



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:13 PM JST

PDB ID : 8ZFG / pdb_00008zfg
EMDB ID : EMD-60060
Title : Structure of the Bacterial Ribosome with hypoxia-induced rRNA modifications
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Ito, T.; Suzuki, T.
Deposited on : 2024-05-07
Resolution : 2.68 Å(reported)
Based on initial model : 7K00

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

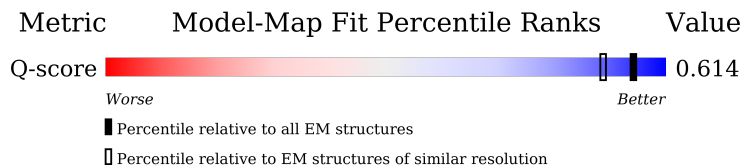
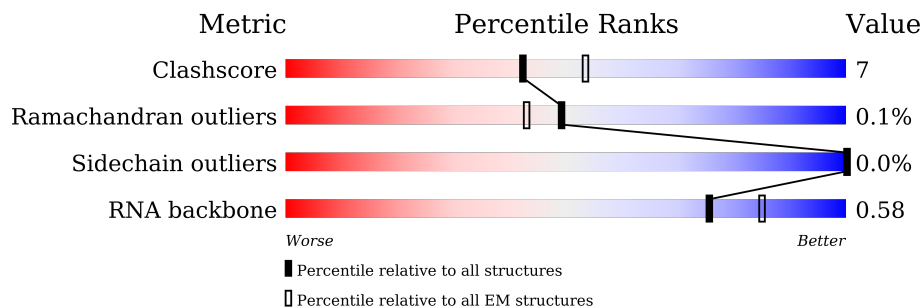
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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

Mol	Chain	Length	Quality of chain
1	A	1542	
2	B	241	
3	C	233	

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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

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Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	66	

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Mol	Chain	Length	Quality of chain
54	Z	77	<div><div></div><div>6%</div><div>52%</div><div>44%</div><div>.</div></div>

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0
			32466	14487	5964	10503	1512		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2761	Total	C	N	O	P	0	0
			59304	26462	10925	19156	2761		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 42 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	51	Total	C	N	O		0	0
			417	269	76	72			

- Molecule 49 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 50 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	6	Total	C	N	O	P	0	0
			130	58	25	41	6		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

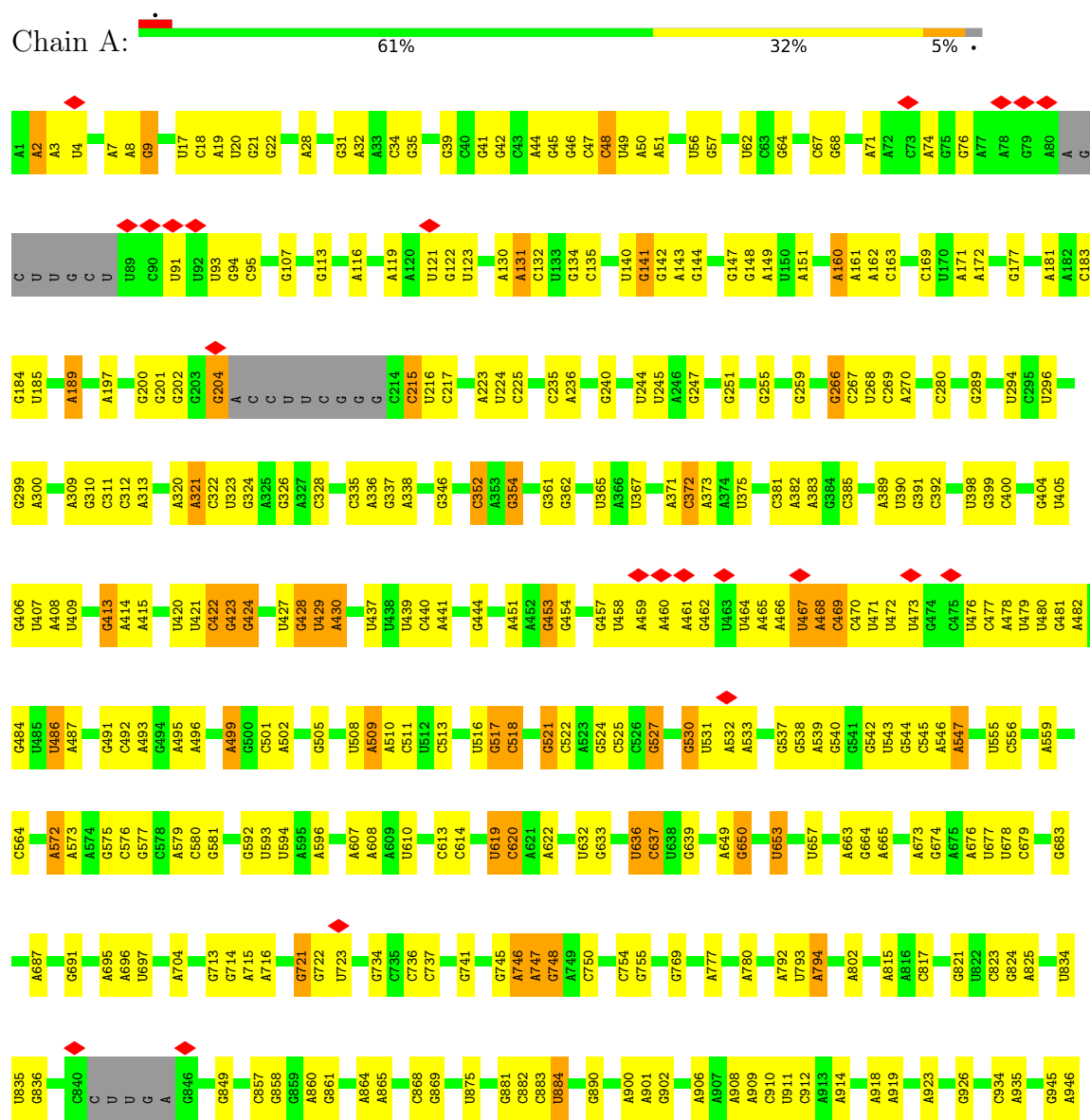
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

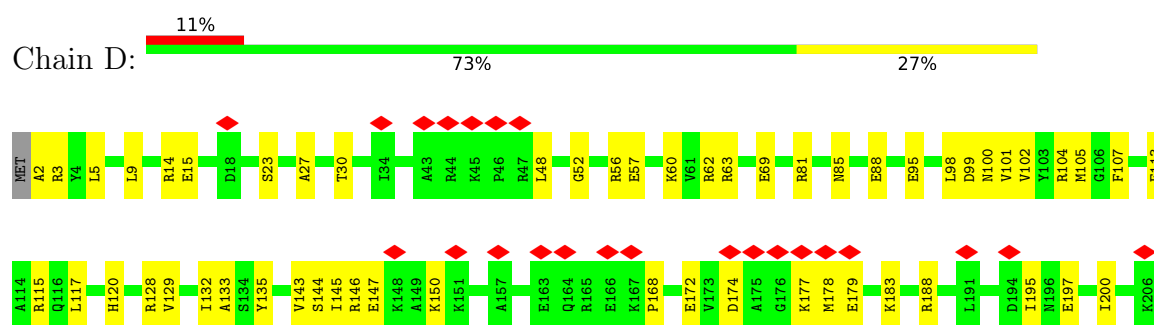
Mol	Chain	Residues	Atoms		AltConf
55	A	121	Total	Mg	0
			121	121	
55	a	340	Total	Mg	0
			340	340	
55	b	7	Total	Mg	0
			7	7	
55	c	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	

3 Residue-property plots

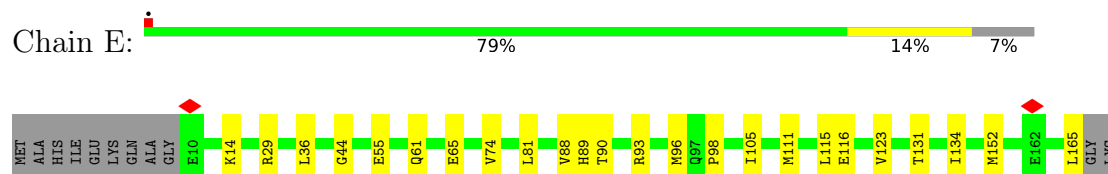
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

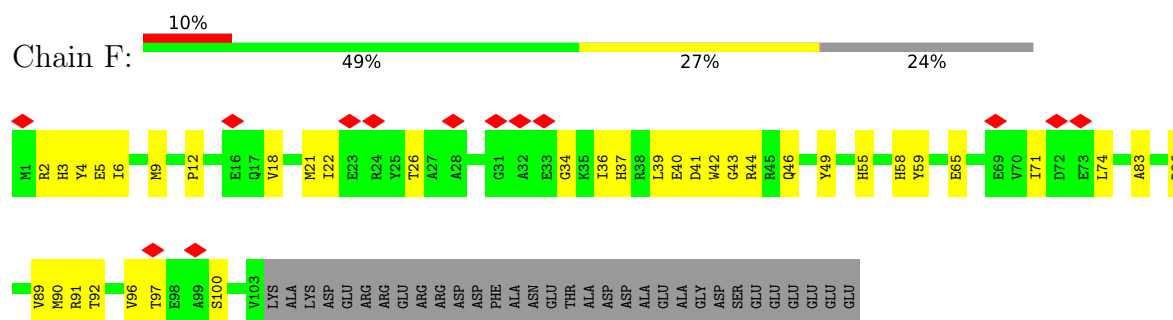




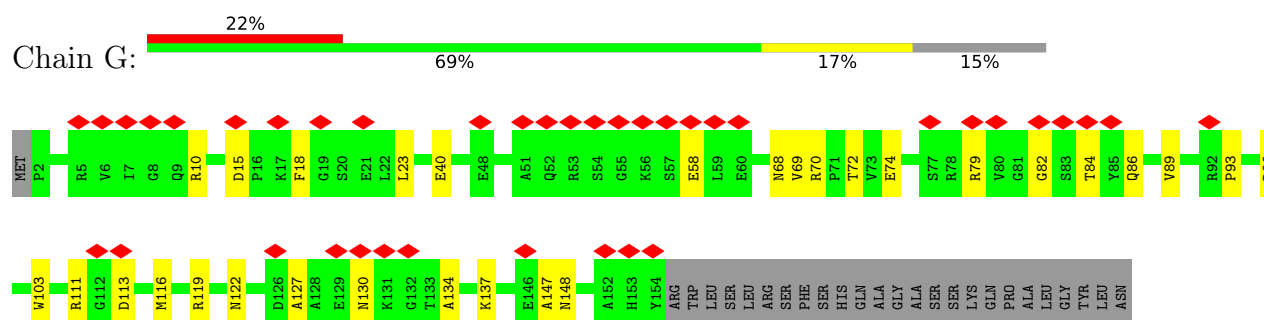
- Molecule 5: Small ribosomal subunit protein uS5



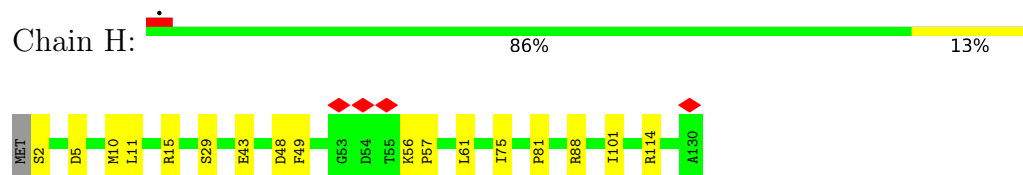
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 7: Small ribosomal subunit protein uS7

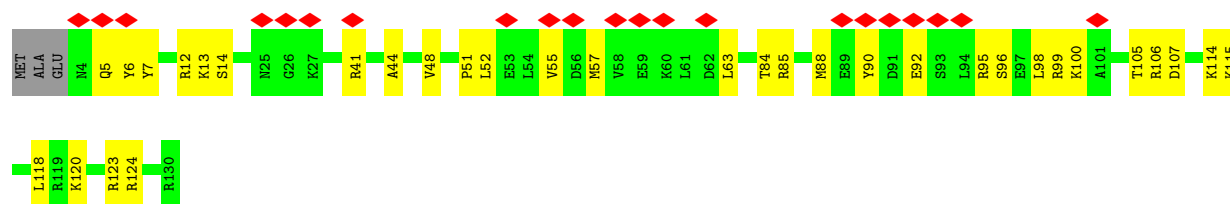


- Molecule 8: Small ribosomal subunit protein uS8



- Molecule 9: Small ribosomal subunit protein uS9

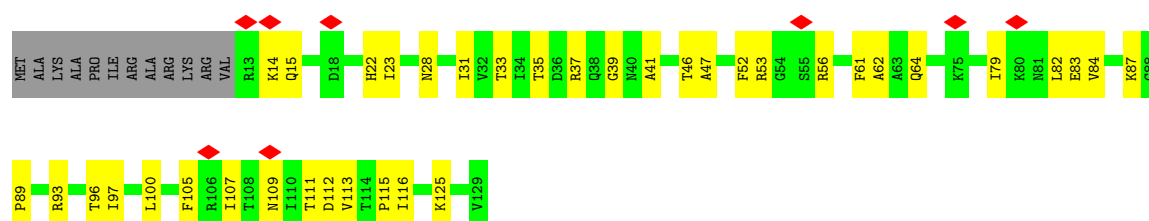




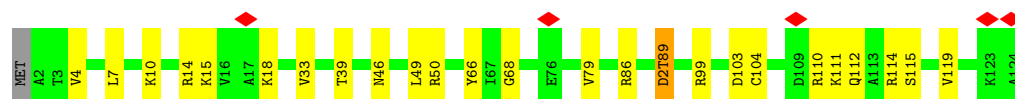
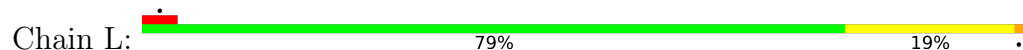
- Molecule 10: Small ribosomal subunit protein uS10



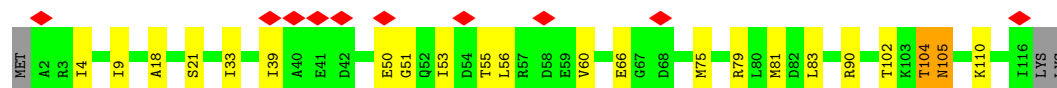
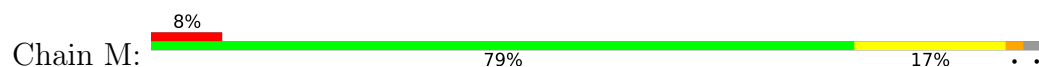
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein uS12

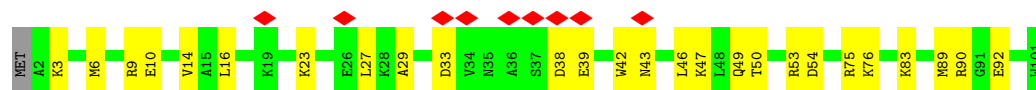


- Molecule 13: Small ribosomal subunit protein uS13

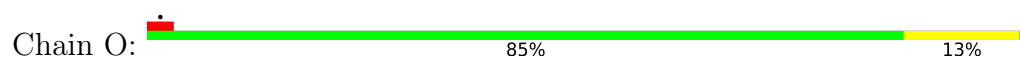


- Molecule 14: Small ribosomal subunit protein uS14

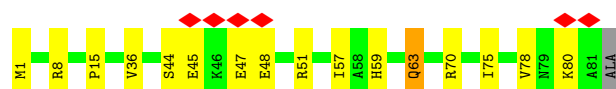
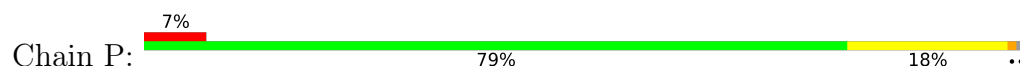




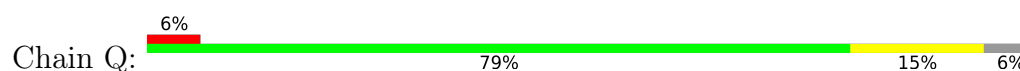
- Molecule 15: Small ribosomal subunit protein uS15



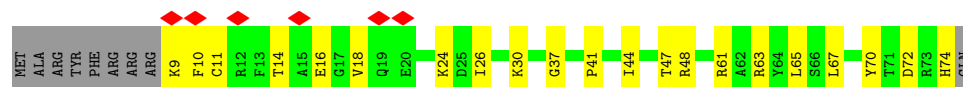
- Molecule 16: Small ribosomal subunit protein bS16



- Molecule 17: Small ribosomal subunit protein uS17



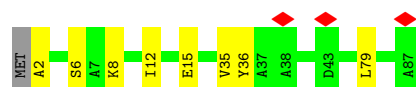
- Molecule 18: Small ribosomal subunit protein bS18



