



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:18 PM EDT

PDB ID : 7UVV / pdb_00007uvv
EMDB ID : EMD-26817
Title : A. baumannii ribosome-Streptothricin-F complex: 70S with P-site tRNA
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2022-05-02
Resolution : 2.50 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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

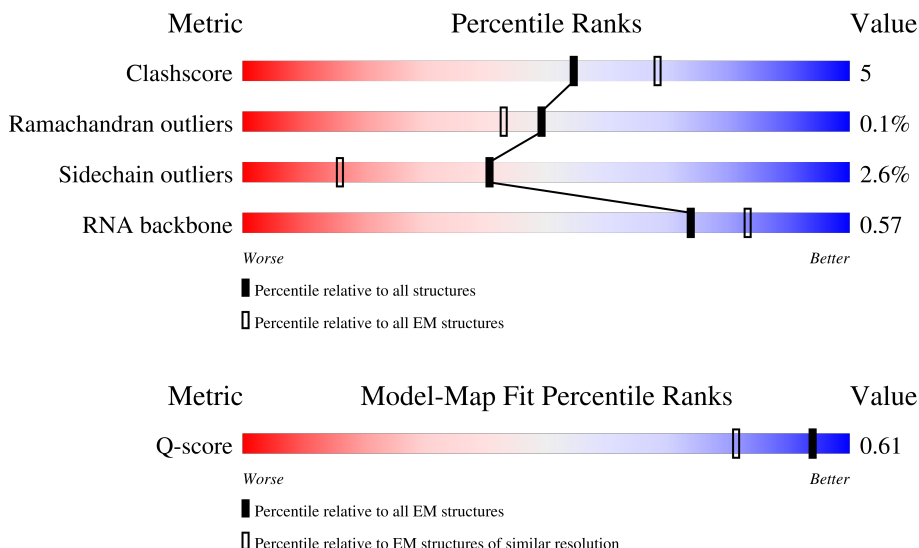
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	0	51	
2	1	44	
3	2	64	

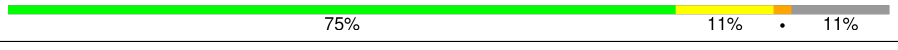
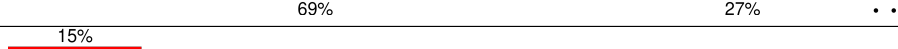
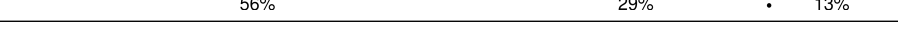
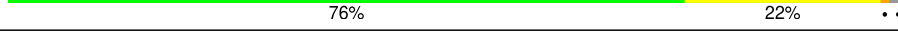
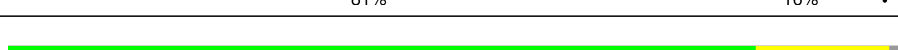
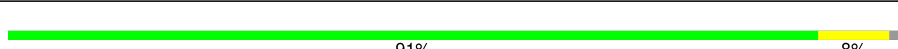
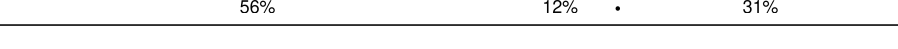
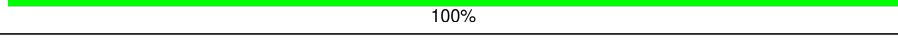
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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	

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Mol	Chain	Length	Quality of chain
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	
52	v	77	
53	w	3	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 138294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	49	Total	C	N	O	S	0	0
			409	263	74	70	2		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2724	Total	C	N	O	P	0	0
			58438	26086	10700	18928	2724		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	45	Total	C	N	O	S	0	0
			334	212	61	60	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	144	Total	C	N	O	S	0	0
			1071	663	213	195			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	117	Total	C	N	O	S	0	0
			919	578	177	164			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	103	Total	C	N	O		0	0
			766	476	142	148			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	83	Total	C	N	O	S	0	0
			620	384	120	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	136	Total	C	N	O	S	0	0
			1073	671	201	194	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total	C	N	O	0	0
			426	273	74	79		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	63	Total	C	N	O	S	0	0
			522	327	105	89	1		

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total	C	N	O	P	S	0	0
			1636	733	291	535	76	1		

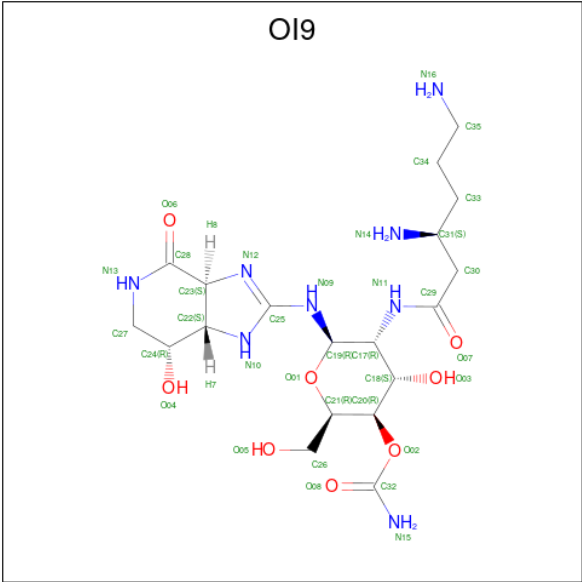
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	

- Molecule 55 is Streptothricin F (CCD ID: OI9) (formula: C₁₉H₃₄N₈O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
55	A	1	Total	C	N	O	0
			35	19	8	8	
55	a	1	Total	C	N	O	0
			35	19	8	8	

3 Residue-property plots [i](#)

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

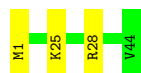
• Molecule 1: 50S ribosomal protein L33

Chain 0:  78% 18% .



• Molecule 2: 50S ribosomal protein L34

Chain 1:  93% 7% .

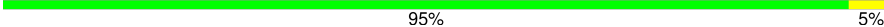


• Molecule 3: 50S ribosomal protein L35

Chain 2:  89% 9% .



• Molecule 4: 50S ribosomal protein L36

Chain 3:  95% 5% .

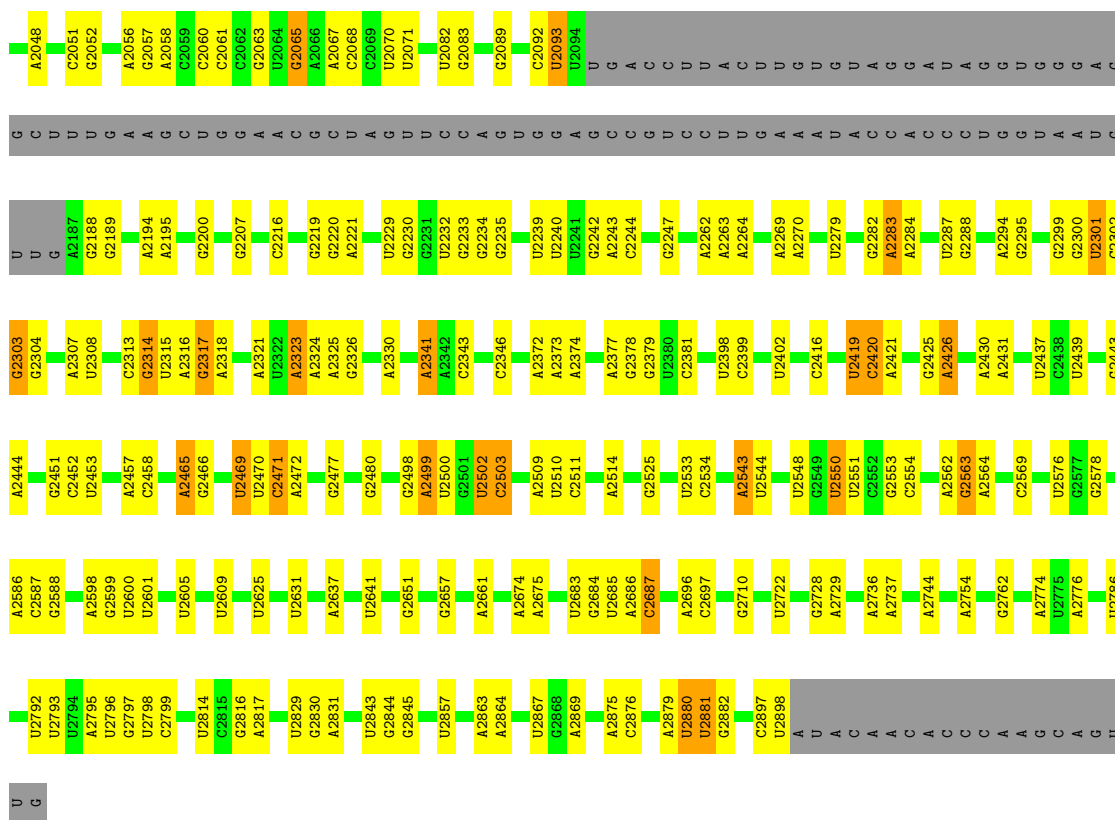


• Molecule 5: 23s ribosomal RNA

Chain A:  68% 23% . 7%



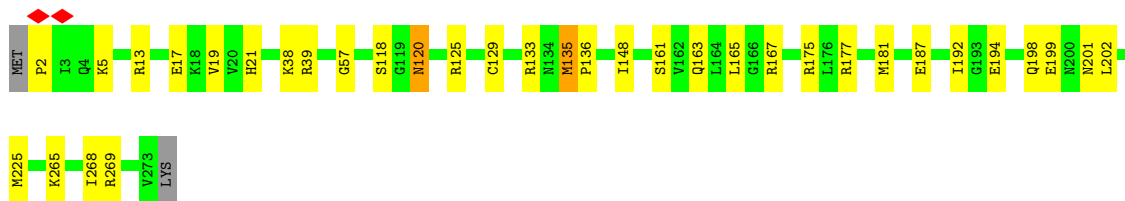
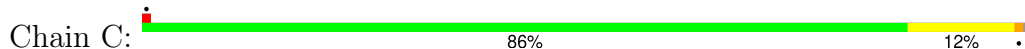
A1915	U1792	A1596	U1502	U1415	G1245	U	G1014	G	A728	U596	U418	U983	
C1916	C1793	U1597	C1503	G1416	A1248	A	G1023	G	G740	A597	C419	U284	A147
G1917	C1796	C1598	U1504	A1422	A1505	U	A1036	U	U741	G598	G423	A285	A148
U1919	A1797	A1606	A1506	C1423	G1251	A	U1030	A	U745	A601	G424	U286	G149
C1920	A1798	A1607	G1507	G1427	G1261	G	A1037	U		U605	C435	U288	U157
	A1799			A1428		C	A1038	C		A606		G989	U158
A1923	G1807		G1510	A1429	G1266	U	G1039	C	G773	A607	C455	U290	G159
A1924			A1511	A1430	A1267	C	C1040	C	G774			G291	C160
G1925	C1812	U1632	G1512	G1431		C	U1043	G	A780	U611	C474	U292	A161
G1926		A1633	C1515	C1432	A1296	U	A1044	A	G782	A612		U293	A162
U1927	A1825	G1634					A1047	C	G783		A478	G297	A170
U1928		A1635	A1518	A1435	A1311	U	G1049	U		G618	A479		C171
G1929	C1828		U1519	A1536	G1312	A	A1051	A	A790		G480	C305	G177
A1932	C1829	A1639	A1520	U1437	U1313	C	G	C	A625	U637	U306	U306	U178
A1933		G1640	G1521	C1438	U1105	C	A1048	C	A630	G482	C307	C307	
A1934	G1835	U1645	G1522	C1315	G1107	A	G1049	A	A631		U308	U308	
U1935	G1836	U1646	A1523	A1316	A1108					G493	G309	G309	A182
		G1647	C1526	A1317	G1109	A			C810				A183
U1951	U1840		U1527	C1442	U1110		A899	G	U811	U498	A313		
	G1841	G1665	G1528	G1445	C1111		C900	C	C812	G499		A313	A188
U1959	G1842		U1529	G1446	G1112		G905	U	A817		G331	G331	A189
A1962	A1843	G1672	A1530	U1447	G1113		A908	A		U503	A332	A332	C190
C1963	G1844			U1448	C1114		A909	G	U825	A504			A198
	G1845	G1680	C1531		C1115				U826		U335	U335	G199
A1966	A1849	U1681	U1532	U1455	U1127		C929	U	G849	U507	U336		
U1967	A1850	C1682	U1533	C1346	G1128	U			U830	C508	C345	C345	A203
G1968		C1683	G1534	U1347	U1129	G	A938	U	A831	A527	G950	G946	A204
	G1853	G1708	U1535	A1348	A1130	C			G832	A528	A347	A347	C205
U1978	A1854	U1709	U1536	A1349	A1131	C	A942	U		G529	A348	A348	A206
			G1537	C1352	C1132	U	G943	U	U837	A531			
G1983			U1538	G1353	G1133	U	A944	U	G838	G532		G351	C215
U1987	G1865	U1718	C1539	U1471	A1140	A	C945	U		U855	U533	G352	C216
G1988	U1866	U1719	G1540	A1472		G	U946	U	G843	U533		C353	
U1989	A1867	G1726	C1541	C1357	G1149	A			A844	A666		A354	G222
	G1868	G1727	G1542			G	U952	U	A845	U544			A223
G2008	C1870	C1731	A1543	A1360	A1166	C	G953	U	U846	C945	A364	A364	
A2009	A1871	U1732	G1544	G1363	U1167	C	C958	U	G546	G546	U365	U365	A228
A2010		U1733			A1168	A			C848	A668	G366	G366	A229
A2011	U1879	G1734	G1558	A1373	C1169	G	G966	U	G854	A675	A367	A367	U235
	G1880	A1735		U1374	U1170	C	U967	U	G855	U684	C368	C368	U236
		G1736	A1564	A1378	U1171	C	G971	U	G856	A561	A370	A370	U236
A2017	A1885			A1381	U1172	C			G857	G568	G371	G371	A240
U2018	A1886	G1742	A1567	U1382	G1173	C	A980	U	G862	U571		G385	U246
C2019			A1568	A1382	U1174	C	G990	U	U707	A572	G395	G395	G255
G2021	G1901	G1749	A1569		A1177	U			U708	A573	A403	A403	G257
U2022	G1902	G1752	A1570	U1400	G1179	A	A993	U	U712		G410	G410	A262
A2026	G1906	G1760	U1576	U1401		A	A997	U	A713	U578	A411	A411	
A2027	U1907		A1577	C1402	G1185	A	A998	U	C715	C579	C412	C412	U278
G2028	A1908	U1578	A1491	G1403	G1186	A	A1006	U	U720	A580	C413	C413	U279
A2029	A1909	A1769	G1579	G1404	G1187	A	U1009	U	C721	A594	A414	A414	A280
	C1910		C1580		U1193	A	C1010	U		G595	G417	G417	A281
G2034	3TD1911	A1776	U1581	G1411	G1187	A			U				G282
U2035		G1497	U1582	C1412	U1193	A			A				
	U1912	G1498	C1583	G1413	U1194	A			G				
	U1913	U1499	A1584	A1414	G1195	C			G				
C2039	A1914	A1500	C1501			G							



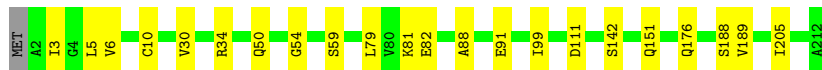
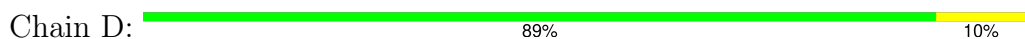
• Molecule 6: 5s ribosomal RNA



• Molecule 7: 50S ribosomal protein L2



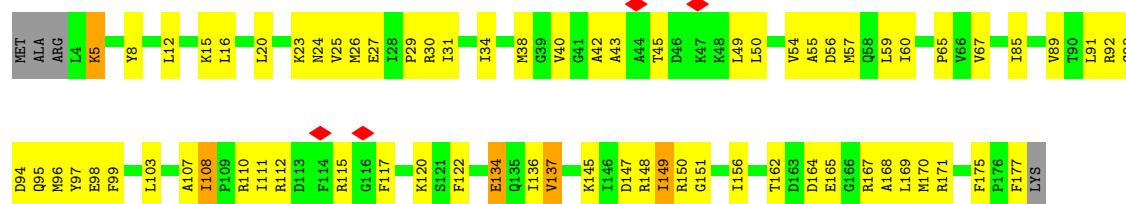
• Molecule 8: 50S ribosomal protein L3



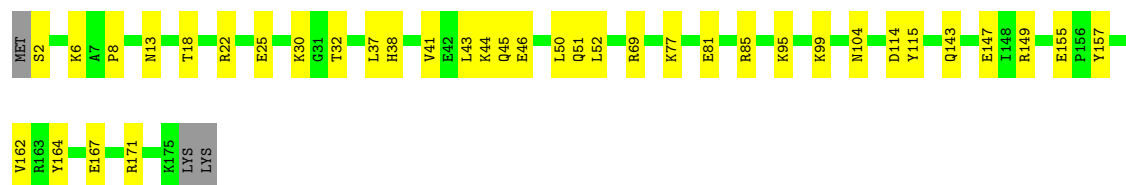
• Molecule 9: 50S ribosomal protein L4

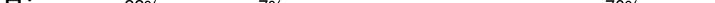
M1	V11	E12	L13	S14	E15	S47	V51	S74	A86	R87	V125	K129	N141	D150	T172	M187	K194	I195	E196	G200
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

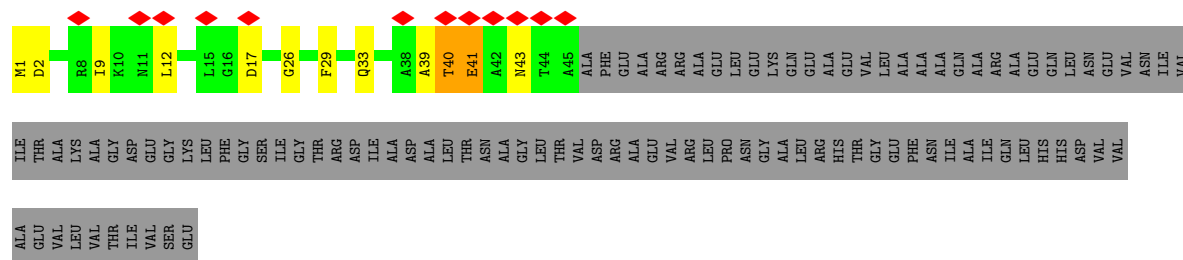
- Chain F: 58% 37%



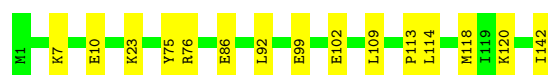
- Chain G: 77% 21%



- Chain H: 



- Chain I: 89% 11%



- Chain J: 81% 17%



- Molecule 15: 50S ribosomal protein L15

Chain K: 92% 7%



- Molecule 16: 50S ribosomal protein L16

Chain L: 87% 13%



- Molecule 17: 50S ribosomal protein L17

Chain M: 90% 5% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 79% 17% 4%



- Molecule 19: 50S ribosomal protein L19

Chain O: 87% 9% 4%



- Molecule 20: 50S ribosomal protein L20

Chain P: 90% 8% 2%



- Molecule 21: 50S ribosomal protein L21

Chain Q: 88% 12%



- Molecule 22: 50S ribosomal protein L22

Chain R: 94% 6%



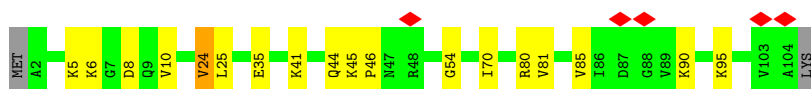
- Molecule 23: 50S ribosomal protein L23

Chain S: 77% 8% 14%



- Molecule 24: 50S ribosomal protein L24

Chain T: 5% 81% 16% ..



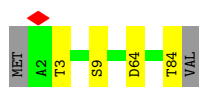
- Molecule 25: 50S ribosomal protein L25

Chain U: 88% 11% .



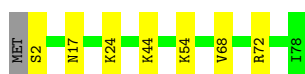
- Molecule 26: 50S ribosomal protein L27

Chain V: 93% 5% .



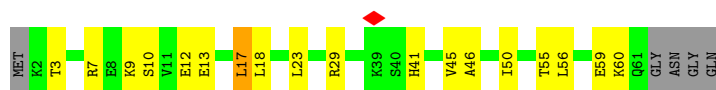
- Molecule 27: 50S ribosomal protein L28

Chain W: 90% 9% .



- Molecule 28: 50S ribosomal protein L29

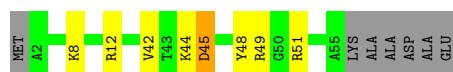
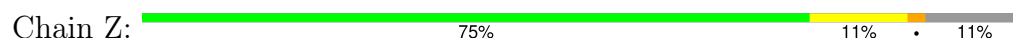
Chain X: 65% 26% 8%



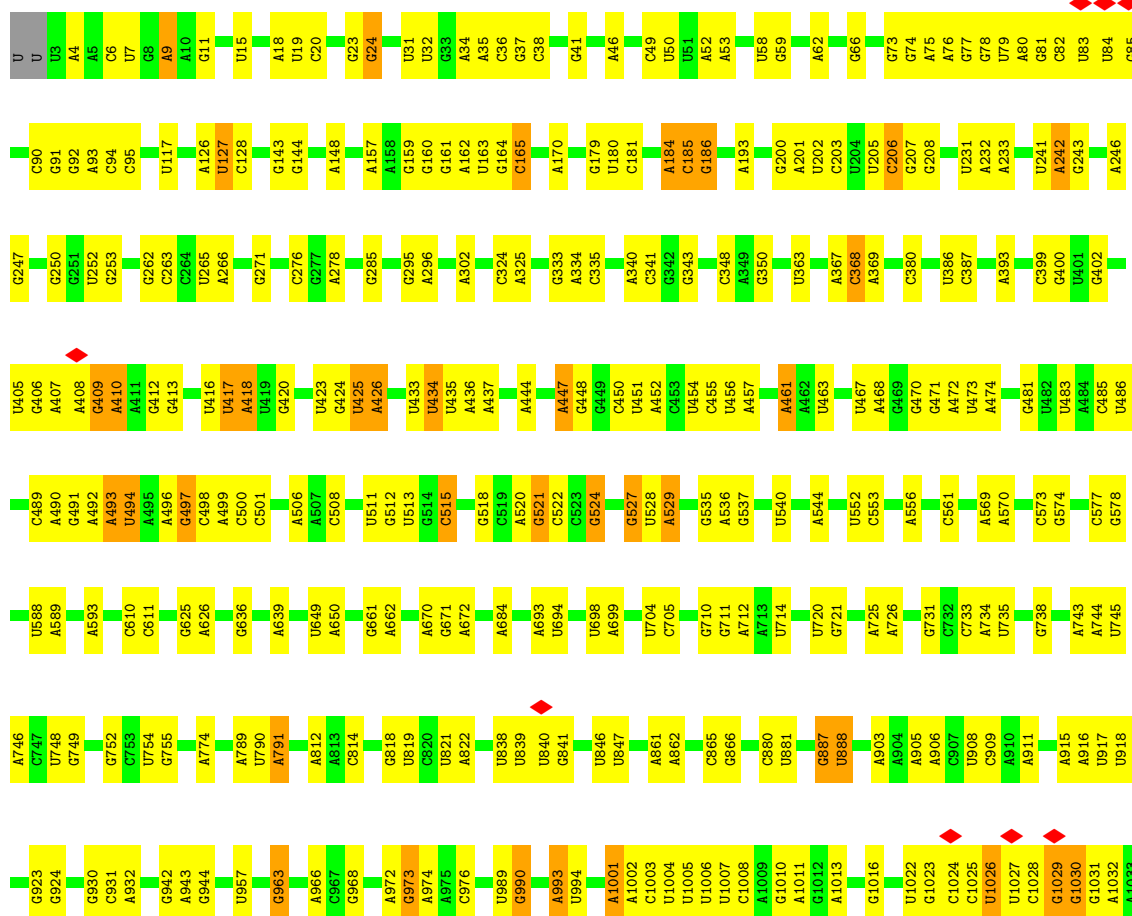
- Molecule 29: 50S ribosomal protein L30

