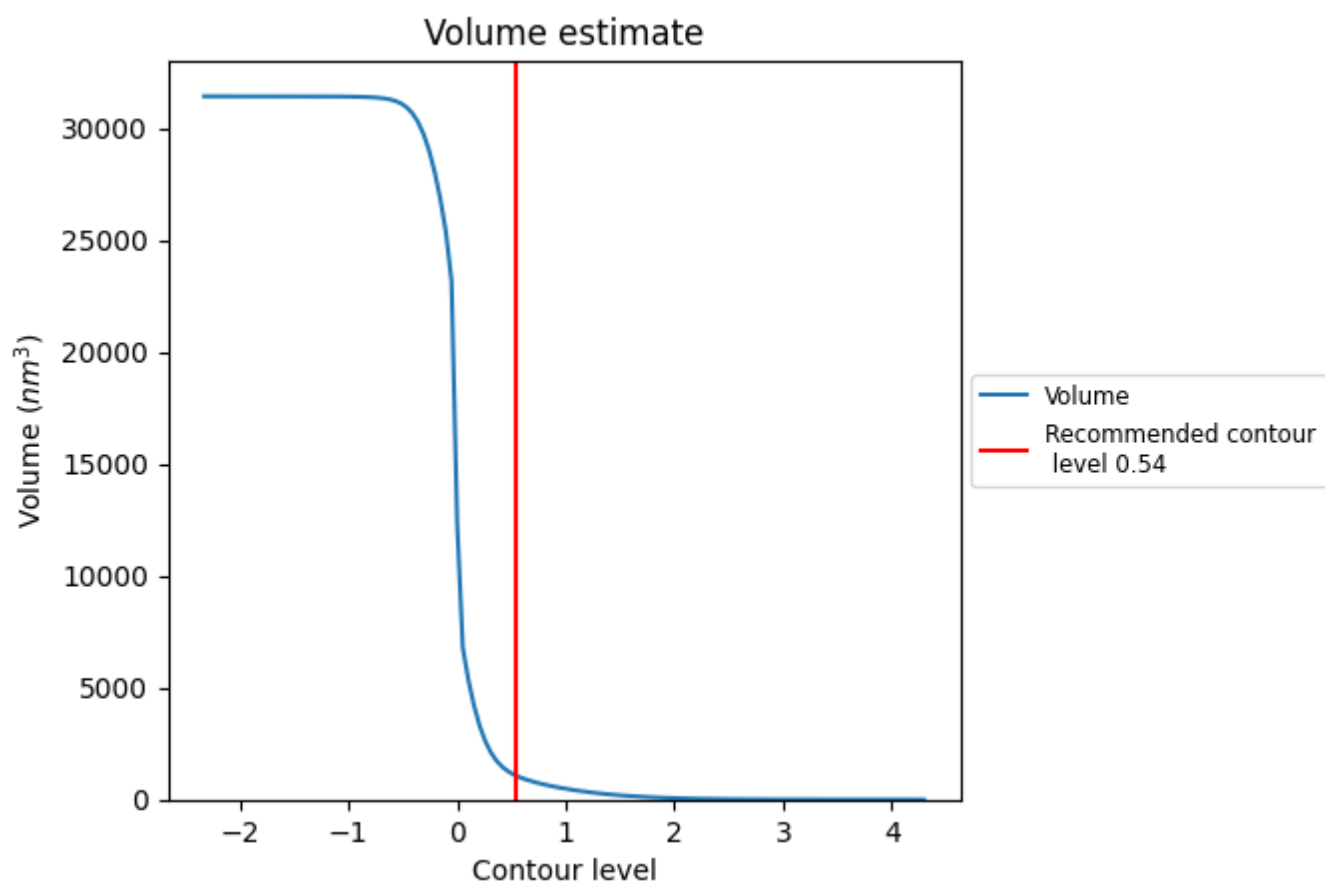
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

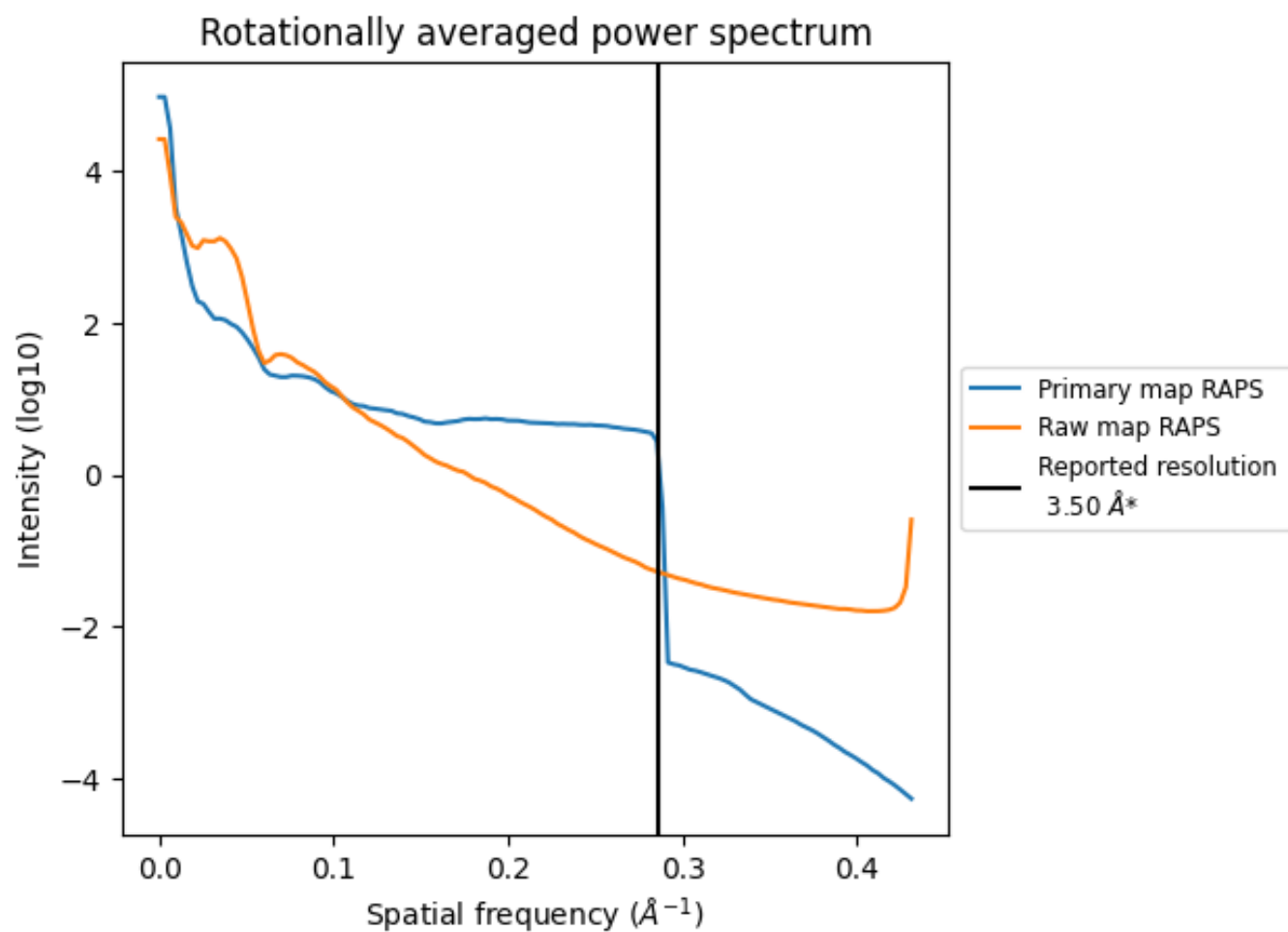
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1075 nm³; this corresponds to an approximate mass of 971 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

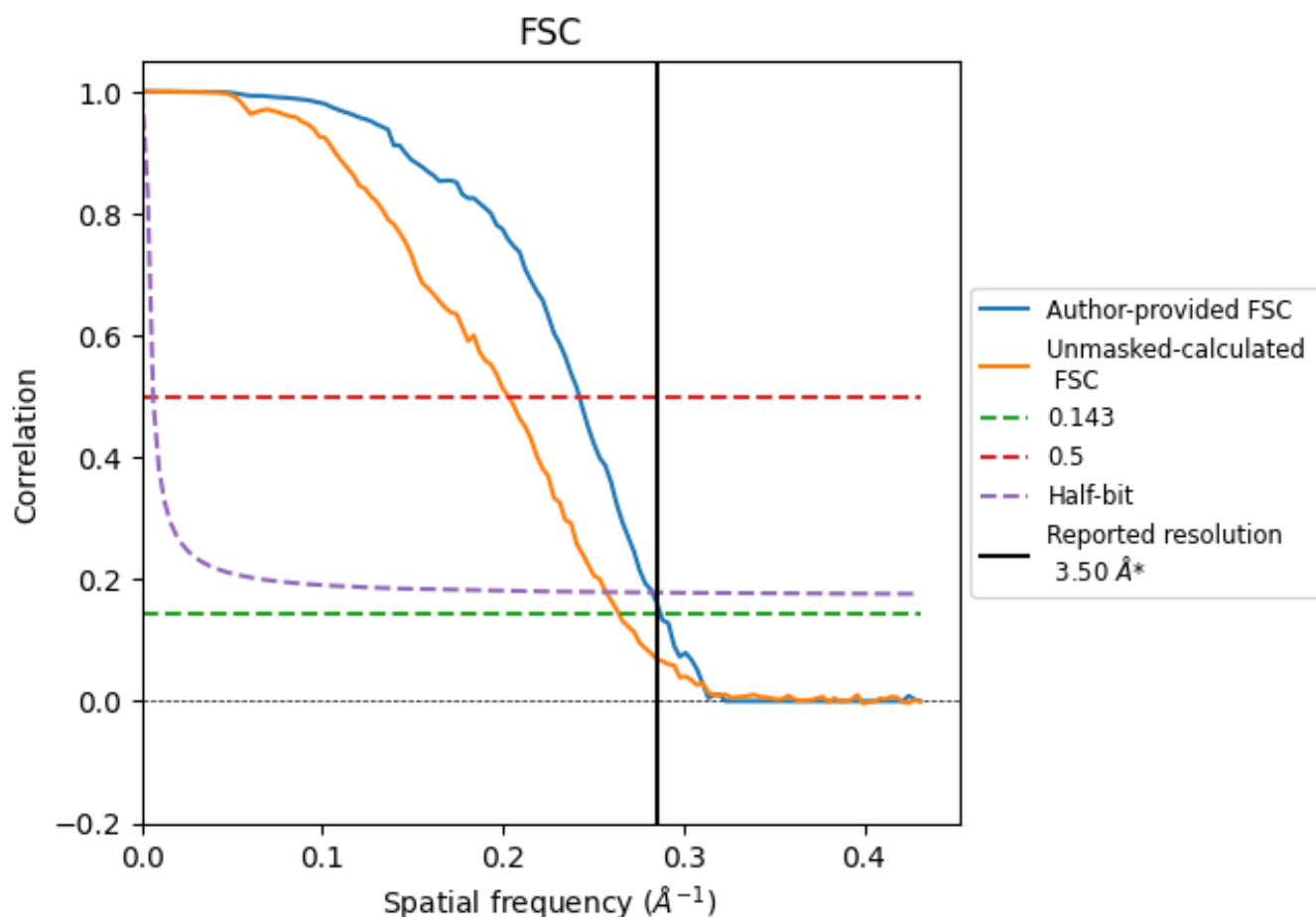


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