- Molecule 19: Small ribosomal subunit protein uS19



- Molecule 20: Small ribosomal subunit protein bS20

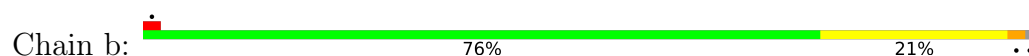


- Molecule 21: Small ribosomal subunit protein bS21

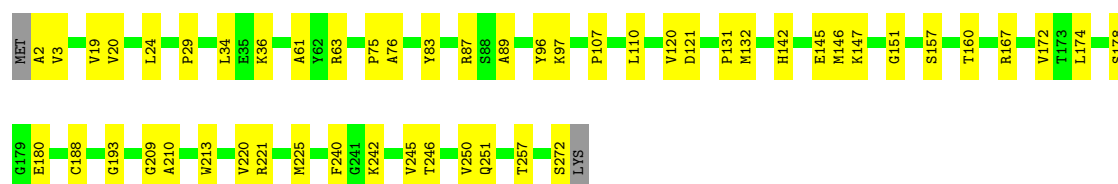
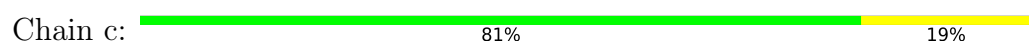
G2625	A2516	U2402	C2295	A2191	U	U	U	G2043	A1912	A1773	C1607	G1519	U1415	G1300
G2626	G2517	C2403	A2298	U2192	U	U	U	C2055	A1913	C1774	A1608	G1524	G1416	A1301
U2629	A2518	U2404	U2299	U2194	G	A	G	G2056	3TD1915	U1779	A1609	A1525	C1417	C1306
G2630	U2522	G2405	C2300	U2195	A	A	G	U1917	A1916	A1786	A1614	G1526	A1419	G1310
A2635	G2523	A2406	U2301	U2197	U	U	U	G1929	U1917	G1790	A1618	A1528	A1420	U1313
G2636	G2525	G2410	U2302	A2198	G	U	G	G1930	G1929	A1791	G1622	G1529	A1427	C1314
U2637	G2529	U2419	U2305	G2204	U	U	U	A2062	U1931	A1794	A1626	C1531	C1428	C1315
G2638	G2535	C2420	G2308	C2208	A	A	C	C2063	G1932	G1795	U1636	A1532	A1434	C1319
C2646	U2536	A2425	U2312	U2209	G	G	C	G2069	A1937	G1797	A1637	C1533	A1435	C1320
U2647	U2537	G2429	G2313	U2210	C	U	C	A2070	A1938	U1798	U1647	U1534	G1436	A1321
G2648	C2538	A2430	A2314	A2211	C	U	C	C2071	A1939	U1796	U1648	A1535	U1437	C1329
C2649	C2539	G2435	G2315	G2216	A	A	A	C2072	U1955	C1800	G1649	G1536	A1439	U1328
U2650	G2545	U2436	A2317	G2217	G	U	G	C2073	U1955	A1801	U1648	G1537	U1440	A1329
G2661	U2546	U2441	A2322	G2225	U	U	C	U2074	C1982	A1802	U1649	G1538	G1441	C1330
U2680	A2547	U2442	G2325	A2225	U	U	C	U2075	G1986	A1803	G1667	U1539	U1442	U1340
C2681	U2548	C2442	G2326	U2233	G	G	C	U2086	C1965	A1808	G1674	G1540	U1443	G1341
A2682	U2552	G2443	C2327	G2234	C	U	C	G2087	A1966	A1809	U1683	C1541	G1444	A1342
C2683	G2553	G2444	U2328	G2235	A	U	A	A2095	G1967	G1816	G1684	U1542	G1445	G1343
U2688	U2554	G2445	U2329	U2236	U	U	G	C2096	A1968	U1827	U1688	G1543	C1446	U1344
U2690	U2555	A2448	U2330	G2237	G	G	A	A2097	A1970	G1828	C1686	A1548	G1452	C1349
C2698	G2556	D5D2449	G2331	G2238	A	U	G	U2099	U1971	A1829	U1686	A1549	U1453	C1350
G2699	C2557	G2455	A2336	U2243	C	C	C	G2100	G1980	G1835	C1704	U1554	G1452	C1351
C2700	A2566	C2456	U2345	U2244	C	U	C	A2101	A1981	G1842	A1705	U1558	U1460	A1353
U2701	G2567	U2457	G2346	U2245	A	A	G	G2102	U1982	C1843	G1715	C1559	A1469	A1354
G2709	U2568	A2469	A2347	G2247	C	U	C	C	G1991	U1847	U1720	G1560	A1470	G1355
G2714	A2572	C2475	U2348	G2251	U	U	U	U	U1991	A1848	G1721	U1563	G1473	A1365
C2723	C2573	A2476	G2349	A2266	U	U	G	A	U1993	U1853	G1724	C1564	U1474	C1370
U2724	U2580	U2477	G2350	A2267	A	A	A	U	U2011	A1854	U1725	G1565	C1480	G1371
A2725	G2581	C2483	C2354	A2268	A	A	G	U	G2012	U1855	C1726	A1566	U1481	U1379
U2726	G2582	G2486	G2361	G2269	U	U	U	U	A2013	U1856	C1727	G1567	G1482	G1383
G2732	U2584	C2486	C2362	A2270	U	U	A	U	A2014	G1857	C1728	A1569	G1483	A1386
A2733	U2585	U2491	G2365	U2271	A	A	C	A	U2015	A1858	U1729	A1570	U1484	C1387
G2740	A2589	U2492	A2369	A2272	C	C	C	U	U2016	U1864	C1730	A1571	U1485	A1392
A2741	C2590	U2493	A2377	A2273	A	A	C	G	A2020	G1869	G1731	U1578	C1493	A1494
G2742	C2591	G2494	A2378	A2274	C	C	C	U	C2023	C1870	U1736	A1583	A1495	U1397
G2744	G2592	MSQ2498	G2383	G2279	C	C	C	A	G2024	A1871	G1737	U1584	A1496	C1398
A2748	A2602	C2499	U2384	A2280	U	U	U	U	C2025	A1872	G1738	C1585	C1497	U1405
G2751	G2603	TKV2501	G2385	G2281	A	A	A	G	U2026	U1883	G1743	G1586	C1498	U1406
U2764	U2604	G2502	A2392	G2282	A	A	A	G	A2030	G1884	A1744	G1588	A1508	G1407
G2775	C2605	A2503	G2393	A2287	U	U	U	U	G2032	U1746	A1745	U1589	A1509	U1508
A2778	U2613	U2504	G2396	A2288	G	G	G	A	A2033	C1902	U1747	U1591	G1510	G1410
	U2615	U2506	G2396	U2291	U	U	U	C	G2038	G1906	C1760	C1592	C1512	U1412
		C2515	G2396	U2292	U2187	U2188	U2189	C	U2039	U1911	C1764	A1597	A1515	C1414
				G2294	G2190			U				A1598		



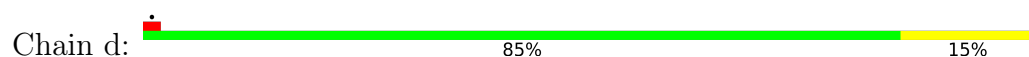
• Molecule 23: 5S rRNA



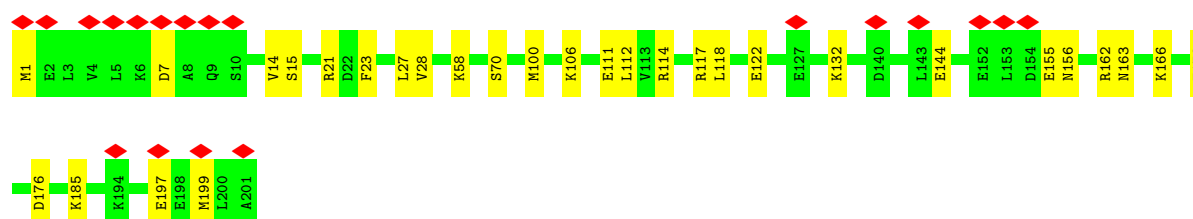
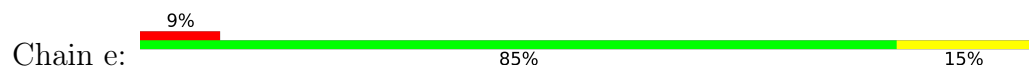
• Molecule 24: Large ribosomal subunit protein uL2



• Molecule 25: Large ribosomal subunit protein uL3

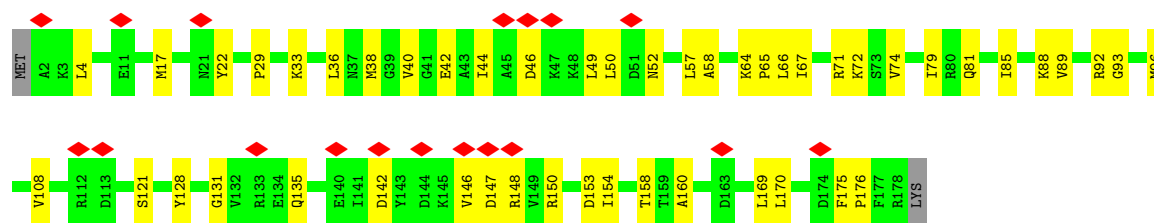


• Molecule 26: Large ribosomal subunit protein uL4

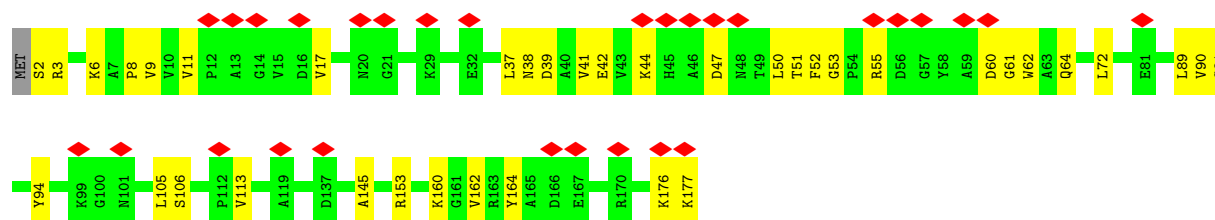
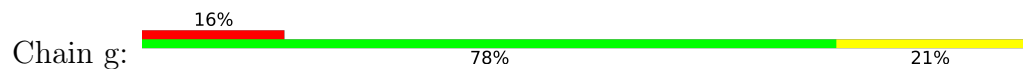


• Molecule 27: Large ribosomal subunit protein uL5

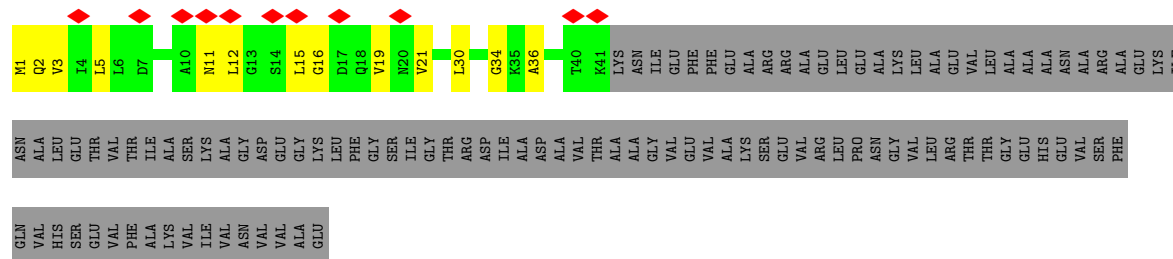




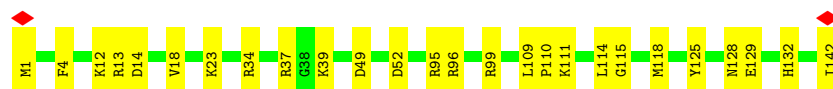
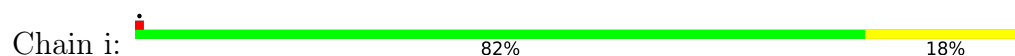
• Molecule 28: Large ribosomal subunit protein uL6



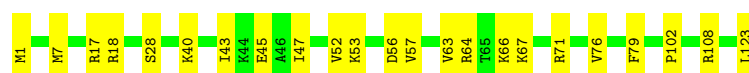
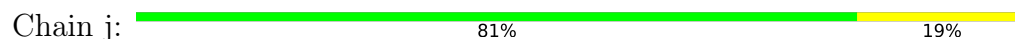
• Molecule 29: Large ribosomal subunit protein bL9



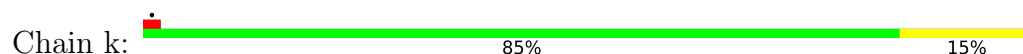
• Molecule 30: Large ribosomal subunit protein uL13



• Molecule 31: Large ribosomal subunit protein uL14

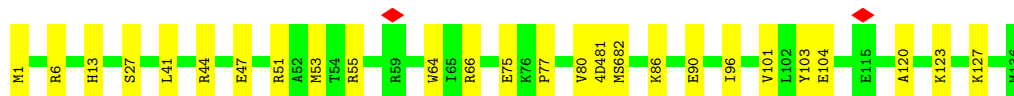
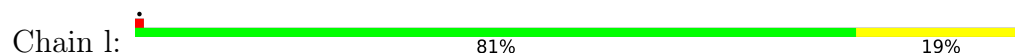


• Molecule 32: Large ribosomal subunit protein uL15

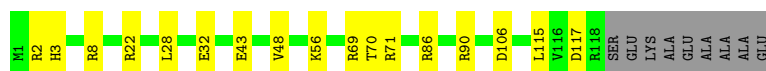
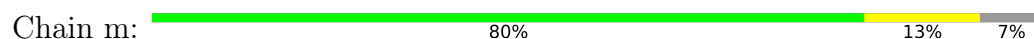




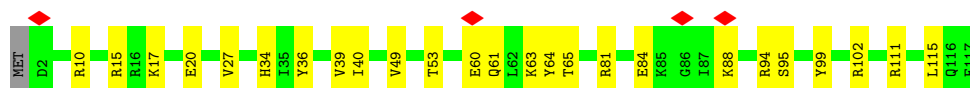
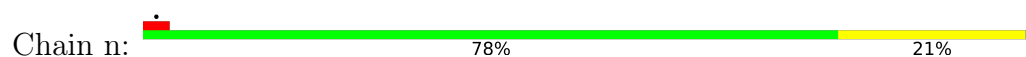
- Molecule 33: Large ribosomal subunit protein uL16



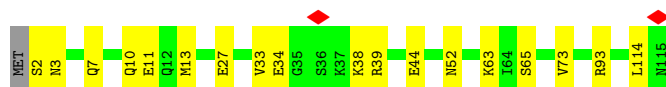
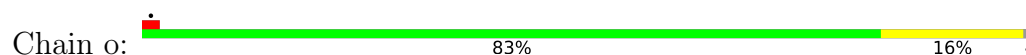
- Molecule 34: Large ribosomal subunit protein bL17



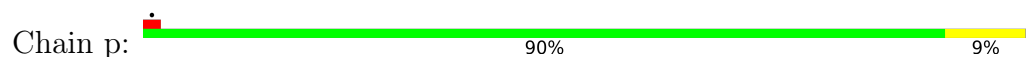
- Molecule 35: Large ribosomal subunit protein uL18



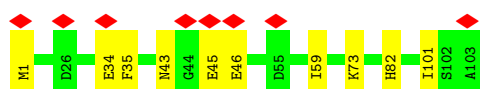
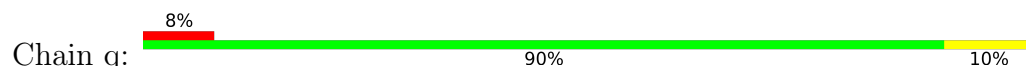
- Molecule 36: Large ribosomal subunit protein bL19



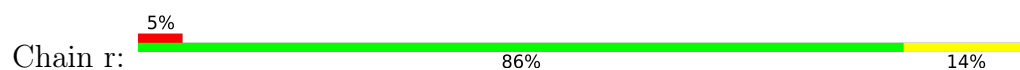
- Molecule 37: Large ribosomal subunit protein bL20



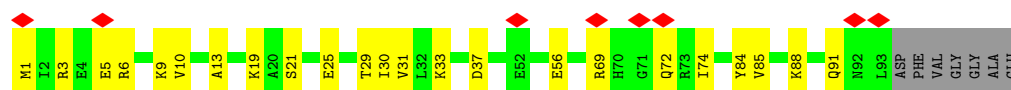
- Molecule 38: Large ribosomal subunit protein bL21



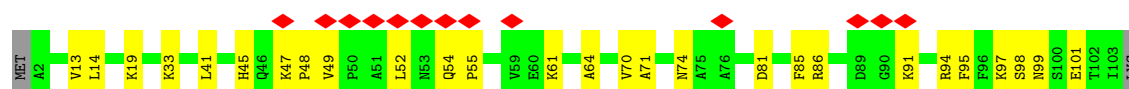
- Molecule 39: Large ribosomal subunit protein uL22



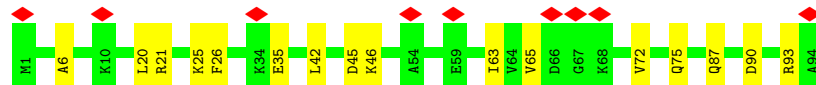
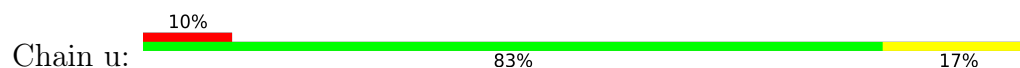
- Molecule 40: Large ribosomal subunit protein uL23



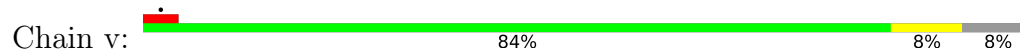
- Molecule 41: Large ribosomal subunit protein uL24



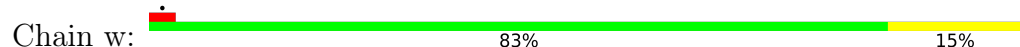
- Molecule 42: Large ribosomal subunit protein bL25



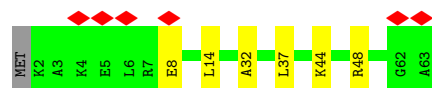
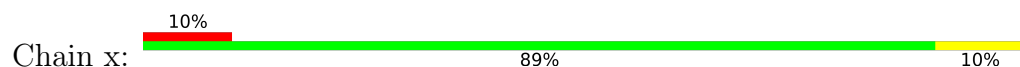
- Molecule 43: Large ribosomal subunit protein bL27