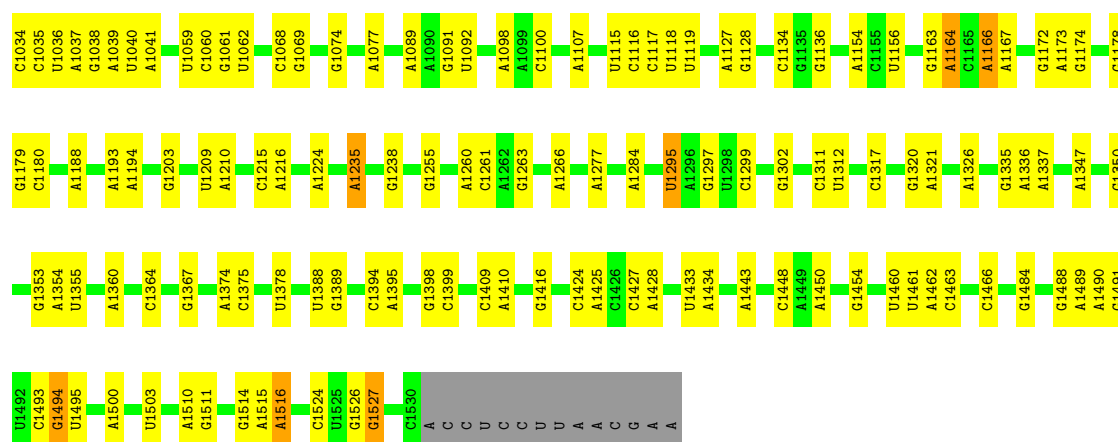


- Molecule 30: 50S ribosomal protein L32

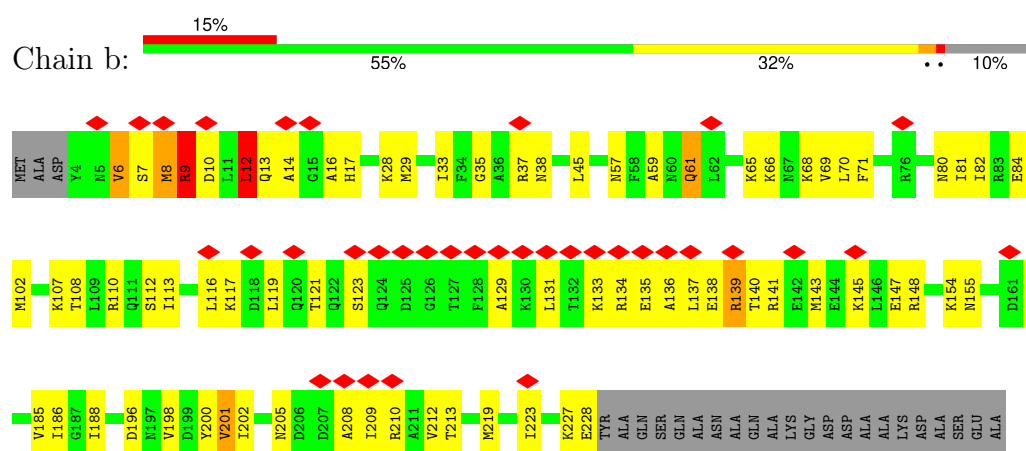


- Molecule 31: 16s Ribosomal RNA

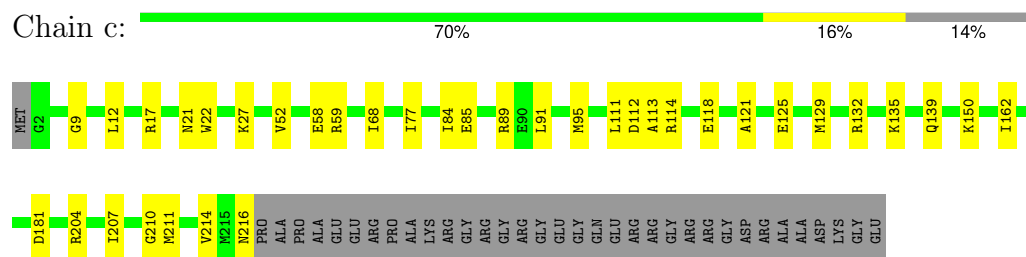




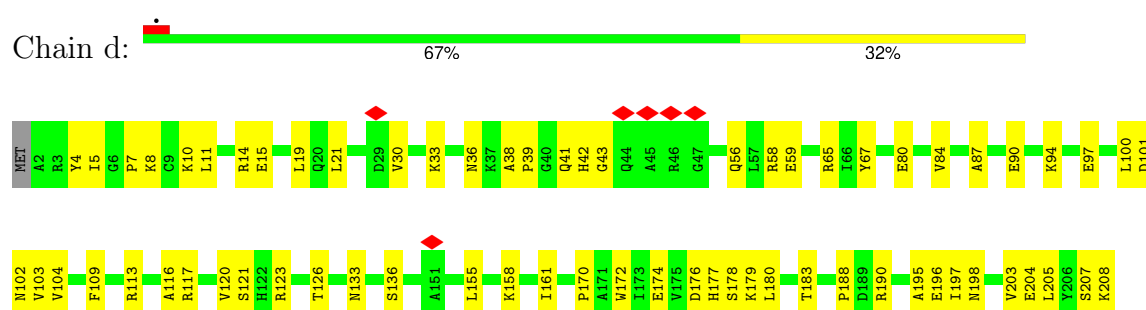
• Molecule 32: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S5

Chain e:  78% 16% 6%



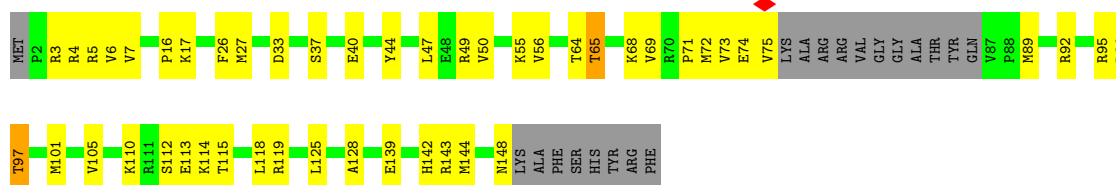
- Molecule 36: 30S ribosomal protein S6

Chain f:  55% 26% 18%



- Molecule 37: 30S ribosomal protein S7

Chain g:  56% 29% 13%



- Molecule 38: 30S ribosomal protein S8

Chain h:  88% 11%



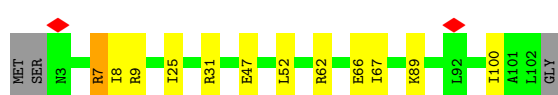
- Molecule 39: 30S ribosomal protein S9

Chain i:  87% 12%



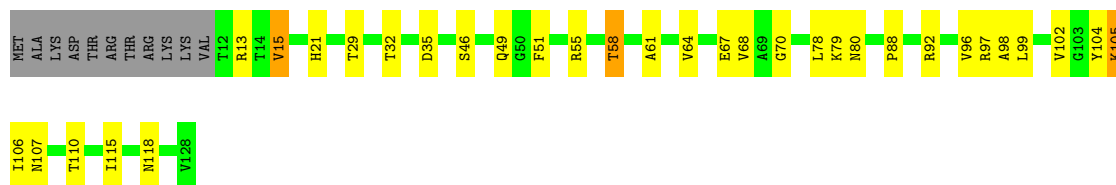
- Molecule 40: 30S ribosomal protein S10

Chain j:  85% 11%



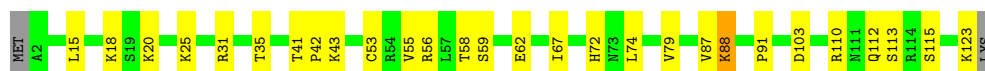
- Molecule 41: 30S ribosomal protein S11

Chain k:  66% 23% 9%



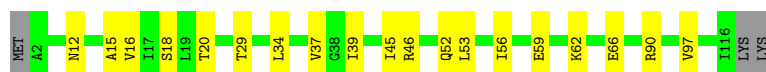
- Molecule 42: 30S ribosomal protein S12

Chain l:  76% 22% ..



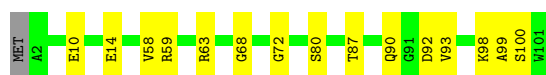
- Molecule 43: 30S ribosomal protein S13

Chain m:  81% 16% .



- Molecule 44: 30S ribosomal protein S14

Chain n:  84% 15% .



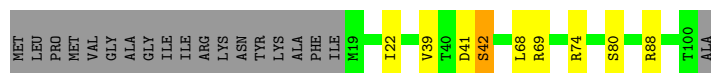
- Molecule 45: 30S ribosomal protein S15

Chain o:  91% 8% .



- Molecule 46: 30S ribosomal protein S16

Chain p:  72% 8% 19%

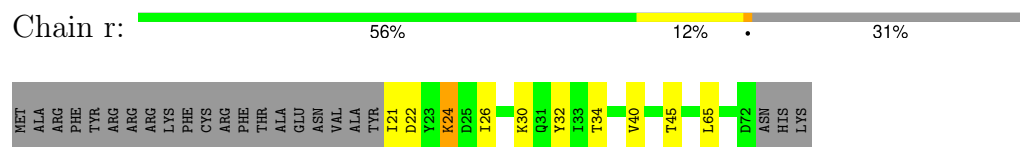


- Molecule 47: 30S ribosomal protein S17

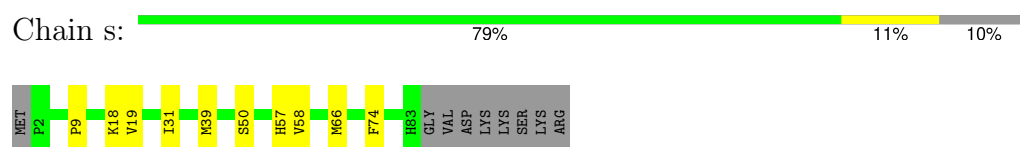
Chain q:  76% 15% 7%



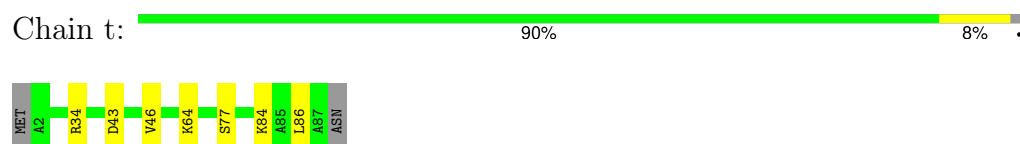
- Molecule 48: 30S ribosomal protein S18



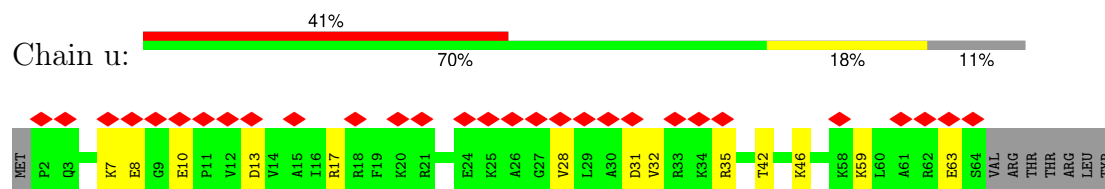
- Molecule 49: 30S ribosomal protein S19



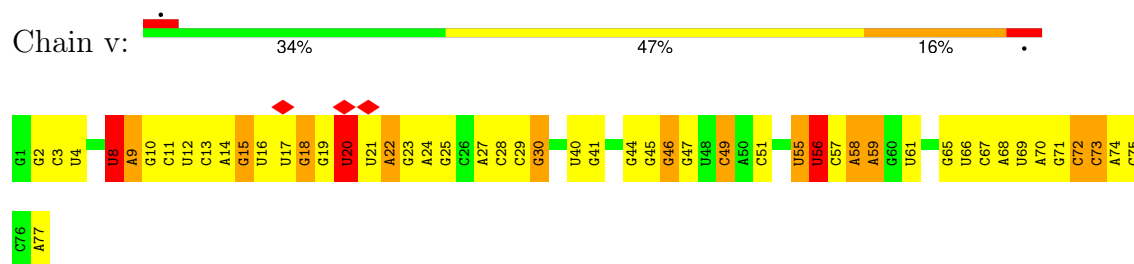
- Molecule 50: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S21



- Molecule 52: tRNA-met



- Molecule 53: mRNA



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53114	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.334	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 6MZ, MA6, 5MC, OMU, 5MU, 2MG, 4OC, OMG, 7MG, 4SU, PSU, 2MA, UR3, OI9, H2U, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.19	0/416	0.44	0/552
2	1	0.18	0/367	0.38	0/481
3	2	0.17	0/515	0.42	0/678
4	3	0.19	0/296	0.36	0/389
5	A	0.20	0/65086	0.32	0/101513
6	B	0.16	0/2739	0.27	0/4266
7	C	0.20	0/2152	0.44	0/2891
8	D	0.19	0/1590	0.38	0/2142
9	E	0.19	0/1537	0.39	0/2073
10	F	0.18	0/1390	0.48	0/1863
11	G	0.17	0/1337	0.41	0/1807
12	H	0.14	0/336	0.44	0/450
13	I	0.19	0/1151	0.42	0/1551
14	J	0.20	0/956	0.40	0/1286
15	K	0.19	0/1079	0.44	0/1439
16	L	0.19	0/1104	0.40	0/1475
17	M	0.21	0/956	0.41	0/1282
18	N	0.17	0/865	0.41	0/1156
19	O	0.18	0/931	0.41	0/1249
20	P	0.21	0/947	0.36	0/1262
21	Q	0.18	0/818	0.37	0/1094
22	R	0.18	0/831	0.36	0/1113
23	S	0.18	0/716	0.37	0/957
24	T	0.14	0/770	0.35	0/1034
25	U	0.18	0/770	0.45	0/1036
26	V	0.20	0/628	0.42	0/839
27	W	0.17	0/642	0.36	0/856
28	X	0.15	0/487	0.36	0/646
29	Y	0.19	0/460	0.34	0/614
30	Z	0.18	0/453	0.36	0/604
31	a	0.18	0/36476	0.30	0/56895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.27	0/1799	0.64	5/2429 (0.2%)
33	c	0.18	0/1714	0.39	0/2304
34	d	0.17	0/1653	0.44	0/2213
35	e	0.19	0/1141	0.38	0/1537
36	f	0.17	0/882	0.45	0/1189
37	g	0.19	0/1087	0.47	0/1456
38	h	0.18	0/993	0.37	0/1331
39	i	0.20	0/1002	0.46	0/1339
40	j	0.19	0/811	0.46	0/1096
41	k	0.18	0/878	0.41	0/1189
42	l	0.18	0/958	0.46	0/1284
43	m	0.18	0/913	0.42	0/1226
44	n	0.19	0/803	0.36	0/1071
45	o	0.18	0/715	0.31	0/958
46	p	0.17	0/655	0.38	0/879
47	q	0.15	0/628	0.38	0/847
48	r	0.17	0/432	0.36	0/583
49	s	0.18	0/664	0.36	0/897
50	t	0.20	0/669	0.35	0/892
51	u	0.13	0/528	0.32	0/697
52	v	0.18	0/1739	0.33	0/2709
53	w	0.14	0/72	0.19	0/110
All	All	0.19	0/149537	0.34	5/223729 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
32	b	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	8	MET	CA-CB-CG	7.32	128.73	114.10
32	b	9	ARG	CA-CB-CG	6.90	127.89	114.10
32	b	12	LEU	CA-C-N	-5.91	112.78	122.54
32	b	12	LEU	C-N-CA	-5.91	112.78	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	8	MET	CB-CG-SD	5.55	129.36	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	51	ALA	Peptide
32	b	139	ARG	Sidechain
32	b	9	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	409	0	437	6	0
2	1	363	0	401	2	0
3	2	509	0	566	4	0
4	3	295	0	326	1	0
5	A	58438	0	29389	334	0
6	B	2450	0	1241	16	0
7	C	2111	0	2176	27	0
8	D	1572	0	1610	11	0
9	E	1516	0	1569	11	0
10	F	1370	0	1420	54	0
11	G	1318	0	1373	22	0
12	H	334	0	363	8	0
13	I	1125	0	1148	10	0
14	J	946	0	1007	19	0
15	K	1071	0	1141	8	0
16	L	1087	0	1162	10	0
17	M	942	0	987	4	0
18	N	857	0	899	14	0
19	O	919	0	973	10	0
20	P	934	0	997	7	0
21	Q	807	0	842	6	0
22	R	826	0	894	4	0
23	S	710	0	768	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	T	766	0	816	11	0
25	U	760	0	783	9	0
26	V	620	0	629	2	0
27	W	632	0	667	3	0
28	X	486	0	528	14	0
29	Y	455	0	476	3	0
30	Z	447	0	435	7	0
31	a	32782	0	16508	244	0
32	b	1769	0	1787	62	0
33	c	1690	0	1774	23	0
34	d	1631	0	1691	42	0
35	e	1129	0	1174	16	0
36	f	867	0	868	19	0
37	g	1073	0	1118	34	0
38	h	985	0	1047	10	0
39	i	991	0	1048	10	0
40	j	801	0	832	7	0
41	k	862	0	877	21	0
42	l	945	0	998	17	0
43	m	903	0	962	11	0
44	n	792	0	833	8	0
45	o	705	0	712	5	0
46	p	644	0	655	6	0
47	q	621	0	665	7	0
48	r	426	0	447	9	0
49	s	646	0	663	4	0
50	t	663	0	715	4	0
51	u	522	0	565	10	0
52	v	1636	0	835	31	0
53	w	65	0	33	0	0
54	3	1	0	0	0	0
55	A	35	0	0	0	0
55	a	35	0	0	0	0
All	All	138294	0	92830	1168	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 5.