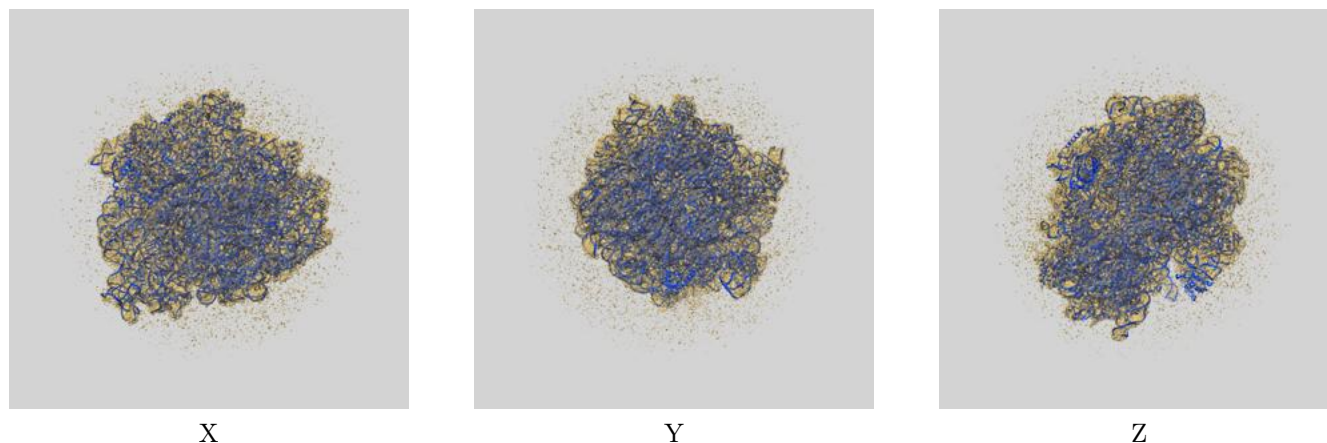
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.13	3.54
Unmasked-calculated*	3.79	4.93	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

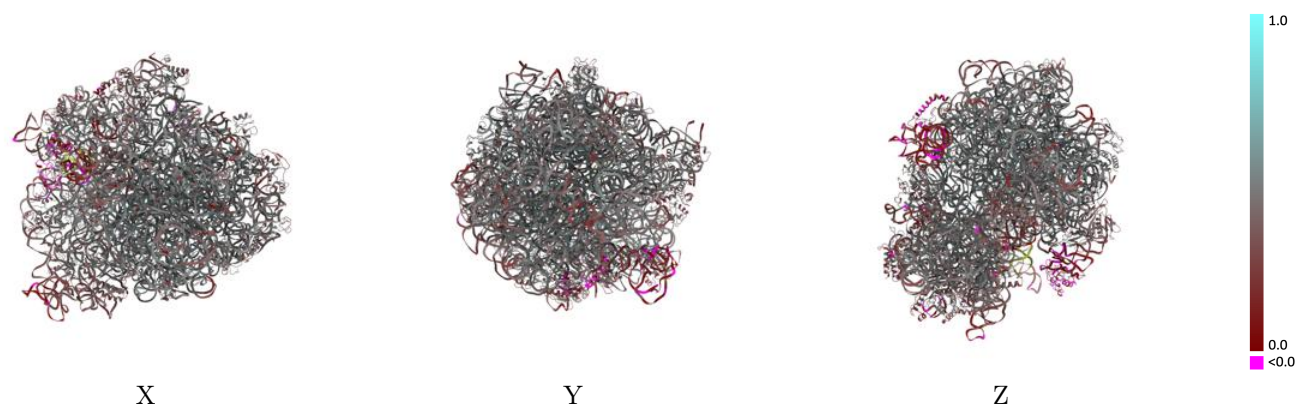
This section contains information regarding the fit between EMDB map EMD-4125 and PDB model 5LZE. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