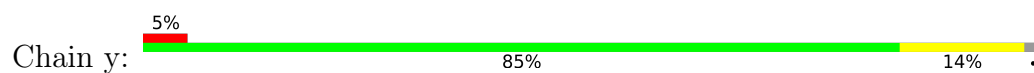
- Molecule 44: Large ribosomal subunit protein bL28



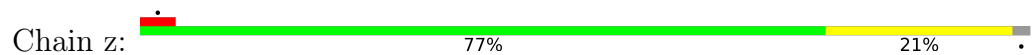
- Molecule 45: Large ribosomal subunit protein uL29



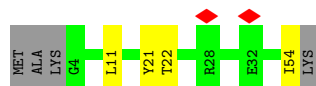
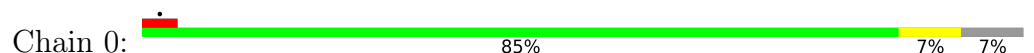
- Molecule 46: Large ribosomal subunit protein uL30



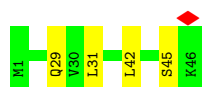
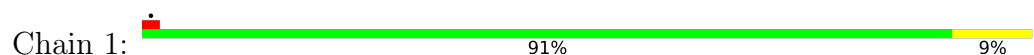
- Molecule 47: Large ribosomal subunit protein bL32



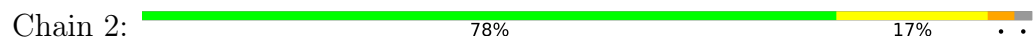
- Molecule 48: Large ribosomal subunit protein bL33



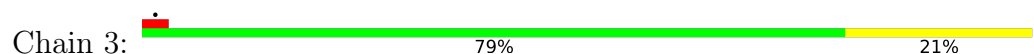
- Molecule 49: Large ribosomal subunit protein bL34



- Molecule 50: Large ribosomal subunit protein bL35



- Molecule 51: Large ribosomal subunit protein bL36A



- Molecule 52: Large ribosomal subunit protein bL31





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174805	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)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.115	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0244	Depositor
Map size (Å)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, D2T, 4D4, MS6, 2MG, OMU, M5Q, TKW, MG, D5D, UR3, 4SU, PSU, 2MA, 1MG, MEQ, OMG, 5MC, OMC, 4OC, MA6, 6MZ, IAS, 3TD, G7M, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	0/36073	0.35	0/56264
2	B	0.27	0/1784	0.37	0/2403
3	C	0.36	0/1651	0.39	0/2225
4	D	0.37	0/1665	0.43	0/2227
5	E	0.41	0/1165	0.42	0/1568
6	F	0.37	0/858	0.46	0/1160
7	G	0.28	0/1219	0.38	0/1635
8	H	0.41	0/989	0.39	0/1326
9	I	0.35	0/1034	0.46	0/1375
10	J	0.35	0/796	0.48	0/1077
11	K	0.38	0/884	0.38	0/1191
12	L	0.44	0/960	0.44	0/1286
13	M	0.35	0/900	0.49	0/1204
14	N	0.37	0/817	0.47	0/1088
15	O	0.40	0/722	0.43	0/964
16	P	0.43	0/653	0.48	0/877
17	Q	0.41	0/650	0.43	0/871
18	R	0.39	0/553	0.46	0/742
19	S	0.33	0/685	0.39	0/922
20	T	0.39	0/676	0.41	0/895
21	U	0.26	0/597	0.44	0/792
22	a	0.55	0/65817	0.36	0/102665
23	b	0.46	0/2850	0.31	0/4444
24	c	0.51	0/2121	0.44	0/2852
25	d	0.50	0/1576	0.42	0/2119
26	e	0.41	0/1571	0.38	0/2113
27	f	0.36	0/1434	0.39	0/1926
28	g	0.34	0/1343	0.45	0/1816
29	h	0.30	0/306	0.44	0/413
30	i	0.46	0/1152	0.39	0/1551
31	j	0.49	0/955	0.40	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.45	0/1062	0.41	0/1413
33	l	0.47	0/1073	0.43	0/1433
34	m	0.50	0/958	0.51	0/1281
35	n	0.38	0/902	0.41	0/1209
36	o	0.48	0/929	0.38	0/1242
37	p	0.51	0/960	0.42	0/1278
38	q	0.45	0/829	0.48	0/1107
39	r	0.46	0/864	0.43	0/1156
40	s	0.39	0/744	0.47	0/994
41	t	0.36	0/787	0.47	0/1051
42	u	0.41	0/766	0.42	0/1025
43	v	0.47	0/599	0.39	0/792
44	w	0.47	0/635	0.40	0/848
45	x	0.35	0/502	0.40	0/667
46	y	0.46	0/453	0.42	0/605
47	z	0.45	0/450	0.39	0/599
48	0	0.39	0/424	0.38	0/565
49	1	0.53	0/380	0.47	0/498
50	2	0.51	0/513	0.52	0/676
51	3	0.49	0/303	0.40	0/397
52	4	0.27	0/488	0.40	0/649
53	X	0.39	0/145	0.32	0/224
54	Z	0.34	0/1725	0.30	0/2687
All	All	0.50	0/150947	0.37	0/225666

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
13	M	0	1
38	q	0	1
50	2	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide
38	q	45	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	369	0
2	B	1753	0	1780	27	0
3	C	1624	0	1696	17	0
4	D	1643	0	1707	43	0
5	E	1152	0	1196	17	0
6	F	839	0	833	26	0
7	G	1203	0	1254	24	0
8	H	979	0	1031	12	0
9	I	1022	0	1070	28	0
10	J	786	0	828	32	0
11	K	877	0	884	27	0
12	L	957	0	1017	21	0
13	M	891	0	952	16	0
14	N	805	0	844	19	0
15	O	714	0	734	9	0
16	P	643	0	661	13	0
17	Q	641	0	682	8	0
18	R	544	0	565	14	0
19	S	668	0	693	16	0
20	T	670	0	719	5	0
21	U	589	0	629	16	0
22	a	59304	0	29821	537	0
23	b	2549	0	1291	16	0
24	c	2082	0	2154	36	0
25	d	1566	0	1618	23	0
26	e	1552	0	1619	23	0
27	f	1410	0	1444	33	0
28	g	1323	0	1371	28	0
29	h	303	0	327	9	0
30	i	1129	0	1162	19	0
31	j	946	0	1023	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	k	1053	0	1129	18	0
33	l	1075	0	1145	19	0
34	m	945	0	989	12	0
35	n	892	0	923	16	0
36	o	917	0	962	14	0
37	p	947	0	1019	10	0
38	q	816	0	839	7	0
39	r	857	0	922	9	0
40	s	738	0	807	19	0
41	t	779	0	831	20	0
42	u	753	0	780	9	0
43	v	592	0	607	4	0
44	w	625	0	652	8	0
45	x	501	0	531	4	0
46	y	449	0	488	6	0
47	z	444	0	458	9	0
48	0	417	0	451	3	0
49	1	377	0	418	3	0
50	2	504	0	572	12	0
51	3	302	0	343	6	0
52	4	480	0	482	13	0
53	X	130	0	66	0	0
54	Z	1645	0	842	17	0
55	A	121	0	0	0	0
55	Z	1	0	0	0	0
55	a	340	0	0	0	0
55	b	7	0	0	0	0
55	c	1	0	0	0	0
55	z	1	0	0	0	0
All	All	140339	0	94220	1542	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 7.