All (1168) 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)
31:a:74:G:H1	31:a:93:A:N6	1.56	1.03
32:b:135:GLU:HG3	32:b:139:ARG:HH12	1.22	1.01
52:v:27:A:H61	52:v:45:G:H1	1.01	0.93
5:A:1036:A:H61	5:A:1113:G:H1	1.04	0.92
32:b:135:GLU:HG3	32:b:139:ARG:NH1	1.90	0.86
5:A:2093:U:H3	5:A:2188:G:H1	0.87	0.84
10:F:38:MET:HG3	10:F:57:MET:HE2	1.59	0.84
10:F:43:ALA:HA	10:F:49:LEU:HD21	1.61	0.83
52:v:27:A:N6	52:v:45:G:H1	1.76	0.82
5:A:1521:G:H1	5:A:1544:G:H22	1.26	0.82
5:A:1036:A:N6	5:A:1113:G:H1	1.77	0.81
31:a:74:G:N2	31:a:93:A:N1	2.28	0.81
43:m:59:GLU:OE1	43:m:62:LYS:NZ	2.13	0.81
8:D:30:VAL:O	8:D:188:SER:OG	1.99	0.80
31:a:417:U:H4'	31:a:418:A:H5''	1.64	0.78
52:v:19:G:H5''	52:v:20:H2U:H52	1.65	0.77
52:v:21:U:H1'	52:v:22:A:H2'	1.65	0.77
5:A:1529:U:H3	5:A:1536:G:H1	1.31	0.77
41:k:80:ASN:HB3	41:k:107:ASN:HD21	1.50	0.76
24:T:45:LYS:HD2	24:T:46:PRO:HD2	1.66	0.76
41:k:13:ARG:NH2	41:k:35:ASP:OD2	2.20	0.74
34:d:8:LYS:HB3	34:d:21:LEU:HD22	1.68	0.74
5:A:1865:G:N2	5:A:1868:A:OP2	2.20	0.74
10:F:34:ILE:HG13	10:F:96:MET:HE2	1.70	0.74
42:l:25:LYS:HE2	42:l:59:SER:HB2	1.70	0.74
35:e:159:SER:OG	35:e:161:GLU:OE2	2.05	0.73
31:a:74:G:H1	31:a:93:A:H61	0.80	0.73
19:O:112:ARG:NH1	31:a:1460:U:OP1	2.21	0.73
18:N:32:THR:HG23	18:N:35:HIS:H	1.53	0.73
52:v:10:G:O6	52:v:46:G:N2	2.20	0.72
32:b:9:ARG:HD2	32:b:13:GLN:HE22	1.54	0.72
32:b:119:LEU:HG	32:b:143:MET:HE2	1.71	0.71
7:C:5:LYS:HD3	7:C:17:GLU:HG3	1.71	0.71
31:a:1036:U:H2'	31:a:1037:A:H8	1.54	0.71
25:U:36:GLY:HA3	25:U:97:ARG:HB2	1.72	0.71
10:F:162:THR:OG1	10:F:164:ASP:OD1	2.09	0.71
5:A:85:C:OP1	28:X:7:ARG:NH2	2.25	0.70
31:a:670:A:H2'	31:a:671:G:C8	2.27	0.70
5:A:1111:C:H2'	5:A:1112:G:C8	2.27	0.70
33:c:114:ARG:NH1	33:c:118:GLU:OE1	2.24	0.70
14:J:65:THR:HG22	14:J:68:GLY:H	1.57	0.70
31:a:1089:A:OP2	37:g:4:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1798:A:H2'	5:A:1799:A:C8	2.27	0.70
11:G:77:LYS:NZ	11:G:81:GLU:OE2	2.20	0.69
5:A:279:U:H3	5:A:366:G:H22	1.40	0.69
43:m:12:ASN:OD1	43:m:46:ARG:NH1	2.26	0.69
7:C:175:ARG:HG3	7:C:181:MET:HE3	1.73	0.69
5:A:1037:A:H61	5:A:1112:G:H1	1.39	0.68
5:A:2469:U:OP1	5:A:2471:C:N4	2.24	0.68
32:b:80:ASN:O	32:b:84:GLU:HG2	1.93	0.68
31:a:148:A:N6	31:a:165:C:O2	2.26	0.68
31:a:207:G:O2'	31:a:208:G:O4'	2.11	0.68
5:A:1471:U:H2'	5:A:1472:A:H8	1.56	0.68
38:h:55:GLU:CD	38:h:56:THR:H	2.02	0.68
35:e:110:MET:HE2	35:e:126:CYS:SG	2.35	0.67
5:A:2287:U:H2'	5:A:2288:G:C8	2.28	0.67
37:g:74:GLU:OE1	37:g:95:ARG:NH1	2.28	0.67
33:c:211:MET:SD	33:c:216:ASN:HB2	2.34	0.67
37:g:74:GLU:HG3	37:g:75:VAL:HG12	1.76	0.67
5:A:854:G:H2'	5:A:855:G:C8	2.29	0.67
31:a:454:U:H3	31:a:470:G:H1	1.40	0.67
31:a:489:C:H2'	31:a:490:A:C8	2.29	0.67
31:a:1022:U:H5''	31:a:1023:G:H5'	1.77	0.67
5:A:1849:A:H2'	5:A:1850:A:C8	2.30	0.67
5:A:2324:A:H2'	5:A:2325:A:C8	2.30	0.67
37:g:26:PHE:HD1	37:g:101:MET:HG2	1.60	0.66
5:A:1577:A:H3'	5:A:1578:A:H8	1.59	0.66
42:l:56:ARG:HG3	42:l:62:GLU:HG2	1.77	0.66
47:q:18:MET:HB2	47:q:21:SER:HB2	1.77	0.66
3:2:24:LYS:NZ	3:2:46:CYS:SG	2.69	0.66
32:b:7:SER:HA	32:b:8:MET:HE3	1.77	0.66
34:d:190:ARG:NH1	34:d:190:ARG:O	2.29	0.66
5:A:1111:C:H2'	5:A:1112:G:H8	1.60	0.66
36:f:26:ILE:HD12	36:f:36:ILE:HG12	1.78	0.66
10:F:8:TYR:HA	10:F:12:LEU:HB2	1.78	0.65
40:j:47:GLU:HG3	40:j:67:ILE:HG23	1.79	0.65
16:L:110:ASN:ND2	16:L:112:ASP:OD2	2.30	0.65
36:f:33:ASP:OD1	36:f:34:GLY:N	2.30	0.65
32:b:112:SER:O	32:b:116:LEU:HD12	1.96	0.65
10:F:56:ASP:OD2	10:F:150:ARG:NH1	2.29	0.64
11:G:104:ASN:ND2	11:G:114:ASP:OD2	2.30	0.64
5:A:204:A:N6	5:A:2426:A:O2'	2.30	0.64
5:A:1506:U:H2'	5:A:1507:G:C8	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1353:G:H2'	31:a:1354:A:C8	2.33	0.64
33:c:150:LYS:HG3	33:c:169:ARG:HB2	1.78	0.64
34:d:67:TYR:HD2	34:d:113:ARG:HH12	1.46	0.64
31:a:423:U:OP2	31:a:424:G:O2'	2.15	0.63
24:T:5:LYS:N	24:T:8:ASP:OD2	2.32	0.63
52:v:69:U:H2'	52:v:70:A:H8	1.64	0.63
32:b:33:ILE:HG22	32:b:35:GLY:H	1.63	0.63
5:A:1104:G:N2	5:A:1105:U:O4	2.30	0.63
5:A:1595:A:H5''	5:A:1596:A:H5'	1.79	0.63
10:F:55:ALA:O	10:F:59:LEU:HD22	1.99	0.63
10:F:147:ASP:OD1	10:F:148:ARG:N	2.29	0.63
31:a:943:A:H2'	31:a:944:G:C8	2.34	0.63
41:k:70:GLY:O	41:k:104:TYR:OH	2.14	0.63
23:S:11:LYS:HA	28:X:29:ARG:HH22	1.64	0.63
7:C:165:LEU:HD11	7:C:181:MET:HE1	1.79	0.62
10:F:56:ASP:O	10:F:60:ILE:HD12	1.98	0.62
37:g:5:ARG:HH22	37:g:7:VAL:HA	1.64	0.62
5:A:2093:U:O4	5:A:2188:G:O6	2.17	0.62
32:b:134:ARG:HA	32:b:137:LEU:HD12	1.81	0.62
33:c:135:LYS:HG2	33:c:168:TYR:HE2	1.64	0.62
34:d:196:GLU:HG2	34:d:197:ILE:HD12	1.81	0.62
41:k:88:PRO:HG3	51:u:32:VAL:HG11	1.80	0.62
31:a:143:G:H2'	31:a:144:G:C8	2.35	0.62
34:d:87:ALA:HB3	34:d:90:GLU:HG2	1.80	0.62
38:h:55:GLU:OE1	38:h:56:THR:N	2.24	0.62
34:d:123:ARG:HG3	34:d:133:ASN:HB3	1.81	0.62
36:f:25:TYR:O	36:f:29:ILE:HD12	1.99	0.62
5:A:2313:C:H2'	5:A:2314:G:C8	2.34	0.61
34:d:11:LEU:HD13	34:d:65:ARG:HG2	1.83	0.61
5:A:545:C:H1'	5:A:546:G:C2	2.36	0.61
5:A:71:G:H2'	5:A:72:C:C6	2.35	0.61
7:C:39:ARG:NH1	7:C:57:GLY:O	2.33	0.61
19:O:109:LYS:HA	19:O:112:ARG:HE	1.66	0.61
5:A:606:A:H2'	5:A:607:A:C8	2.36	0.61
9:E:86:ALA:O	9:E:87:ARG:NH1	2.33	0.61
31:a:77:G:H2'	31:a:78:G:H8	1.66	0.61
37:g:97:THR:HG22	37:g:101:MET:HE3	1.83	0.61
31:a:1127:A:H2'	31:a:1128:G:H8	1.65	0.61
31:a:1428:A:H2	31:a:1466:C:H42	1.47	0.61
31:a:79:U:H2'	31:a:80:A:C8	2.36	0.61
18:N:68:GLU:O	18:N:72:LYS:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:399:C:OP1	34:d:136:SER:OG	2.18	0.60
31:a:1527:G:O6	51:u:46:LYS:NZ	2.33	0.60
47:q:69:SER:OG	47:q:70:LYS:N	2.34	0.60
52:v:8:4SU:O2'	52:v:49:C:O2	2.12	0.60
5:A:2543:A:H2'	5:A:2544:U:C6	2.37	0.60
34:d:56:GLN:HB3	34:d:205:LEU:HG	1.83	0.60
5:A:1428:A:H2'	5:A:1429:A:C8	2.37	0.60
31:a:714:U:H4'	41:k:118:ASN:HD22	1.66	0.60
18:N:44:ASP:OD2	18:N:47:LYS:NZ	2.35	0.60
33:c:181:ASP:HB2	33:c:207:ILE:HG13	1.83	0.60
37:g:64:THR:HG22	37:g:68:LYS:NZ	2.16	0.60
5:A:141:U:H2'	5:A:142:A:H8	1.67	0.60
20:P:86:ALA:HB2	20:P:116:ALA:HB2	1.83	0.60
5:A:1854:A:H61	5:A:1880:G:H1'	1.65	0.59
31:a:160:G:H2'	31:a:161:G:H8	1.67	0.59
51:u:59:LYS:NZ	51:u:63:GLU:OE2	2.30	0.59
31:a:77:G:H2'	31:a:78:G:C8	2.38	0.59
36:f:35:GLN:HB2	36:f:37:HIS:CD2	2.37	0.59
5:A:1647:G:O2'	17:M:106:ASP:OD2	2.16	0.59
32:b:28:LYS:NZ	32:b:196:ASP:OD2	2.28	0.59
47:q:51:ASN:HB2	47:q:53:VAL:HG23	1.85	0.59
7:C:165:LEU:HD11	7:C:181:MET:CE	2.32	0.59
37:g:68:LYS:HE2	37:g:128:ALA:HA	1.85	0.59
5:A:12:A:H2'	5:A:13:A:C8	2.38	0.59
5:A:71:G:H2'	5:A:72:C:H6	1.66	0.59
31:a:295:G:H2'	31:a:296:A:C8	2.37	0.59
10:F:170:MET:HB3	10:F:175:PHE:HB3	1.85	0.59
31:a:1454:G:OP1	50:t:34:ARG:NE	2.35	0.59
18:N:68:GLU:CD	18:N:68:GLU:H	2.11	0.59
22:R:69:LEU:HD13	22:R:107:VAL:HG11	1.84	0.58
31:a:80:A:H2'	31:a:81:G:C8	2.38	0.58
31:a:333:G:H2'	31:a:334:A:C8	2.37	0.58
5:A:141:U:H2'	5:A:142:A:C8	2.38	0.58
31:a:498:C:H2'	31:a:499:A:H8	1.68	0.58
37:g:55:LYS:HE2	37:g:55:LYS:N	2.19	0.58
5:A:1854:A:N6	5:A:1880:G:H1'	2.18	0.58
31:a:80:A:H2'	31:a:81:G:H8	1.68	0.58
32:b:135:GLU:HA	32:b:138:GLU:HG2	1.85	0.58
5:A:1749:G:N2	5:A:1752:G:OP2	2.32	0.58
5:A:1581:U:H5'	5:A:1582:U:OP1	2.04	0.58
5:A:2308:U:H5'	10:F:85:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:1:MET:HE1	16:L:45:ARG:HG2	1.85	0.58
5:A:2325:A:H2'	5:A:2326:G:C8	2.37	0.58
38:h:78:ARG:NH1	38:h:80:SER:O	2.37	0.58
41:k:21:HIS:HB2	41:k:32:THR:HG22	1.86	0.58
6:B:41:C:O2	10:F:92:ARG:NH1	2.37	0.57
10:F:134:GLU:HB3	10:F:136:ILE:HG12	1.86	0.57
31:a:184:A:C5	50:t:84:LYS:HD3	2.39	0.57
31:a:471:G:H2'	31:a:472:A:C8	2.39	0.57
5:A:2844:G:O2'	5:A:2864:A:N6	2.36	0.57
23:S:87:LYS:HE2	23:S:87:LYS:HA	1.86	0.57
35:e:161:GLU:CD	35:e:161:GLU:H	2.12	0.57
5:A:1464:A:H2'	5:A:1465:A:C8	2.40	0.57
5:A:1634:G:H2'	5:A:1635:A:C8	2.40	0.57
31:a:79:U:H2'	31:a:80:A:H8	1.69	0.57
5:A:1172:U:H2'	5:A:1173:G:C4	2.39	0.57
5:A:2060:C:H2'	5:A:2061:C:C6	2.40	0.57
6:B:112:A:H2'	6:B:113:G:C8	2.39	0.57
5:A:2048:A:H4'	8:D:151:GLN:O	2.03	0.57
5:A:2082:U:H2'	5:A:2083:G:C8	2.40	0.57
31:a:73:G:H2'	31:a:74:G:C8	2.40	0.57
31:a:499:A:OP1	42:l:115:SER:OG	2.16	0.57
10:F:136:ILE:HG13	10:F:137:VAL:HG23	1.86	0.57
21:Q:42:VAL:HG22	21:Q:47:ILE:HG23	1.85	0.57
5:A:591:U:H2'	5:A:592:U:C6	2.40	0.57
5:A:2314:G:H2'	5:A:2315:U:O4'	2.04	0.57
31:a:1024:C:H2'	31:a:1025:C:C6	2.39	0.57
31:a:1036:U:H2'	31:a:1037:A:C8	2.39	0.57
32:b:17:HIS:HB3	32:b:45:LEU:HD21	1.86	0.57
32:b:186:ILE:HG22	32:b:200:TYR:HB2	1.86	0.57
36:f:13:ASP:OD2	36:f:13:ASP:N	2.33	0.57
37:g:139:GLU:O	37:g:143:ARG:HG2	2.05	0.57
5:A:1719:U:O4	5:A:1734:G:N2	2.38	0.57
31:a:498:C:H2'	31:a:499:A:C8	2.40	0.57
31:a:1424:C:H2'	31:a:1425:A:H8	1.69	0.56
34:d:174:GLU:OE1	34:d:174:GLU:N	2.37	0.56
5:A:780:A:C2	7:C:225:MET:HG2	2.40	0.56
5:A:1471:U:H2'	5:A:1472:A:C8	2.37	0.56
31:a:1364:C:H5''	39:i:114:LEU:HD12	1.88	0.56
13:I:75:TYR:CE1	13:I:86:GLU:HG3	2.40	0.56
36:f:12:PRO:HD2	36:f:44:ARG:HH12	1.70	0.56
52:v:9:A:H2'	52:v:11:C:H41	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:368:C:H4'	5:A:369:G:O5'	2.05	0.56
10:F:5:LYS:HE2	10:F:97:TYR:CE2	2.41	0.56
31:a:661:G:H22	31:a:738:G:H1	1.53	0.56
52:v:69:U:H2'	52:v:70:A:C8	2.40	0.56
5:A:293:U:H3	5:A:351:G:H1	1.53	0.56
5:A:1718:A:N6	5:A:1734:G:O2'	2.39	0.56
31:a:1001:A:N6	31:a:1023:G:H1'	2.19	0.56
34:d:203:VAL:O	34:d:207:SER:OG	2.18	0.56
5:A:280:A:H2'	5:A:281:A:C8	2.40	0.56
5:A:2631:U:O2'	8:D:82:GLU:OE1	2.18	0.56
31:a:733:C:H2'	31:a:734:A:C8	2.40	0.56
1:0:46:LYS:NZ	1:0:46:LYS:HB3	2.20	0.56
24:T:25:LEU:HD11	24:T:35:GLU:HG3	1.88	0.56
25:U:62:GLU:O	25:U:62:GLU:HG2	2.06	0.56
31:a:1164:A:O2'	31:a:1166:A:OP2	2.24	0.56
31:a:1320:G:H2'	31:a:1321:A:C8	2.41	0.56
25:U:53:LYS:HA	25:U:56:GLU:OE1	2.06	0.56
31:a:1034:C:H2'	31:a:1035:C:C6	2.41	0.56
7:C:133:ARG:HA	7:C:167:ARG:HD3	1.88	0.56
28:X:12:GLU:H	28:X:12:GLU:CD	2.14	0.56
32:b:37:ARG:CZ	32:b:38:ASN:HB2	2.35	0.56
37:g:72:MET:HG2	37:g:73:VAL:HG23	1.88	0.55
39:i:40:GLU:OE2	39:i:44:MET:HE1	2.06	0.55
5:A:579:C:H2'	5:A:580:A:C8	2.42	0.55
31:a:1074:G:N2	31:a:1077:A:OP2	2.33	0.55
5:A:482:A:H5''	24:T:45:LYS:HD3	1.88	0.55
31:a:9:A:H2'	35:e:123:LEU:HD22	1.88	0.55
9:E:141:ASN:O	9:E:141:ASN:ND2	2.39	0.55
31:a:725:A:H2'	31:a:726:A:C8	2.42	0.55
31:a:743:A:H2'	31:a:744:A:C8	2.42	0.55
32:b:169:ASP:OD2	32:b:170:HIS:N	2.40	0.55
36:f:5:GLU:HG3	36:f:63:ASN:ND2	2.21	0.55
48:r:21:ILE:HD12	48:r:22:ASP:H	1.71	0.55
1:0:28:GLU:H	1:0:28:GLU:CD	2.14	0.55
5:A:1036:A:H4'	25:U:49:ARG:HD3	1.88	0.55
5:A:2063:G:H1	5:A:2439:U:H3	1.53	0.55
19:O:27:ASP:OD2	19:O:92:ARG:HA	2.06	0.55
31:a:1263:G:N2	31:a:1266:A:OP2	2.30	0.55
32:b:69:VAL:HG22	32:b:162:ALA:HB3	1.88	0.55
5:A:2294:A:H61	5:A:2314:G:H1	1.54	0.55
5:A:2637:A:P	13:I:76:ARG:HH21	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:33:ALA:HB2	16:L:105:GLU:HG2	1.89	0.55
31:a:671:G:H2'	31:a:672:A:H8	1.72	0.55
31:a:1068:C:H2'	31:a:1069:G:H8	1.72	0.55
32:b:9:ARG:HD2	32:b:13:GLN:NE2	2.20	0.55
5:A:830:U:H2'	5:A:831:A:C8	2.42	0.55
5:A:2287:U:H2'	5:A:2288:G:H8	1.72	0.55
33:c:77:ILE:HA	33:c:84:ILE:HG23	1.88	0.55
32:b:9:ARG:NH1	32:b:13:GLN:NE2	2.55	0.54
52:v:19:G:H5'	52:v:20:H2U:H2'	1.88	0.54
45:o:8:ARG:O	45:o:12:ILE:HG13	2.06	0.54
6:B:38:U:N3	6:B:42:G:OP2	2.36	0.54
7:C:198:GLN:HG3	7:C:199:GLU:OE1	2.08	0.54
43:m:39:ILE:HD11	43:m:52:GLN:HB3	1.89	0.54
32:b:96:HIS:CE1	32:b:148:ARG:HE	2.23	0.54
5:A:286:U:H2'	5:A:287:G:C8	2.43	0.54
35:e:80:LEU:HB2	35:e:97:PRO:HG3	1.87	0.54
39:i:47:ARG:O	39:i:51:GLU:HG2	2.08	0.54
5:A:2067:A:H2'	5:A:2068:C:C6	2.43	0.54
8:D:34:ARG:NH2	8:D:54:GLY:O	2.36	0.54
10:F:91:LEU:HD12	10:F:95:GLN:HB3	1.89	0.54
34:d:38:ALA:HB3	34:d:43:GLY:HA2	1.90	0.54
46:p:22:ILE:HG12	46:p:39:VAL:HG22	1.90	0.54
37:g:55:LYS:HE2	37:g:55:LYS:H	1.72	0.54
5:A:1733:U:H3'	5:A:1734:G:C8	2.43	0.54
10:F:110:ARG:HB3	10:F:137:VAL:HG13	1.89	0.54
12:H:9:ILE:HB	12:H:12:LEU:HB2	1.90	0.54
5:A:1411:G:H2'	5:A:1412:C:C6	2.43	0.54
10:F:112:ARG:H	10:F:112:ARG:HD2	1.74	0.54
11:G:164:TYR:HB2	11:G:167:GLU:HB2	1.89	0.54
25:U:76:VAL:HG12	25:U:97:ARG:HA	1.88	0.54
34:d:97:GLU:OE1	34:d:102:ASN:ND2	2.41	0.54
41:k:49:GLN:HE21	41:k:68:VAL:HG21	1.72	0.53
31:a:1424:C:H2'	31:a:1425:A:C8	2.43	0.53
45:o:53:ARG:O	45:o:57:ILE:HG12	2.08	0.53
32:b:59:ALA:HB2	32:b:219:MET:HE1	1.89	0.53
35:e:12:GLU:HG2	35:e:38:VAL:HG12	1.91	0.53
12:H:9:ILE:HD12	12:H:12:LEU:HD22	1.90	0.53
36:f:21:MET:O	36:f:24:ARG:HG2	2.08	0.53
36:f:41:ASP:OD2	36:f:43:GLY:N	2.29	0.53
5:A:1432:C:HO2'	5:A:1512:G:HO2'	1.57	0.53
5:A:1866:U:H2'	5:A:1867:A:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2341:A:N3	5:A:2377:A:H2'	2.24	0.53
31:a:1100:C:H4'	32:b:99:LEU:HD23	1.91	0.53
5:A:1261:G:O2'	5:A:2008:G:O6	2.26	0.53
5:A:2687:C:HO2'	5:A:2867:U:HO2'	1.53	0.53
7:C:120:ASN:OD1	7:C:120:ASN:N	2.41	0.53
31:a:1215:C:H2'	31:a:1216:A:C8	2.43	0.53
48:r:26:ILE:H	48:r:26:ILE:HD12	1.73	0.53
5:A:1437:U:H2'	5:A:1438:C:C6	2.44	0.53
15:K:95:GLU:CD	15:K:95:GLU:H	2.16	0.53
5:A:1479:U:H2'	5:A:1480:A:C8	2.43	0.53
32:b:208:ALA:O	32:b:212:VAL:HG12	2.08	0.53
5:A:1521:G:H1	5:A:1544:G:N2	2.01	0.52
5:A:1840:U:H2'	5:A:1841:G:H8	1.74	0.52
5:A:1910:C:H2'	5:A:1911:3TD:H6	1.90	0.52
32:b:81:ILE:HD11	32:b:209:ILE:HG23	1.92	0.52
34:d:15:GLU:OE2	34:d:65:ARG:NH1	2.42	0.52
49:s:50:SER:HB3	49:s:57:HIS:HB3	1.90	0.52
5:A:997:A:H2'	5:A:998:A:C8	2.45	0.52
5:A:1102:U:N3	5:A:1103:A:N7	2.58	0.52
31:a:333:G:H2'	31:a:334:A:H8	1.73	0.52
32:b:175:ILE:HD12	32:b:185:VAL:HG11	1.91	0.52
32:b:123:SER:HB2	32:b:143:MET:SD	2.49	0.52
38:h:10:MET:HG3	38:h:27:MET:SD	2.49	0.52
5:A:1500:A:H2'	5:A:1501:C:C6	2.44	0.52
5:A:2426:A:H2'	5:A:2426:A:N3	2.23	0.52
19:O:2:SER:O	19:O:2:SER:OG	2.25	0.52
31:a:451:U:C2	31:a:452:A:C8	2.97	0.52
38:h:30:SER:HB3	38:h:33:LYS:HE3	1.92	0.52
5:A:2188:G:H2'	5:A:2189:G:C8	2.44	0.52
13:I:114:LEU:HG	13:I:118:MET:HE2	1.92	0.52
28:X:41:HIS:O	28:X:45:VAL:HG23	2.10	0.52
31:a:698:U:OP1	31:a:699:A:O2'	2.20	0.52
31:a:1007:U:H3	31:a:1016:G:H1	1.56	0.52
52:v:55:5MU:O2'	52:v:56:PSU:O4'	2.27	0.52
5:A:308:U:H2'	5:A:309:G:O4'	2.10	0.52
15:K:6:ASN:OD1	15:K:6:ASN:N	2.43	0.52
28:X:13:GLU:O	28:X:17:LEU:HD22	2.10	0.52
34:d:176:ASP:OD1	34:d:178:SER:OG	2.26	0.52
31:a:733:C:H2'	31:a:734:A:H8	1.73	0.52
33:c:22:TRP:CG	33:c:59:ARG:HD2	2.44	0.52
37:g:5:ARG:NH2	37:g:6:VAL:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:17:ARG:HG2	14:J:17:ARG:HH11	1.74	0.52
31:a:231:U:H2'	31:a:232:A:H8	1.74	0.52
32:b:71:PHE:HB3	32:b:82:ILE:HD11	1.91	0.52
46:p:41:ASP:OD1	46:p:42:SER:N	2.42	0.52
52:v:9:A:O2'	52:v:10:G:N7	2.43	0.52
5:A:2879:A:OP2	30:Z:49:ARG:NH1	2.42	0.52
10:F:93:GLY:O	10:F:96:MET:HG3	2.09	0.52
31:a:905:A:H2'	31:a:906:A:H8	1.75	0.52
33:c:129:MET:HE2	33:c:132:ARG:HD3	1.92	0.52
10:F:29:PRO:HB2	10:F:169:LEU:HD22	1.91	0.52
10:F:122:PHE:CZ	10:F:170:MET:HE1	2.45	0.52
31:a:206:C:H4'	31:a:207:G:H5'	1.92	0.52
36:f:3:HIS:NE2	36:f:65:GLU:OE2	2.43	0.52
5:A:199:G:O2'	5:A:675:A:N1	2.43	0.51
7:C:135:MET:HE3	7:C:136:PRO:HD2	1.92	0.51
14:J:104:ARG:N	14:J:122:LEU:OXT	2.43	0.51
31:a:989:U:H4'	31:a:990:G:O5'	2.10	0.51
32:b:117:LYS:O	32:b:121:THR:HG23	2.10	0.51
5:A:830:U:H2'	5:A:831:A:H8	1.76	0.51
10:F:40:VAL:HG23	10:F:43:ALA:HB2	1.92	0.51
38:h:114:ASP:OD2	38:h:118:ARG:NH2	2.43	0.51
5:A:279:U:H3	5:A:366:G:H1	1.59	0.51
5:A:811:U:H2'	5:A:812:C:H6	1.76	0.51
31:a:1001:A:H2'	31:a:1002:A:O4'	2.09	0.51
32:b:134:ARG:O	32:b:137:LEU:HB2	2.10	0.51
34:d:109:PHE:CE2	34:d:180:LEU:HB3	2.46	0.51
5:A:637:U:H2'	5:A:638:C:C6	2.46	0.51
31:a:711:G:H2'	31:a:712:A:C8	2.45	0.51
34:d:15:GLU:OE2	34:d:58:ARG:NH2	2.28	0.51
3:2:33:THR:OG1	5:A:2416:C:OP1	2.20	0.51
5:A:9:G:H2'	5:A:10:U:C6	2.45	0.51
5:A:161:A:H2'	5:A:162:A:C8	2.46	0.51
5:A:1050:U:H3	5:A:1103:A:H61	1.57	0.51
6:B:26:C:OP1	18:N:32:THR:HG21	2.11	0.51
23:S:11:LYS:HA	28:X:29:ARG:NH2	2.25	0.51
28:X:55:THR:O	28:X:59:GLU:HG3	2.11	0.51
30:Z:51:ARG:HB3	30:Z:51:ARG:CZ	2.41	0.51
32:b:137:LEU:O	32:b:140:THR:OG1	2.22	0.51
41:k:79:LYS:HE3	41:k:79:LYS:HA	1.91	0.51
33:c:21:ASN:HB3	33:c:58:GLU:OE1	2.11	0.51
5:A:2239:U:H2'	5:A:2240:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:155:GLU:OE1	11:G:157:TYR:N	2.43	0.51
31:a:75:A:H61	31:a:92:G:H1	1.59	0.51
31:a:1038:G:H2'	31:a:1039:A:C8	2.45	0.51
36:f:17:GLN:O	36:f:21:MET:HG2	2.11	0.51
5:A:12:A:H2'	5:A:13:A:H8	1.74	0.50
31:a:1173:A:H2'	31:a:1174:G:C8	2.46	0.50
41:k:115:ILE:HD12	51:u:31:ASP:HB2	1.93	0.50
5:A:2301:U:C2	10:F:151:GLY:HA3	2.46	0.50
31:a:1029:G:H3'	31:a:1030:G:O4'	2.11	0.50
31:a:1488:G:H2'	31:a:1489:A:C8	2.47	0.50
41:k:97:ARG:NH1	51:u:13:ASP:OD2	2.44	0.50
5:A:1185:G:H5'	15:K:34:GLY:HA2	1.93	0.50
31:a:693:A:H2'	31:a:694:U:H6	1.76	0.50
31:a:710:G:H2'	31:a:711:G:C8	2.47	0.50
5:A:862:G:H2'	5:A:863:C:C6	2.47	0.50
5:A:1483:U:H3	5:A:1496:G:H1	1.58	0.50
32:b:198:VAL:HB	32:b:201:VAL:HG13	1.93	0.50
5:A:579:C:H2'	5:A:580:A:H8	1.75	0.50
31:a:1002:A:C5	31:a:1003:C:H1'	2.47	0.50
31:a:1010:G:N2	31:a:1013:A:OP2	2.37	0.50
31:a:1524:C:OP2	51:u:42:THR:HG22	2.11	0.50
32:b:164:PHE:HD1	32:b:186:ILE:HG13	1.77	0.50
5:A:413:C:H2'	5:A:414:A:C8	2.47	0.50
5:A:740:G:H2'	5:A:741:U:C6	2.47	0.50
5:A:1798:A:H2'	5:A:1799:A:H8	1.77	0.50
7:C:177:ARG:HB3	7:C:177:ARG:NH1	2.27	0.50
51:u:31:ASP:O	51:u:35:ARG:HG2	2.12	0.50
5:A:9:G:H2'	5:A:10:U:H6	1.75	0.50
31:a:973:G:OP2	31:a:1355:U:O2'	2.29	0.50
35:e:164:GLN:NE2	38:h:115:ARG:HD2	2.27	0.50
40:j:8:ILE:HG12	40:j:100:ILE:HG12	1.93	0.50
43:m:37:VAL:HG21	43:m:56:ILE:HD13	1.93	0.50
5:A:2188:G:H2'	5:A:2189:G:H8	1.76	0.50
5:A:2587:C:H2'	5:A:2588:G:C8	2.47	0.50
11:G:44:LYS:HD3	11:G:46:GLU:HG2	1.93	0.50
34:d:170:PRO:HB3	34:d:172:TRP:CH2	2.46	0.50
36:f:95:ALA:C	36:f:96:ILE:HD13	2.37	0.50
37:g:112:SER:O	37:g:113:GLU:HB3	2.12	0.50
41:k:98:ALA:O	41:k:102:VAL:HG23	2.12	0.50
1:0:28:GLU:OE1	1:0:28:GLU:N	2.34	0.49
5:A:292:U:H2'	5:A:293:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:347:A:H1'	5:A:348:A:H2	1.76	0.49
5:A:2324:A:H2'	5:A:2325:A:H8	1.75	0.49
5:A:2793:U:O4	5:A:2797:G:N2	2.34	0.49
31:a:649:U:O4	31:a:749:G:O2'	2.22	0.49
34:d:101:ASP:OD2	34:d:101:ASP:N	2.42	0.49
36:f:42:TRP:HB2	36:f:59:TYR:HB2	1.93	0.49
37:g:65:THR:O	37:g:69:VAL:HG23	2.12	0.49
51:u:28:VAL:O	51:u:32:VAL:HG23	2.12	0.49
5:A:687:A:H2'	5:A:688:U:C6	2.47	0.49
32:b:147:GLU:OE1	32:b:154:LYS:NZ	2.45	0.49
34:d:172:TRP:CD1	34:d:188:PRO:HD3	2.48	0.49
52:v:19:G:C4	52:v:57:C:H1'	2.47	0.49
52:v:44:G:H2'	52:v:45:G:C8	2.47	0.49
31:a:58:U:H2'	31:a:59:G:C8	2.47	0.49
31:a:908:U:H2'	31:a:909:C:C6	2.46	0.49
41:k:49:GLN:NE2	41:k:68:VAL:HG21	2.28	0.49
31:a:200:G:H2'	31:a:201:A:H8	1.76	0.49
31:a:202:U:H2'	31:a:203:C:C6	2.48	0.49
42:l:123:LYS:NZ	42:l:123:LYS:HB3	2.26	0.49
5:A:2553:G:H2'	5:A:2554:C:C6	2.48	0.49
13:I:7:LYS:HB2	13:I:10:GLU:HG3	1.95	0.49
5:A:101:U:H2'	5:A:102:A:C8	2.47	0.49
5:A:158:U:H2'	5:A:159:G:H8	1.76	0.49
31:a:536:A:H2'	31:a:537:G:H8	1.78	0.49
31:a:1374:A:H5'	37:g:92:ARG:HH22	1.77	0.49
34:d:87:ALA:O	34:d:90:GLU:HG3	2.13	0.49
52:v:74:A:H5'	52:v:75:C:H5'	1.94	0.49
5:A:286:U:H2'	5:A:287:G:H8	1.78	0.49
5:A:844:A:H4'	5:A:845:A:O5'	2.12	0.49
5:A:1428:A:H2'	5:A:1429:A:H8	1.76	0.49
5:A:2070:U:H2'	5:A:2071:U:C6	2.47	0.49
8:D:6:VAL:HG11	8:D:79:LEU:HD11	1.93	0.49
14:J:69:ILE:HD11	14:J:103:THR:HG21	1.95	0.49
34:d:161:ILE:HD11	34:d:177:HIS:ND1	2.28	0.49
36:f:18:VAL:O	36:f:22:VAL:HG13	2.11	0.49
41:k:92:ARG:O	41:k:96:VAL:HG23	2.12	0.49
5:A:1792:U:H2'	5:A:1793:C:H6	1.78	0.49
10:F:108:ILE:HD11	10:F:117:PHE:CZ	2.48	0.49
51:u:7:LYS:HB2	51:u:10:GLU:HB2	1.94	0.49
5:A:1400:U:H2'	5:A:1401:U:C6	2.48	0.49
5:A:2533:U:H2'	5:A:2534:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:112:A:H2'	6:B:113:G:H8	1.78	0.49
16:L:30:GLY:HA2	16:L:107:GLU:HB2	1.95	0.49
28:X:46:ALA:O	28:X:50:ILE:HG13	2.12	0.49
30:Z:42:VAL:HG12	30:Z:48:TYR:HB2	1.94	0.49
31:a:231:U:H2'	31:a:232:A:C8	2.47	0.49
31:a:818:G:H2'	31:a:819:U:H6	1.78	0.49
31:a:1311:C:H2'	31:a:1312:U:C6	2.47	0.49
31:a:1374:A:C5	37:g:7:VAL:HG11	2.48	0.49
32:b:61:GLN:O	32:b:65:LYS:HD2	2.12	0.49
40:j:89:LYS:HZ2	40:j:89:LYS:C	2.20	0.49
43:m:37:VAL:HG23	43:m:59:GLU:HG3	1.95	0.49
5:A:637:U:H2'	5:A:638:C:H6	1.77	0.49
5:A:811:U:H2'	5:A:812:C:C6	2.48	0.49
5:A:1356:G:H2'	5:A:1357:C:C6	2.48	0.49
5:A:1381:A:H2'	5:A:1382:U:C6	2.47	0.49
31:a:447:A:OP2	46:p:88:ARG:NH1	2.26	0.49
5:A:578:U:H2'	5:A:579:C:C6	2.48	0.48
5:A:1568:A:H2'	5:A:1569:A:C8	2.48	0.48
5:A:1792:U:H2'	5:A:1793:C:C6	2.48	0.48
6:B:111:C:H2'	6:B:112:A:H8	1.78	0.48
10:F:164:ASP:OD1	10:F:165:GLU:N	2.46	0.48
31:a:1007:U:H2'	31:a:1008:C:C6	2.48	0.48
37:g:27:MET:SD	37:g:40:GLU:HG2	2.53	0.48
5:A:1503:C:H4'	5:A:1505:A:C8	2.48	0.48
5:A:2502:U:O2'	5:A:2503:C:OP1	2.26	0.48
6:B:28:C:H1'	6:B:55:A:H61	1.78	0.48
31:a:818:G:H2'	31:a:819:U:C6	2.48	0.48
43:m:39:ILE:HD12	43:m:56:ILE:HD11	1.94	0.48
11:G:143:GLN:O	11:G:147:GLU:HG3	2.13	0.48
31:a:1059:U:H2'	31:a:1060:C:C6	2.48	0.48
32:b:141:ARG:O	32:b:145:LYS:HE2	2.13	0.48
34:d:155:LEU:HA	34:d:158:LYS:HG2	1.95	0.48
36:f:87:ASN:OD1	36:f:87:ASN:N	2.47	0.48
5:A:2242:G:H2'	5:A:2243:A:C8	2.48	0.48
6:B:52:G:H21	10:F:26:MET:HE1	1.78	0.48
7:C:187:GLU:HA	7:C:187:GLU:OE1	2.12	0.48
31:a:536:A:H2'	31:a:537:G:C8	2.48	0.48
41:k:97:ARG:CZ	41:k:97:ARG:HB2	2.44	0.48
5:A:2219:G:O3'	7:C:265:LYS:NZ	2.46	0.48
31:a:19:U:H2'	31:a:20:C:C6	2.48	0.48
31:a:1347:A:O2'	37:g:33:ASP:OD2	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:57:ASN:O	32:b:61:GLN:OE1	2.31	0.48
41:k:46:SER:HB3	41:k:61:ALA:HB1	1.96	0.48
49:s:66:MET:HG2	49:s:74:PHE:CZ	2.47	0.48
5:A:478:A:H4'	5:A:479:A:OP1	2.14	0.48
5:A:568:G:H2'	5:A:2026:6MZ:N7	2.28	0.48
5:A:1924:A:H2'	5:A:1925:G:O4'	2.13	0.48
5:A:2843:U:H2'	5:A:2844:G:O4'	2.13	0.48
11:G:115:TYR:OH	11:G:147:GLU:OE2	2.27	0.48
31:a:529:A:N6	31:a:1203:G:O2'	2.45	0.48
33:c:121:ALA:O	33:c:125:GLU:HG2	2.11	0.48
37:g:114:LYS:O	37:g:119:ARG:NH1	2.46	0.48
5:A:908:A:H2'	5:A:909:A:C8	2.49	0.48
5:A:1879:U:H2'	5:A:1880:G:O4'	2.12	0.48
5:A:1935:5MU:OP1	5:A:2600:U:O2'	2.31	0.48
13:I:92:LEU:HD21	13:I:99:GLU:OE2	2.14	0.48
20:P:111:GLU:OE2	20:P:114:LYS:NZ	2.45	0.48
52:v:24:A:H2'	52:v:25:G:C8	2.49	0.48
5:A:157:U:H2'	5:A:158:U:C6	2.48	0.48
5:A:2247:OMG:O6	26:V:3:THR:OG1	2.28	0.48
5:A:2373:A:H2'	5:A:2374:A:C8	2.48	0.48
28:X:7:ARG:HD3	28:X:56:LEU:HD11	1.96	0.48
31:a:265:U:H2'	31:a:266:A:C8	2.48	0.48
31:a:1004:U:H2'	31:a:1005:U:H6	1.78	0.48
32:b:154:LYS:HG3	32:b:155:ASN:OD1	2.14	0.48
46:p:68:LEU:HD12	46:p:69:ARG:N	2.29	0.48
52:v:22:A:N6	52:v:47:G:H2'	2.28	0.48
5:A:2295:G:C2	5:A:2314:G:C2	3.02	0.48
7:C:135:MET:HE3	7:C:136:PRO:CD	2.44	0.48
8:D:50:GLN:HG3	8:D:82:GLU:HG3	1.96	0.48
31:a:588:U:H2'	31:a:589:A:C8	2.49	0.48
5:A:100:A:H2'	5:A:101:U:C6	2.49	0.48
5:A:847:A:H2'	5:A:848:C:C6	2.48	0.48
5:A:1464:A:H2'	5:A:1465:A:H8	1.77	0.48
5:A:2880:U:H2'	5:A:2881:U:C6	2.48	0.48
31:a:473:U:H2'	31:a:474:A:C8	2.49	0.48
32:b:131:LEU:CB	32:b:139:ARG:HH21	2.26	0.48
5:A:158:U:H2'	5:A:159:G:C8	2.49	0.47
5:A:2021:C:H2'	5:A:2022:U:C6	2.50	0.47
5:A:2242:G:H2'	5:A:2243:A:H8	1.79	0.47
12:H:1:MET:HE3	12:H:26:GLY:HA3	1.96	0.47
31:a:577:C:H2'	31:a:578:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:625:G:H2'	31:a:626:A:C8	2.49	0.47
31:a:1035:C:H2'	31:a:1036:U:C6	2.49	0.47
31:a:1040:U:HO2'	31:a:1041:A:H8	1.59	0.47
34:d:176:ASP:OD2	34:d:179:LYS:NZ	2.42	0.47
5:A:1437:U:H2'	5:A:1438:C:H6	1.79	0.47
6:B:60:U:H2'	6:B:61:C:H6	1.78	0.47
14:J:104:ARG:HG3	14:J:107:ARG:HD3	1.96	0.47
31:a:450:C:H2'	31:a:451:U:H6	1.79	0.47
31:a:671:G:H2'	31:a:672:A:C8	2.49	0.47
35:e:159:SER:OG	35:e:162:GLU:OE1	2.32	0.47
47:q:22:ILE:HG13	47:q:47:ALA:HB3	1.95	0.47
5:A:284:U:H2'	5:A:285:A:H8	1.80	0.47
5:A:2510:U:H2'	5:A:2511:C:H6	1.79	0.47
5:A:2586:A:H2'	5:A:2587:C:C6	2.50	0.47
6:B:52:G:H21	10:F:26:MET:CE	2.26	0.47
20:P:44:GLN:OE1	21:Q:77:MET:HE3	2.13	0.47
34:d:80:GLU:O	34:d:84:VAL:HG23	2.15	0.47
39:i:51:GLU:OE2	39:i:56:THR:OG1	2.32	0.47
50:t:43:ASP:OD1	50:t:46:VAL:HG23	2.15	0.47
5:A:1037:A:N6	5:A:1112:G:H1	2.10	0.47
5:A:2034:G:H2'	5:A:2035:U:O4'	2.14	0.47
5:A:2323:A:H2'	5:A:2324:A:C8	2.49	0.47
41:k:15:VAL:O	41:k:78:LEU:HB3	2.14	0.47
5:A:1917:G:H2'	5:A:1918:G:H8	1.78	0.47
5:A:2419:U:H4'	5:A:2420:C:O5'	2.14	0.47
5:A:2798:U:H2'	5:A:2799:C:C6	2.49	0.47
10:F:57:MET:HB2	10:F:65:PRO:HG3	1.96	0.47
13:I:120:LYS:HE3	13:I:120:LYS:HB3	1.64	0.47
31:a:1001:A:C6	31:a:1023:G:H1'	2.49	0.47
34:d:190:ARG:HH22	34:d:195:ALA:HA	1.80	0.47
5:A:1193:U:H2'	5:A:1194:U:C6	2.50	0.47
11:G:52:LEU:HD23	11:G:69:ARG:HA	1.95	0.47
19:O:109:LYS:HB3	19:O:112:ARG:HH21	1.80	0.47
21:Q:45:ASP:OD2	21:Q:45:ASP:N	2.33	0.47
31:a:232:A:H2'	31:a:233:A:C8	2.50	0.47
31:a:744:A:H2'	31:a:745:U:H6	1.80	0.47
33:c:132:ARG:HG2	33:c:132:ARG:HH11	1.80	0.47
5:A:353:C:H2'	5:A:354:A:C8	2.50	0.47
5:A:707:U:H2'	5:A:708:U:C6	2.49	0.47
5:A:2294:A:N1	5:A:2314:G:N2	2.62	0.47
5:A:2550:U:H2'	5:A:2551:U:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2674:A:H2'	5:A:2675:A:C8	2.48	0.47
7:C:163:GLN:OE1	7:C:163:GLN:HA	2.12	0.47
14:J:17:ARG:HG2	14:J:17:ARG:NH1	2.27	0.47
15:K:138:GLU:HA	15:K:138:GLU:OE2	2.15	0.47
31:a:242:A:C2	31:a:278:A:C5	3.03	0.47
31:a:511:U:C2	31:a:512:G:C8	3.02	0.47
31:a:1005:U:H2'	31:a:1006:U:C6	2.50	0.47
31:a:1011:A:C2	31:a:1216:A:H1'	2.50	0.47
31:a:1461:U:H2'	31:a:1462:A:H8	1.80	0.47
35:e:150:GLU:CD	35:e:150:GLU:H	2.22	0.47
41:k:67:GLU:HG3	41:k:98:ALA:HB1	1.97	0.47
42:l:53:CYS:HB2	42:l:67:ILE:HD11	1.96	0.47
44:n:63:ARG:NH1	44:n:68:GLY:O	2.46	0.47
44:n:87:THR:HG22	44:n:93:VAL:HG23	1.96	0.47
15:K:117:GLU:HA	15:K:117:GLU:OE2	2.14	0.47
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.96	0.47
31:a:454:U:H2'	31:a:455:C:H6	1.80	0.47
31:a:905:A:H2'	31:a:906:A:C8	2.49	0.47
39:i:54:GLU:HA	39:i:54:GLU:OE1	2.14	0.47
5:A:110:A:OP2	5:A:110:A:H8	1.98	0.47
5:A:745:U:H4'	22:R:92:ARG:HH12	1.78	0.47
5:A:2736:A:H2'	5:A:2737:A:C8	2.49	0.47
5:A:2797:G:H2'	5:A:2798:U:C6	2.50	0.47
5:A:2798:U:H2'	5:A:2799:C:H6	1.80	0.47
9:E:1:MET:N	9:E:13:LEU:H	2.13	0.47
13:I:114:LEU:O	13:I:118:MET:HG3	2.14	0.47
15:K:4:ARG:HB2	15:K:7:GLU:HG3	1.97	0.47
5:A:1194:U:H2'	5:A:1195:C:H6	1.80	0.47
5:A:2469:U:O2	5:A:2469:U:H2'	2.15	0.47
14:J:64:ARG:HB2	14:J:83:ALA:HB3	1.97	0.47
25:U:27:GLU:HA	25:U:27:GLU:OE1	2.13	0.47
34:d:174:GLU:OE2	34:d:183:THR:OG1	2.33	0.47
5:A:103:U:H2'	5:A:104:C:O4'	2.15	0.46
5:A:2315:U:O2'	5:A:2317:G:N7	2.49	0.46
5:A:2470:U:OP2	5:A:2471:C:N4	2.41	0.46
7:C:118:SER:HB2	7:C:129:CYS:HB3	1.97	0.46
7:C:201:ASN:OD1	7:C:202:LEU:HD12	2.15	0.46
31:a:76:A:N1	31:a:91:G:O6	2.48	0.46
31:a:578:G:OP1	45:o:65:LYS:NZ	2.47	0.46
31:a:839:U:H1'	31:a:841:G:H1	1.79	0.46
31:a:943:A:H2'	31:a:944:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:227:LYS:NZ	32:b:228:GLU:OE1	2.32	0.46
34:d:109:PHE:HE2	34:d:180:LEU:HB3	1.78	0.46
42:l:110:ARG:NH2	42:l:112:GLN:O	2.42	0.46
5:A:605:U:C5	5:A:618:G:C5	3.03	0.46
5:A:666:A:H2'	5:A:668:A:H62	1.80	0.46
5:A:1928:A:H2'	5:A:1929:G:O4'	2.15	0.46
5:A:2586:A:H2'	5:A:2587:C:H6	1.79	0.46
8:D:111:ASP:OD1	8:D:176:GLN:HG2	2.15	0.46
14:J:97:ARG:NH1	31:a:335:C:OP2	2.49	0.46
31:a:78:G:H2'	31:a:79:U:C6	2.51	0.46
32:b:29:MET:O	32:b:33:ILE:HG12	2.15	0.46
35:e:114:LEU:HD13	35:e:122:VAL:HG11	1.96	0.46
43:m:53:LEU:HD23	43:m:53:LEU:HA	1.79	0.46