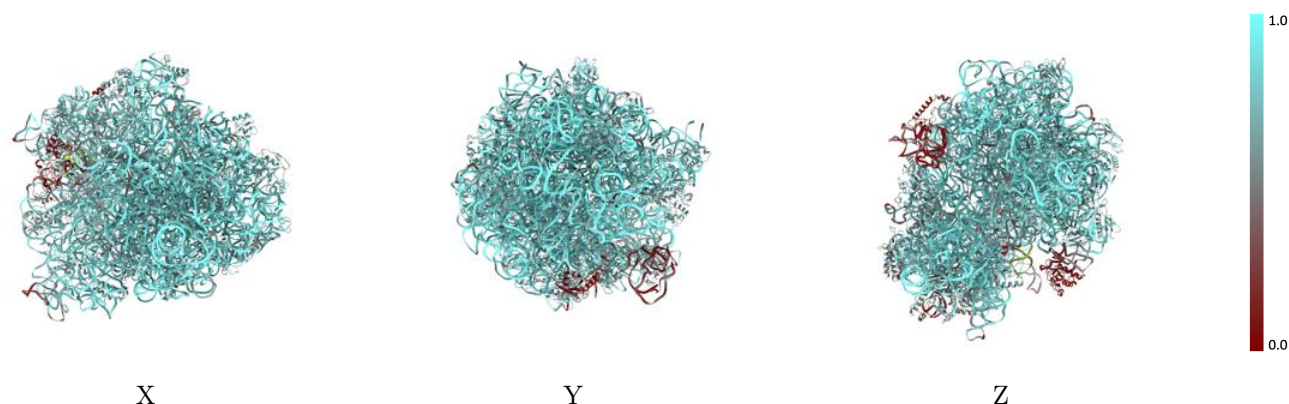
The images above show the 3D surface view of the map at the recommended contour level 0.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



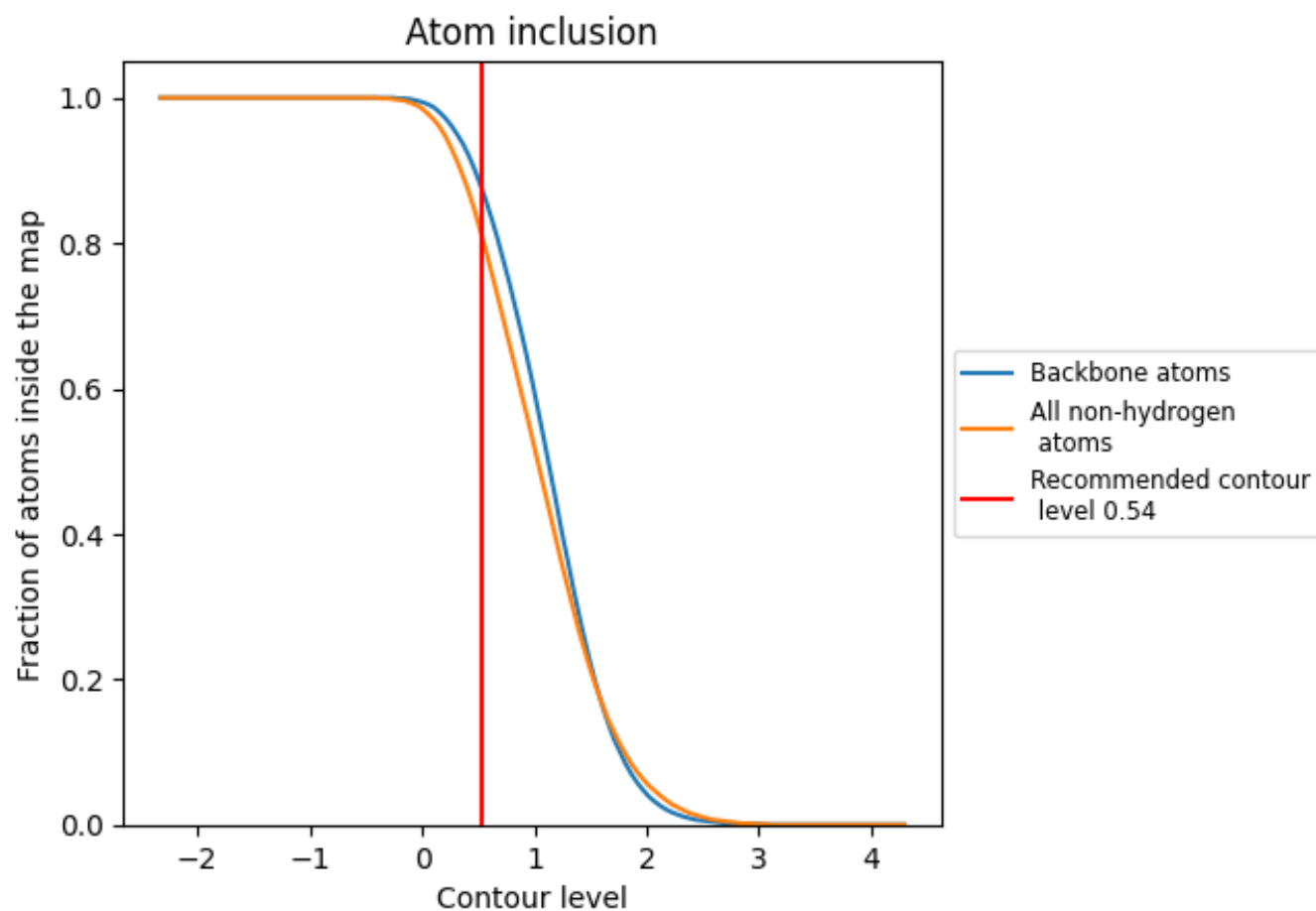
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.54).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.4310