All (1542) 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)
22:a:881:G:H1	22:a:895:U:H3	1.12	0.98
22:a:1047:G:HO2'	22:a:1110:G:H1	1.05	0.92
22:a:1534:U:H3	22:a:1537:G:H1	1.17	0.90
1:A:677:U:H3	1:A:713:G:H22	1.16	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:G:H1	1:A:93:U:H3	0.88	0.88
25:d:61:THR:HG22	25:d:63:PRO:HD2	1.56	0.88
2:B:97:LEU:H	2:B:100:MET:HE3	1.38	0.87
1:A:1086:U:H3	1:A:1099:G:H22	1.23	0.87
22:a:2100:G:H1	22:a:2189:U:H3	0.90	0.87
3:C:35:SER:OG	3:C:59:ARG:NH2	2.10	0.85
10:J:26:VAL:HG12	10:J:30:LYS:HZ2	1.41	0.84
18:R:9:LYS:HD3	18:R:10:PHE:H	1.41	0.84
1:A:664:G:H22	1:A:741:G:H1	1.24	0.83
22:a:2102:G:H1	22:a:2187:U:H3	0.83	0.83
22:a:1607:C:N4	22:a:1622:G:OP2	2.12	0.83
22:a:287:G:N1	22:a:353:C:N3	2.27	0.81
22:a:1434:A:H2'	22:a:1435:G:H8	1.46	0.79
23:b:1:U:H2'	23:b:2:G:H8	1.48	0.78
1:A:1009:U:O2	1:A:1020:G:N2	2.15	0.78
22:a:287:G:N2	22:a:353:C:O2	2.17	0.77
22:a:2102:G:N2	22:a:2187:U:O2	2.17	0.77
2:B:15:HIS:HB3	2:B:43:LEU:HD11	1.66	0.77
27:f:158:THR:HG22	27:f:160:ALA:H	1.48	0.76
8:H:48:ASP:OD1	8:H:49:PHE:N	2.18	0.76
22:a:1534:U:O2	22:a:1537:G:O6	2.03	0.76
7:G:93:PRO:HA	7:G:96:ARG:HD3	1.67	0.76
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.18	0.76
1:A:428:G:H1'	1:A:430:A:C8	2.20	0.76
10:J:6:ILE:HB	10:J:76:ILE:HB	1.67	0.75
22:a:545:U:O2	22:a:548:G:O6	2.05	0.75
7:G:68:ASN:HD21	7:G:130:ASN:HB2	1.51	0.75
22:a:1434:A:H2'	22:a:1435:G:C8	2.22	0.74
22:a:881:G:O6	22:a:895:U:O4	2.06	0.74
19:S:11:ILE:HD12	19:S:38:SER:HB3	1.70	0.74
14:N:39:GLU:O	14:N:43:ASN:ND2	2.20	0.74
27:f:92:ARG:HA	27:f:96:MET:HE3	1.69	0.73
24:c:142:HIS:ND1	24:c:193:GLY:O	2.18	0.73
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.19	0.73
1:A:42:G:H21	1:A:622:A:H8	1.36	0.73
11:K:37:ARG:NH1	11:K:83:GLU:OE2	2.22	0.72
1:A:76:G:O6	1:A:93:U:O4	2.07	0.72
32:k:91:ASP:OD1	32:k:92:LEU:N	2.21	0.72
2:B:117:LEU:HB3	2:B:141:LEU:HD12	1.71	0.71
22:a:1007:C:OP1	30:i:37:ARG:NH2	2.22	0.71
46:y:11:ARG:HH11	46:y:16:ARG:HH22	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.71	0.71
52:4:59:ARG:HA	52:4:62:LYS:HE3	1.72	0.71
24:c:2:ALA:N	24:c:20:VAL:O	2.23	0.71
40:s:69:ARG:HH22	40:s:72:GLN:HG2	1.53	0.71
7:G:79:ARG:HH11	7:G:82:GLY:H	1.35	0.71
3:C:110:GLU:HB2	3:C:144:LEU:HD22	1.73	0.71
22:a:1417:C:HO2'	22:a:1587:G:HO2'	1.32	0.70
1:A:1040:U:H2'	1:A:1041:G:H8	1.56	0.70
22:a:2635:A:O2'	25:d:81:GLU:OE1	2.09	0.70
29:h:5:LEU:HD11	29:h:12:LEU:HD11	1.74	0.70
7:G:72:THR:HG22	7:G:96:ARG:HH12	1.56	0.70
22:a:2477:U:O2	51:3:4:ARG:NH2	2.24	0.70
22:a:2683:C:H4'	25:d:13:ARG:NH1	2.06	0.70
1:A:673:A:H2'	1:A:674:G:C8	2.27	0.70
36:o:10:GLN:HA	36:o:13:MET:HG3	1.73	0.69
38:q:1:MET:SD	38:q:43:ASN:ND2	2.65	0.69
1:A:537:G:OP1	12:L:110:ARG:NH2	2.25	0.69
31:j:1:MET:SD	31:j:67:LYS:NZ	2.66	0.69
1:A:714:G:H2'	1:A:715:A:C8	2.28	0.69
22:a:2102:G:O6	22:a:2187:U:O4	2.11	0.69
1:A:1004:A:O2'	1:A:1036:A:N6	2.26	0.68
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.75	0.68
27:f:33:LYS:HA	27:f:96:MET:HE2	1.75	0.68
22:a:639:U:H2'	22:a:640:C:C6	2.28	0.68
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.27	0.68
1:A:1130:A:O2'	9:I:5:GLN:NE2	2.27	0.68
28:g:2:SER:OG	28:g:3:ARG:N	2.26	0.68
13:M:39:ILE:HD12	13:M:56:LEU:HD11	1.76	0.68
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.25	0.68
9:I:106:ARG:NH1	9:I:107:ASP:O	2.27	0.68
43:v:10:THR:HG22	43:v:12:ASN:H	1.59	0.67
1:A:1350:A:OP2	9:I:120:LYS:NZ	2.25	0.67
1:A:413:G:N2	1:A:428:G:H2'	2.09	0.67
1:A:544:G:OP1	4:D:56:ARG:NH2	2.26	0.67
22:a:287:G:O6	22:a:353:C:N4	2.23	0.67
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.28	0.67
22:a:284:U:H2'	22:a:285:G:C8	2.30	0.67
54:Z:48:U:H4'	54:Z:49:C:H5'	1.75	0.67
1:A:946:A:H2'	1:A:947:G:C8	2.29	0.66
1:A:1033:G:H2'	1:A:1034:G:H8	1.60	0.66
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:67:ASP:OD1	39:r:68:ASP:N	2.29	0.66
5:E:88:VAL:HG12	5:E:93:ARG:HG2	1.78	0.66
22:a:2095:A:O5'	29:h:11:ASN:ND2	2.26	0.66
1:A:736:C:OP1	18:R:61:ARG:NH1	2.28	0.66
6:F:3:HIS:ND1	6:F:65:GLU:OE2	2.28	0.66
10:J:25:ILE:HD13	10:J:90:LEU:HD23	1.77	0.66
47:z:54:VAL:HG23	47:z:55:ILE:HG12	1.78	0.66
1:A:653:U:OP1	8:H:56:LYS:NZ	2.21	0.65
30:i:128:ASN:O	30:i:128:ASN:ND2	2.29	0.65
22:a:534:U:O2'	37:p:49:ASP:OD2	2.07	0.65
23:b:1:U:H2'	23:b:2:G:C8	2.30	0.65
36:o:2:SER:OG	36:o:3:ASN:N	2.29	0.65
1:A:1009:U:O4	1:A:1020:G:O6	2.15	0.64
1:A:910:C:OP2	12:L:18:LYS:NZ	2.30	0.64
4:D:105:MET:HE1	4:D:143:VAL:HB	1.80	0.64
4:D:99:ASP:OD1	4:D:100:ASN:N	2.30	0.64
22:a:1870:C:HO2'	22:a:1871:A:H8	1.46	0.64
7:G:148:ASN:OD1	11:K:56:ARG:NH2	2.31	0.64
2:B:129:LEU:HD23	2:B:133:GLU:HB3	1.80	0.64
25:d:4:LEU:HD22	25:d:32:ASN:HD22	1.62	0.64
13:M:83:LEU:HD11	19:S:66:MET:HG2	1.80	0.63
40:s:3:ARG:NH2	40:s:5:GLU:OE2	2.31	0.63
4:D:101:VAL:HG12	4:D:105:MET:HE2	1.81	0.63
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.80	0.63
50:2:24:HIS:ND1	50:2:25:LYS:O	2.30	0.63
54:Z:51:U:H3	54:Z:65:G:H1	1.46	0.63
22:a:870:U:OP1	33:l:6:ARG:NH1	2.31	0.63
33:l:75:GLU:HB2	33:l:90:GLU:HG3	1.79	0.63
1:A:509:A:H8	1:A:543:U:O2'	1.81	0.63
1:A:1130:A:H2'	1:A:1131:G:H8	1.64	0.63
4:D:145:ILE:HD13	4:D:178:MET:HB3	1.78	0.63
6:F:5:GLU:OE1	18:R:24:LYS:NZ	2.30	0.63
22:a:1026:G:H2'	22:a:1027:A:H8	1.64	0.63
3:C:19:ASN:O	3:C:40:ARG:NH2	2.31	0.63
33:l:53:MET:HG3	33:l:120:ALA:HB2	1.81	0.63
1:A:1038:C:H2'	1:A:1039:G:H8	1.62	0.63
1:A:509:A:C8	1:A:543:U:O2'	2.52	0.62
22:a:848:C:H2'	22:a:849:A:H8	1.63	0.62
1:A:492:C:H2'	1:A:493:A:C8	2.34	0.62
22:a:172:A:H2'	22:a:173:A:C8	2.33	0.62
22:a:2830:C:H5''	25:d:56:LYS:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2523:G:HO2'	22:a:2764:A:HO2'	1.47	0.62
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.82	0.62
11:K:23:ILE:HG21	11:K:96:THR:HG21	1.81	0.62
22:a:172:A:H2'	22:a:173:A:H8	1.65	0.62
22:a:307:G:N1	22:a:310:A:OP2	2.27	0.62
28:g:41:VAL:O	28:g:55:ARG:NH1	2.32	0.62
1:A:713:G:H2'	1:A:714:G:C8	2.34	0.62
9:I:92:GLU:H	9:I:92:GLU:CD	2.08	0.62
29:h:1:MET:N	29:h:21:VAL:O	2.33	0.62
31:j:108:ARG:NH2	36:o:34:GLU:OE2	2.33	0.62
1:A:1030:U:O2'	1:A:1031:C:O5'	2.16	0.61
1:A:486:U:H2'	1:A:487:A:H8	1.65	0.61
8:H:5:ASP:OD1	8:H:81:PRO:HD3	2.00	0.61
22:a:742:A:H2'	22:a:743:A:C8	2.34	0.61
22:a:1296:G:OP1	22:a:2709:G:O2'	2.18	0.61
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.80	0.61
9:I:12:ARG:HG3	9:I:13:LYS:H	1.65	0.61
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.81	0.61
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.82	0.61
22:a:1704:C:H2'	22:a:1705:A:H8	1.64	0.61
1:A:404:G:OP2	4:D:115:ARG:NH2	2.30	0.61
1:A:950:U:O4	13:M:104:THR:HG21	2.01	0.61
22:a:856:G:H2'	22:a:857:G:C8	2.34	0.61
22:a:1030:C:OP2	33:l:127:LYS:NZ	2.33	0.61
26:e:23:PHE:HB2	26:e:111:GLU:OE2	2.01	0.61
1:A:427:U:H3'	1:A:428:G:H5''	1.82	0.61
1:A:1033:G:H2'	1:A:1034:G:C8	2.36	0.61
22:a:184:C:H2'	22:a:185:G:H8	1.66	0.61
22:a:284:U:O2	22:a:356:G:O6	2.19	0.61
1:A:1004:A:H2'	1:A:1005:A:O4'	2.01	0.61
22:a:276:U:O2'	22:a:277:G:O5'	2.19	0.61
6:F:12:PRO:O	6:F:44:ARG:NH2	2.33	0.60
30:i:23:LYS:NZ	30:i:142:ILE:OXT	2.33	0.60
22:a:1469:A:H2'	22:a:1470:A:C8	2.37	0.60
22:a:2547:A:H2'	22:a:2548:U:C6	2.36	0.60
1:A:429:U:H5'	4:D:9:LEU:HD12	1.84	0.60
1:A:502:A:OP1	12:L:115:SER:OG	2.14	0.60
1:A:1040:U:H2'	1:A:1041:G:C8	2.35	0.60
14:N:46:LEU:HD13	14:N:49:GLN:HE21	1.66	0.60
22:a:183:C:H42	22:a:213:A:H61	1.49	0.60
11:K:14:LYS:HD2	11:K:15:GLN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:358:U:H2'	22:a:359:G:H8	1.65	0.60
34:m:32:GLU:HG2	34:m:115:LEU:HD12	1.84	0.60
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.60
22:a:2099:U:H3	22:a:2190:G:H1	1.50	0.60
46:y:11:ARG:NH1	46:y:16:ARG:HH22	2.00	0.60
1:A:202:G:H21	1:A:466:A:H61	1.50	0.60
12:L:14:ARG:HH12	12:L:15:LYS:HE2	1.66	0.60
14:N:29:ALA:O	14:N:33:ASP:HB2	2.00	0.60
21:U:49:LYS:O	21:U:53:VAL:HG23	2.02	0.60
22:a:1870:C:O2'	22:a:1871:A:H8	1.83	0.60
1:A:451:A:N6	1:A:480:U:O2'	2.33	0.59
1:A:823:C:HO2'	8:H:2:SER:N	1.99	0.59
24:c:132:MET:HE1	24:c:174:LEU:HD21	1.83	0.59
33:l:41:LEU:HG	33:l:96:ILE:HG13	1.83	0.59
1:A:1009:U:H3	1:A:1020:G:H1	0.70	0.59
22:a:2328:A:H2'	22:a:2329:U:C6	2.37	0.59
25:d:108:ASP:OD1	25:d:173:GLN:HA	2.02	0.59
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.59
22:a:1548:A:H2'	22:a:1549:A:C8	2.36	0.59
1:A:437:U:O2'	4:D:120:HIS:ND1	2.35	0.59
22:a:243:U:OP2	50:2:8:ARG:NH1	2.35	0.59
25:d:56:LYS:HB2	25:d:59:ARG:HB2	1.84	0.59
1:A:1029:U:H3	1:A:1032:G:H1	1.48	0.59
22:a:126:A:OP1	49:1:45:SER:OG	2.19	0.59
22:a:396:G:OP2	44:w:10:LYS:NZ	2.34	0.59
22:a:1799:G:O2'	24:c:180:GLU:OE2	2.16	0.59
2:B:120:GLN:OE1	2:B:137:ARG:NH1	2.36	0.59
1:A:428:G:O2'	1:A:429:U:O5'	2.18	0.59
22:a:2478:A:OP2	51:3:2:LYS:NZ	2.30	0.59
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.17	0.59
22:a:2365:G:N7	50:2:39:LYS:NZ	2.44	0.59
22:a:2327:A:H2'	22:a:2328:A:C8	2.37	0.59
27:f:42:GLU:OE1	27:f:148:ARG:NH2	2.36	0.59
25:d:35:THR:HG22	25:d:73:VAL:HG21	1.85	0.58
27:f:44:ILE:HD11	27:f:79:ILE:HG22	1.85	0.58
1:A:147:G:H2'	1:A:148:G:C8	2.38	0.58
22:a:1141:U:H4'	22:a:1142:A:O4'	2.03	0.58
42:u:45:ASP:OD1	42:u:46:LYS:N	2.36	0.58
52:4:11:GLU:HA	52:4:25:ARG:HA	1.85	0.58
10:J:88:MET:HE3	10:J:88:MET:HA	1.85	0.58
12:L:68:GLY:O	12:L:99:ARG:NH1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:50:LEU:HD21	27:f:67:ILE:HD12	1.84	0.58
28:g:8:PRO:HB3	28:g:51:THR:HG22	1.84	0.58
22:a:1794:A:H2'	22:a:1795:C:C6	2.38	0.58
31:j:45:GLU:N	31:j:45:GLU:OE1	2.36	0.58
34:m:2:ARG:HD2	34:m:2:ARG:O	2.03	0.58
3:C:11:ARG:NH2	3:C:175:LEU:O	2.37	0.58
3:C:47:LEU:HD21	3:C:87:LEU:HD11	1.85	0.58
26:e:15:SER:N	26:e:197:GLU:OE2	2.35	0.58
52:4:58:ASP:OD1	52:4:59:ARG:N	2.36	0.58
2:B:217:VAL:O	2:B:221:VAL:HG12	2.03	0.58
22:a:276:U:O2'	22:a:277:G:O4'	2.16	0.58
22:a:1799:G:N7	24:c:178:SER:OG	2.34	0.58
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.86	0.58
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.84	0.58
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.85	0.58
22:a:1871:A:H2'	22:a:1872:A:C8	2.39	0.58
1:A:1006:G:O6	1:A:1023:U:O2	2.22	0.58
22:a:910:A:H2'	22:a:911:A:C8	2.39	0.58
33:l:1:MET:HE1	33:l:44:ARG:HA	1.85	0.58
1:A:28:A:O2'	1:A:296:U:OP1	2.16	0.58
22:a:320:A:N3	26:e:163:ASN:ND2	2.46	0.58
1:A:1098:C:O2'	21:U:71:TYR:O	2.17	0.57
5:E:55:GLU:N	5:E:55:GLU:OE2	2.36	0.57
13:M:33:ILE:HD13	13:M:60:VAL:HG22	1.86	0.57
31:j:18:ARG:HB2	31:j:45:GLU:OE1	2.04	0.57
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.31	0.57
6:F:21:MET:HE1	6:F:83:ALA:HB3	1.87	0.57
22:a:2845:U:H5''	36:o:52:ASN:O	2.04	0.57
22:a:364:C:H2'	22:a:365:U:C6	2.39	0.57
54:Z:24:C:H2'	54:Z:25:U:C6	2.40	0.57
1:A:1125:U:H4'	10:J:7:ARG:HH12	1.69	0.57
10:J:47:GLU:OE1	14:N:76:LYS:NZ	2.36	0.57
22:a:2291:U:H2'	22:a:2292:U:C6	2.39	0.57
1:A:407:U:O2'	4:D:113:GLU:HG2	2.05	0.57
1:A:423:G:O2'	1:A:424:G:O4'	2.19	0.57
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.87	0.57
22:a:64:A:H2'	22:a:65:U:C6	2.39	0.57
28:g:42:GLU:OE2	28:g:55:ARG:NH1	2.38	0.57
22:a:1802:A:H2'	22:a:1803:A:C8	2.40	0.57
1:A:134:G:O6	16:P:1:MET:HE2	2.05	0.57
1:A:459:A:H2'	1:A:460:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:G:H2'	1:A:525:C:C6	2.40	0.57
10:J:26:VAL:HG12	10:J:30:LYS:NZ	2.17	0.57