52:v:40:U:H2'	52:v:41:G:H8	1.80	0.46
5:A:1583:C:H3'	5:A:1584:A:H8	1.81	0.46
5:A:2220:G:OP1	7:C:265:LYS:NZ	2.47	0.46
14:J:17:ARG:HH11	14:J:47:ILE:HG23	1.80	0.46
10:F:50:LEU:O	10:F:54:VAL:HG13	2.15	0.46
10:F:120:LYS:HD2	10:F:167:ARG:HH22	1.81	0.46
29:Y:5:LYS:HG2	29:Y:36:GLU:HG2	1.97	0.46
5:A:1348:A:H2'	5:A:1349:A:C8	2.51	0.46
5:A:1885:A:H2'	5:A:1886:A:C8	2.51	0.46
10:F:30:ARG:HG2	10:F:31:ILE:H	1.81	0.46
19:O:116:LYS:HB3	19:O:116:LYS:HE3	1.68	0.46
22:R:68:ASP:OD1	22:R:68:ASP:N	2.48	0.46
31:a:887:G:H1'	31:a:903:A:N6	2.30	0.46
33:c:211:MET:O	33:c:211:MET:HG3	2.15	0.46
39:i:34:GLU:CD	39:i:34:GLU:H	2.23	0.46
5:A:1403:U:H2'	5:A:1404:G:C8	2.50	0.46
31:a:200:G:H2'	31:a:201:A:C8	2.51	0.46
1:O:19:THR:OG1	1:O:20:THR:N	2.49	0.46
5:A:90:G:OP1	24:T:90:LYS:NZ	2.46	0.46
5:A:215:C:H2'	5:A:216:C:H6	1.79	0.46
5:A:2330:A:H5'	18:N:13:LYS:HG2	1.98	0.46
10:F:50:LEU:HD11	10:F:67:VAL:HG11	1.97	0.46
31:a:18:A:H8	31:a:1077:A:O2'	1.99	0.46
31:a:200:G:C8	31:a:461:A:N1	2.84	0.46
5:A:953:G:N7	16:L:14:LYS:NZ	2.62	0.46
31:a:754:U:H2'	31:a:755:G:O4'	2.15	0.46
33:c:85:GLU:OE2	33:c:89:ARG:NH1	2.48	0.46
5:A:2247:OMG:HM23	5:A:2247:OMG:HI'	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:120:LYS:HA	10:F:167:ARG:NH2	2.31	0.46
11:G:77:LYS:HE3	11:G:77:LYS:HB3	1.70	0.46
31:a:367:A:H2'	31:a:368:C:O4'	2.15	0.46
31:a:409:G:O6	34:d:33:LYS:HD2	2.16	0.46
16:L:112:ASP:O	16:L:116:GLU:HG3	2.15	0.46
31:a:942:G:C2	31:a:943:A:C8	3.04	0.46
32:b:8:MET:O	32:b:12:LEU:HB2	2.16	0.46
32:b:139:ARG:H	32:b:139:ARG:HD2	1.81	0.46
35:e:15:VAL:HB	35:e:35:LEU:HD23	1.97	0.46
41:k:105:LYS:NZ	41:k:106:ILE:O	2.49	0.46
31:a:74:G:H2'	31:a:75:A:C8	2.51	0.45
31:a:425:U:H1'	31:a:426:A:H5''	1.97	0.45
5:A:161:A:H2'	5:A:162:A:H8	1.80	0.45
5:A:413:C:H2'	5:A:414:A:H8	1.81	0.45
5:A:714:A:OP2	45:o:88:ARG:NH2	2.49	0.45
5:A:1790:A:H2'	5:A:1791:C:H6	1.81	0.45
11:G:45:GLN:HB3	11:G:50:LEU:HG	1.98	0.45
31:a:37:G:H2'	31:a:38:C:C6	2.52	0.45
38:h:10:MET:SD	38:h:33:LYS:HG2	2.55	0.45
44:n:90:GLN:NE2	44:n:92:ASP:OD2	2.50	0.45
5:A:1479:U:H2'	5:A:1480:A:H8	1.80	0.45
5:A:1542:A:H2'	5:A:1543:A:C8	2.51	0.45
31:a:91:G:H2'	31:a:92:G:C8	2.52	0.45
31:a:745:U:C2	31:a:746:A:C8	3.04	0.45
31:a:887:G:H4'	31:a:888:U:O5'	2.16	0.45
32:b:6:VAL:HG12	32:b:10:ASP:HB3	1.96	0.45
40:j:66:GLU:HB3	44:n:99:ALA:HB2	1.97	0.45
41:k:55:ARG:O	41:k:58:THR:OG1	2.26	0.45
5:A:2229:U:H2'	5:A:2230:G:C8	2.51	0.45
9:E:187:MET:HE3	9:E:187:MET:HB2	1.87	0.45
19:O:91:ARG:HG2	19:O:115:GLU:HG2	1.99	0.45
31:a:163:U:H2'	31:a:164:G:H8	1.81	0.45
31:a:1068:C:H2'	31:a:1069:G:C8	2.51	0.45
31:a:1295:U:C5	37:g:114:LYS:HD2	2.51	0.45
45:o:5:ASN:OD1	45:o:8:ARG:NH2	2.50	0.45
5:A:740:G:H2'	5:A:741:U:H6	1.81	0.45
10:F:168:ALA:O	10:F:171:ARG:HG2	2.16	0.45
11:G:2:SER:O	11:G:6:LYS:HG2	2.16	0.45
11:G:99:LYS:HE3	11:G:99:LYS:HB2	1.55	0.45
18:N:29:VAL:HG11	18:N:102:ILE:HD13	1.98	0.45
32:b:209:ILE:O	32:b:213:THR:OG1	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:113:LYS:HB2	39:i:116:LEU:HD12	1.98	0.45
42:l:56:ARG:HB3	42:l:56:ARG:NH1	2.31	0.45
48:r:34:THR:HG22	48:r:40:VAL:HG22	1.99	0.45
5:A:306:U:H2'	5:A:307:C:C6	2.52	0.45
7:C:135:MET:HE2	7:C:192:ILE:HG12	1.99	0.45
10:F:60:ILE:HG22	10:F:99:PHE:HE1	1.81	0.45
31:a:161:G:H2'	31:a:162:A:H8	1.81	0.45
31:a:163:U:H2'	31:a:164:G:C8	2.52	0.45
31:a:880:C:O2'	31:a:881:U:H5'	2.17	0.45
31:a:1510:A:H2'	31:a:1511:G:C8	2.51	0.45
32:b:119:LEU:HD12	32:b:119:LEU:HA	1.82	0.45
52:v:29:C:H2'	52:v:30:G:H8	1.81	0.45
5:A:482:A:H4'	24:T:44:GLN:O	2.16	0.45
5:A:1853:G:H22	5:A:1880:G:H2'	1.81	0.45
8:D:81:LYS:HB2	8:D:81:LYS:HE2	1.56	0.45
9:E:141:ASN:O	9:E:141:ASN:CG	2.59	0.45
12:H:40:THR:HG22	12:H:43:ASN:HB2	1.98	0.45
31:a:473:U:H2'	31:a:474:A:H8	1.81	0.45
31:a:846:U:H2'	31:a:847:U:C6	2.51	0.45
31:a:1326:A:OP1	43:m:29:THR:OG1	2.31	0.45
32:b:9:ARG:O	32:b:13:GLN:OE1	2.34	0.45
46:p:74:ARG:HD2	46:p:74:ARG:HA	1.55	0.45
17:M:72:ASN:HB3	17:M:75:THR:HB	1.98	0.45
31:a:511:U:N3	31:a:512:G:N7	2.65	0.45
5:A:365:U:O2'	5:A:366:G:OP2	2.26	0.45
5:A:1103:A:N3	5:A:1103:A:H2'	2.32	0.45
14:J:105:GLU:N	14:J:105:GLU:OE2	2.49	0.45
16:L:57:ARG:O	16:L:57:ARG:HD3	2.17	0.45
19:O:92:ARG:HD3	19:O:116:LYS:NZ	2.31	0.45
25:U:53:LYS:HA	25:U:53:LYS:HD2	1.65	0.45
31:a:470:G:H2'	31:a:471:G:C8	2.52	0.45
38:h:39:VAL:HG21	38:h:111:ILE:HG22	1.99	0.45
48:r:32:TYR:HE1	48:r:45:THR:HG21	1.82	0.45
5:A:1039:G:H2'	5:A:1040:C:C6	2.52	0.45
5:A:2294:A:N6	5:A:2314:G:H1	2.14	0.45
18:N:56:ASP:OD1	18:N:57:ALA:N	2.50	0.45
31:a:200:G:C4	31:a:201:A:C8	3.04	0.45
37:g:144:MET:SD	37:g:148:ASN:ND2	2.90	0.45
5:A:198:A:H2'	5:A:199:G:N3	2.32	0.44
5:A:287:G:H2'	5:A:288:U:H6	1.82	0.44
5:A:990:G:OP2	20:P:51:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1790:A:H2'	5:A:1791:C:C6	2.53	0.44
10:F:24:ASN:HB3	10:F:27:GLU:HG3	1.99	0.44
30:Z:45:ASP:OD2	30:Z:45:ASP:N	2.46	0.44
31:a:1163:G:N1	31:a:1166:A:OP1	2.50	0.44
42:l:31:ARG:HH21	42:l:58:THR:HG21	1.82	0.44
14:J:7:MET:HE1	14:J:44:LYS:HG3	1.99	0.44
31:a:271:G:H5'	47:q:17:LYS:HG3	1.99	0.44
31:a:412:G:H2'	31:a:413:G:H8	1.83	0.44
31:a:521:G:H2'	31:a:522:C:C6	2.52	0.44
31:a:838:U:H2'	31:a:839:U:O4'	2.17	0.44
32:b:135:GLU:O	32:b:139:ARG:HD2	2.17	0.44
34:d:116:ALA:O	34:d:120:VAL:HG23	2.17	0.44
37:g:47:LEU:O	37:g:50:VAL:HG12	2.16	0.44
5:A:1169:C:H3'	5:A:1170:U:H4'	1.99	0.44
6:B:43:A:C4	6:B:44:A:C8	3.05	0.44
18:N:40:VAL:HG23	18:N:77:ILE:HD11	1.99	0.44
32:b:219:MET:O	32:b:223:ILE:HD12	2.18	0.44
36:f:44:ARG:HE	36:f:44:ARG:HB2	1.55	0.44
42:l:43:LYS:HE3	42:l:91:PRO:HG3	2.00	0.44
52:v:67:C:H2'	52:v:68:A:C8	2.53	0.44
5:A:279:U:H3	5:A:366:G:N2	2.12	0.44
5:A:418:U:H2'	5:A:419:C:C6	2.52	0.44
5:A:1497:G:C2	5:A:1498:G:C8	3.05	0.44
5:A:2587:C:H2'	5:A:2588:G:H8	1.81	0.44
9:E:15:GLU:HA	9:E:15:GLU:OE2	2.17	0.44
10:F:5:LYS:HE2	10:F:97:TYR:CD2	2.52	0.44
25:U:77:LYS:NZ	25:U:77:LYS:HB2	2.32	0.44
31:a:436:A:C4	31:a:437:A:C8	3.05	0.44
31:a:472:A:H2'	31:a:473:U:C6	2.53	0.44
31:a:744:A:H2'	31:a:745:U:C6	2.53	0.44
31:a:861:A:H2'	31:a:862:A:C8	2.51	0.44
32:b:136:ALA:HA	32:b:139:ARG:HD3	1.99	0.44
34:d:19:LEU:HB2	34:d:21:LEU:CD1	2.48	0.44
41:k:51:PHE:HE2	41:k:64:VAL:HG21	1.83	0.44
5:A:498:U:H2'	5:A:499:G:O4'	2.18	0.44
5:A:1411:G:H2'	5:A:1412:C:H6	1.82	0.44
10:F:42:ALA:O	10:F:45:THR:OG1	2.32	0.44
31:a:386:U:H2'	31:a:387:C:C6	2.53	0.44
31:a:734:A:H2'	31:a:735:U:H6	1.82	0.44
42:l:18:LYS:HA	42:l:18:LYS:HD3	1.83	0.44
5:A:944:A:H2'	5:A:945:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1314:C:O2'	5:A:1315:C:H5'	2.18	0.44
5:A:1506:U:H2'	5:A:1507:G:H8	1.80	0.44
5:A:1529:U:H2'	5:A:1530:A:C8	2.52	0.44
5:A:2795:A:H2'	5:A:2797:G:OP2	2.18	0.44
14:J:13:ASN:O	14:J:13:ASN:ND2	2.50	0.44
16:L:54:ILE:HG22	16:L:64:ILE:HD11	1.98	0.44
31:a:180:U:C2	31:a:181:C:C5	3.05	0.44
38:h:115:ARG:HG2	38:h:115:ARG:HH11	1.83	0.44
11:G:85:ARG:HD2	11:G:85:ARG:HA	1.74	0.44
25:U:6:LEU:HD13	25:U:6:LEU:HA	1.88	0.44
52:v:18:G:N7	52:v:57:C:N4	2.65	0.44
5:A:655:U:H2'	5:A:656:U:C6	2.53	0.44
5:A:945:C:H2'	5:A:946:U:C6	2.53	0.44
31:a:435:U:C2	31:a:436:A:C8	3.05	0.44
31:a:1031:G:H2'	31:a:1032:A:H8	1.82	0.44
32:b:81:ILE:HG21	32:b:213:THR:HA	2.00	0.44
40:j:31:ARG:HB2	40:j:31:ARG:NH1	2.32	0.44
5:A:1311:A:H2'	5:A:1312:G:H8	1.83	0.44
11:G:38:HIS:HB3	11:G:41:VAL:HG12	1.99	0.44
23:S:53:GLU:HB3	23:S:87:LYS:HB3	2.00	0.44
29:Y:15:ARG:HG3	29:Y:53:MET:HE1	2.00	0.44
31:a:23:G:H2'	31:a:24:G:C8	2.53	0.44
31:a:748:U:H2'	31:a:749:G:O4'	2.18	0.44
35:e:100:GLU:OE2	35:e:101:GLY:N	2.51	0.44
31:a:588:U:H2'	31:a:589:A:H8	1.83	0.43
31:a:839:U:H1'	31:a:841:G:N1	2.33	0.43
32:b:16:ALA:HA	32:b:205:ASN:HB3	2.00	0.43
5:A:2465:A:N6	5:A:2477:G:O2'	2.45	0.43
6:B:60:U:H2'	6:B:61:C:C6	2.53	0.43
7:C:199:GLU:OE1	7:C:199:GLU:N	2.52	0.43
10:F:94:ASP:O	10:F:98:GLU:HG2	2.18	0.43
31:a:993:A:H2'	31:a:994:U:C6	2.53	0.43
31:a:1374:A:C6	37:g:7:VAL:HG21	2.53	0.43
5:A:177:G:H2'	5:A:178:U:C6	2.53	0.43
5:A:189:A:H2'	5:A:190:C:C6	2.54	0.43
5:A:845:A:OP2	5:A:846:U:H5	2.01	0.43
5:A:2243:A:H2'	5:A:2244:C:H6	1.84	0.43
31:a:405:U:H2'	31:a:406:G:O4'	2.17	0.43
31:a:1040:U:O2'	31:a:1041:A:H5''	2.18	0.43
32:b:166:ILE:O	32:b:188:ILE:HB	2.18	0.43
37:g:26:PHE:CD1	37:g:101:MET:HG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:26:LEU:HD12	39:i:61:LEU:HD12	1.99	0.43
5:A:592:U:H2'	5:A:593:C:C6	2.53	0.43
5:A:652:U:H5'	5:A:653:A:H5'	1.99	0.43
11:G:18:THR:HG23	11:G:25:GLU:HB3	2.00	0.43
11:G:171:ARG:HE	11:G:171:ARG:HB3	1.45	0.43
13:I:23:LYS:NZ	13:I:142:ILE:O	2.43	0.43
31:a:400:G:OP2	34:d:117:ARG:NH2	2.42	0.43
31:a:470:G:H2'	31:a:471:G:H8	1.82	0.43
31:a:1462:A:H2'	31:a:1463:C:H6	1.82	0.43
48:r:26:ILE:HG22	48:r:30:LYS:HE2	2.00	0.43
5:A:46:G:H2'	5:A:47:U:C6	2.53	0.43
5:A:846:U:H2'	5:A:847:A:H8	1.83	0.43
6:B:59:C:H2'	6:B:60:U:H6	1.84	0.43
11:G:95:LYS:HB2	11:G:95:LYS:HE2	1.80	0.43
30:Z:44:LYS:HB2	30:Z:44:LYS:HE2	1.80	0.43
33:c:91:LEU:O	33:c:95:MET:HG3	2.18	0.43
33:c:112:ASP:OD2	33:c:113:ALA:N	2.51	0.43
34:d:90:GLU:O	34:d:94:LYS:HG3	2.19	0.43
52:v:18:G:N2	52:v:58:A:H4'	2.33	0.43
5:A:1038:G:H2'	5:A:1039:G:H8	1.84	0.43
11:G:22:ARG:NH1	11:G:37:LEU:HB3	2.34	0.43
11:G:30:LYS:HA	11:G:30:LYS:HD3	1.77	0.43
12:H:9:ILE:HG21	12:H:12:LEU:HD13	2.01	0.43
29:Y:10:LYS:HB2	29:Y:53:MET:HB2	2.01	0.43
31:a:161:G:H2'	31:a:162:A:C8	2.54	0.43
31:a:1433:U:H2'	31:a:1434:A:C8	2.53	0.43
33:c:135:LYS:O	33:c:139:GLN:HG2	2.18	0.43
2:1:1:MET:HE2	2:1:1:MET:HB3	1.85	0.43
5:A:37:G:H2'	5:A:38:C:C6	2.54	0.43
5:A:1427:G:H2'	5:A:1428:A:C8	2.54	0.43
5:A:2510:U:H2'	5:A:2511:C:C6	2.53	0.43
27:W:17:ASN:O	27:W:24:LYS:HA	2.19	0.43
31:a:610:C:H2'	31:a:611:C:C6	2.53	0.43
31:a:930:G:O6	37:g:3:ARG:NH2	2.52	0.43
31:a:1335:G:H2'	31:a:1336:A:C8	2.54	0.43
32:b:14:ALA:HA	32:b:210:ARG:NH1	2.34	0.43
4:3:16:VAL:HG22	4:3:25:VAL:HG22	2.01	0.43
5:A:596:U:H2'	5:A:597:A:H8	1.84	0.43
5:A:706:G:H2'	5:A:707:U:C6	2.53	0.43
5:A:713:A:H8	5:A:713:A:OP1	2.02	0.43
6:B:64:A:N6	6:B:104:U:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:2:ASP:HB3	12:H:39:ALA:HB3	2.00	0.43
14:J:4:THR:HG22	14:J:5:GLU:HG2	1.99	0.43
24:T:41:LYS:HE3	24:T:41:LYS:HB2	1.91	0.43
31:a:456:U:H2'	31:a:457:A:H8	1.83	0.43
31:a:1030:G:H2'	31:a:1031:G:H8	1.83	0.43
42:l:72:HIS:ND1	42:l:74:LEU:HB2	2.34	0.43
42:l:87:VAL:O	42:l:88:LYS:HB3	2.19	0.43
5:A:1416:G:H1'	5:A:1489:A:N6	2.34	0.43
5:A:2533:U:H2'	5:A:2534:C:H6	1.84	0.43
9:E:14:SER:N	9:E:196:GLU:OE1	2.52	0.43
11:G:25:GLU:OE2	11:G:32:THR:HG23	2.18	0.43
14:J:109:GLU:CD	14:J:109:GLU:N	2.77	0.43
31:a:450:C:H2'	31:a:451:U:C6	2.53	0.43
31:a:1388:U:H2'	31:a:1389:G:C8	2.53	0.43
36:f:100:SER:OG	36:f:101:LEU:N	2.52	0.43
52:v:71:G:O2'	52:v:72:C:H5'	2.19	0.43
5:A:2563:G:H2'	5:A:2564:A:C8	2.54	0.43
31:a:485:C:H2'	31:a:486:U:H6	1.84	0.43
31:a:500:C:OP2	42:l:113:SER:OG	2.35	0.43
36:f:38:ARG:NH1	36:f:98:GLU:O	2.40	0.43
48:r:65:LEU:HD23	48:r:65:LEU:HA	1.89	0.43
5:A:189:A:H2'	5:A:190:C:H6	1.83	0.42
5:A:1403:U:H2'	5:A:1404:G:H8	1.83	0.42
7:C:268:ILE:HG13	7:C:269:ARG:N	2.34	0.42
8:D:88:ALA:O	8:D:91:GLU:HG3	2.19	0.42
10:F:31:ILE:O	10:F:31:ILE:HG13	2.19	0.42
13:I:109:LEU:HD23	13:I:109:LEU:HA	1.84	0.42
23:S:1:MET:HE2	23:S:4:GLU:HG2	2.01	0.42
31:a:74:G:H2'	31:a:75:A:H8	1.84	0.42
31:a:1260:A:H2'	31:a:1261:C:C6	2.54	0.42
33:c:111:LEU:HD12	33:c:204:ARG:HG2	2.00	0.42
5:A:353:C:H2'	5:A:354:A:H8	1.83	0.42
5:A:837:U:H2'	5:A:838:C:C6	2.54	0.42
5:A:1708:G:H2'	5:A:1709:U:C6	2.54	0.42
5:A:1919:U:H2'	5:A:1920:C:C6	2.54	0.42
7:C:161:SER:O	7:C:177:ARG:HD3	2.19	0.42
10:F:136:ILE:C	10:F:137:VAL:HG23	2.44	0.42
31:a:35:A:H2'	31:a:36:C:C6	2.54	0.42
31:a:888:U:OP2	31:a:903:A:N6	2.46	0.42
31:a:1490:A:H8	31:a:1490:A:OP2	2.02	0.42
33:c:169:ARG:HG2	33:c:170:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:70:MET:HE2	35:e:70:MET:HB3	1.83	0.42
43:m:16:VAL:O	43:m:20:THR:HG23	2.19	0.42
5:A:1520:A:H2'	5:A:1521:G:C8	2.53	0.42
9:E:1:MET:HE3	9:E:1:MET:HA	2.01	0.42
23:S:7:TYR:CE1	28:X:23:LEU:HD13	2.54	0.42
27:W:44:LYS:HD3	27:W:44:LYS:HA	1.80	0.42
31:a:127:U:H2'	31:a:128:C:C6	2.54	0.42
32:b:129:ALA:HA	32:b:133:LYS:NZ	2.34	0.42
33:c:210:GLY:O	33:c:214:VAL:HG23	2.20	0.42
34:d:176:ASP:OD2	34:d:179:LYS:HB2	2.19	0.42
36:f:44:ARG:HG2	36:f:56:LYS:NZ	2.35	0.42
37:g:17:LYS:HD3	37:g:44:TYR:CE2	2.54	0.42
5:A:1166:A:H2'	5:A:1167:U:C6	2.55	0.42
5:A:1919:U:O2'	52:v:12:U:O2'	2.36	0.42
10:F:5:LYS:HE2	10:F:97:TYR:HE2	1.85	0.42
11:G:8:PRO:HB3	11:G:51:GLN:HG2	2.01	0.42
12:H:41:GLU:H	12:H:41:GLU:HG3	1.52	0.42
21:Q:2:TYR:HB3	21:Q:15:VAL:HG12	2.02	0.42
31:a:433:U:H2'	31:a:434:U:C6	2.54	0.42
31:a:470:G:C2	31:a:471:G:C5	3.08	0.42
31:a:552:U:H2'	31:a:553:C:C6	2.55	0.42
32:b:107:LYS:HD2	32:b:110:ARG:HH22	1.84	0.42
44:n:10:GLU:HG3	44:n:63:ARG:HD2	2.00	0.42
5:A:478:A:N3	5:A:480:G:H5''	2.35	0.42
5:A:1870:C:H2'	5:A:1871:G:O4'	2.19	0.42
7:C:2:PRO:HD2	7:C:19:VAL:HG13	2.02	0.42
7:C:265:LYS:H	7:C:265:LYS:HG2	1.58	0.42
10:F:103:LEU:HD22	10:F:107:ALA:HB3	2.01	0.42
31:a:1117:C:H2'	31:a:1118:U:C6	2.54	0.42
33:c:17:ARG:HE	33:c:17:ARG:HB3	1.63	0.42
34:d:102:ASN:OD1	34:d:113:ARG:NH2	2.53	0.42
40:j:7:ARG:HD3	40:j:9:ARG:NH2	2.35	0.42
5:A:597:A:H2'	5:A:598:G:H8	1.85	0.42
5:A:1680:G:H2'	5:A:1681:U:C6	2.54	0.42
14:J:51:ARG:HA	14:J:51:ARG:HD3	1.77	0.42
16:L:76:GLU:HB2	16:L:91:GLU:HG3	2.00	0.42
31:a:497:G:H2'	31:a:498:C:C6	2.54	0.42
31:a:704:U:H2'	31:a:705:C:C6	2.54	0.42
31:a:1163:G:H1'	31:a:1167:A:N6	2.35	0.42
37:g:72:MET:HE2	37:g:142:HIS:CG	2.55	0.42
48:r:26:ILE:HD12	48:r:26:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:533:U:O2'	20:P:49:ASP:OD2	2.23	0.42
5:A:2060:C:H2'	5:A:2061:C:H6	1.81	0.42
5:A:2239:U:H2'	5:A:2240:U:H6	1.84	0.42
5:A:2301:U:O2	10:F:151:GLY:HA3	2.20	0.42
5:A:2792:U:O2'	5:A:2793:U:H5''	2.20	0.42
8:D:81:LYS:HE3	8:D:205:ILE:HD11	2.01	0.42
10:F:112:ARG:H	10:F:112:ARG:CD	2.31	0.42
17:M:33:LEU:HD13	17:M:114:GLU:HB2	2.01	0.42
31:a:81:G:H2'	31:a:82:C:C6	2.55	0.42
31:a:1427:C:H2'	31:a:1428:A:C8	2.55	0.42
33:c:9:GLY:HA2	33:c:12:LEU:HD12	2.02	0.42
41:k:99:LEU:HD12	41:k:99:LEU:HA	1.82	0.42
44:n:98:LYS:HE3	44:n:98:LYS:HB3	1.84	0.42
5:A:188:A:H2'	5:A:189:A:C8	2.55	0.42
5:A:2683:U:H2'	5:A:2684:G:O4'	2.20	0.42
9:E:47:SER:O	9:E:51:VAL:HG23	2.20	0.42
14:J:104:ARG:HH11	14:J:104:ARG:HG2	1.85	0.42
21:Q:1:MET:HE2	21:Q:1:MET:HB2	1.85	0.42
31:a:976:C:O2	44:n:59:ARG:NH1	2.52	0.42
31:a:1154:A:C2	31:a:1178:G:C4	3.08	0.42
32:b:102:MET:HE2	32:b:102:MET:HB2	1.81	0.42
33:c:52:VAL:HG13	33:c:68:ILE:HG23	2.01	0.42
34:d:4:TYR:O	34:d:5:ILE:HD13	2.20	0.42
48:r:22:ASP:OD1	48:r:22:ASP:N	2.51	0.42
2:1:25:LYS:HA	2:1:28:ARG:NH1	2.35	0.42
5:A:843:G:N3	5:A:843:G:H5''	2.35	0.42
5:A:1840:U:H2'	5:A:1841:G:C8	2.55	0.42
5:A:2696:A:H2'	5:A:2697:C:C6	2.54	0.42
10:F:24:ASN:OD1	10:F:25:VAL:N	2.52	0.42
27:W:68:VAL:O	27:W:72:ARG:HG3	2.20	0.42
28:X:18:LEU:HD11	28:X:50:ILE:HG23	2.02	0.42
31:a:917:U:H2'	31:a:918:U:C6	2.55	0.42
35:e:43:GLY:O	35:e:73:VAL:N	2.49	0.42
37:g:49:ARG:HH21	37:g:118:LEU:HD13	1.84	0.42
37:g:101:MET:O	37:g:105:VAL:HG22	2.18	0.42
42:l:110:ARG:HE	42:l:110:ARG:HB3	1.62	0.42
52:v:72:C:HO2'	52:v:73:C:H6	1.64	0.42
5:A:281:A:H2'	5:A:282:G:O4'	2.19	0.42
5:A:1050:U:H3	5:A:1103:A:N6	2.17	0.42
5:A:1665:G:O2'	5:A:1987:U:O4	2.33	0.42
5:A:2830:G:H2'	5:A:2875:A:H61	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2897:C:H2'	5:A:2898:U:O4'	2.20	0.42
10:F:23:LYS:HD3	10:F:23:LYS:HA	1.78	0.42
18:N:13:LYS:HE3	18:N:13:LYS:HB2	1.86	0.42
31:a:185:C:H4'	31:a:186:G:O5'	2.20	0.42
31:a:454:U:H2'	31:a:455:C:C6	2.54	0.42
32:b:113:ILE:HA	32:b:116:LEU:HD13	2.02	0.42
52:v:40:U:H2'	52:v:41:G:C8	2.54	0.42
5:A:782:G:H5'	5:A:783:G:OP1	2.19	0.41
5:A:1499:U:H2'	5:A:1500:A:C8	2.55	0.41
5:A:1502:U:O2'	5:A:1505:A:H1'	2.20	0.41
5:A:1518:A:H4'	5:A:1519:U:H3'	2.01	0.41
10:F:12:LEU:HA	10:F:15:LYS:HE3	2.02	0.41
10:F:115:ARG:HD2	10:F:177:PHE:CE2	2.55	0.41
10:F:115:ARG:HD2	10:F:177:PHE:HE2	1.84	0.41
10:F:171:ARG:HE	10:F:171:ARG:HB3	1.58	0.41
31:a:179:G:C5	31:a:180:U:C6	3.08	0.41
34:d:19:LEU:HB2	34:d:21:LEU:HD11	2.02	0.41
5:A:630:A:H2'	5:A:631:A:C8	2.55	0.41
5:A:2262:A:H4'	5:A:2263:A:N3	2.35	0.41
5:A:2302:C:H3'	5:A:2303:G:H5''	2.02	0.41
5:A:2550:U:H2'	5:A:2551:U:H6	1.85	0.41
8:D:5:LEU:HD21	8:D:99:ILE:HG22	2.01	0.41
24:T:10:VAL:HG12	24:T:70:ILE:HA	2.02	0.41
31:a:75:A:N6	31:a:92:G:H1	2.17	0.41
31:a:821:U:H2'	31:a:822:A:H8	1.85	0.41
44:n:72:GLY:O	44:n:80:SER:HA	2.20	0.41
48:r:22:ASP:OD2	48:r:24:LYS:HG3	2.20	0.41
51:u:17:ARG:HE	51:u:17:ARG:HB3	1.68	0.41
52:v:24:A:H62	52:v:47:G:H22	1.67	0.41
5:A:1423:C:O2'	5:A:1567:A:OP2	2.29	0.41
5:A:1430:G:H2'	5:A:1431:G:H8	1.85	0.41
5:A:1828:C:H2'	5:A:1829:C:O4'	2.21	0.41
5:A:2282:G:H4'	5:A:2283:A:O4'	2.19	0.41
6:B:111:C:H2'	6:B:112:A:C8	2.56	0.41
19:O:113:ILE:HD12	19:O:113:ILE:N	2.35	0.41
28:X:60:LYS:HE3	28:X:60:LYS:HB2	1.86	0.41
31:a:506:A:N3	31:a:540:U:O2'	2.49	0.41
37:g:16:PRO:HG3	39:i:41:THR:HG23	2.02	0.41
37:g:50:VAL:HG23	37:g:125:LEU:HG	2.02	0.41
43:m:90:ARG:HA	43:m:90:ARG:HD2	1.83	0.41
52:v:55:5MU:OP2	52:v:55:5MU:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:417:C:H2'	5:A:418:U:C6	2.55	0.41
5:A:966:G:H2'	5:A:967:U:C6	2.56	0.41
5:A:1177:A:H2'	5:A:1178:C:C6	2.55	0.41
31:a:1374:A:N6	37:g:7:VAL:HG21	2.35	0.41
34:d:7:PRO:HB2	34:d:10:LYS:HG3	2.02	0.41
40:j:52:LEU:HD23	40:j:62:ARG:HD3	2.02	0.41
1:0:47:GLU:HG2	1:0:48:ALA:N	2.36	0.41
5:A:2457:A:H2'	5:A:2458:C:C6	2.55	0.41
6:B:46:U:H2'	6:B:47:C:C6	2.54	0.41
17:M:106:ASP:OD1	17:M:106:ASP:N	2.53	0.41
24:T:6:LYS:O	24:T:24:VAL:HG22	2.21	0.41
31:a:207:G:O2'	31:a:208:G:O5'	2.37	0.41
31:a:250:G:OP1	47:q:69:SER:OG	2.38	0.41
31:a:1493:C:H2'	31:a:1494:G:O4'	2.20	0.41
32:b:133:LYS:HD3	32:b:133:LYS:HA	1.89	0.41
34:d:14:ARG:HD2	34:d:39:PRO:HD2	2.02	0.41
42:l:20:LYS:HE2	42:l:20:LYS:HB2	1.62	0.41
5:A:1639:A:H2'	5:A:1640:G:O4'	2.21	0.41
5:A:2269:A:H2'	5:A:2270:A:C8	2.56	0.41
5:A:2299:G:H2'	5:A:2300:G:C8	2.56	0.41
23:S:6:ILE:HD13	23:S:6:ILE:HA	1.86	0.41
31:a:90:C:H2'	31:a:91:G:C8	2.56	0.41
31:a:467:U:C2	31:a:468:A:C8	3.09	0.41
31:a:1025:C:H2'	31:a:1026:U:O4'	2.21	0.41
5:A:712:U:H5'	5:A:713:A:OP2	2.21	0.41
5:A:1036:A:N1	5:A:1113:G:N2	2.51	0.41
5:A:2373:A:O2'	18:N:116:PHE:OXT	2.20	0.41
11:G:149:ARG:HG3	11:G:162:VAL:O	2.20	0.41
22:R:72:SER:OG	22:R:73:THR:N	2.53	0.41
24:T:46:PRO:HB3	24:T:54:GLY:H	1.85	0.41
31:a:76:A:H2	31:a:91:G:H1	1.63	0.41
31:a:1118:U:H2'	31:a:1119:U:C6	2.55	0.41
31:a:1488:G:H2'	31:a:1489:A:H8	1.85	0.41
32:b:169:ASP:OD2	32:b:169:ASP:C	2.64	0.41
42:l:79:VAL:O	42:l:103:ASP:HB2	2.20	0.41
49:s:18:LYS:HD2	49:s:31:ILE:HG23	2.02	0.41
52:v:58:A:H1'	52:v:59:A:H2'	2.03	0.41
7:C:21:HIS:NE2	7:C:199:GLU:OE2	2.40	0.41
9:E:129:LYS:HD3	9:E:129:LYS:HA	1.86	0.41
10:F:57:MET:SD	10:F:89:VAL:HG23	2.60	0.41
31:a:447:A:H5'	46:p:88:ARG:HH22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:515:C:O2'	31:a:527:G:N2	2.53	0.41
31:a:789:A:H1'	31:a:791:A:N7	2.35	0.41
31:a:1115:U:H2'	31:a:1116:C:H6	1.85	0.41
3:2:13:ARG:HD2	15:K:65:LYS:HG2	2.02	0.41
5:A:287:G:H2'	5:A:288:U:C6	2.55	0.41
5:A:720:A:H2'	5:A:721:C:C6	2.55	0.41
5:A:869:U:H2'	5:A:870:U:C6	2.55	0.41
5:A:1316:A:C4	5:A:1317:A:C8	3.09	0.41
5:A:1352:C:H2'	5:A:1353:G:O4'	2.20	0.41
5:A:1441:C:H2'	5:A:1442:C:C6	2.55	0.41
5:A:1597:U:H2'	5:A:1598:C:H6	1.86	0.41
5:A:1917:G:H2'	5:A:1918:G:C8	2.55	0.41
5:A:2641:U:H4'	5:A:2728:G:O2'	2.21	0.41
10:F:108:ILE:O	10:F:111:ILE:HG22	2.21	0.41
10:F:149:ILE:H	10:F:149:ILE:HG13	1.61	0.41
12:H:29:PHE:O	12:H:33:GLN:HG3	2.20	0.41
14:J:69:ILE:CD1	14:J:103:THR:HG21	2.51	0.41
28:X:9:LYS:HE3	28:X:13:GLU:OE1	2.20	0.41
31:a:75:A:H2'	31:a:76:A:C8	2.56	0.41
31:a:94:C:C2	31:a:95:C:C5	3.08	0.41
31:a:456:U:H2'	31:a:457:A:C8	2.56	0.41
31:a:493:A:H5'	31:a:494:U:OP2	2.21	0.41
31:a:734:A:H2'	31:a:735:U:C6	2.56	0.41
31:a:865:C:H2'	31:a:866:G:O4'	2.21	0.41
31:a:915:A:H2'	31:a:916:A:C8	2.56	0.41
31:a:1235:A:H2	31:a:1238:G:N3	2.19	0.41
31:a:1409:C:H2'	31:a:1410:A:C8	2.55	0.41
37:g:71:PRO:O	37:g:96:ARG:HD2	2.21	0.41
52:v:28:C:H2'	52:v:29:C:H6	1.86	0.41
5:A:727:G:OP1	7:C:13:ARG:HG2	2.21	0.41
5:A:1430:G:H2'	5:A:1431:G:C8	2.56	0.41
5:A:1569:A:H2'	5:A:1570:A:C8	2.56	0.41
5:A:1577:A:H3'	5:A:1578:A:C8	2.49	0.41
5:A:1681:U:H2'	5:A:1682:A:C8	2.56	0.41
5:A:1708:G:H2'	5:A:1709:U:H6	1.85	0.41
5:A:1867:A:H2'	5:A:1868:A:C8	2.56	0.41
16:L:14:LYS:HE3	16:L:14:LYS:HB2	1.76	0.41
18:N:28:CYS:HA	18:N:92:ASP:HB3	2.03	0.41
19:O:40:ARG:CZ	19:O:40:ARG:HB2	2.51	0.41
24:T:80:ARG:HB2	24:T:95:LYS:HG3	2.03	0.41
32:b:9:ARG:CD	32:b:13:GLN:HE22	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:105:ILE:HB	35:e:123:LEU:HD23	2.03	0.41
1:0:5:ILE:HD13	1:0:47:GLU:HG3	2.03	0.40
5:A:98:A:H1'	5:A:99:A:C8	2.56	0.40
5:A:1835:G:C2	5:A:1836:G:C8	3.09	0.40
26:V:64:ASP:O	26:V:84:THR:HG22	2.21	0.40
31:a:252:U:H2'	31:a:253:G:H8	1.85	0.40
31:a:1172:G:H2'	31:a:1173:A:H8	1.85	0.40
33:c:27:LYS:HB2	33:c:27:LYS:HE2	1.87	0.40
34:d:41:GLN:OE1	34:d:42:HIS:NE2	2.54	0.40
34:d:100:LEU:O	34:d:104:VAL:HG23	2.21	0.40
49:s:9:PRO:HB3	49:s:39:MET:HE3	2.02	0.40
50:t:86:LEU:HA	50:t:86:LEU:HD12	1.78	0.40
5:A:831:A:H2'	5:A:832:G:C8	2.57	0.40
5:A:846:U:H2'	5:A:847:A:C8	2.56	0.40
7:C:125:ARG:HA	7:C:125:ARG:NE	2.35	0.40
18:N:19:ILE:HG21	18:N:26:ARG:HG3	2.03	0.40
28:X:10:SER:OG	28:X:12:GLU:OE2	2.29	0.40
32:b:66:LYS:HA	32:b:66:LYS:HE2	2.02	0.40
35:e:155:LYS:HG3	35:e:156:ARG:N	2.37	0.40
47:q:30:VAL:O	47:q:38:SER:HA	2.21	0.40
52:v:15:G:H22	52:v:49:C:H42	1.69	0.40
3:2:48:MET:HE3	3:2:48:MET:HB3	1.78	0.40
5:A:215:C:H2'	5:A:216:C:C6	2.56	0.40
5:A:1038:G:H2'	5:A:1039:G:C8	2.57	0.40
5:A:1344:C:C2	5:A:1345:C:C5	3.09	0.40
5:A:1682:A:H2'	5:A:1683:C:H6	1.87	0.40
5:A:1849:A:H2'	5:A:1850:A:H8	1.83	0.40
5:A:1962:A:N3	5:A:2588:G:O2'	2.53	0.40
5:A:2010:A:H2'	5:A:2011:A:C8	2.56	0.40
5:A:2451:G:H2'	5:A:2452:C:C6	2.56	0.40
9:E:150:ASP:OD2	9:E:194:LYS:HE3	2.22	0.40
18:N:76:LEU:HD12	18:N:76:LEU:HA	1.88	0.40
30:Z:12:ARG:HE	30:Z:12:ARG:HB3	1.75	0.40
31:a:94:C:H2'	31:a:95:C:H6	1.87	0.40
32:b:179:LYS:HB3	32:b:179:LYS:HE3	1.88	0.40
43:m:15:ALA:HA	43:m:45:ILE:HD11	2.03	0.40
5:A:142:A:H2'	5:A:143:C:H6	1.87	0.40
5:A:527:A:H5'	13:I:113:PRO:HG3	2.02	0.40
5:A:1047:A:H2'	5:A:1048:G:H8	1.86	0.40
5:A:1193:U:C2	5:A:1194:U:C5	3.09	0.40
14:J:17:ARG:NH1	14:J:47:ILE:HG23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:131:LYS:HE2	15:K:131:LYS:HB3	1.73	0.40
20:P:58:ARG:HA	20:P:61:TRP:CE3	2.57	0.40
31:a:31:U:O2'	31:a:32:U:H5'	2.20	0.40
31:a:963:2MG:HM21	39:i:127:LYS:HD2	2.02	0.40
32:b:68:LYS:HD3	32:b:92:PRO:HD3	2.04	0.40
34:d:59:GLU:OE2	34:d:198:ASN:HB3	2.21	0.40
5:A:182:A:H2'	5:A:183:A:C8	2.57	0.40
5:A:1445:G:O2'	5:A:1446:C:H5'	2.21	0.40
5:A:1491:A:H2'	5:A:1493:C:C5	2.57	0.40
5:A:1912:A:H2'	5:A:1913:PSU:C6	2.55	0.40
5:A:2232:U:H2'	5:A:2233:G:O4'	2.21	0.40
5:A:2509:A:H2'	5:A:2510:U:C6	2.56	0.40
14:J:79:PHE:HZ	14:J:122:LEU:HD21	1.87	0.40
30:Z:8:LYS:HB2	30:Z:8:LYS:HE2	1.97	0.40
31:a:75:A:H2'	31:a:76:A:H8	1.87	0.40
31:a:409:G:H4'	31:a:410:A:H5''	2.04	0.40
31:a:491:G:O2'	31:a:493:A:H1'	2.22	0.40
31:a:693:A:H2'	31:a:694:U:C6	2.55	0.40
42:l:41:THR:HA	42:l:42:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	47/51 (92%)	47 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	270/274 (98%)	262 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
10	F	172/178 (97%)	160 (93%)	9 (5%)	3 (2%)	7	13
11	G	172/177 (97%)	166 (96%)	5 (3%)	1 (1%)	21	38
12	H	43/148 (29%)	43 (100%)	0	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	120 (100%)	0	0	100	100
15	K	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18	34
17	M	117/125 (94%)	114 (97%)	3 (3%)	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	12	24
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100
24	T	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
25	U	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
26	V	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	207 (93%)	16 (7%)	0	100	100
33	c	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
34	d	205/208 (99%)	200 (98%)	5 (2%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
36	f	102/127 (80%)	99 (97%)	3 (3%)	0	100	100
37	g	132/156 (85%)	126 (96%)	5 (4%)	1 (1%)	16	31
38	h	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
39	i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	j	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
41	k	115/128 (90%)	109 (95%)	6 (5%)	0	100	100
42	l	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
43	m	113/118 (96%)	110 (97%)	2 (2%)	1 (1%)	14	27
44	n	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
45	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
48	r	50/75 (67%)	48 (96%)	2 (4%)	0	100	100
49	s	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	59 (97%)	2 (3%)	0	100	100
All	All	5402/5872 (92%)	5252 (97%)	142 (3%)	8 (0%)	49	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	L	79	LEU
10	F	137	VAL
11	G	13	ASN
43	m	66	GLU
10	F	5	LYS
10	F	134	GLU
21	Q	52	PRO
37	g	89	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	45/47 (96%)	43 (96%)	2 (4%)	25	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	51 (98%)	1 (2%)	50	76
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	213 (98%)	5 (2%)	44	72
8	D	166/167 (99%)	161 (97%)	5 (3%)	36	64
9	E	155/155 (100%)	151 (97%)	4 (3%)	40	68
10	F	144/147 (98%)	138 (96%)	6 (4%)	26	52
11	G	139/142 (98%)	138 (99%)	1 (1%)	76	89
12	H	34/112 (30%)	31 (91%)	3 (9%)	9	20
13	I	118/118 (100%)	117 (99%)	1 (1%)	73	88
14	J	103/103 (100%)	99 (96%)	4 (4%)	28	55
15	K	106/108 (98%)	105 (99%)	1 (1%)	70	87
16	L	113/113 (100%)	111 (98%)	2 (2%)	51	77
17	M	96/101 (95%)	95 (99%)	1 (1%)	68	86
18	N	83/85 (98%)	78 (94%)	5 (6%)	17	36
19	O	99/102 (97%)	98 (99%)	1 (1%)	68	86
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	82 (98%)	2 (2%)	43	70
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	75 (97%)	2 (3%)	40	68
24	T	83/85 (98%)	80 (96%)	3 (4%)	31	58
25	U	79/80 (99%)	78 (99%)	1 (1%)	61	82
26	V	62/64 (97%)	61 (98%)	1 (2%)	55	79
27	W	69/70 (99%)	67 (97%)	2 (3%)	37	65
28	X	53/56 (95%)	51 (96%)	2 (4%)	29	56
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	46/50 (92%)	45 (98%)	1 (2%)	45	73
32	b	185/200 (92%)	177 (96%)	8 (4%)	26	51
33	c	175/198 (88%)	173 (99%)	2 (1%)	65	84
34	d	170/171 (99%)	163 (96%)	7 (4%)	27	53
35	e	113/120 (94%)	111 (98%)	2 (2%)	51	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	94/111 (85%)	91 (97%)	3 (3%)	34	62
37	g	113/128 (88%)	107 (95%)	6 (5%)	20	42
38	h	108/109 (99%)	106 (98%)	2 (2%)	50	76
39	i	99/100 (99%)	98 (99%)	1 (1%)	68	86
40	j	89/91 (98%)	87 (98%)	2 (2%)	45	73
41	k	88/98 (90%)	83 (94%)	5 (6%)	18	39
42	l	104/106 (98%)	100 (96%)	4 (4%)	29	56
43	m	95/98 (97%)	92 (97%)	3 (3%)	34	62
44	n	81/82 (99%)	78 (96%)	3 (4%)	30	57
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	61 (97%)	2 (3%)	34	62
47	q	71/76 (93%)	67 (94%)	4 (6%)	19	39
48	r	46/66 (70%)	45 (98%)	1 (2%)	45	73
49	s	70/78 (90%)	68 (97%)	2 (3%)	37	65
50	t	65/67 (97%)	63 (97%)	2 (3%)	35	62
51	u	54/62 (87%)	53 (98%)	1 (2%)	50	76
All	All	4473/4756 (94%)	4357 (97%)	116 (3%)	41	68