0	 0.7590	 0.4790
1	 0.6740	 0.4220
2	 0.7890	 0.4900
3	 0.7740	 0.5000
4	 0.7470	 0.4460
6	 0.5670	 0.2940
A	 0.8820	 0.4550
B	 0.8910	 0.4310
C	 0.7780	 0.4880
D	 0.7480	 0.4730
E	 0.6990	 0.4310
F	 0.6480	 0.3800
G	 0.6580	 0.3740
H	 0.1840	 0.2040
I	 0.0350	 0.0820
J	 0.7500	 0.4570
K	 0.7390	 0.4600
L	 0.7400	 0.4530
M	 0.7520	 0.4700
N	 0.7560	 0.4760
O	 0.7020	 0.4210
P	 0.7160	 0.4340
Q	 0.7740	 0.4800
R	 0.7390	 0.4440
S	 0.7360	 0.4760
T	 0.6820	 0.4270
U	 0.6800	 0.4120
V	 0.7110	 0.4190
W	 0.7550	 0.4780
X	 0.7550	 0.4720
Y	 0.6500	 0.3680
Z	 0.7510	 0.4610
a	 0.8740	 0.4340
b	 0.5090	 0.3320



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Chain	Atom inclusion	Q-score
c	 0.6780	 0.4250
d	 0.5410	 0.3280
e	 0.7130	 0.4380
f	 0.6880	 0.3830
g	 0.6420	 0.3680
h	 0.7230	 0.4440
i	 0.6820	 0.3960
j	 0.5890	 0.3720
k	 0.7340	 0.4260
l	 0.6710	 0.4280
m	 0.6680	 0.3770
n	 0.7460	 0.4330
o	 0.7350	 0.4180
p	 0.6160	 0.3500
q	 0.6560	 0.3810
r	 0.7310	 0.4280
s	 0.6850	 0.3910
t	 0.6800	 0.3680
u	 0.5560	 0.2790
v	 0.8330	 0.4270
w	 0.2740	 0.3240
x	 0.3140	 0.2170
y	 0.5940	 0.3130