1:A:683:G:N2	11:K:39:GLY:O	2.38	0.57
22:a:2100:G:O6	22:a:2189:U:O4	2.21	0.57
1:A:1038:C:H2'	1:A:1039:G:C8	2.39	0.57
5:E:81:LEU:HB2	5:E:98:PRO:HG3	1.86	0.56
22:a:276:U:O2	22:a:362:A:N6	2.38	0.56
22:a:820:A:H4'	22:a:836:G:H22	1.70	0.56
22:a:1340:U:OP1	40:s:19:LYS:NZ	2.38	0.56
22:a:2788:C:H2'	22:a:2789:C:C6	2.40	0.56
22:a:1197:G:H2'	22:a:1198:U:H6	1.70	0.56
22:a:2799:A:O2'	22:a:2800:A:H5''	2.05	0.56
25:d:46:ARG:NH1	25:d:85:ALA:O	2.34	0.56
1:A:135:C:O2	16:P:1:MET:N	2.38	0.56
1:A:398:U:H2'	1:A:399:G:H8	1.70	0.56
1:A:451:A:H61	1:A:480:U:HO2'	1.51	0.56
1:A:1030:U:O2'	1:A:1031:C:O2	2.22	0.56
1:A:1391:U:H2'	1:A:1392:G:C8	2.39	0.56
6:F:46:GLN:HE22	6:F:55:HIS:HB3	1.70	0.56
42:u:35:GLU:N	42:u:35:GLU:OE1	2.39	0.56
33:l:47:GLU:OE1	33:l:51:ARG:NH2	2.38	0.56
52:4:11:GLU:OE1	52:4:23:LYS:HG3	2.05	0.56
22:a:163:C:H2'	22:a:164:C:C6	2.40	0.56
22:a:742:A:H2'	22:a:743:A:H8	1.69	0.56
1:A:131:A:H2'	1:A:132:C:C6	2.40	0.56
23:b:66:A:N6	23:b:107:G:H2'	2.19	0.56
7:G:147:ALA:O	11:K:56:ARG:NH1	2.38	0.56
11:K:35:THR:HG22	11:K:41:ALA:HA	1.88	0.56
22:a:848:C:H2'	22:a:849:A:C8	2.40	0.56
1:A:399:G:H2'	1:A:400:C:C6	2.41	0.56
1:A:501:C:H2'	1:A:502:A:C8	2.41	0.56
30:i:34:ARG:HG3	30:i:39:LYS:HB2	1.88	0.56
38:q:1:MET:HE3	38:q:101:ILE:HB	1.86	0.56
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.56
21:U:5:LYS:O	21:U:18:ARG:NH2	2.33	0.56
1:A:1034:G:H2'	1:A:1035:A:C8	2.40	0.56
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.39	0.56
12:L:4:VAL:HG23	17:Q:34:TYR:HB3	1.88	0.56
22:a:1590:A:H2'	22:a:1591:A:H8	1.71	0.56
41:t:86:ARG:HG3	41:t:95:PHE:CD1	2.40	0.56
1:A:1314:C:H2'	1:A:1315:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:THR:HG21	10:J:90:LEU:HD22	1.87	0.55
22:a:1508:A:O2'	22:a:1509:A:O4'	2.25	0.55
1:A:518:C:H2'	1:A:530:G:C8	2.41	0.55
1:A:613:C:OP1	4:D:81:ARG:NH2	2.34	0.55
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.42	0.55
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.88	0.55
22:a:1980:G:O2'	22:a:1982:U:OP2	2.21	0.55
5:E:165:LEU:O	8:H:114:ARG:NH1	2.39	0.55
1:A:525:C:OP1	12:L:86:ARG:NH2	2.34	0.55
1:A:1314:C:OP2	19:S:4:SER:OG	2.13	0.55
2:B:116:ASP:O	2:B:120:GLN:HG3	2.06	0.55
1:A:309:A:H2'	1:A:310:G:H8	1.70	0.55
22:a:2012:G:N7	39:r:16:LYS:NZ	2.52	0.55
22:a:2243:U:H2'	22:a:2244:U:C6	2.42	0.55
27:f:46:ASP:HB3	27:f:49:LEU:HG	1.88	0.55
1:A:464:U:N3	1:A:467:U:OP2	2.25	0.55
11:K:22:HIS:HB2	11:K:33:THR:HG22	1.89	0.55
40:s:6:ARG:NH2	40:s:37:ASP:OD2	2.39	0.55
1:A:923:A:O2'	1:A:1399:C:OP2	2.24	0.55
2:B:87:CYS:SG	2:B:221:VAL:HG11	2.47	0.55
21:U:4:ILE:HG13	21:U:19:PHE:HA	1.89	0.55
22:a:1667:G:O2'	22:a:1991:U:O4	2.24	0.55
1:A:459:A:H2'	1:A:460:A:H8	1.71	0.55
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.88	0.55
22:a:1149:G:H2'	22:a:1150:C:C6	2.42	0.55
22:a:1797:G:HO2'	24:c:257:THR:HG1	1.55	0.55
22:a:1930:G:O2'	22:a:1968:G:O6	2.24	0.55
22:a:2809:A:H2'	22:a:2810:A:C8	2.41	0.55
22:a:1494:A:H2'	22:a:1495:A:C8	2.42	0.55
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.35	0.55
1:A:736:C:H2'	1:A:737:C:C6	2.42	0.54
3:C:186:THR:HG22	3:C:199:LYS:HG2	1.88	0.54
10:J:71:LEU:O	10:J:72:ARG:NH1	2.35	0.54
22:a:2299:U:OP1	27:f:72:LYS:NZ	2.40	0.54
1:A:413:G:H21	1:A:428:G:H8	1.54	0.54
2:B:136:MET:HG3	2:B:139:ARG:HH21	1.73	0.54
3:C:36:ASP:OD1	3:C:59:ARG:NH2	2.29	0.54
20:T:35:VAL:HG11	20:T:79:LEU:HD13	1.89	0.54
22:a:1212:G:O2'	22:a:1236:G:N2	2.38	0.54
22:a:2071:A:H2'	22:a:2072:C:C6	2.42	0.54
30:i:125:TYR:HH	30:i:132:HIS:CD2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:G:H2'	1:A:338:A:C8	2.43	0.54
1:A:746:A:H2'	1:A:747:A:C8	2.43	0.54
22:a:3:U:H2'	22:a:4:U:C6	2.42	0.54
22:a:100:U:O2	41:t:91:LYS:NZ	2.40	0.54
30:i:95:ARG:NH1	30:i:96:ARG:HH12	2.05	0.54
33:l:27:SER:N	33:l:104:GLU:OE1	2.35	0.54
1:A:45:G:H2'	1:A:46:G:H8	1.73	0.54
1:A:539:A:H2'	1:A:540:G:C8	2.42	0.54
1:A:546:A:P	4:D:69:GLU:HB3	2.46	0.54
10:J:30:LYS:HB2	10:J:31:ARG:HH12	1.71	0.54
16:P:44:SER:OG	16:P:47:GLU:OE2	2.19	0.54
22:a:1342:A:O2'	22:a:1344:U:OP2	2.22	0.54
28:g:60:ASP:O	28:g:62:TRP:N	2.39	0.54
18:R:9:LYS:CD	18:R:10:PHE:H	2.15	0.54
22:a:191:A:H2'	22:a:192:C:C6	2.41	0.54
22:a:1724:G:H1	22:a:1736:U:H3	1.55	0.54
28:g:42:GLU:O	28:g:52:PHE:HA	2.08	0.54
35:n:27:VAL:HG21	35:n:40:ILE:HD12	1.90	0.54
40:s:13:ALA:HB3	40:s:33:LYS:HD2	1.89	0.54
41:t:33:LYS:HB3	41:t:64:ALA:HB1	1.90	0.54
45:x:8:GLU:OE2	45:x:8:GLU:N	2.34	0.54
10:J:10:LEU:HD12	10:J:22:THR:HG22	1.89	0.54
22:a:358:U:H2'	22:a:359:G:C8	2.42	0.54
22:a:1386:C:H2'	22:a:1387:A:C8	2.43	0.54
25:d:48:ILE:HG23	25:d:84:LEU:HD11	1.88	0.54
47:z:52:ARG:HH21	47:z:54:VAL:HG12	1.73	0.54
1:A:413:G:H21	1:A:428:G:H2'	1.71	0.54
13:M:81:MET:HE2	22:a:888:C:N3	2.23	0.54
19:S:41:PHE:N	19:S:44:MET:SD	2.73	0.54
22:a:1405:U:H2'	22:a:1406:U:C6	2.43	0.54
24:c:157:SER:O	24:c:160:THR:OG1	2.25	0.54
1:A:864:A:H4'	5:E:90:THR:HG23	1.90	0.54
1:A:1130:A:H2'	1:A:1131:G:C8	2.42	0.54
22:a:286:U:H2'	22:a:287:G:H8	1.72	0.54
22:a:1567:G:OP2	24:c:83:TYR:OH	2.21	0.54
1:A:375:U:OP1	16:P:70:ARG:NH2	2.37	0.53
1:A:1371:G:OP1	9:I:14:SER:OG	2.21	0.53
22:a:807:U:OP2	32:k:41:ARG:NH1	2.41	0.53
22:a:879:G:H2'	22:a:880:G:H8	1.73	0.53
22:a:1720:U:H2'	22:a:1721:G:O4'	2.08	0.53
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:78:VAL:O	16:P:80:LYS:NZ	2.42	0.53
22:a:729:G:H5''	22:a:730:A:H5''	1.89	0.53
45:x:32:ALA:HB2	45:x:37:LEU:HD23	1.90	0.53
1:A:223:A:H2'	1:A:224:U:C6	2.43	0.53
1:A:1311:A:OP1	52:4:59:ARG:NH1	2.40	0.53
7:G:15:ASP:N	7:G:15:ASP:OD2	2.41	0.53
22:a:888:C:H2'	22:a:889:C:C6	2.43	0.53
22:a:2030:6MZ:H2	22:a:2499:C:H5''	1.90	0.53
28:g:42:GLU:N	28:g:53:GLY:O	2.34	0.53
39:r:88:ARG:HG3	39:r:94:ASP:OD1	2.08	0.53
1:A:1533:C:H4'	1:A:1534:A:C8	2.44	0.53
12:L:99:ARG:NE	12:L:104:CYS:SG	2.81	0.53
34:m:22:ARG:HG3	34:m:70:THR:HA	1.90	0.53
22:a:903:C:H2'	22:a:904:G:H8	1.74	0.53
1:A:269:C:H2'	1:A:270:A:H8	1.73	0.53
24:c:145:GLU:HG2	24:c:151:GLY:C	2.33	0.53
4:D:104:ARG:HG3	4:D:168:PRO:HG2	1.90	0.53
22:a:577:G:O2'	22:a:1254:A:OP1	2.27	0.53
22:a:641:U:O2'	22:a:2350:C:OP1	2.27	0.53
52:4:16:CYS:HA	52:4:34:LEU:HB2	1.90	0.53
1:A:399:G:H2'	1:A:400:C:H6	1.73	0.53
14:N:46:LEU:HD13	14:N:49:GLN:NE2	2.23	0.53
28:g:60:ASP:OD1	28:g:61:GLY:N	2.38	0.53
31:j:17:ARG:HD3	31:j:47:ILE:HG23	1.90	0.53
40:s:21:SER:O	40:s:25:GLU:HG2	2.09	0.53
6:F:37:HIS:CD2	6:F:65:GLU:HG2	2.44	0.53
22:a:5:A:H2'	22:a:6:A:C8	2.44	0.53
22:a:1800:C:H3'	24:c:146:MET:HE1	1.91	0.53
28:g:38:ASN:ND2	28:g:64:GLN:OE1	2.27	0.53
22:a:24:G:O2'	39:r:78:GLU:O	2.27	0.53
22:a:720:U:H2'	22:a:721:A:C8	2.44	0.53
22:a:849:A:H2'	22:a:850:U:C6	2.44	0.53
22:a:1597:A:H5''	22:a:1598:A:H5'	1.91	0.53
38:q:35:PHE:HB2	38:q:59:ILE:HB	1.90	0.53
40:s:56:GLU:OE2	40:s:56:GLU:N	2.41	0.53
1:A:695:A:H2'	1:A:696:A:C8	2.44	0.52
2:B:97:LEU:N	2:B:100:MET:HE3	2.17	0.52
4:D:197:GLU:HA	4:D:200:ILE:HD13	1.90	0.52
18:R:16:GLU:HG3	18:R:18:VAL:HG23	1.91	0.52
22:a:84:A:N1	22:a:98:G:O2'	2.40	0.52
22:a:1856:U:H2'	22:a:1857:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2430:A:N3	22:a:2430:A:H2'	2.23	0.52
33:l:53:MET:HE1	33:l:103:TYR:CD1	2.45	0.52
35:n:34:HIS:O	35:n:102:ARG:NH1	2.43	0.52
44:w:74:ARG:NH1	44:w:76:GLU:OE2	2.43	0.52
1:A:407:U:H2'	1:A:408:A:C8	2.45	0.52
1:A:636:U:O2'	1:A:637:C:H5'	2.09	0.52
6:F:49:TYR:OH	6:F:86:ARG:NH1	2.42	0.52
22:a:1245:G:OP1	32:k:13:LYS:NZ	2.33	0.52
22:a:2394:C:H5''	32:k:63:LYS:HE2	1.90	0.52
22:a:2637:U:H5''	25:d:83:ARG:HH11	1.74	0.52
23:b:52:A:N7	35:n:64:TYR:OH	2.38	0.52
25:d:184:ARG:NH1	36:o:7:GLN:OE1	2.42	0.52
1:A:470:C:H2'	1:A:471:U:H6	1.74	0.52
1:A:1023:U:H2'	1:A:1024:G:C8	2.44	0.52
22:a:1649:G:O2'	34:m:106:ASP:OD2	2.17	0.52
22:a:2483:C:N3	33:l:123:LYS:NZ	2.57	0.52
22:a:2502:G:H5''	22:a:2503:2MA:H5''	1.90	0.52
26:e:7:ASP:OD2	26:e:122:GLU:N	2.42	0.52
28:g:89:LEU:HD22	28:g:162:VAL:HG22	1.90	0.52
34:m:69:ARG:O	34:m:70:THR:OG1	2.23	0.52
51:3:18:LYS:HE2	51:3:21:GLY:HA2	1.91	0.52
22:a:948:C:H1'	22:a:984:A:C8	2.44	0.52
22:a:1292:G:H2'	22:a:1293:C:C6	2.45	0.52
22:a:2537:U:H2'	22:a:2538:C:C6	2.44	0.52
26:e:27:LEU:HD11	26:e:100:MET:HG2	1.92	0.52
34:m:86:ARG:NE	34:m:117:ASP:OD2	2.42	0.52
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.43	0.52
10:J:37:ARG:HB3	10:J:75:ASP:HB2	1.91	0.52
22:a:593:U:H2'	22:a:594:U:C6	2.44	0.52
22:a:1864:U:OP1	22:a:2410:G:O2'	2.20	0.52
30:i:114:LEU:HG	30:i:118:MET:HE3	1.90	0.52
1:A:423:G:O2'	1:A:424:G:O5'	2.27	0.52
1:A:1035:A:O2'	1:A:1036:A:H5''	2.10	0.52
1:A:1179:A:OP2	9:I:99:ARG:NH2	2.42	0.52
22:a:545:U:O2	22:a:548:G:C6	2.63	0.52
22:a:882:G:O6	22:a:894:U:O2	2.27	0.52
22:a:1570:A:H2'	22:a:1571:A:C8	2.44	0.52
41:t:54:GLN:HG2	41:t:55:PRO:HD3	1.92	0.52
1:A:653:U:H5'	8:H:56:LYS:NZ	2.25	0.52
22:a:184:C:H2'	22:a:185:G:C8	2.44	0.52
24:c:145:GLU:HB2	24:c:188:CYS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:44:LYS:O	45:x:48:ARG:HG2	2.08	0.52
46:y:3:LYS:HE2	46:y:40:ASP:HB3	1.91	0.52
1:A:1363:A:O2'	1:A:1365:G:N7	2.34	0.52
6:F:96:VAL:HG12	6:F:96:VAL:O	2.09	0.52
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.92	0.52
22:a:210:C:OP1	49:1:29:GLN:NE2	2.40	0.52
1:A:312:C:H2'	1:A:313:A:C8	2.45	0.52
22:a:644:A:H2'	22:a:645:C:O4'	2.10	0.52
29:h:2:GLN:HA	29:h:2:GLN:OE1	2.10	0.52
35:n:99:TYR:OH	35:n:111:ARG:NH1	2.43	0.52
37:p:86:ALA:HB2	37:p:116:ALA:HB2	1.93	0.52
1:A:555:U:H2'	1:A:556:C:C6	2.44	0.51
10:J:52:LEU:HD11	10:J:59:LYS:HD2	1.91	0.51
22:a:720:U:H2'	22:a:721:A:H8	1.75	0.51
1:A:409:U:P	4:D:23:SER:HG	2.33	0.51
11:K:52:PHE:O	11:K:53:ARG:HD2	2.09	0.51
1:A:407:U:H2'	1:A:408:A:H8	1.74	0.51
2:B:184:PHE:HD1	2:B:198:PHE:HB2	1.74	0.51
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.92	0.51
22:a:347:A:H2'	22:a:348:A:C8	2.46	0.51
22:a:721:A:H2'	22:a:722:A:C8	2.46	0.51
22:a:1266:G:O2'	22:a:2012:G:O6	2.21	0.51
22:a:1534:U:C4	22:a:1535:A:H1'	2.46	0.51
22:a:703:U:H2'	22:a:704:G:O4'	2.11	0.51
22:a:2030:6MZ:C2	22:a:2499:C:H5''	2.40	0.51
22:a:2646:C:OP2	22:a:2732:G:O2'	2.26	0.51
26:e:7:ASP:CG	26:e:122:GLU:H	2.19	0.51
30:i:109:LEU:O	30:i:111:LYS:NZ	2.37	0.51
22:a:1156:A:C8	37:p:51:ARG:HG2	2.46	0.51
1:A:900:A:H2'	1:A:901:A:C8	2.45	0.51
22:a:1535:A:O2'	22:a:1537:G:N1	2.43	0.51
22:a:1636:U:H2'	22:a:1637:A:C8	2.46	0.51
30:i:4:PHE:O	37:p:64:ARG:NH2	2.40	0.51
1:A:201:G:O2'	1:A:469:C:O2'	2.23	0.51
1:A:1356:G:H2'	1:A:1357:A:H8	1.75	0.51
8:H:10:MET:HE3	8:H:61:LEU:HD11	1.91	0.51
22:a:1684:G:H2'	22:a:1685:C:H6	1.75	0.51
24:c:272:SER:O	24:c:272:SER:OG	2.25	0.51
42:u:20:LEU:HD22	42:u:25:LYS:HB2	1.93	0.51
1:A:580:C:H2'	1:A:581:G:O4'	2.11	0.51
22:a:361:G:H8	22:a:361:G:OP2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:639:U:H2'	22:a:640:C:H6	1.71	0.51
42:u:63:ILE:HG22	42:u:65:VAL:HG13	1.92	0.51
1:A:45:G:H2'	1:A:46:G:C8	2.46	0.51
1:A:390:U:H2'	1:A:391:G:C8	2.46	0.51
1:A:470:C:H2'	1:A:471:U:C6	2.45	0.51
11:K:84:VAL:HG11	11:K:97:ILE:HG12	1.92	0.51
17:Q:11:ARG:H	17:Q:23:VAL:HG13	1.75	0.51
22:a:640:C:H2'	22:a:641:U:C6	2.46	0.51
22:a:995:C:OP2	37:p:54:LYS:NZ	2.37	0.51
22:a:1684:G:H2'	22:a:1685:C:C6	2.46	0.51
24:c:121:ASP:OD2	24:c:121:ASP:N	2.36	0.51
1:A:1151:A:HO2'	1:A:1152:A:H8	1.58	0.51
22:a:139:U:C4	40:s:1:MET:HE1	2.45	0.51
22:a:171:U:H2'	22:a:172:A:H8	1.75	0.51