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	44	ILE
1	0	50	ILE
3	2	64	ILE
7	C	38	LYS
7	C	120	ASN
7	C	135	MET
7	C	148	ILE
7	C	194	GLU
8	D	3	ILE
8	D	10	CYS
8	D	59	SER
8	D	142	SER
8	D	189	VAL
9	E	11	VAL
9	E	74	SER

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Mol	Chain	Res	Type
9	E	125	VAL
9	E	172	THR
10	F	16	LEU
10	F	20	LEU
10	F	108	ILE
10	F	145	LYS
10	F	149	ILE
10	F	156	ILE
11	G	43	LEU
12	H	17	ASP
12	H	40	THR
12	H	41	GLU
13	I	102	GLU
14	J	28	SER
14	J	65	THR
14	J	80	ASP
14	J	105	GLU
15	K	70	SER
16	L	25	SER
16	L	80	GLU
17	M	116	VAL
18	N	29	VAL
18	N	42	SER
18	N	55	LEU
18	N	67	ILE
18	N	102	ILE
19	O	83	VAL
21	Q	34	THR
21	Q	53	VAL
23	S	49	LEU
23	S	62	THR
24	T	24	VAL
24	T	81	VAL
24	T	85	VAL
25	U	73	VAL
26	V	9	SER
27	W	2	SER
27	W	54	LYS
28	X	3	THR
28	X	17	LEU
30	Z	45	ASP
32	b	6	VAL

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Mol	Chain	Res	Type
32	b	12	LEU
32	b	61	GLN
32	b	70	LEU
32	b	108	THR
32	b	163	LEU
32	b	201	VAL
32	b	202	ILE
33	c	162	ILE
33	c	165	THR
34	d	30	VAL
34	d	36	ASN
34	d	103	VAL
34	d	121	SER
34	d	126	THR
34	d	204	GLU
34	d	208	LYS
35	e	23	VAL
35	e	33	THR
36	f	13	ASP
36	f	58	HIS
36	f	64	VAL
37	g	37	SER
37	g	56	VAL
37	g	65	THR
37	g	97	THR
37	g	110	LYS
37	g	115	THR
38	h	68	GLU
38	h	107	THR
39	i	27	VAL
40	j	7	ARG
40	j	25	ILE
41	k	15	VAL
41	k	29	THR
41	k	58	THR
41	k	105	LYS
41	k	110	THR
42	l	15	LEU
42	l	35	THR
42	l	55	VAL
42	l	88	LYS
43	m	18	SER

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Mol	Chain	Res	Type
43	m	34	LEU
43	m	97	VAL
44	n	14	GLU
44	n	58	VAL
44	n	100	SER
46	p	42	SER
46	p	80	SER
47	q	10	THR
47	q	24	VAL
47	q	39	ILE
47	q	69	SER
48	r	24	LYS
49	s	19	VAL
49	s	58	VAL
50	t	64	LYS
50	t	77	SER
51	u	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	86	ASN
7	C	198	GLN
7	C	200	ASN
8	D	133	GLN
8	D	153	GLN
9	E	138	ASN
9	E	141	ASN
9	E	165	HIS
10	F	37	ASN
11	G	64	GLN
11	G	106	ASN
13	I	47	HIS
18	N	35	HIS
21	Q	48	GLN
22	R	62	ASN
24	T	21	GLN
27	W	16	ASN
27	W	35	HIS
27	W	36	HIS
32	b	13	GLN
32	b	20	HIS

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Mol	Chain	Res	Type
32	b	21	GLN
32	b	53	ASN
33	c	28	GLN
36	f	52	ASN
37	g	32	GLN
37	g	51	GLN
37	g	148	ASN
40	j	58	ASN
43	m	76	ASN
48	r	31	GLN
51	u	43	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	184 (12%)	0
5	A	2720/2918 (93%)	369 (13%)	18 (0%)
52	v	76/77 (98%)	28 (36%)	0
53	w	2/3 (66%)	0	0
6	B	114/115 (99%)	11 (9%)	1 (0%)
All	All	4439/4657 (95%)	592 (13%)	19 (0%)

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	41	U
5	A	53	G
5	A	56	A
5	A	67	G
5	A	78	A
5	A	81	A
5	A	82	G
5	A	104	C
5	A	109	G
5	A	110	A
5	A	125	A
5	A	126	A
5	A	127	U
5	A	138	A
5	A	147	A

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Mol	Chain	Res	Type
5	A	149	G
5	A	170	A
5	A	171	C
5	A	188	A
5	A	203	A
5	A	206	A
5	A	222	G
5	A	223	A
5	A	228	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	246	U
5	A	255	G
5	A	257	G
5	A	262	A
5	A	278	U
5	A	279	U
5	A	290	U
5	A	297	G
5	A	305	C
5	A	313	A
5	A	331	G
5	A	332	A
5	A	335	U
5	A	336	U
5	A	345	C
5	A	347	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	385	G
5	A	395	G
5	A	403	A
5	A	410	G
5	A	411	A
5	A	423	G
5	A	435	C
5	A	455	C

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Mol	Chain	Res	Type
5	A	474	C
5	A	479	A
5	A	480	G
5	A	493	G
5	A	503	U
5	A	504	A
5	A	508	C
5	A	529	G
5	A	530	C
5	A	531	A
5	A	544	U
5	A	545	C
5	A	546	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	595	G
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	635	A
5	A	643	U
5	A	649	G
5	A	651	U
5	A	666	A
5	A	684	U
5	A	713	A
5	A	715	C
5	A	728	A
5	A	745	U
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	790	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U

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Mol	Chain	Res	Type
5	A	826	U
5	A	843	G
5	A	845	A
5	A	857	G
5	A	864	A
5	A	900	C
5	A	905	G
5	A	908	A
5	A	929	C
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1037	A
5	A	1043	A
5	A	1044	G
5	A	1051	A
5	A	1104	G
5	A	1105	U
5	A	1106	C
5	A	1107	G
5	A	1108	A
5	A	1109	G
5	A	1113	G
5	A	1115	C
5	A	1127	U
5	A	1128	G
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1140	A
5	A	1149	G

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Mol	Chain	Res	Type
5	A	1166	A
5	A	1170	U
5	A	1173	G
5	A	1174	U
5	A	1245	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1296	A
5	A	1316	A
5	A	1324	U
5	A	1333	G
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1381	A
5	A	1411	G
5	A	1412	C
5	A	1414	A
5	A	1415	U
5	A	1422	A
5	A	1423	C
5	A	1428	A
5	A	1432	C
5	A	1435	A
5	A	1446	C
5	A	1447	G
5	A	1448	U
5	A	1455	U
5	A	1456	C
5	A	1462	G
5	A	1477	U
5	A	1478	G
5	A	1483	U
5	A	1485	A
5	A	1488	C
5	A	1489	A
5	A	1492	U

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Mol	Chain	Res	Type
5	A	1504	U
5	A	1505	A
5	A	1507	G
5	A	1510	G
5	A	1515	C
5	A	1520	A
5	A	1523	A
5	A	1526	C
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1538	A
5	A	1539	G
5	A	1540	C
5	A	1543	A
5	A	1544	G
5	A	1558	G
5	A	1564	A
5	A	1567	A
5	A	1576	U
5	A	1577	A
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1606	A
5	A	1607	A
5	A	1616	A
5	A	1632	U
5	A	1645	U
5	A	1646	U
5	A	1672	G
5	A	1726	C
5	A	1727	G
5	A	1731	C
5	A	1732	C
5	A	1734	G
5	A	1736	G
5	A	1742	G

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Mol	Chain	Res	Type
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1807	G
5	A	1812	C
5	A	1825	A
5	A	1829	C
5	A	1843	A
5	A	1844	A
5	A	1845	G
5	A	1865	G
5	A	1872	A
5	A	1901	C
5	A	1902	G
5	A	1906	G
5	A	1908	A
5	A	1909	A
5	A	1910	C
5	A	1915	A
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1932	A
5	A	1934	A
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1983	G
5	A	1987	U
5	A	1989	U
5	A	2017	A
5	A	2018	U
5	A	2019	C
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A

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Mol	Chain	Res	Type
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2092	C
5	A	2093	U
5	A	2194	A
5	A	2195	A
5	A	2200	G
5	A	2207	G
5	A	2216	C
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2264	A
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2307	A
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2318	A
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2372	A
5	A	2378	G
5	A	2379	G
5	A	2381	C
5	A	2398	U
5	A	2399	C
5	A	2402	U

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Mol	Chain	Res	Type
5	A	2420	C
5	A	2421	A
5	A	2425	G
5	A	2426	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2465	A
5	A	2466	G
5	A	2469	U
5	A	2471	C
5	A	2472	A
5	A	2480	G
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2514	A
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2569	C
5	A	2578	G
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2609	U
5	A	2625	U
5	A	2651	G
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2744	A
5	A	2754	A
5	A	2762	G

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Mol	Chain	Res	Type
5	A	2774	A
5	A	2776	A
5	A	2786	U
5	A	2796	U
5	A	2814	U
5	A	2816	G
5	A	2817	A
5	A	2829	U
5	A	2831	A
5	A	2845	G
5	A	2857	U
5	A	2863	A
5	A	2869	A
5	A	2876	C
5	A	2880	U
5	A	2881	U
5	A	2882	G
6	B	22	G
6	B	39	C
6	B	42	G
6	B	51	A
6	B	54	G
6	B	65	G
6	B	67	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	106	A
31	a	4	A
31	a	6	C
31	a	7	U
31	a	9	A
31	a	11	G
31	a	15	U
31	a	24	G
31	a	34	A
31	a	41	G
31	a	46	A
31	a	49	C
31	a	50	U
31	a	52	A
31	a	53	A

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Mol	Chain	Res	Type
31	a	62	A
31	a	66	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	117	U
31	a	126	A
31	a	127	U
31	a	157	A
31	a	159	G
31	a	165	C
31	a	170	A
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A
31	a	205	U
31	a	206	C
31	a	241	U
31	a	242	A
31	a	243	G
31	a	246	A
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	302	A
31	a	324	C
31	a	325	A
31	a	340	A
31	a	341	C
31	a	343	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	369	A
31	a	380	C
31	a	393	A
31	a	402	G
31	a	407	A

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Mol	Chain	Res	Type
31	a	408	A
31	a	409	G
31	a	410	A
31	a	416	U
31	a	417	U
31	a	418	A
31	a	420	G
31	a	425	U
31	a	426	A
31	a	434	U
31	a	444	A
31	a	447	A
31	a	448	G
31	a	461	A
31	a	463	U
31	a	481	G
31	a	483	U
31	a	492	A
31	a	493	A
31	a	494	U
31	a	496	A
31	a	497	G
31	a	501	C
31	a	508	C
31	a	515	C
31	a	518	G
31	a	520	A
31	a	521	G
31	a	524	7MG
31	a	527	G
31	a	528	U
31	a	529	A
31	a	535	G
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	574	G
31	a	593	A
31	a	636	G

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Mol	Chain	Res	Type
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	720	U
31	a	721	G
31	a	731	G
31	a	752	G
31	a	774	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	840	U
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	957	U
31	a	963	2MG
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	990	G
31	a	993	A
31	a	1001	A
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1061	G
31	a	1062	U
31	a	1091	G
31	a	1092	U
31	a	1098	A
31	a	1107	A

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Mol	Chain	Res	Type
31	a	1134	C
31	a	1136	G
31	a	1156	U
31	a	1164	A
31	a	1166	A
31	a	1179	G
31	a	1180	C
31	a	1188	A
31	a	1193	A
31	a	1194	A
31	a	1209	U
31	a	1210	A
31	a	1224	A
31	a	1235	A
31	a	1255	G
31	a	1277	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1302	G
31	a	1317	C
31	a	1337	A
31	a	1350	G
31	a	1360	A
31	a	1367	G
31	a	1375	C
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1398	G
31	a	1416	G
31	a	1443	A
31	a	1448	C
31	a	1450	A
31	a	1484	G
31	a	1491	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1514	G
31	a	1516	MA6

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Mol	Chain	Res	Type
31	a	1526	G
31	a	1527	G
52	v	2	G
52	v	3	C
52	v	4	U
52	v	8	4SU
52	v	9	A
52	v	13	C
52	v	14	A
52	v	15	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	20	H2U
52	v	22	A
52	v	23	G
52	v	30	G
52	v	46	G
52	v	49	C
52	v	51	C
52	v	55	5MU
52	v	56	PSU
52	v	58	A
52	v	59	A
52	v	61	U
52	v	65	G
52	v	66	U
52	v	72	C
52	v	73	C
52	v	77	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	109	G
5	A	256	C
5	A	364	A
5	A	365	U
5	A	368	C
5	A	424	G
5	A	478	A
5	A	507	U

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Mol	Chain	Res	Type
5	A	782	G
5	A	844	A
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	1187	G
5	A	1519	U
5	A	2419	U
5	A	2443	G
5	A	2502	U
6	B	86	U

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

28 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$
5	PSU	A	2576	5	18,21,22	1.12	2 (11%)	21,30,33	2.02	6 (28%)
5	PSU	A	2453	5	18,21,22	1.07	1 (5%)	21,30,33	2.03	6 (28%)
31	PSU	a	513	31	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
5	OMG	A	2247	5,52	23,26,27	0.53	0	32,38,41	0.47	0
5	2MG	A	2441	5	23,26,27	0.52	0	33,38,41	0.46	0
5	5MU	A	1935	5	19,22,23	0.52	0	27,32,35	0.49	0
52	4SU	v	8	52	18,21,22	4.44	8 (44%)	25,30,33	2.30	4 (16%)
5	PSU	A	1913	5	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
5	3TD	A	1911	5	19,22,23	4.39	6 (31%)	23,32,35	1.75	3 (13%)
31	MA6	a	1516	31	23,26,27	1.43	4 (17%)	33,38,41	3.29	12 (36%)
5	PSU	A	2500	5	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
31	7MG	a	524	31	23,26,27	1.08	1 (4%)	27,39,42	0.89	2 (7%)
5	PSU	A	2601	5	18,21,22	1.08	1 (5%)	21,30,33	1.97	3 (14%)
31	4OC	a	1399	31	20,23,24	3.12	8 (40%)	25,32,35	0.97	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	7MG	A	2065	5	23,26,27	1.05	1 (4%)	27,39,42	0.93	2 (7%)
52	PSU	v	56	52	18,21,22	1.12	1 (5%)	21,30,33	1.83	5 (23%)
31	MA6	a	1515	31	23,26,27	1.42	4 (17%)	33,38,41	3.22	12 (36%)
52	H2U	v	20	52	18,21,22	0.55	0	19,30,33	0.99	1 (5%)
31	2MG	a	1204	31	23,26,27	0.48	0	33,38,41	0.49	0
31	2MG	a	963	31	23,26,27	0.49	0	33,38,41	0.50	0
5	6MZ	A	2026	5	22,25,26	2.48	4 (18%)	29,36,39	3.47	11 (37%)
5	PSU	A	952	5	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
52	5MU	v	55	52	19,22,23	0.47	0	27,32,35	0.71	0
5	PSU	A	1907	5	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
5	OMU	A	2548	5	19,22,23	3.02	8 (42%)	25,31,34	1.87	5 (20%)
31	UR3	a	1495	31	19,22,23	2.88	7 (36%)	26,32,35	1.63	3 (11%)
5	2MA	A	2499	5	22,25,26	3.87	9 (40%)	32,37,40	2.59	11 (34%)
31	5MC	a	964	31	19,22,23	0.58	0	26,32,35	0.63	0