29:h:34:GLY:O	29:h:36:ALA:N	2.44	0.51
1:A:715:A:H2'	1:A:716:A:C8	2.45	0.50
1:A:1166:G:N1	1:A:1169:A:OP2	2.45	0.50
10:J:27:GLU:O	10:J:31:ARG:HG2	2.12	0.50
22:a:2038:G:H2'	22:a:2039:U:O4'	2.10	0.50
1:A:215:C:H1'	1:A:465:A:N6	2.26	0.50
1:A:1218:C:H2'	1:A:1219:A:C8	2.47	0.50
1:A:1268:G:H2'	1:A:1269:A:C8	2.46	0.50
10:J:30:LYS:HB2	10:J:31:ARG:NH1	2.26	0.50
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.76	0.50
22:a:365:U:H2'	22:a:366:C:C6	2.46	0.50
22:a:1028:A:N3	22:a:2486:C:O2'	2.42	0.50
39:r:4:ILE:HG13	39:r:106:VAL:HG22	1.93	0.50
1:A:1530:G:O6	21:U:46:LYS:NZ	2.28	0.50
15:O:14:GLU:HG2	15:O:84:ARG:HH21	1.76	0.50
46:y:41:THR:HG22	46:y:43:ALA:H	1.75	0.50
22:a:1484:U:H2'	22:a:1485:U:C6	2.46	0.50
22:a:1614:A:H8	22:a:1614:A:P	2.34	0.50
22:a:1182:G:H2'	22:a:1183:U:O4'	2.11	0.50
24:c:240:PHE:O	24:c:242:LYS:NZ	2.37	0.50
30:i:110:PRO:O	30:i:115:GLY:HA3	2.11	0.50
42:u:72:VAL:HG12	42:u:93:ARG:HA	1.92	0.50
1:A:522:C:OP2	12:L:66:TYR:OH	2.25	0.50
1:A:543:U:OP1	4:D:14:ARG:HD2	2.11	0.50
22:a:2514:U:H2'	22:a:2515:C:C6	2.47	0.50
28:g:38:ASN:HD22	28:g:64:GLN:CD	2.18	0.50
52:4:16:CYS:SG	52:4:17:SER:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:G:O2'	1:A:48:C:N4	2.45	0.50
1:A:1119:C:OP1	9:I:85:ARG:NH1	2.36	0.50
1:A:1287:A:H2'	1:A:1288:A:C8	2.47	0.50
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.45	0.50
18:R:37:GLY:O	18:R:63:ARG:NH2	2.45	0.50
22:a:1746:A:H2'	22:a:1747:U:C6	2.46	0.50
22:a:2266:A:H4'	22:a:2267:A:N3	2.26	0.50
39:r:2:GLU:HA	39:r:108:SER:HB3	1.94	0.50
1:A:202:G:O2'	1:A:468:A:N3	2.39	0.50
1:A:405:U:OP2	4:D:3:ARG:NH1	2.45	0.50
1:A:754:C:O5'	15:O:72:ARG:NH2	2.45	0.50
1:A:1010:U:H2'	1:A:1011:C:H6	1.77	0.50
1:A:1169:A:H2'	1:A:1170:A:C8	2.47	0.50
3:C:142:MET:HA	3:C:142:MET:HE3	1.93	0.50
9:I:44:ALA:O	9:I:48:VAL:HG23	2.12	0.50
22:a:182:A:H2'	22:a:183:C:H6	1.76	0.50
2:B:48:PRO:O	2:B:51:ASN:N	2.45	0.50
6:F:26:THR:HG22	6:F:36:ILE:HG12	1.92	0.50
10:J:42:LEU:HB2	10:J:71:LEU:HB3	1.94	0.50
10:J:99:GLN:OE1	10:J:99:GLN:HA	2.12	0.50
14:N:38:ASP:OD2	14:N:39:GLU:N	2.45	0.50
22:a:2:G:H2'	22:a:3:U:C6	2.47	0.50
22:a:219:A:N3	22:a:234:U:O2'	2.38	0.50
22:a:272:A:H2'	22:a:273:G:C8	2.46	0.50
22:a:359:G:H2'	22:a:360:U:H6	1.77	0.50
22:a:1000:A:H2'	22:a:1001:A:C8	2.47	0.50
1:A:171:A:H2'	1:A:172:A:C8	2.47	0.49
1:A:780:A:H5''	11:K:125:LYS:HD3	1.94	0.49
22:a:106:C:H2'	22:a:107:G:H8	1.77	0.49
22:a:547:A:H3'	22:a:548:G:C8	2.47	0.49
22:a:1526:C:H2'	22:a:1527:G:O4'	2.12	0.49
22:a:2698:U:H2'	22:a:2699:C:C6	2.47	0.49
26:e:176:ASP:N	26:e:176:ASP:OD1	2.43	0.49
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.42	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
22:a:1527:G:N1	22:a:1544:A:OP2	2.37	0.49
22:a:2100:G:N2	22:a:2189:U:O2	2.32	0.49
22:a:2246:G:H2'	22:a:2247:A:C8	2.47	0.49
22:a:2798:U:H4'	22:a:2799:A:H5'	1.95	0.49
41:t:47:LYS:HD3	41:t:48:PRO:HD2	1.94	0.49
1:A:64:G:OP1	1:A:382:A:N6	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:G:H4'	1:A:1513:A:H4'	1.94	0.49
1:A:1041:G:H2'	1:A:1042:A:C8	2.46	0.49
22:a:1278:C:H2'	22:a:1279:G:H8	1.77	0.49
22:a:1315:C:O2'	22:a:1392:A:N3	2.40	0.49
29:h:12:LEU:HD13	29:h:19:VAL:HG21	1.94	0.49
42:u:21:ARG:HE	42:u:87:GLN:HA	1.77	0.49
1:A:983:A:H5'	1:A:984:C:OP2	2.12	0.49
22:a:17:G:H2'	22:a:18:U:C6	2.47	0.49
22:a:286:U:H2'	22:a:287:G:C8	2.47	0.49
22:a:631:A:OP2	50:2:23:LYS:NZ	2.44	0.49
22:a:1790:C:H2'	22:a:1791:A:C5	2.47	0.49
22:a:2557:G:H2'	22:a:2558:C:C6	2.47	0.49
27:f:74:VAL:H	27:f:79:ILE:HG13	1.76	0.49
28:g:47:ASP:N	28:g:47:ASP:OD1	2.44	0.49
19:S:18:LYS:HG2	19:S:31:LEU:HD23	1.93	0.49
22:a:183:C:H42	22:a:213:A:N6	2.10	0.49
22:a:782:A:C2	24:c:225:MET:HG2	2.48	0.49
22:a:1168:G:H1	22:a:1181:U:H3	1.59	0.49
25:d:108:ASP:N	25:d:204:LYS:O	2.42	0.49
30:i:49:ASP:OD1	30:i:118:MET:HG3	2.13	0.49
1:A:184:G:H2'	1:A:185:U:C6	2.47	0.49
1:A:619:U:O2	1:A:619:U:H2'	2.12	0.49
9:I:123:ARG:NH1	9:I:124:ARG:O	2.43	0.49
18:R:26:ILE:HG22	18:R:30:LYS:HE3	1.94	0.49
22:a:645:C:H2'	22:a:647:G:C8	2.48	0.49
22:a:1028:A:H2'	22:a:1029:A:C8	2.48	0.49
22:a:2312:U:H5'	27:f:85:ILE:HD11	1.95	0.49
26:e:173:THR:HA	26:e:199:MET:HE1	1.94	0.49
1:A:204:G:C5	1:A:465:A:C6	3.00	0.49
1:A:215:C:H1'	1:A:465:A:H62	1.77	0.49
1:A:216:U:H2'	1:A:217:C:C6	2.46	0.49
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.49
1:A:1010:U:H2'	1:A:1011:C:C6	2.47	0.49
1:A:1062:U:H2'	1:A:1063:C:C6	2.47	0.49
13:M:75:MET:HE2	13:M:75:MET:HA	1.94	0.49
21:U:21:ARG:O	21:U:25:LYS:HG2	2.12	0.49
22:a:1534:U:C2	22:a:1537:G:O6	2.65	0.49
22:a:1683:U:H2'	22:a:1684:G:H8	1.78	0.49
22:a:2362:C:OP1	50:2:40:ARG:NE	2.42	0.49
22:a:2602:A:H5'	22:a:2603:G:OP1	2.13	0.49
22:a:2804:U:H2'	22:a:2805:C:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:42:C:C5	27:f:66:LEU:HD22	2.47	0.49
1:A:476:U:H2'	1:A:477:C:C6	2.48	0.49
1:A:663:A:H5'	1:A:836:G:OP1	2.12	0.49
1:A:1507:A:H2'	1:A:1508:A:C8	2.48	0.49
22:a:850:U:O2	46:y:47:MET:HE2	2.13	0.49
22:a:2505:G:N2	22:a:2506:U:O4	2.36	0.49
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.93	0.49
40:s:5:GLU:HG2	40:s:6:ARG:N	2.27	0.49
2:B:120:GLN:HB3	2:B:125:THR:HB	1.94	0.49
7:G:111:ARG:NH2	7:G:122:ASN:HB3	2.28	0.49
22:a:278:A:C6	22:a:362:A:C8	3.00	0.49
22:a:299:A:N3	22:a:319:G:O2'	2.40	0.49
22:a:306:U:H2'	22:a:307:G:O4'	2.12	0.49
22:a:1636:U:H2'	22:a:1637:A:H8	1.78	0.49
27:f:40:VAL:HG12	27:f:40:VAL:O	2.13	0.49
40:s:69:ARG:NH1	40:s:72:GLN:HA	2.28	0.49
4:D:144:SER:HB3	4:D:179:GLU:HG3	1.95	0.49
4:D:150:LYS:NZ	4:D:177:LYS:O	2.45	0.49
22:a:881:G:N1	22:a:895:U:N3	2.37	0.49
22:a:1212:G:H1'	22:a:1237:A:N6	2.28	0.49
22:a:2591:C:H2'	22:a:2592:G:C8	2.47	0.49
47:z:43:ILE:HG22	47:z:49:TYR:HB2	1.94	0.49
1:A:408:A:O3'	4:D:23:SER:OG	2.30	0.48
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.94	0.48
22:a:282:A:H2'	22:a:283:G:C8	2.48	0.48
22:a:2554:U:H2'	22:a:2555:U:C6	2.48	0.48
25:d:16:THR:OG1	25:d:18:ASP:OD1	2.20	0.48
40:s:69:ARG:HH12	40:s:72:GLN:HA	1.78	0.48
1:A:49:U:C2	1:A:361:G:N2	2.81	0.48
1:A:1360:A:OP2	14:N:75:ARG:NH2	2.45	0.48
17:Q:9:GLN:HE22	17:Q:79:VAL:HG21	1.78	0.48
22:a:2478:A:H5'	51:3:32:LYS:HE2	1.94	0.48
33:l:64:TRP:HB2	33:l:104:GLU:HB2	1.95	0.48
54:Z:51:U:H2'	54:Z:52:C:C6	2.49	0.48
1:A:945:G:C2	1:A:946:A:C8	3.01	0.48
1:A:1071:C:H2'	1:A:1072:G:C8	2.49	0.48
1:A:1527:U:H2'	1:A:1528:U:C6	2.47	0.48
1:A:255:G:OP1	17:Q:71:LYS:NZ	2.38	0.48
1:A:371:A:H2'	1:A:372:C:O4'	2.14	0.48
13:M:66:GLU:H	13:M:66:GLU:CD	2.21	0.48
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:221:A:N1	22:a:265:A:O2'	2.45	0.48
22:a:1704:C:H2'	22:a:1705:A:C8	2.47	0.48
22:a:2636:C:H2'	22:a:2637:U:C6	2.48	0.48
1:A:1144:G:N2	1:A:1146:A:H62	2.11	0.48
1:A:1441:A:C4	36:o:114:LEU:HD11	2.49	0.48
9:I:57:MET:HE1	9:I:90:TYR:HE2	1.78	0.48
10:J:77:VAL:HG22	10:J:78:GLU:HG2	1.96	0.48
14:N:47:LYS:HA	14:N:50:THR:HG22	1.96	0.48
22:a:1715:G:O2'	22:a:1743:G:O6	2.28	0.48
41:t:13:VAL:HA	41:t:70:VAL:HG12	1.96	0.48
1:A:362:G:N2	1:A:365:U:OP2	2.45	0.48
1:A:1404:C:H2'	1:A:1405:G:C8	2.48	0.48
6:F:18:VAL:HG21	6:F:58:HIS:CD2	2.49	0.48
19:S:20:GLU:HA	19:S:23:VAL:HG12	1.96	0.48
22:a:351:C:H2'	22:a:352:A:C8	2.49	0.48
22:a:1590:A:H2'	22:a:1591:A:C8	2.48	0.48
22:a:2567:G:H2'	22:a:2568:U:C6	2.48	0.48
22:a:2808:G:O2'	22:a:2890:G:O6	2.31	0.48
35:n:60:GLU:OE2	35:n:61:GLN:NE2	2.47	0.48
22:a:357:C:H2'	22:a:358:U:C6	2.49	0.48
23:b:48:U:H2'	23:b:49:C:C6	2.49	0.48
23:b:106:G:H2'	23:b:107:G:O4'	2.14	0.48
30:i:14:ASP:O	30:i:52:ASP:HB3	2.13	0.48
1:A:148:G:O2'	1:A:1446:A:N3	2.37	0.48
1:A:405:U:C5	4:D:5:LEU:HD11	2.49	0.48
22:a:1529:G:H2'	22:a:1530:G:H8	1.78	0.48
22:a:2074:U:H2'	22:a:2075:U:C6	2.48	0.48
27:f:93:GLY:O	27:f:96:MET:HB3	2.13	0.48
28:g:176:LYS:O	28:g:177:LYS:HG2	2.14	0.48
1:A:1120:C:H2'	1:A:1121:U:H6	1.79	0.48
10:J:7:ARG:HB2	10:J:101:SER:OG	2.14	0.48
15:O:18:ASP:HB3	15:O:21:ASP:HB2	1.96	0.48
22:a:1281:G:H2'	22:a:1282:U:C6	2.48	0.48
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.95	0.48
1:A:204:G:N2	1:A:465:A:H2'	2.29	0.48
1:A:1225:A:H2'	1:A:1226:C:C5	2.49	0.48
1:A:1373:G:N7	9:I:13:LYS:NZ	2.62	0.48
20:T:12:ILE:O	20:T:15:GLU:HG3	2.14	0.48
22:a:1441:G:H2'	22:a:1442:U:C6	2.48	0.48
22:a:1794:A:H2'	22:a:1795:C:H6	1.78	0.48
22:a:2216:G:H2'	22:a:2217:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.49	0.48
1:A:1004:A:C6	1:A:1026:G:H1'	2.49	0.47
1:A:1076:U:OP1	2:B:174:LYS:NZ	2.29	0.47
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.95	0.47
12:L:39:THR:HG21	12:L:49:LEU:HB3	1.96	0.47
54:Z:64:G:H2'	54:Z:65:G:H8	1.80	0.47
1:A:352:C:H4'	1:A:354:G:OP1	2.14	0.47
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.47
4:D:85:ASN:HB3	4:D:88:GLU:HG3	1.96	0.47
22:a:1538:G:OP2	22:a:1538:G:H8	1.96	0.47
1:A:736:C:H2'	1:A:737:C:H6	1.78	0.47
1:A:1026:G:O6	1:A:1035:A:N1	2.47	0.47
1:A:1280:A:OP2	10:J:9:ARG:NH2	2.47	0.47
22:a:2273:A:H2'	22:a:2274:A:C8	2.50	0.47
25:d:1:MET:HB3	25:d:205:PRO:HG2	1.96	0.47
34:m:71:ARG:HD2	34:m:71:ARG:HA	1.65	0.47
1:A:160:A:H2'	1:A:161:A:O4'	2.14	0.47
1:A:633:G:OP2	8:H:88:ARG:NH2	2.48	0.47
5:E:81:LEU:HD11	5:E:96:MET:HB3	1.95	0.47
11:K:87:LYS:HB2	11:K:113:VAL:HG23	1.95	0.47
22:a:191:A:H2'	22:a:192:C:H6	1.80	0.47
22:a:711:G:C6	22:a:721:A:C6	3.02	0.47
22:a:2308:G:H2'	22:a:2308:G:N3	2.29	0.47
22:a:2804:U:H2'	22:a:2805:C:C6	2.49	0.47
26:e:1:MET:HB3	26:e:14:VAL:HG23	1.97	0.47
14:N:3:LYS:HB2	14:N:6:MET:HG2	1.96	0.47
22:a:721:A:H2'	22:a:722:A:H8	1.80	0.47
22:a:1428:C:C5	22:a:1569:A:H5''	2.50	0.47
22:a:1589:U:H2'	22:a:1590:A:H8	1.79	0.47
27:f:58:ALA:HB2	27:f:65:PRO:HD3	1.96	0.47
47:z:33:THR:OG1	47:z:51:GLY:HA2	2.15	0.47
54:Z:1:C:H2'	54:Z:2:G:C8	2.50	0.47
1:A:17:U:H2'	1:A:18:C:C6	2.49	0.47
1:A:1273:C:H2'	1:A:1274:A:O4'	2.14	0.47
7:G:40:GLU:OE1	9:I:41:ARG:NH1	2.48	0.47
22:a:1796:U:H2'	22:a:1797:G:C8	2.50	0.47
22:a:2786:U:H2'	22:a:2787:C:H6	1.80	0.47
31:j:63:VAL:HG23	31:j:64:ARG:HG3	1.97	0.47
1:A:1119:C:H2'	1:A:1120:C:H6	1.78	0.47
1:A:1134:G:H2'	1:A:1135:U:O4'	2.15	0.47
1:A:1510:C:H2'	1:A:1511:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:174:ASP:OD2	4:D:177:LYS:HG2	2.15	0.47
16:P:45:GLU:OE2	16:P:45:GLU:HA	2.14	0.47
22:a:851:C:H2'	22:a:852:U:H6	1.80	0.47
22:a:910:A:C8	33:l:13:HIS:CD2	3.02	0.47
22:a:1412:U:H2'	22:a:1413:A:C8	2.49	0.47
22:a:1842:G:H2'	22:a:1843:C:C6	2.49	0.47
22:a:2515:C:H2'	22:a:2516:A:H8	1.80	0.47
22:a:2843:G:H2'	22:a:2844:G:H8	1.79	0.47
25:d:184:ARG:NH1	36:o:11:GLU:OE1	2.47	0.47
31:j:76:VAL:HG12	36:o:73:VAL:HB	1.97	0.47
1:A:161:A:H2'	1:A:162:A:C8	2.49	0.47
1:A:967:5MC:OP2	1:A:968:A:O2'	2.22	0.47
22:a:207:A:H2'	22:a:208:C:O4'	2.15	0.47
22:a:1026:G:H2'	22:a:1027:A:C8	2.48	0.47
35:n:88:LYS:O	35:n:88:LYS:HG2	2.14	0.47
4:D:102:VAL:HG13	4:D:107:PHE:HB2	1.97	0.47
22:a:150:U:H2'	22:a:151:C:C6	2.50	0.47
24:c:3:VAL:HG22	24:c:19:VAL:HG22	1.97	0.47
1:A:451:A:N6	1:A:480:U:HO2'	2.11	0.47
7:G:68:ASN:ND2	7:G:127:ALA:O	2.47	0.47
7:G:79:ARG:HA	7:G:84:THR:HA	1.97	0.47
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.50	0.47
22:a:5:A:H2'	22:a:6:A:H8	1.80	0.47
22:a:340:A:O2'	26:e:162:ARG:NH1	2.48	0.47
22:a:597:G:O2'	32:k:11:GLY:O	2.24	0.47
22:a:636:G:OP1	32:k:129:LYS:NZ	2.39	0.47
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.50	0.47