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
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5,52	-	1/9/27/28	0/3/3/3
5	2MG	A	2441	5	-	2/9/27/28	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
52	4SU	v	8	52	-	2/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	0/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	0/11/29/30	0/3/3/3
5	PSU	A	2500	5	-	1/7/25/26	0/2/2/2
31	7MG	a	524	31	-	3/7/37/38	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
52	PSU	v	56	52	-	4/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
52	H2U	v	20	52	-	1/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
31	2MG	a	963	31	-	2/9/27/28	0/3/3/3
5	6MZ	A	2026	5	-	1/9/27/28	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
52	5MU	v	55	52	-	3/7/25/26	0/2/2/2
5	PSU	A	1907	5	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	2MA	A	2499	5	-	2/7/25/26	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.21	1.49	1.35
5	A	2499	2MA	C4-N3	11.70	1.49	1.34
5	A	1911	3TD	C2-N1	10.48	1.50	1.37
5	A	2026	6MZ	C6-N6	9.74	1.45	1.34
52	v	8	4SU	C2-N1	9.61	1.53	1.38
52	v	8	4SU	C4-N3	8.82	1.46	1.37
52	v	8	4SU	C5-C4	7.34	1.51	1.42
31	a	1495	UR3	C2-N1	7.13	1.48	1.38
52	v	8	4SU	C2-N3	7.10	1.50	1.38
5	A	2548	OMU	C2-N1	7.02	1.49	1.38
5	A	2499	2MA	C2-N3	6.99	1.46	1.34
5	A	2499	2MA	C6-N1	6.86	1.44	1.35
31	a	1399	4OC	C4-N3	6.78	1.44	1.32
31	a	1495	UR3	C6-C5	6.70	1.50	1.35
5	A	2548	OMU	C2-N3	6.69	1.49	1.38
52	v	8	4SU	C6-C5	6.45	1.50	1.35
31	a	1399	4OC	C6-C5	6.30	1.49	1.35
31	a	1399	4OC	C2-N3	6.00	1.48	1.36
5	A	2499	2MA	C2-N1	5.98	1.44	1.34
5	A	1911	3TD	C6-N1	5.70	1.45	1.36
5	A	2548	OMU	C6-C5	5.58	1.48	1.35
31	a	1495	UR3	C2-N3	5.51	1.49	1.39
5	A	1911	3TD	C2-N3	4.97	1.49	1.38
52	v	8	4SU	C4-S4	-4.93	1.60	1.68
31	a	1399	4OC	C4-N4	4.71	1.45	1.36
5	A	2499	2MA	C5-C6	4.58	1.53	1.41
31	a	524	7MG	C5-N7	4.49	1.41	1.35
5	A	2065	7MG	C5-N7	4.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1399	4OC	C2-N1	4.18	1.48	1.40
5	A	2548	OMU	C4-N3	4.08	1.45	1.38
31	a	1516	MA6	C6-N6	3.96	1.47	1.36
31	a	1515	MA6	C6-N6	3.94	1.47	1.36
52	v	56	PSU	C6-C5	3.73	1.39	1.35
31	a	1399	4OC	C5-C4	3.61	1.49	1.41
5	A	1907	PSU	C6-C5	3.57	1.39	1.35
5	A	1913	PSU	C6-C5	3.55	1.39	1.35
5	A	2499	2MA	C6-N6	-3.48	1.25	1.34
31	a	513	PSU	C6-C5	3.45	1.39	1.35
5	A	2601	PSU	C6-C5	3.43	1.39	1.35
5	A	2576	PSU	C6-C5	3.42	1.39	1.35
5	A	2500	PSU	C6-C5	3.40	1.39	1.35
5	A	952	PSU	C6-C5	3.32	1.39	1.35
5	A	2453	PSU	C6-C5	3.28	1.38	1.35
31	a	1495	UR3	C6-N1	3.27	1.45	1.38
31	a	1399	4OC	C6-N1	3.26	1.45	1.38
5	A	2026	6MZ	C5-C4	-3.18	1.33	1.39
5	A	2026	6MZ	C5-N7	-3.16	1.33	1.39
5	A	2548	OMU	O4-C4	-3.13	1.18	1.24
31	a	1515	MA6	C5-C4	-3.02	1.33	1.39
31	a	1516	MA6	C5-C4	-3.01	1.33	1.39
5	A	1911	3TD	C4-N3	2.99	1.46	1.40
31	a	1399	4OC	O2-C2	-2.89	1.18	1.23
5	A	2548	OMU	C6-N1	2.75	1.44	1.38
5	A	2548	OMU	O2-C2	-2.68	1.18	1.23
5	A	2499	2MA	C4-N9	-2.64	1.32	1.37
52	v	8	4SU	O2-C2	-2.62	1.18	1.23
5	A	2026	6MZ	C8-N9	-2.61	1.33	1.37
52	v	8	4SU	C6-N1	2.59	1.44	1.38
5	A	2499	2MA	C5-N7	-2.57	1.34	1.39
31	a	1516	MA6	C5-N7	-2.53	1.34	1.39
31	a	1515	MA6	C5-N7	-2.45	1.34	1.39
31	a	1495	UR3	C4-N3	2.40	1.45	1.40
5	A	2548	OMU	C5-C4	2.31	1.48	1.43
31	a	1516	MA6	C8-N9	-2.29	1.33	1.37
5	A	1911	3TD	O2-C2	-2.28	1.19	1.23
31	a	1495	UR3	C5-C4	2.25	1.49	1.43
31	a	1515	MA6	C8-N9	-2.22	1.33	1.37
5	A	2499	2MA	C8-N7	2.16	1.35	1.31
31	a	1495	UR3	O2-C2	-2.05	1.18	1.22
5	A	2576	PSU	O4'-C1'	-2.02	1.41	1.43

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	N1-C6-N6	-11.86	102.40	116.86
31	a	1515	MA6	N1-C6-N6	-11.53	102.81	116.86
5	A	2026	6MZ	C4-N9-C1'	-9.89	103.49	126.63
5	A	2026	6MZ	C1'-N9-C8	9.82	148.88	127.09
31	a	1516	MA6	C5-C6-N6	8.03	138.03	125.33
52	v	8	4SU	C4-N3-C2	-7.94	119.70	127.31
31	a	1515	MA6	C5-C6-N6	7.73	137.56	125.33
5	A	2499	2MA	C1'-N9-C8	-6.72	112.18	127.09
5	A	2499	2MA	N9-C8-N7	-6.00	105.42	113.94
5	A	2548	OMU	C4-N3-C2	-5.85	119.35	126.61
31	a	1495	UR3	C4-N3-C2	-5.76	119.95	124.58
31	a	1516	MA6	N1-C2-N3	-5.67	120.00	128.58
5	A	2026	6MZ	C5-C4-N3	-5.62	118.98	126.72
31	a	1515	MA6	N1-C2-N3	-5.59	120.11	128.58
5	A	2026	6MZ	N1-C2-N3	-5.47	120.31	128.58
5	A	1911	3TD	N1-C2-N3	5.47	120.10	116.13
52	v	8	4SU	C5-C4-N3	5.44	119.81	114.75
5	A	2601	PSU	C4-N3-C2	-5.16	119.27	126.37
5	A	2499	2MA	C4-N9-C8	5.11	111.10	105.74
5	A	2453	PSU	C4-N3-C2	-5.06	119.40	126.37
5	A	2453	PSU	N1-C2-N3	5.05	120.50	115.17
5	A	2576	PSU	N1-C2-N3	5.05	120.50	115.17
5	A	2499	2MA	C5-C4-N3	-5.04	121.87	127.18
5	A	952	PSU	N1-C2-N3	5.03	120.48	115.17
5	A	952	PSU	C4-N3-C2	-5.03	119.44	126.37
5	A	2601	PSU	N1-C2-N3	4.91	120.35	115.17
5	A	2576	PSU	C4-N3-C2	-4.88	119.65	126.37
5	A	1907	PSU	C4-N3-C2	-4.85	119.69	126.37
5	A	2500	PSU	C4-N3-C2	-4.85	119.69	126.37
31	a	1515	MA6	C5-C4-N3	-4.84	120.05	126.72
31	a	1516	MA6	C5-C4-N3	-4.83	120.06	126.72
5	A	1913	PSU	C4-N3-C2	-4.79	119.78	126.37
5	A	1907	PSU	N1-C2-N3	4.77	120.20	115.17
5	A	2500	PSU	N1-C2-N3	4.76	120.18	115.17
31	a	513	PSU	N1-C2-N3	4.72	120.14	115.17
31	a	513	PSU	C4-N3-C2	-4.71	119.89	126.37
5	A	1913	PSU	N1-C2-N3	4.66	120.09	115.17
52	v	56	PSU	N1-C2-N3	4.58	120.00	115.17
52	v	56	PSU	C4-N3-C2	-4.51	120.16	126.37
5	A	2026	6MZ	C4-C5-C6	4.45	120.48	116.78
31	a	1515	MA6	N9-C8-N7	-4.38	107.72	113.94
31	a	1516	MA6	N9-C8-N7	-4.32	107.81	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2499	2MA	C4-N9-C1'	4.31	136.72	126.63
31	a	1515	MA6	C4-C5-C6	4.15	120.20	115.91
5	A	2548	OMU	N3-C2-N1	4.10	120.22	114.89
31	a	1516	MA6	C4-C5-C6	4.09	120.13	115.91
5	A	1911	3TD	C4-N3-C2	-3.98	120.40	124.61
5	A	2026	6MZ	N9-C8-N7	-3.87	108.45	113.94
52	v	8	4SU	N3-C2-N1	3.80	119.83	114.89
52	v	8	4SU	C5-C4-S4	-3.77	120.00	124.31
5	A	2548	OMU	C5-C4-N3	3.71	120.00	114.80
31	a	1495	UR3	C5-C4-N3	3.66	119.86	115.04
5	A	2026	6MZ	N3-C4-N9	3.56	133.23	127.17
5	A	2026	6MZ	C2-N3-C4	3.53	120.45	111.83
5	A	2499	2MA	N3-C4-N9	3.50	131.44	126.99
31	a	1516	MA6	C2-N1-C6	3.48	120.32	111.83
31	a	1515	MA6	C2-N1-C6	3.41	120.17	111.83
5	A	2499	2MA	C5-N7-C8	3.41	108.81	103.45
31	a	1516	MA6	C2-N3-C4	3.31	119.92	111.83
5	A	2499	2MA	N3-C2-N1	-3.31	119.94	125.77
31	a	1515	MA6	C2-N3-C4	3.28	119.84	111.83
52	v	20	H2U	C5-C4-N3	-3.27	113.21	116.69
31	a	513	PSU	O2-C2-N1	-3.06	119.63	122.79
31	a	1515	MA6	N3-C4-N9	3.06	132.37	127.17
5	A	2453	PSU	O2-C2-N1	-2.99	119.70	122.79
31	a	1516	MA6	C5-N7-C8	2.94	108.07	103.45
31	a	1516	MA6	N3-C4-N9	2.93	132.15	127.17
31	a	1515	MA6	C5-N7-C8	2.91	108.03	103.45
5	A	2548	OMU	O4-C4-C5	-2.89	120.19	125.16
5	A	2026	6MZ	C5-N7-C8	2.86	107.95	103.45
5	A	1911	3TD	C1'-C5-C4	2.85	121.93	117.61
5	A	1907	PSU	O2-C2-N1	-2.82	119.88	122.79
5	A	952	PSU	O2-C2-N1	-2.74	119.97	122.79
5	A	2576	PSU	O2-C2-N1	-2.72	119.99	122.79
5	A	2500	PSU	O2-C2-N1	-2.69	120.01	122.79
5	A	1913	PSU	O2-C2-N1	-2.67	120.03	122.79
31	a	1515	MA6	C4-N9-C8	2.61	108.48	105.74
5	A	2576	PSU	C6-N1-C2	-2.61	120.27	122.69
52	v	56	PSU	O2-C2-N1	-2.59	120.12	122.79
31	a	513	PSU	C6-N1-C2	-2.56	120.31	122.69
5	A	2499	2MA	CM2-C2-N1	2.54	120.92	117.13
52	v	56	PSU	C6-N1-C2	-2.49	120.38	122.69
31	a	1399	4OC	C6-C5-C4	2.49	120.00	117.00
5	A	2576	PSU	O4'-C1'-C2'	2.45	108.53	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	C4-N9-C8	2.44	108.30	105.74
5	A	2601	PSU	O2-C2-N1	-2.44	120.28	122.79
5	A	1913	PSU	C6-N1-C2	-2.41	120.45	122.69
5	A	2065	7MG	C5-C4-N9	2.39	109.40	106.33
5	A	2453	PSU	C6-C5-C4	2.38	119.78	118.17
52	v	56	PSU	O4'-C1'-C2'	2.36	108.41	105.15
31	a	513	PSU	O4'-C1'-C2'	2.30	108.34	105.15
31	a	524	7MG	C4-C5-N7	2.29	108.08	105.38
31	a	524	7MG	C5-C4-N9	2.28	109.26	106.33
5	A	2499	2MA	C4-C5-N7	-2.28	107.98	110.58
5	A	1907	PSU	C6-N1-C2	-2.28	120.58	122.69
5	A	2453	PSU	C6-N1-C2	-2.24	120.61	122.69
5	A	2065	7MG	C4-C5-N7	2.24	108.03	105.38
5	A	2026	6MZ	C5-C6-N1	2.23	120.55	118.15
31	a	1516	MA6	C4-C5-N7	-2.23	108.03	110.58
5	A	2548	OMU	O2-C2-N1	-2.22	119.91	122.80
5	A	2500	PSU	C6-N1-C2	-2.20	120.65	122.69
5	A	952	PSU	C6-N1-C2	-2.20	120.65	122.69
5	A	1907	PSU	C6-C5-C4	2.14	119.61	118.17
31	a	1495	UR3	C6-N1-C2	-2.13	120.06	121.80
5	A	2499	2MA	N6-C6-N1	2.09	119.85	117.03
31	a	1515	MA6	C4-C5-N7	-2.09	108.19	110.58
5	A	2026	6MZ	C4-C5-N7	-2.09	108.19	110.58
5	A	2576	PSU	C6-C5-C4	2.07	119.57	118.17
5	A	2453	PSU	O4'-C1'-C2'	2.06	108.00	105.15

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
52	v	56	PSU	O4'-C1'-C5-C4
52	v	56	PSU	O4'-C1'-C5-C6
5	A	2247	OMG	C1'-C2'-O2'-CM2
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
52	v	8	4SU	C3'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	a	524	7MG	O4'-C4'-C5'-O5'
5	A	2441	2MG	C3'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	56	PSU	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	963	2MG	C3'-C4'-C5'-O5'
5	A	2500	PSU	O4'-C4'-C5'-O5'
52	v	56	PSU	O4'-C4'-C5'-O5'
52	v	55	5MU	C4'-C5'-O5'-P
5	A	2026	6MZ	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
31	a	524	7MG	C4'-C5'-O5'-P
5	A	2441	2MG	O4'-C4'-C5'-O5'
5	A	2065	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2247	OMG	2	0
5	A	1935	5MU	1	0
52	v	8	4SU	1	0
5	A	1913	PSU	1	0
5	A	1911	3TD	1	0
52	v	56	PSU	1	0
52	v	20	H2U	2	0
31	a	963	2MG	1	0
5	A	2026	6MZ	1	0
52	v	55	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	OI9	a	1601	-	36,37,37	1.40	6 (16%)	37,52,52	1.60	4 (10%)
55	OI9	A	3001	-	36,37,37	1.40	6 (16%)	37,52,52	1.56	5 (13%)

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
55	OI9	a	1601	-	-	5/22/67/67	0/3/3/3
55	OI9	A	3001	-	-	6/22/67/67	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3001	OI9	C28-N13	3.96	1.40	1.33
55	a	1601	OI9	C28-N13	3.82	1.40	1.33
55	a	1601	OI9	C24-C22	-3.68	1.50	1.53
55	A	3001	OI9	C27-C24	3.64	1.55	1.52
55	a	1601	OI9	C27-C24	3.42	1.55	1.52
55	a	1601	OI9	C27-N13	3.17	1.49	1.46
55	A	3001	OI9	C27-N13	2.99	1.49	1.46
55	A	3001	OI9	C24-C22	-2.63	1.50	1.53
55	A	3001	OI9	C32-N15	2.30	1.37	1.33
55	A	3001	OI9	C29-N11	2.29	1.38	1.34
55	a	1601	OI9	C29-N11	2.13	1.38	1.34
55	a	1601	OI9	C23-C28	-2.03	1.48	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A	3001	OI9	C24-C27-N13	6.67	116.63	109.83
55	a	1601	OI9	C24-C27-N13	6.34	116.29	109.83
55	a	1601	OI9	O06-C28-N13	4.03	127.87	122.41
55	A	3001	OI9	C30-C29-N11	-3.28	111.78	116.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	a	1601	OI9	C30-C29-N11	-3.15	111.95	116.25
55	A	3001	OI9	O06-C28-N13	2.70	126.07	122.41
55	a	1601	OI9	C22-N10-C25	-2.58	107.86	112.17
55	A	3001	OI9	C22-N10-C25	-2.40	108.15	112.17
55	A	3001	OI9	O01-C19-C17	2.33	110.56	108.97

There are no chirality outliers.

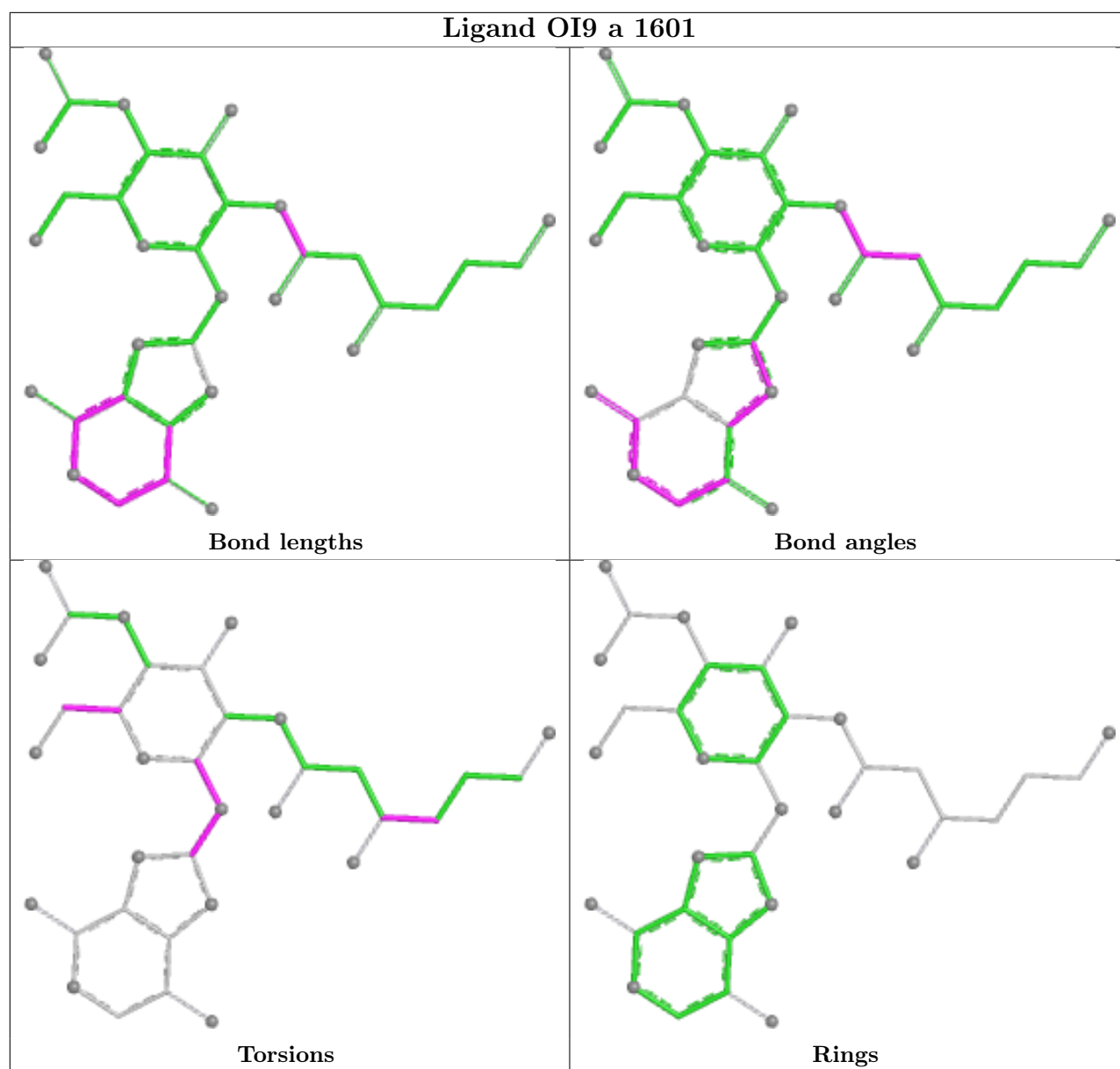
All (11) torsion outliers are listed below:

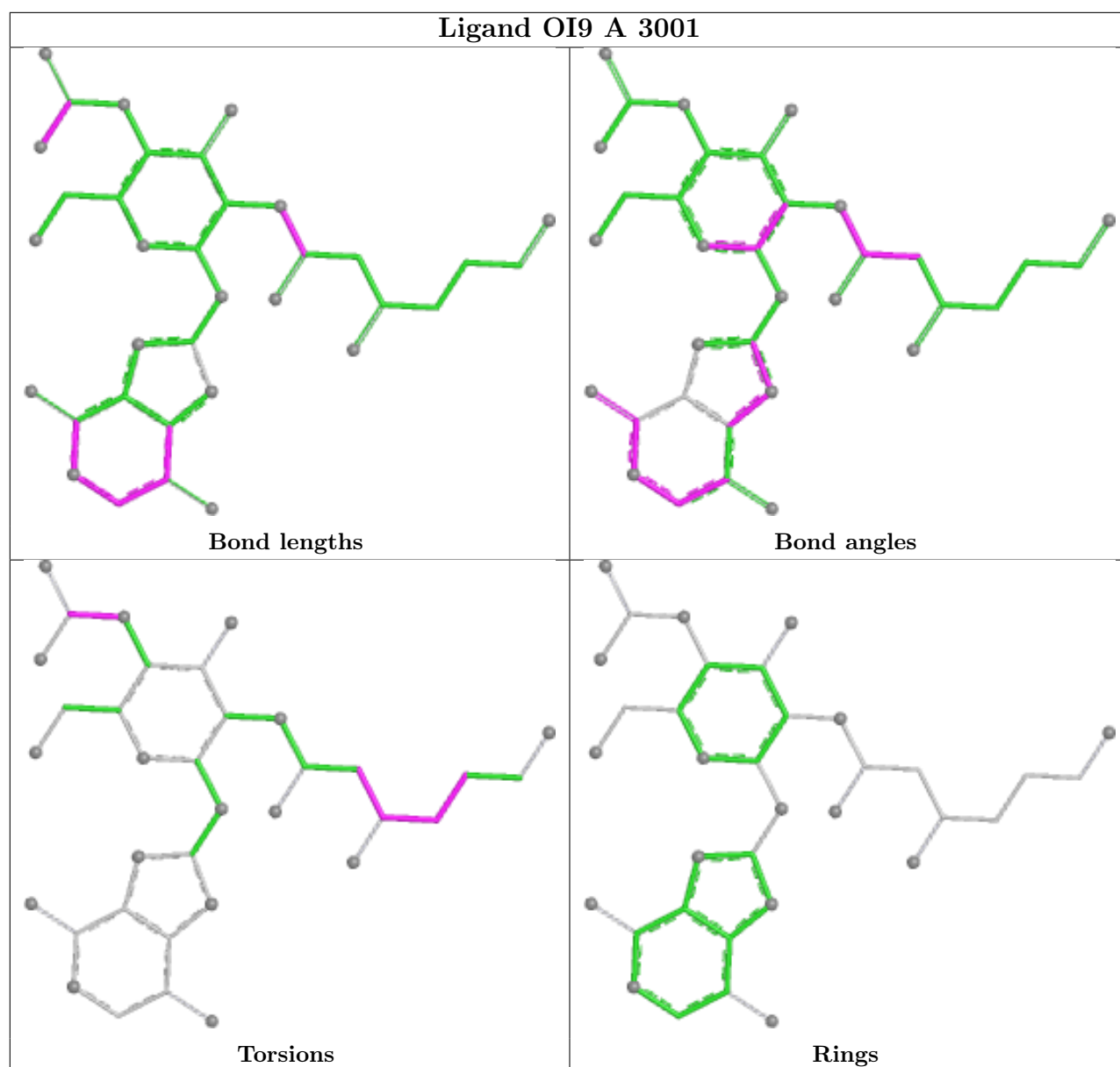
Mol	Chain	Res	Type	Atoms
55	A	3001	OI9	C30-C31-C33-C34
55	A	3001	OI9	N15-C32-O02-C20
55	A	3001	OI9	O08-C32-O02-C20
55	a	1601	OI9	O01-C21-C26-O05
55	a	1601	OI9	C20-C21-C26-O05
55	A	3001	OI9	C29-C30-C31-C33
55	A	3001	OI9	C29-C30-C31-N14
55	a	1601	OI9	O01-C19-N09-C25
55	a	1601	OI9	N12-C25-N09-C19
55	a	1601	OI9	N14-C31-C33-C34
55	A	3001	OI9	C31-C33-C34-C35

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

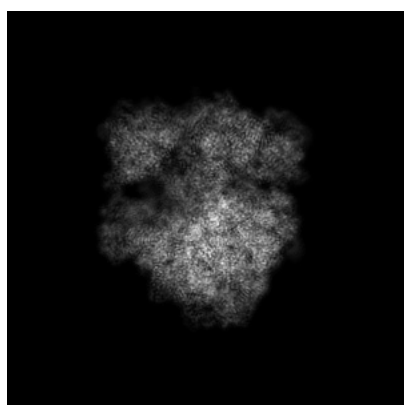
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26817. These allow visual inspection of the internal detail of the map and identification of artifacts.