1:A:113:G:H1'	1:A:354:G:H5'	1.97	0.46
1:A:299:G:H2'	1:A:300:A:C8	2.50	0.46
1:A:1118:U:H2'	1:A:1119:C:H6	1.80	0.46
9:I:114:LYS:NZ	9:I:118:LEU:O	2.44	0.46
10:J:7:ARG:HD3	10:J:75:ASP:OD1	2.14	0.46
22:a:347:A:H2'	22:a:348:A:H8	1.80	0.46
22:a:871:U:H2'	22:a:872:U:C6	2.51	0.46
32:k:57:LEU:HD22	50:2:54:ASP:HB3	1.97	0.46
54:Z:24:C:H2'	54:Z:25:U:H6	1.79	0.46
1:A:1226:C:O2'	13:M:102:THR:O	2.25	0.46
22:a:483:A:C8	41:t:45:HIS:HD2	2.33	0.46
22:a:568:U:OP1	32:k:36:LYS:HE2	2.15	0.46
22:a:1558:C:O4'	22:a:1560:G:C8	2.68	0.46
22:a:1827:U:OP2	24:c:221:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:C:N3	16:P:1:MET:HG2	2.31	0.46
1:A:977:A:O2'	1:A:979:C:OP2	2.34	0.46
17:Q:58:VAL:HB	17:Q:80:GLU:HG3	1.97	0.46
22:a:548:G:H5''	22:a:549:G:OP2	2.16	0.46
23:b:24:G:N7	23:b:56:G:H2'	2.30	0.46
1:A:632:U:H5''	1:A:633:G:C8	2.51	0.46
6:F:2:ARG:HD3	6:F:91:ARG:HD3	1.98	0.46
10:J:9:ARG:HB2	10:J:99:GLN:HB2	1.95	0.46
22:a:279:A:H2'	22:a:280:U:O4'	2.15	0.46
22:a:880:G:H2'	22:a:881:G:H8	1.81	0.46
33:l:66:ARG:HB2	33:l:101:VAL:O	2.16	0.46
41:t:98:SER:OG	41:t:98:SER:O	2.29	0.46
4:D:15:GLU:OE1	4:D:63:ARG:NH1	2.49	0.46
11:K:89:PRO:HB3	21:U:32:VAL:HG21	1.97	0.46
16:P:75:ILE:HA	16:P:78:VAL:HG12	1.98	0.46
22:a:476:G:N1	22:a:479:A:OP2	2.46	0.46
22:a:1484:U:H2'	22:a:1485:U:H6	1.80	0.46
23:b:29:A:H2'	23:b:30:C:C6	2.51	0.46
1:A:613:C:H2'	1:A:614:C:C6	2.51	0.46
1:A:824:G:H2'	1:A:825:A:H8	1.81	0.46
1:A:1032:G:H2'	1:A:1033:G:O4'	2.16	0.46
1:A:1496:C:H2'	1:A:1497:G:O4'	2.16	0.46
2:B:130:THR:C	2:B:132:LYS:H	2.24	0.46
7:G:18:PHE:CE1	7:G:58:GLU:HG3	2.51	0.46
9:I:12:ARG:O	9:I:13:LYS:C	2.59	0.46
22:a:2316:G:H2'	22:a:2317:A:H8	1.80	0.46
22:a:2743:U:OP1	51:3:34:LYS:NZ	2.33	0.46
24:c:75:PRO:HG2	24:c:97:LYS:HG3	1.97	0.46
24:c:132:MET:O	24:c:167:ARG:NH2	2.48	0.46
50:2:32:ILE:O	50:2:32:ILE:HG13	2.15	0.46
1:A:215:C:H2'	1:A:216:U:C6	2.51	0.46
1:A:864:A:H2'	1:A:865:A:C8	2.50	0.46
2:B:104:TRP:HA	2:B:107:VAL:HG22	1.96	0.46
22:a:287:G:H2'	22:a:288:U:C6	2.50	0.46
22:a:624:C:O2'	22:a:657:U:OP1	2.29	0.46
22:a:657:U:H2'	22:a:658:U:C6	2.50	0.46
22:a:2566:A:N1	31:j:28:SER:OG	2.44	0.46
22:a:2740:A:H2'	22:a:2741:A:C8	2.50	0.46
28:g:90:VAL:HG12	28:g:91:GLY:N	2.31	0.46
32:k:30:THR:HG22	32:k:33:ARG:H	1.80	0.46
33:l:77:PRO:HG2	33:l:80:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:17:LYS:O	35:n:20:GLU:HG2	2.15	0.46
1:A:107:G:H1	20:T:6:SER:HG	1.60	0.46
1:A:1071:C:H2'	1:A:1072:G:H8	1.80	0.46
4:D:129:VAL:HG21	4:D:146:ARG:HH11	1.81	0.46
22:a:183:C:N4	22:a:213:A:H61	2.11	0.46
22:a:1528:A:OP2	22:a:1543:G:N2	2.49	0.46
27:f:71:ARG:O	27:f:81:GLN:NE2	2.47	0.46
28:g:94:TYR:HA	28:g:106:SER:O	2.16	0.46
54:Z:10:G:N2	54:Z:27:G:H1'	2.31	0.46
1:A:486:U:H2'	1:A:487:A:C8	2.47	0.46
1:A:1240:U:C5	7:G:116:MET:HG2	2.51	0.46
5:E:89:HIS:O	5:E:90:THR:C	2.59	0.46
22:a:580:U:H2'	22:a:581:C:C6	2.50	0.46
22:a:2233:U:H2'	22:a:2234:G:C8	2.50	0.46
22:a:2849:U:OP1	36:o:93:ARG:NH2	2.28	0.46
28:g:38:ASN:OD1	28:g:39:ASP:N	2.48	0.46
52:4:12:ILE:HG13	52:4:13:THR:N	2.31	0.46
1:A:999:C:H2'	1:A:1000:A:C8	2.51	0.46
1:A:1035:A:C4	1:A:1036:A:C2	3.04	0.46
2:B:57:LEU:HD13	2:B:217:VAL:HG13	1.98	0.46
11:K:109:ASN:OD1	21:U:5:LYS:HD2	2.15	0.46
22:a:58:G:H2'	22:a:59:U:C6	2.51	0.46
22:a:2783:U:H2'	22:a:2784:U:C6	2.51	0.46
42:u:26:PHE:CE1	42:u:42:LEU:HB2	2.50	0.46
10:J:21:ALA:O	10:J:25:ILE:HG12	2.16	0.45
22:a:875:G:H2'	22:a:876:C:C6	2.51	0.45
40:s:31:VAL:HG22	40:s:84:TYR:CD1	2.51	0.45
41:t:74:ASN:ND2	41:t:81:ASP:OD1	2.50	0.45
52:4:35:ASP:OD1	52:4:36:VAL:N	2.49	0.45
1:A:244:U:O4	1:A:906:A:H1'	2.16	0.45
1:A:382:A:H2'	1:A:383:A:C8	2.50	0.45
2:B:45:LYS:HG3	2:B:49:MET:HE3	1.98	0.45
3:C:111:LEU:O	3:C:204:LYS:NZ	2.38	0.45
13:M:79:ARG:NE	19:S:65:GLU:OE1	2.43	0.45
22:a:250:G:H2'	22:a:251:A:C8	2.51	0.45
22:a:367:G:H2'	22:a:368:A:C8	2.51	0.45
22:a:989:G:OP2	46:y:12:SER:OG	2.21	0.45
22:a:2251:OMG:HM23	22:a:2251:OMG:H1'	1.73	0.45
32:k:108:ALA:HB3	32:k:125:LEU:HD22	1.97	0.45
34:m:8:ARG:HD2	34:m:43:GLU:HG2	1.98	0.45
1:A:324:G:N2	1:A:326:G:H3'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:A:O2'	1:A:794:A:N7	2.44	0.45
1:A:1376:U:O4	7:G:10:ARG:NH1	2.49	0.45
5:E:61:GLN:O	5:E:65:GLU:HG2	2.16	0.45
22:a:638:G:H2'	22:a:639:U:C6	2.52	0.45
28:g:37:LEU:HD23	28:g:37:LEU:HA	1.76	0.45
42:u:75:GLN:HB3	42:u:90:ASP:HB3	1.98	0.45
44:w:72:ARG:NH1	44:w:78:TYR:OH	2.48	0.45
9:I:6:TYR:CE2	9:I:90:TYR:HD1	2.35	0.45
22:a:876:C:H2'	22:a:877:A:O4'	2.16	0.45
24:c:246:THR:HG23	24:c:250:VAL:O	2.17	0.45
26:e:117:ARG:HA	26:e:185:LYS:HD3	1.97	0.45
27:f:153:ASP:OD1	27:f:153:ASP:N	2.49	0.45
31:j:40:LYS:HE3	31:j:57:VAL:HG12	1.99	0.45
1:A:398:U:H2'	1:A:399:G:C8	2.48	0.45
1:A:499:A:H61	1:A:547:A:H5''	1.81	0.45
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.47	0.45
22:a:987:C:O2'	22:a:1000:A:N3	2.48	0.45
22:a:1447:C:H2'	22:a:1448:G:H8	1.82	0.45
22:a:1774:C:H2'	22:a:1774:C:O2	2.17	0.45
22:a:2020:A:H5'	47:z:9:THR:CG2	2.45	0.45
47:z:38:HIS:ND1	47:z:39:LEU:O	2.49	0.45
1:A:390:U:H2'	1:A:391:G:H8	1.81	0.45
1:A:575:G:O2'	1:A:821:G:OP2	2.25	0.45
1:A:1317:C:O2	19:S:37:ARG:NH2	2.43	0.45
12:L:110:ARG:NH1	12:L:112:GLN:O	2.50	0.45
14:N:90:ARG:HD2	14:N:92:GLU:OE1	2.16	0.45
22:a:955:PSU:OP1	33:l:86:LYS:NZ	2.36	0.45
39:r:20:VAL:HG11	39:r:44:ALA:HA	1.99	0.45
41:t:14:LEU:HD11	41:t:71:ALA:HB2	1.97	0.45
1:A:381:C:H2'	1:A:382:A:O4'	2.16	0.45
1:A:1037:C:H2'	1:A:1038:C:H6	1.80	0.45
6:F:4:TYR:CE2	6:F:71:ILE:HG13	2.52	0.45
15:O:14:GLU:HG2	15:O:84:ARG:NH2	2.32	0.45
22:a:373:U:O2'	22:a:423:A:H1'	2.16	0.45
22:a:1480:C:H2'	22:a:1481:U:O4'	2.17	0.45
22:a:2196:C:H2'	22:a:2197:U:C6	2.52	0.45
28:g:2:SER:O	28:g:6:LYS:HG2	2.17	0.45
2:B:188:ASP:OD1	2:B:189:THR:N	2.42	0.45
3:C:120:ILE:O	3:C:124:LEU:HG	2.17	0.45
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.98	0.45
22:a:722:A:H2'	22:a:723:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:851:C:H2'	22:a:852:U:C6	2.52	0.45
22:a:1447:C:H2'	22:a:1448:G:C8	2.52	0.45
22:a:2097:A:H2'	22:a:2098:U:C6	2.52	0.45
1:A:687:A:C2	1:A:704:A:C5	3.05	0.45
1:A:901:A:O2'	1:A:1513:A:OP1	2.30	0.45
6:F:6:ILE:HG12	6:F:89:VAL:HG22	1.99	0.45
9:I:57:MET:HE1	9:I:90:TYR:CE2	2.51	0.45
14:N:10:GLU:O	14:N:14:VAL:HG23	2.17	0.45
18:R:41:PRO:HD2	18:R:44:ILE:HD12	1.98	0.45
22:a:820:A:H4'	22:a:836:G:N2	2.31	0.45
22:a:910:A:C4	33:l:13:HIS:CD2	3.05	0.45
22:a:1529:G:H2'	22:a:1530:G:C8	2.52	0.45
22:a:1796:U:H2'	22:a:1797:G:H8	1.81	0.45
22:a:2681:C:OP2	25:d:114:LYS:NZ	2.31	0.45
23:b:2:G:H2'	23:b:3:C:C6	2.52	0.45
1:A:216:U:H4'	1:A:464:U:H4'	1.99	0.45
1:A:472:U:H2'	1:A:473:U:C6	2.52	0.45
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.45
1:A:1314:C:H2'	1:A:1315:U:H6	1.80	0.45
1:A:1314:C:OP1	19:S:6:LYS:NZ	2.37	0.45
19:S:45:ILE:HD12	19:S:45:ILE:H	1.82	0.45
22:a:414:C:H2'	22:a:415:A:C8	2.51	0.45
22:a:881:G:O6	22:a:895:U:C4	2.69	0.45
22:a:1197:G:H2'	22:a:1198:U:C6	2.51	0.45
22:a:2812:G:H2'	22:a:2813:A:C8	2.52	0.45
49:1:31:LEU:HD22	49:1:42:LEU:HD13	1.98	0.45
52:4:11:GLU:HG2	52:4:25:ARG:HG2	1.99	0.45
1:A:420:U:O2'	1:A:423:G:O6	2.25	0.44
1:A:592:G:H2'	1:A:593:U:C6	2.51	0.44
1:A:696:A:H2'	1:A:697:U:H6	1.81	0.44
5:E:131:THR:HG22	5:E:131:THR:O	2.16	0.44
7:G:86:GLN:HA	7:G:86:GLN:OE1	2.17	0.44
13:M:90:ARG:HA	13:M:90:ARG:HD2	1.78	0.44
22:a:419:U:H2'	22:a:420:C:C6	2.52	0.44
22:a:594:U:H2'	22:a:595:C:C6	2.52	0.44
22:a:1045:C:O2	22:a:1047:G:N2	2.50	0.44
22:a:1853:A:H2'	22:a:1854:A:C8	2.53	0.44
23:b:39:A:H2'	23:b:40:U:C6	2.52	0.44
26:e:21:ARG:NH1	26:e:106:LYS:HD2	2.32	0.44
27:f:17:MET:SD	27:f:22:TYR:HB2	2.57	0.44
1:A:312:C:H2'	1:A:313:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:A:H2'	1:A:947:G:H8	1.75	0.44
1:A:1157:A:C2	1:A:1181:G:C4	3.06	0.44
1:A:1180:A:OP1	9:I:105:THR:OG1	2.22	0.44
1:A:1526:G:H2'	1:A:1527:U:C6	2.52	0.44
6:F:3:HIS:O	6:F:92:THR:N	2.43	0.44
6:F:9:MET:SD	6:F:86:ARG:HB3	2.57	0.44
8:H:43:GLU:HG3	8:H:101:ILE:HD13	1.98	0.44
13:M:18:ALA:O	13:M:21:SER:HB3	2.16	0.44
21:U:7:ARG:H	21:U:10:GLU:CD	2.25	0.44
22:a:863:A:H2'	22:a:864:G:H8	1.81	0.44
22:a:1932:A:H2'	22:a:1933:G:O4'	2.16	0.44
22:a:2420:C:H4'	48:0:54:ILE:HG21	1.98	0.44
22:a:2680:U:O2'	22:a:2681:C:H5'	2.16	0.44
29:h:3:VAL:CG2	29:h:36:ALA:HB1	2.47	0.44
54:Z:15:G:N2	54:Z:22:A:N3	2.66	0.44
3:C:17:PRO:HG2	3:C:54:ARG:NH2	2.32	0.44
4:D:60:LYS:HE3	4:D:195:ILE:HG22	1.99	0.44
10:J:32:THR:HG21	10:J:83:THR:HA	1.98	0.44
17:Q:48:ASP:OD1	17:Q:75:LEU:HD13	2.17	0.44
22:a:634:C:H2'	22:a:635:C:C6	2.52	0.44
22:a:813:U:H2'	22:a:814:C:C6	2.51	0.44
22:a:879:G:H2'	22:a:880:G:C8	2.50	0.44
22:a:1496:A:H2'	22:a:1498:C:C5	2.52	0.44
22:a:2584:U:H2'	22:a:2585:U:H2'	1.99	0.44
1:A:67:C:H2'	1:A:68:G:C8	2.52	0.44
1:A:266:G:H3'	17:Q:69:LYS:HB2	1.99	0.44
1:A:335:C:H2'	1:A:336:A:C8	2.52	0.44
1:A:501:C:H2'	1:A:502:A:H8	1.80	0.44
1:A:1526:G:H2'	1:A:1527:U:H6	1.83	0.44
22:a:84:A:H4'	22:a:85:G:O5'	2.17	0.44
22:a:613:A:H8	22:a:613:A:OP1	2.00	0.44
22:a:836:G:C5	22:a:837:C:C5	3.05	0.44
22:a:910:A:C5	33:l:13:HIS:CD2	3.05	0.44
22:a:1397:U:OP2	22:a:1398:C:N4	2.36	0.44
22:a:2314:A:H2'	22:a:2315:G:H8	1.82	0.44
26:e:111:GLU:OE2	26:e:114:ARG:NH2	2.35	0.44
32:k:30:THR:HG21	32:k:34:GLY:O	2.17	0.44
35:n:15:ARG:NH2	35:n:95:SER:OG	2.51	0.44
43:v:17:GLU:O	43:v:19:LYS:NZ	2.49	0.44
1:A:408:A:H5'	4:D:113:GLU:HG3	1.99	0.44
21:U:49:LYS:HE2	21:U:49:LYS:HB2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1354:A:OP1	24:c:36:LYS:NZ	2.50	0.44
22:a:2545:G:H2'	22:a:2546:U:O4'	2.17	0.44
27:f:108:VAL:HG11	27:f:176:PRO:HG2	2.00	0.44
31:j:79:PHE:HE2	31:j:102:PRO:HG2	1.83	0.44
1:A:189:A:H8	1:A:189:A:OP2	2.01	0.44
1:A:389:A:H3'	1:A:390:U:H6	1.82	0.44
1:A:408:A:H2'	1:A:409:U:C6	2.51	0.44
1:A:1127:G:H5'	1:A:1280:A:O2'	2.17	0.44
10:J:83:THR:O	10:J:87:LEU:HG	2.18	0.44
13:M:51:GLY:O	13:M:55:THR:HG23	2.17	0.44
22:a:2:G:H2'	22:a:3:U:H6	1.82	0.44
24:c:24:LEU:HD13	24:c:83:TYR:HB2	1.99	0.44
28:g:52:PHE:CZ	28:g:72:LEU:HD22	2.53	0.44
34:m:56:LYS:NZ	34:m:90:ARG:O	2.43	0.44
35:n:53:THR:HB	35:n:65:THR:HB	1.99	0.44
1:A:461:A:H2'	1:A:462:G:H8	1.83	0.44
1:A:1279:G:P	10:J:9:ARG:HH12	2.40	0.44
2:B:27:MET:HE2	2:B:188:ASP:O	2.18	0.44
2:B:71:GLY:O	2:B:93:ASN:HA	2.18	0.44
5:E:36:LEU:HD22	5:E:134:ILE:HG13	2.00	0.44
22:a:363:G:H2'	22:a:364:C:C6	2.53	0.44
22:a:499:U:H2'	22:a:500:G:O4'	2.18	0.44
22:a:784:G:H5'	22:a:785:G:OP1	2.17	0.44
22:a:849:A:H2'	22:a:850:U:H6	1.83	0.44
22:a:1437:C:H2'	22:a:1438:U:C6	2.53	0.44
22:a:1473:G:H2'	22:a:1474:U:C6	2.53	0.44
22:a:1637:A:H5'	22:a:1760:C:O2'	2.18	0.44
22:a:1744:A:H3'	22:a:1745:A:H8	1.83	0.44
24:c:87:ARG:HG3	24:c:89:ALA:H	1.83	0.44
27:f:38:MET:HE3	27:f:57:LEU:HD22	2.00	0.44
27:f:147:ASP:N	27:f:147:ASP:OD1	2.51	0.44
29:h:15:LEU:HD23	29:h:16:GLY:N	2.32	0.44
1:A:235:C:H2'	1:A:236:A:C8	2.53	0.44
2:B:9:MET:HE1	2:B:46:THR:HG21	2.00	0.44
3:C:73:PRO:HG3	3:C:105:GLU:HG2	2.00	0.44
22:a:197:A:N6	22:a:2430:A:O2'	2.49	0.44
22:a:1199:U:H1'	37:p:4:VAL:HG22	2.00	0.44
22:a:1319:C:O2'	22:a:1320:C:H5'	2.18	0.44
22:a:1446:C:H2'	22:a:1447:C:C6	2.52	0.44
22:a:1511:G:H2'	22:a:1512:C:H6	1.83	0.44
37:p:49:ASP:HA	37:p:52:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:6:GLN:O	44:w:74:ARG:NH1	2.41	0.44
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.44