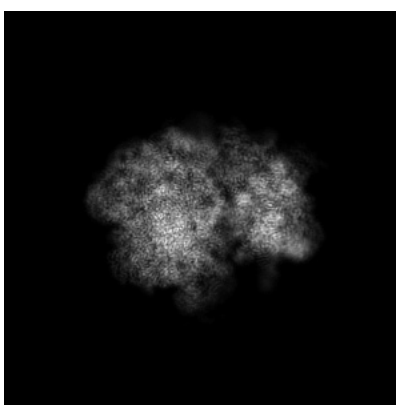
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

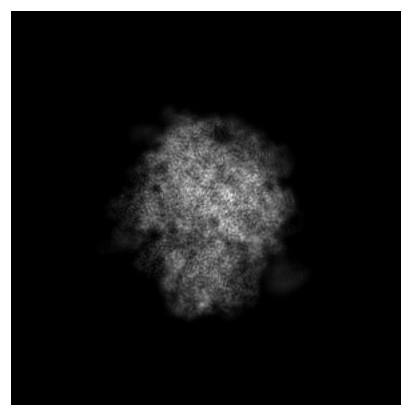
6.1.1 Primary map



X



Y



Z

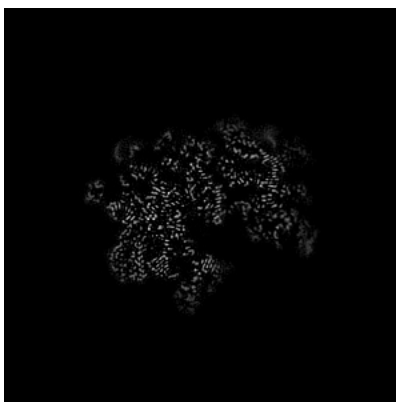
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

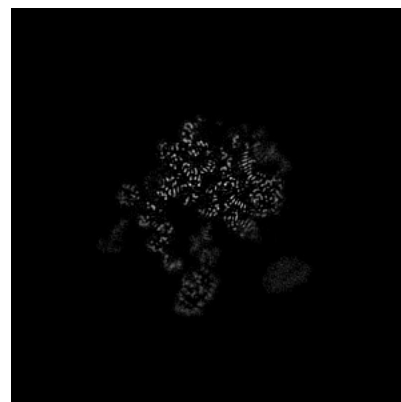
6.2.1 Primary map



X Index: 256



Y Index: 256

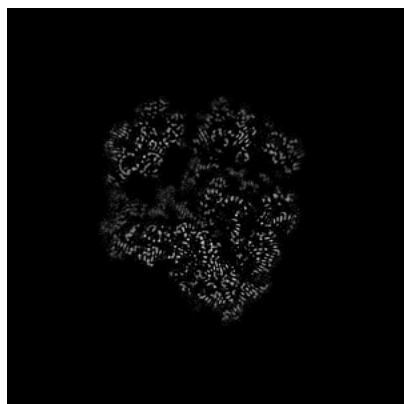


Z Index: 256

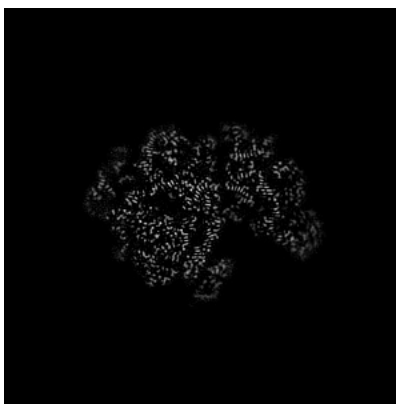
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 248



Y Index: 275

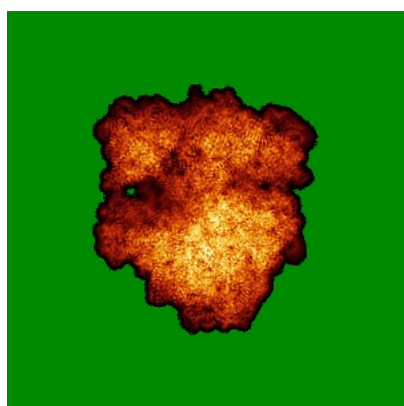


Z Index: 218

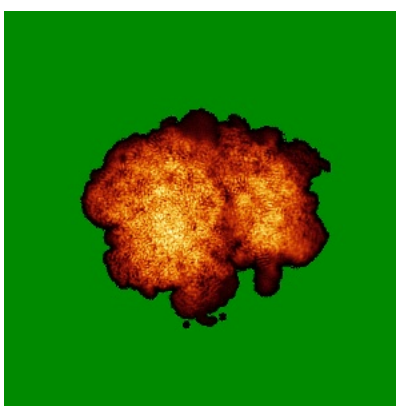
The images above show the largest variance slices of the map in three orthogonal directions.

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

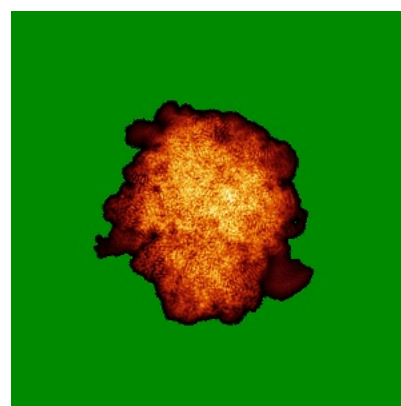
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

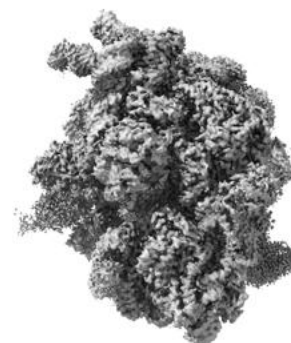
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

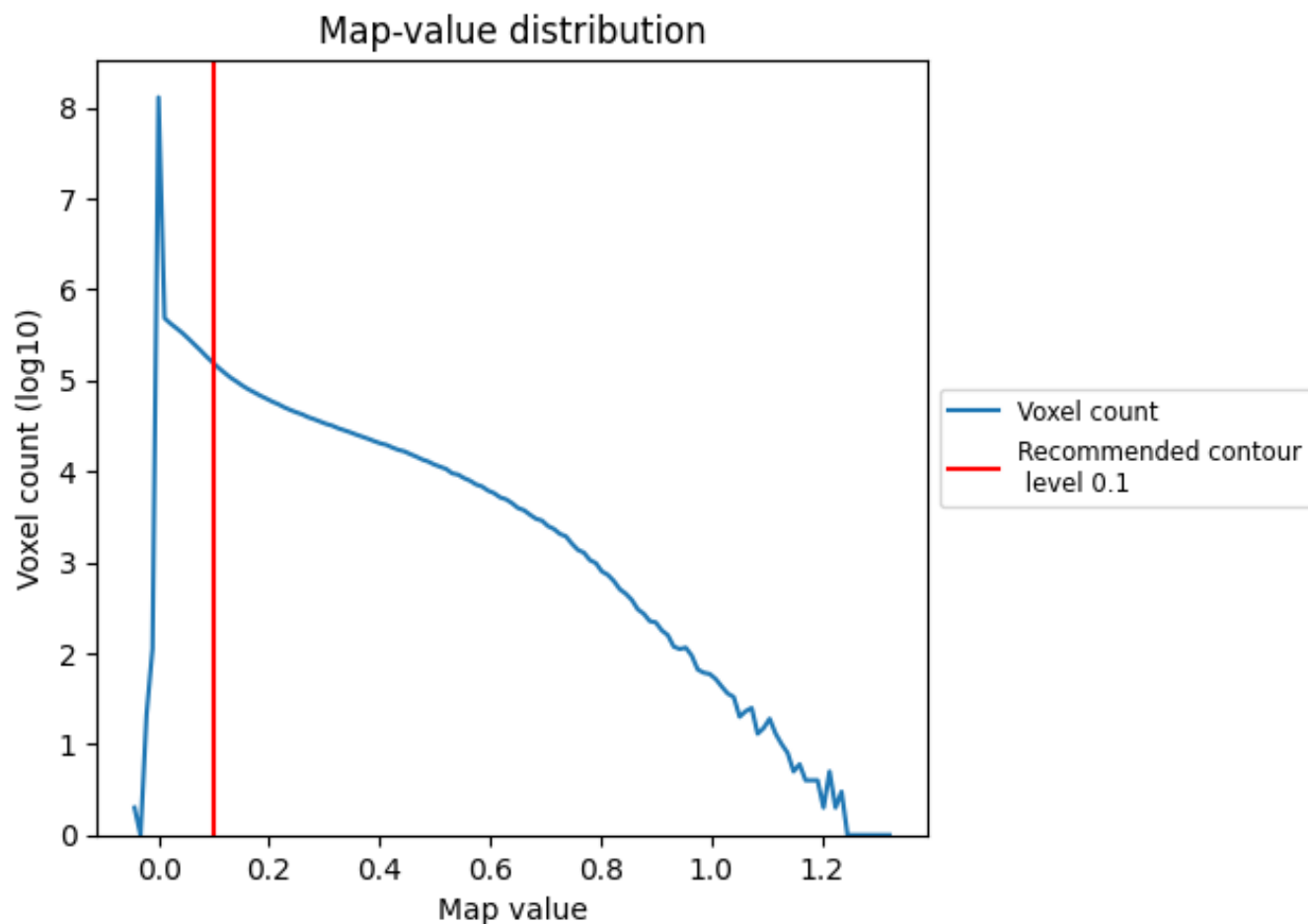
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

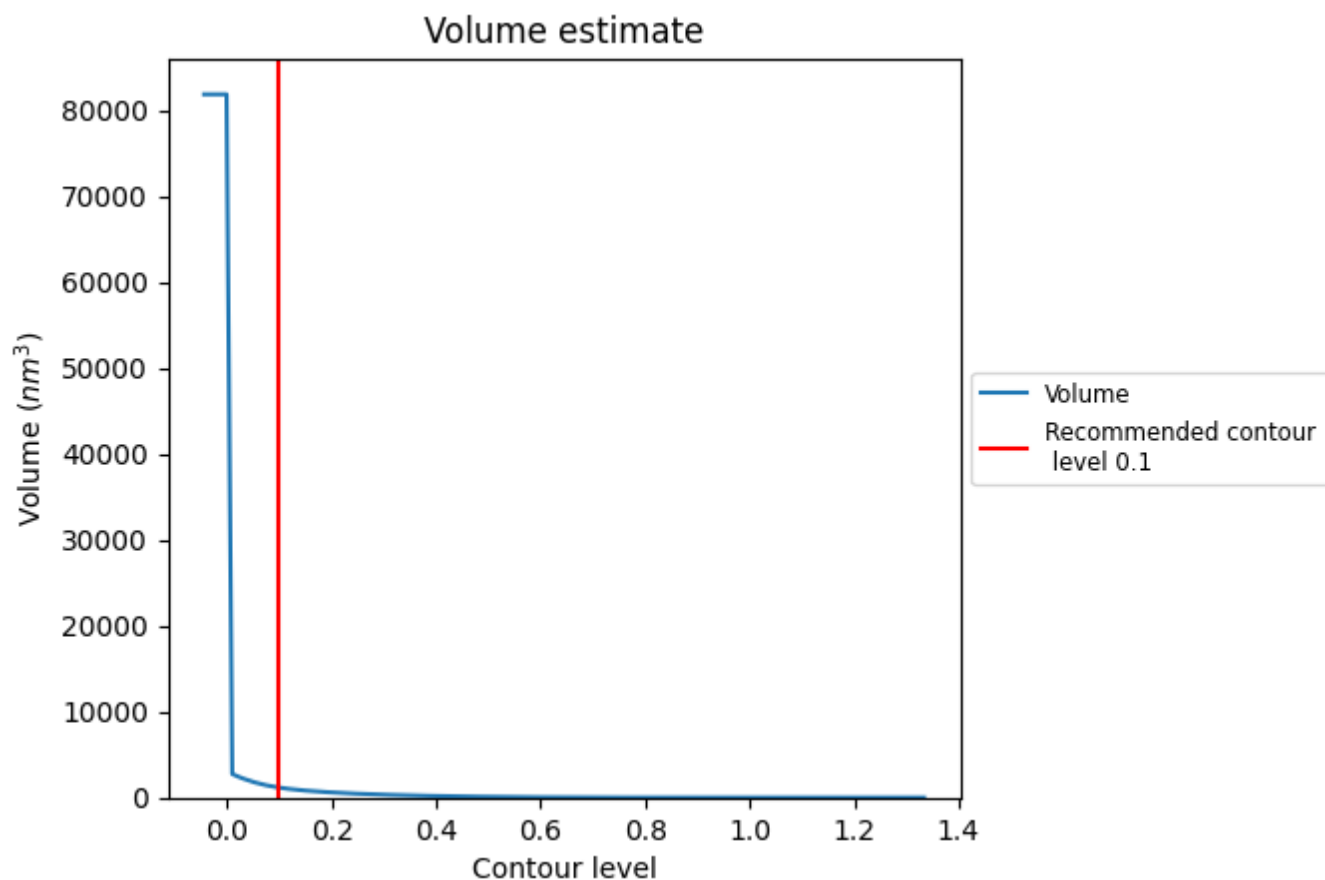
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

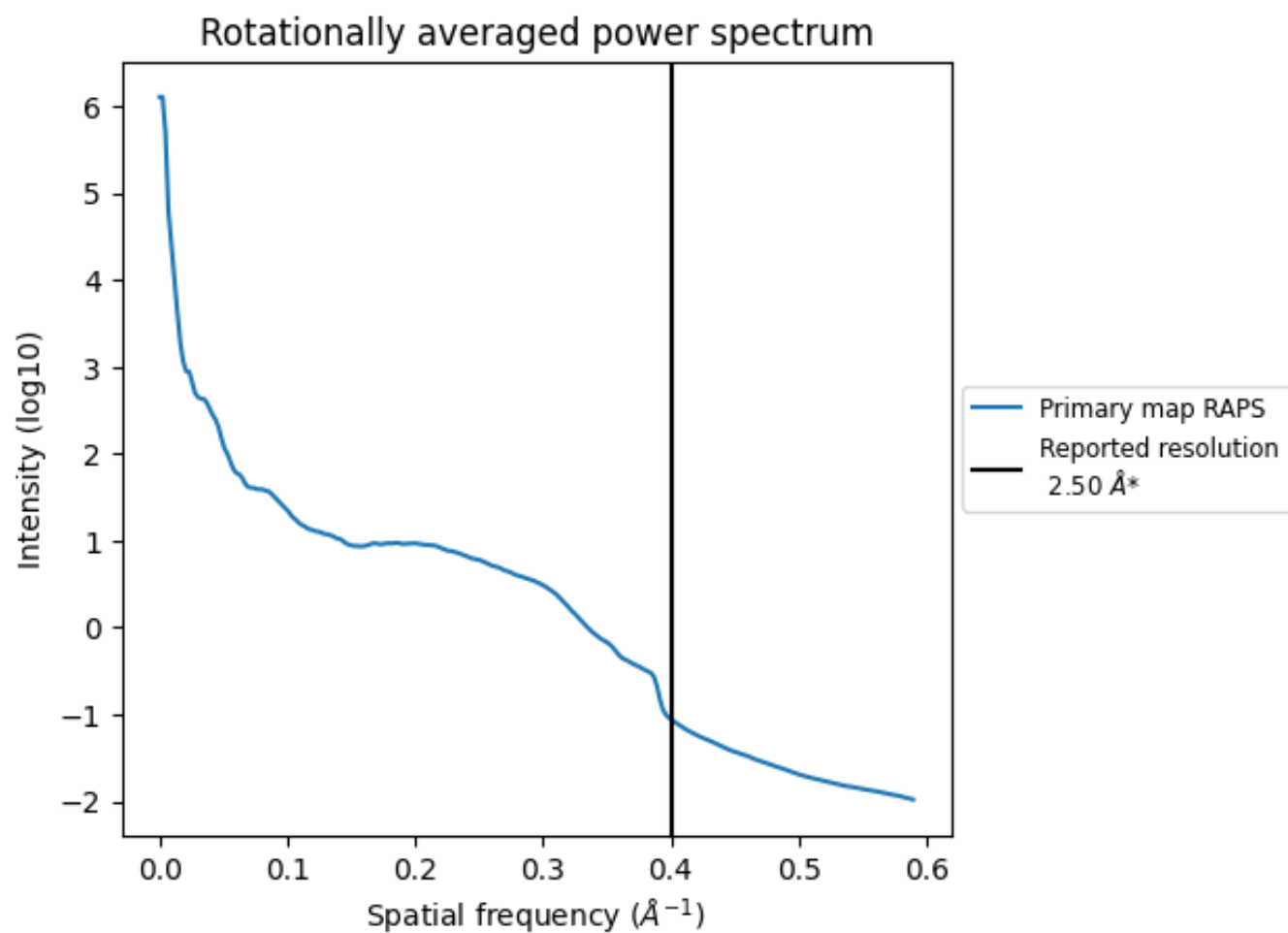
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1161 nm^3 ; this corresponds to an approximate mass of 1049 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

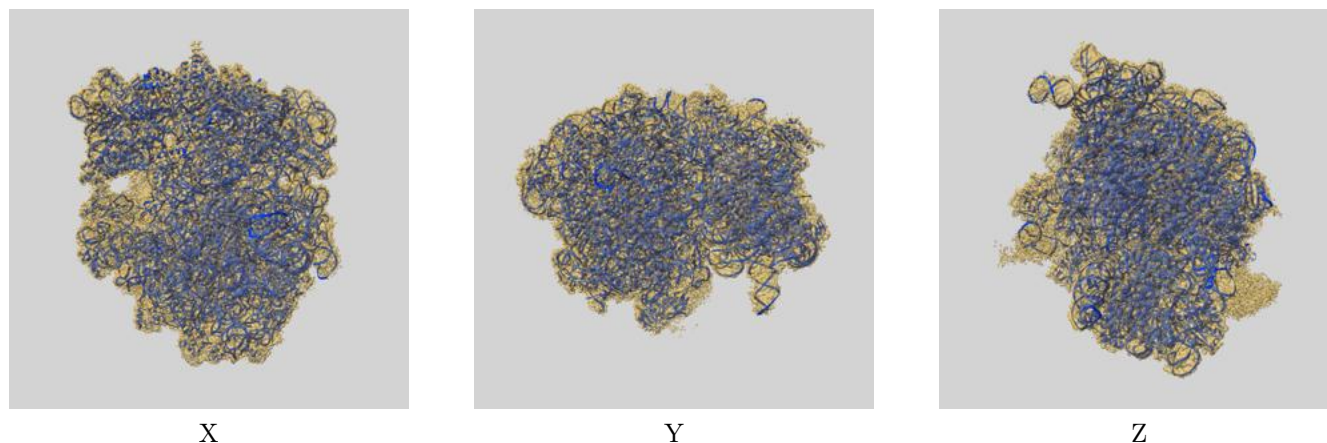
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

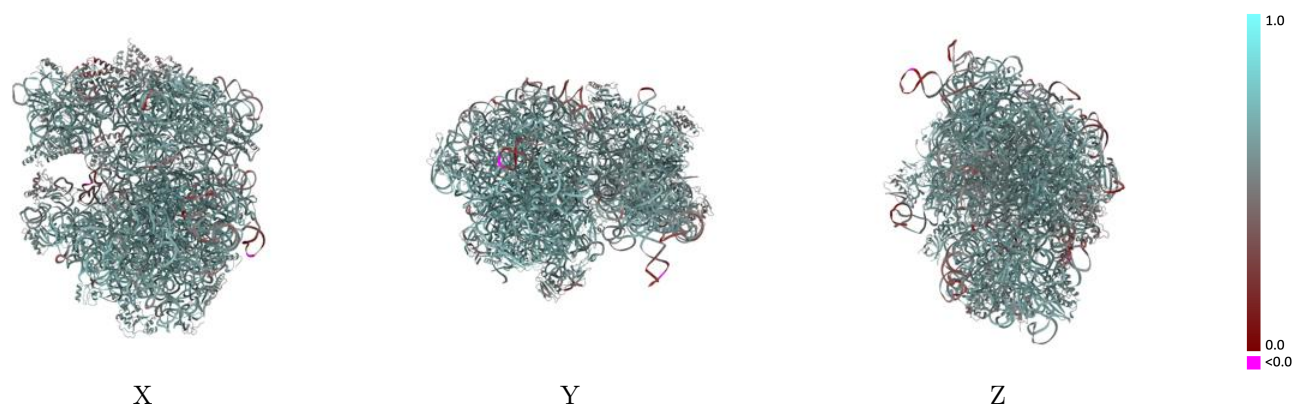
This section contains information regarding the fit between EMDB map EMD-26817 and PDB model 7UVV. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



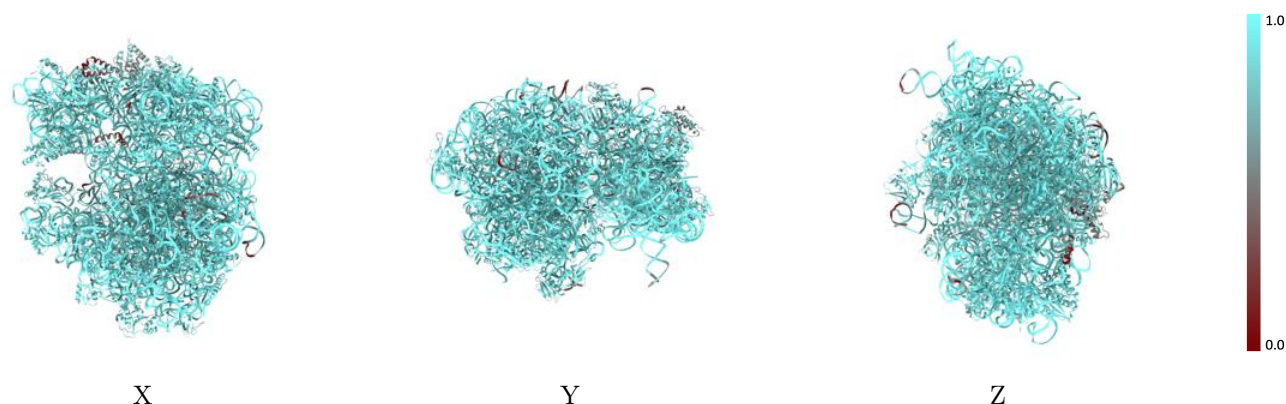
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



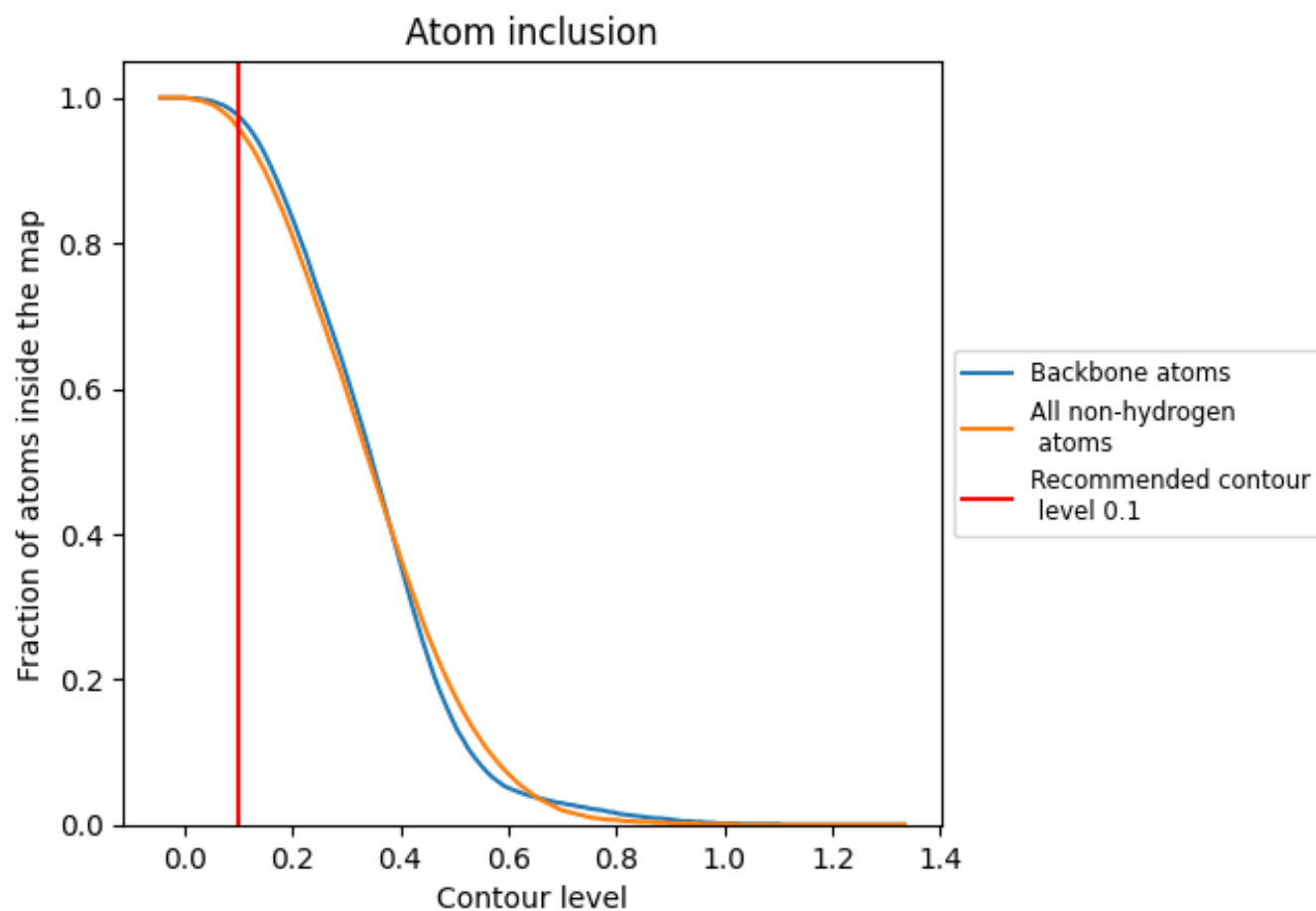
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.6100
0	 0.9420	 0.6300
1	 0.9800	 0.6820
2	 0.9880	 0.6850
3	 0.9830	 0.6510
A	 0.9800	 0.6310
B	 0.9940	 0.5840
C	 0.9660	 0.6530
D	 0.9690	 0.6670
E	 0.9430	 0.6340
F	 0.8420	 0.4770
G	 0.9080	 0.5420
H	 0.6560	 0.4650
I	 0.9730	 0.6590
J	 0.9270	 0.6370
K	 0.9780	 0.6550
L	 0.9580	 0.6500
M	 0.9790	 0.6680
N	 0.9630	 0.5890
O	 0.9370	 0.6360
P	 0.9960	 0.6770
Q	 0.9680	 0.6520
R	 0.9720	 0.6600
S	 0.9080	 0.6070
T	 0.8660	 0.5670
U	 0.9460	 0.6200
V	 0.9620	 0.6670
W	 0.9510	 0.6550
X	 0.8820	 0.5320
Y	 0.9690	 0.6600
Z	 0.9650	 0.6570
a	 0.9810	 0.5930
b	 0.6180	 0.4670
c	 0.9310	 0.5970
d	 0.8350	 0.4910



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Chain	Atom inclusion	Q-score
e	 0.9650	 0.6170
f	 0.8580	 0.5330
g	 0.8210	 0.5110
h	 0.9620	 0.6270
i	 0.9570	 0.6190
j	 0.9050	 0.5820
k	 0.9020	 0.5520
l	 0.9020	 0.5990
m	 0.9640	 0.6070
n	 0.9440	 0.6220
o	 0.9560	 0.6180
p	 0.9700	 0.6210
q	 0.9370	 0.5870
r	 0.9320	 0.5960
s	 0.9780	 0.6260
t	 0.9690	 0.6030
u	 0.4820	 0.4710
v	 0.8700	 0.4420
w	 1.0000	 0.6210