1:A:593:U:H2'	1:A:594:U:C6	2.53	0.44
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.44
1:A:1176:A:H2'	1:A:1177:G:C8	2.52	0.44
1:A:1220:G:P	14:N:53:ARG:HH12	2.41	0.44
1:A:1530:G:H2'	1:A:1531:A:C8	2.53	0.44
2:B:58:ASN:ND2	2:B:223:GLU:OE1	2.49	0.44
16:P:48:GLU:OE1	16:P:51:ARG:HB2	2.18	0.44
22:a:2072:C:H2'	22:a:2073:C:H6	1.83	0.44
24:c:210:ALA:HA	24:c:213:TRP:CE3	2.53	0.44
27:f:52:ASN:HB3	27:f:150:ARG:NH2	2.33	0.44
30:i:96:ARG:HD3	30:i:99:ARG:HG3	2.00	0.44
35:n:115:LEU:HD23	35:n:115:LEU:HA	1.78	0.44
41:t:99:ASN:C	41:t:99:ASN:OD1	2.61	0.44
42:u:6:ALA:HB3	42:u:65:VAL:HG12	2.00	0.44
52:4:12:ILE:HG13	52:4:13:THR:H	1.83	0.44
1:A:908:A:H2'	1:A:909:A:C8	2.53	0.43
1:A:1122:U:H2'	1:A:1123:U:C6	2.53	0.43
22:a:1445:G:C5	22:a:1446:C:C5	3.05	0.43
22:a:1730:C:O2'	22:a:1731:G:O5'	2.35	0.43
22:a:1773:A:C8	22:a:1829:A:C8	3.05	0.43
22:a:2843:G:H2'	22:a:2844:G:C8	2.53	0.43
24:c:76:ALA:HB2	24:c:96:TYR:CD1	2.53	0.43
26:e:144:GLU:OE1	26:e:144:GLU:N	2.51	0.43
40:s:88:LYS:HB2	40:s:91:GLN:HE21	1.83	0.43
1:A:140:U:H2'	1:A:141:G:O4'	2.17	0.43
1:A:1494:G:O2'	22:a:1912:A:O2'	2.35	0.43
6:F:22:ILE:HG23	6:F:39:LEU:HD11	1.99	0.43
6:F:37:HIS:O	6:F:97:THR:HG22	2.18	0.43
11:K:100:LEU:HA	11:K:100:LEU:HD23	1.75	0.43
21:U:31:GLU:OE2	21:U:35:ARG:NE	2.51	0.43
22:a:157:C:H2'	22:a:158:U:O4'	2.18	0.43
22:a:282:A:N6	22:a:359:G:O6	2.52	0.43
22:a:438:G:H2'	22:a:439:A:C8	2.53	0.43
22:a:1168:G:H2'	22:a:1169:A:H8	1.83	0.43
22:a:1354:A:H2'	22:a:1355:G:O4'	2.18	0.43
22:a:1511:G:H2'	22:a:1512:C:C6	2.52	0.43
22:a:1870:C:O2'	22:a:1871:A:O4'	2.36	0.43
26:e:58:LYS:NZ	26:e:70:SER:O	2.47	0.43
28:g:9:VAL:HG13	28:g:50:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:p:20:GLN:OE1	38:q:73:LYS:NZ	2.51	0.43
1:A:619:U:H2'	1:A:619:U:OP1	2.18	0.43
1:A:691:G:OP2	11:K:28:ASN:ND2	2.50	0.43
1:A:883:C:O2'	1:A:884:U:H5'	2.18	0.43
1:A:1014:A:C2	1:A:1219:A:H1'	2.53	0.43
1:A:1037:C:H2'	1:A:1038:C:C6	2.53	0.43
13:M:104:THR:HG22	13:M:105:ASN:N	2.33	0.43
14:N:47:LYS:O	14:N:50:THR:HG22	2.18	0.43
22:a:272:A:H2'	22:a:273:G:H8	1.82	0.43
22:a:500:G:N1	22:a:503:A:OP2	2.49	0.43
22:a:839:U:H2'	22:a:840:C:C6	2.53	0.43
22:a:1548:A:H2'	22:a:1549:A:H8	1.80	0.43
22:a:1736:U:H2'	22:a:1737:G:O4'	2.17	0.43
23:b:45:A:C4	23:b:46:A:C8	3.06	0.43
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.53	0.43
26:e:155:GLU:HG2	26:e:156:ASN:N	2.33	0.43
30:i:1:MET:HE2	37:p:97:ASP:OD1	2.18	0.43
41:t:99:ASN:O	41:t:101:GLU:N	2.52	0.43
3:C:142:MET:HG3	3:C:170:GLU:OE1	2.18	0.43
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.82	0.43
18:R:65:LEU:HD23	18:R:65:LEU:HA	1.85	0.43
22:a:372:G:O2'	22:a:400:G:O6	2.34	0.43
22:a:881:G:N2	22:a:895:U:O2	2.47	0.43
22:a:909:A:H2'	22:a:912:C:H5	1.83	0.43
22:a:1242:U:H2'	22:a:1243:C:C6	2.53	0.43
22:a:1902:C:H4'	24:c:242:LYS:O	2.18	0.43
22:a:2086:U:H2'	22:a:2087:G:C8	2.54	0.43
27:f:65:PRO:HA	27:f:89:VAL:HG12	2.00	0.43
28:g:153:ARG:HB2	28:g:153:ARG:CZ	2.48	0.43
44:w:56:MET:HE3	44:w:56:MET:HB2	1.85	0.43
50:2:62:LEU:HB3	50:2:65:ALA:HB2	2.00	0.43
1:A:676:A:H5''	11:K:115:PRO:HB3	2.01	0.43
1:A:1029:U:H2'	1:A:1030:U:O4'	2.18	0.43
22:a:242:G:O2'	22:a:254:G:O6	2.30	0.43
22:a:323:C:C4	22:a:333:G:C8	3.06	0.43
22:a:2025:C:H2'	22:a:2026:U:C6	2.53	0.43
27:f:170:LEU:O	27:f:175:PHE:HB2	2.19	0.43
32:k:93:ASN:OD1	32:k:94:THR:N	2.52	0.43
36:o:33:VAL:HG22	36:o:38:LYS:HG3	2.00	0.43
39:r:109:ASP:OD1	39:r:110:ARG:N	2.52	0.43
40:s:6:ARG:O	40:s:10:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:G:OP1	36:o:39:ARG:NH1	2.46	0.43
1:A:1162:C:H2'	1:A:1163:A:H8	1.84	0.43
1:A:1390:U:H2'	1:A:1391:U:C6	2.54	0.43
1:A:1463:U:H2'	1:A:1464:U:C6	2.53	0.43
12:L:10:LYS:HB3	12:L:10:LYS:HE3	1.84	0.43
22:a:273:G:C6	22:a:274:C:C4	3.06	0.43
22:a:1115:G:O2'	22:a:1116:G:H5''	2.19	0.43
26:e:166:LYS:HB2	26:e:166:LYS:HE2	1.86	0.43
44:w:15:GLY:HA3	44:w:29:PHE:HE2	1.84	0.43
12:L:111:LYS:HA	12:L:114:ARG:CG	2.49	0.43
22:a:634:C:H2'	22:a:635:C:H6	1.83	0.43
22:a:1444:G:C4	22:a:1445:G:C8	3.06	0.43
22:a:2314:A:H2'	22:a:2315:G:C8	2.54	0.43
22:a:2649:C:H2'	22:a:2650:U:H6	1.84	0.43
37:p:17:ILE:HD13	37:p:17:ILE:HA	1.91	0.43
1:A:135:C:H42	16:P:1:MET:HG3	1.83	0.43
1:A:649:A:H2'	1:A:650:G:O4'	2.19	0.43
3:C:164:ARG:NH1	3:C:166:GLU:OE2	2.49	0.43
18:R:47:THR:HG22	18:R:48:ARG:O	2.18	0.43
22:a:794:A:H2'	22:a:795:C:C6	2.54	0.43
22:a:822:G:H2'	22:a:823:C:C6	2.53	0.43
22:a:1446:C:H2'	22:a:1447:C:H6	1.83	0.43
24:c:61:ALA:O	24:c:63:ARG:NH2	2.49	0.43
26:e:23:PHE:HE1	26:e:28:VAL:HG21	1.82	0.43
27:f:135:GLN:HG3	27:f:150:ARG:O	2.19	0.43
1:A:460:A:H2'	1:A:461:A:C8	2.53	0.43
1:A:510:A:H8	1:A:542:G:H21	1.66	0.43
1:A:1039:G:H2'	1:A:1040:U:C6	2.54	0.43
1:A:1477:U:H2'	1:A:1478:U:C6	2.53	0.43
4:D:57:GLU:HG3	4:D:200:ILE:HD11	2.01	0.43
22:a:887:U:O2'	22:a:888:C:H3'	2.19	0.43
22:a:1473:G:H2'	22:a:1474:U:H6	1.84	0.43
22:a:2469:A:H4'	33:l:55:ARG:HD2	2.00	0.43
22:a:2700:A:H2'	22:a:2701:U:C6	2.53	0.43
31:j:66:LYS:HB3	31:j:66:LYS:HE3	1.71	0.43
31:j:71:ARG:NH2	31:j:123:LEU:O	2.41	0.43
35:n:63:LYS:HG3	35:n:64:TYR:N	2.33	0.43
1:A:538:G:H2'	1:A:539:A:H8	1.84	0.43
1:A:678:U:H2'	1:A:679:C:H6	1.83	0.43
4:D:99:ASP:OD2	4:D:133:ALA:HB1	2.17	0.43
4:D:188:ARG:NH2	4:D:195:ILE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:111:MET:HE2	5:E:111:MET:HB3	1.89	0.43
7:G:74:GLU:O	7:G:89:VAL:N	2.41	0.43
22:a:170:U:H2'	22:a:171:U:C6	2.53	0.43
22:a:545:U:H3'	22:a:546:U:C6	2.54	0.43
22:a:1438:U:H2'	22:a:1439:A:H8	1.84	0.43
22:a:1495:A:H2'	22:a:1496:A:C8	2.54	0.43
22:a:1685:C:H2'	22:a:1686:C:H6	1.84	0.43
22:a:2011:U:H2'	22:a:2012:G:O4'	2.19	0.43
22:a:2818:U:H2'	22:a:2819:G:H8	1.83	0.43
23:b:28:C:OP1	35:n:36:TYR:OH	2.36	0.43
27:f:64:LYS:HD3	52:4:5:ILE:HD12	2.00	0.43
45:x:14:LEU:HD23	45:x:14:LEU:HA	1.80	0.43
1:A:918:A:H2'	1:A:919:A:C8	2.54	0.42
1:A:1121:U:H2'	1:A:1122:U:C6	2.54	0.42
7:G:23:LEU:HD12	7:G:23:LEU:HA	1.82	0.42
9:I:96:SER:HB3	9:I:100:LYS:NZ	2.34	0.42
15:O:3:LEU:HD23	15:O:3:LEU:HA	1.90	0.42
22:a:171:U:H2'	22:a:172:A:C8	2.54	0.42
22:a:782:A:N7	24:c:220:VAL:HG21	2.34	0.42
22:a:863:A:H2'	22:a:864:G:C8	2.54	0.42
22:a:892:A:H2'	22:a:893:C:C6	2.54	0.42
22:a:1683:U:H2'	22:a:1684:G:C8	2.54	0.42
22:a:1914:C:H2'	22:a:1915:3TD:H6	2.01	0.42
22:a:2847:U:H2'	22:a:2848:G:O4'	2.19	0.42
28:g:145:ALA:HB1	28:g:164:TYR:HE1	1.84	0.42
30:i:12:LYS:HD3	30:i:12:LYS:HA	1.91	0.42
1:A:184:G:H2'	1:A:185:U:H6	1.84	0.42
1:A:868:C:H2'	1:A:869:G:O4'	2.19	0.42
1:A:1509:C:C2	1:A:1510:C:C5	3.08	0.42
22:a:479:A:N3	22:a:481:G:H5''	2.34	0.42
22:a:503:A:H4'	22:a:504:A:H3'	2.02	0.42
22:a:1039:A:H2'	22:a:1040:A:O4'	2.19	0.42
22:a:2455:G:H2'	22:a:2456:C:C6	2.54	0.42
28:g:50:LEU:HD13	28:g:72:LEU:HD23	2.00	0.42
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.42
1:A:678:U:H2'	1:A:679:C:C6	2.54	0.42
1:A:1026:G:O6	1:A:1035:A:C6	2.72	0.42
1:A:1268:G:H1'	1:A:1326:U:O2'	2.19	0.42
12:L:114:ARG:HB3	12:L:119:VAL:HB	2.01	0.42
22:a:644:A:C2	22:a:2369:A:H1'	2.54	0.42
22:a:1292:G:H2'	22:a:1293:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2314:A:OP1	27:f:88:LYS:NZ	2.52	0.42
22:a:2589:A:H2'	22:a:2590:A:C8	2.55	0.42
22:a:2625:G:H2'	22:a:2626:C:O4'	2.19	0.42
22:a:2901:C:N4	22:a:2902:C:H41	2.17	0.42
24:c:132:MET:HE2	24:c:172:VAL:HG21	2.01	0.42
41:t:41:LEU:HA	41:t:61:LYS:O	2.18	0.42
1:A:522:C:H41	12:L:50:ARG:NH2	2.17	0.42
1:A:1118:U:H2'	1:A:1119:C:C6	2.54	0.42
1:A:1250:A:H2'	1:A:1251:A:C8	2.54	0.42
1:A:1333:A:H2'	1:A:1334:G:O4'	2.19	0.42
22:a:288:U:H2'	22:a:289:G:C8	2.54	0.42
22:a:645:C:H2'	22:a:647:G:N7	2.34	0.42
22:a:1585:C:H2'	22:a:1586:A:O4'	2.19	0.42
22:a:1589:U:H2'	22:a:1590:A:C8	2.55	0.42
22:a:2522:U:O2'	22:a:2647:U:OP1	2.25	0.42
22:a:2591:C:H2'	22:a:2592:G:H8	1.84	0.42
26:e:132:LYS:HD3	26:e:132:LYS:HA	1.88	0.42
38:q:46:GLU:OE2	38:q:46:GLU:N	2.52	0.42
1:A:142:G:H3'	1:A:143:A:H8	1.85	0.42
1:A:323:U:H2'	1:A:324:G:O4'	2.19	0.42
1:A:508:U:H1'	1:A:509:A:H2	1.84	0.42
1:A:750:C:O2	15:O:23:GLY:HA3	2.20	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:1206:G:H2'	1:A:1207:2MG:O4'	2.19	0.42
1:A:1530:G:H2'	1:A:1531:A:H8	1.85	0.42
15:O:79:THR:HA	15:O:82:ILE:HG12	2.02	0.42
22:a:1179:G:H2'	22:a:1180:U:C6	2.54	0.42
22:a:1370:C:H2'	22:a:1371:G:O4'	2.19	0.42
22:a:1406:U:H2'	22:a:1407:G:C8	2.55	0.42
22:a:1413:A:H2'	22:a:1414:C:C6	2.55	0.42
22:a:1509:A:HO2'	22:a:1510:G:H8	1.64	0.42
22:a:2064:C:H2'	22:a:2065:C:C6	2.54	0.42
22:a:2193:G:H2'	22:a:2194:U:C6	2.53	0.42
22:a:2820:A:H4'	34:m:3:HIS:CD2	2.54	0.42
22:a:2820:A:N3	22:a:2820:A:H2'	2.34	0.42
25:d:13:ARG:HD2	25:d:15:PHE:CE2	2.55	0.42
34:m:28:LEU:HD23	34:m:48:VAL:HG21	2.01	0.42
1:A:223:A:H2'	1:A:224:U:H6	1.83	0.42
1:A:268:U:H2'	1:A:269:C:C6	2.55	0.42
1:A:471:U:H2'	1:A:472:U:C6	2.55	0.42
1:A:834:U:H2'	1:A:835:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:U:H2'	1:A:1122:U:H6	1.85	0.42
1:A:1263:C:H2'	1:A:1264:U:H6	1.85	0.42
1:A:1326:U:H2'	1:A:1327:C:H6	1.85	0.42
4:D:48:LEU:HD22	4:D:52:GLY:HA3	2.02	0.42
9:I:96:SER:O	9:I:100:LYS:HE2	2.19	0.42
22:a:64:A:H2'	22:a:65:U:H6	1.84	0.42
22:a:305:C:H2'	22:a:306:U:C6	2.54	0.42
22:a:608:A:H2'	22:a:609:A:C8	2.54	0.42
22:a:2395:C:H2'	22:a:2396:G:O4'	2.18	0.42
22:a:2538:C:H2'	22:a:2539:C:H6	1.85	0.42
22:a:2783:U:H2'	22:a:2784:U:H6	1.83	0.42
22:a:2795:C:H2'	22:a:2796:U:C6	2.55	0.42
28:g:11:VAL:HG11	28:g:17:VAL:HG21	2.00	0.42
32:k:55:MET:HE2	32:k:55:MET:HB2	1.86	0.42
1:A:460:A:H2'	1:A:461:A:H8	1.84	0.42
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.42
1:A:1147:C:O2'	9:I:7:TYR:OH	2.30	0.42
7:G:79:ARG:NH1	7:G:82:GLY:H	2.08	0.42
9:I:6:TYR:HE2	9:I:90:TYR:HD1	1.67	0.42
16:P:59:HIS:O	16:P:63:GLN:HG2	2.19	0.42
22:a:273:G:H2'	22:a:274:C:C6	2.54	0.42
22:a:1535:A:H3'	22:a:1535:A:N3	2.35	0.42
22:a:1592:C:H2'	22:a:1593:A:C8	2.54	0.42
28:g:160:LYS:HE2	28:g:160:LYS:HB3	1.69	0.42
30:i:13:ARG:HH11	30:i:49:ASP:HB3	1.83	0.42
30:i:129:GLU:N	30:i:129:GLU:OE1	2.53	0.42
33:l:53:MET:CG	33:l:120:ALA:HB2	2.49	0.42
36:o:27:GLU:HB2	36:o:44:GLU:HG3	2.01	0.42
54:Z:44:A:H2'	54:Z:45:A:C8	2.55	0.42
1:A:151:A:OP2	1:A:169:C:N4	2.53	0.42
1:A:444:G:C6	1:A:491:G:C6	3.08	0.42
1:A:1027:C:N4	1:A:1035:A:H61	2.17	0.42
13:M:50:GLU:O	13:M:53:ILE:HG22	2.19	0.42
16:P:36:VAL:HG11	16:P:57:ILE:CD1	2.50	0.42
22:a:2537:U:H2'	22:a:2538:C:H6	1.84	0.42
1:A:1003:G:N2	1:A:1005:A:H5'	2.35	0.42
6:F:42:TRP:HB2	6:F:59:TYR:HB2	2.02	0.42
12:L:111:LYS:HA	12:L:114:ARG:HG3	2.00	0.42
22:a:273:G:H2'	22:a:274:C:H6	1.84	0.42
22:a:404:A:H1'	22:a:405:U:OP2	2.20	0.42
22:a:577:G:H2'	22:a:578:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:675:A:N3	22:a:2443:C:O2'	2.50	0.42
22:a:2615:U:C2	47:z:4:GLN:HA	2.54	0.42
22:a:2723:C:H2'	22:a:2724:U:O4'	2.20	0.42
22:a:2848:G:O2'	22:a:2867:G:N2	2.43	0.42
23:b:48:U:H2'	23:b:49:C:H6	1.85	0.42
30:i:18:VAL:HG21	30:i:142:ILE:HD12	2.01	0.42
40:s:30:ILE:HG13	40:s:85:VAL:HB	2.01	0.42
1:A:2:A:H2'	1:A:2:A:OP2	2.20	0.42
1:A:123:U:OP1	1:A:311:C:O2'	2.36	0.42
1:A:404:G:N7	4:D:2:ALA:HB3	2.34	0.42
7:G:70:ARG:HD2	7:G:96:ARG:HB3	2.02	0.42
14:N:16:LEU:HD12	14:N:54:ASP:HB2	2.01	0.42
14:N:23:LYS:HE3	14:N:27:LEU:HD11	2.02	0.42
14:N:42:TRP:O	14:N:46:LEU:HD23	2.20	0.42
19:S:27:ASP:C	19:S:28:LYS:HD3	2.45	0.42
19:S:46:GLY:HA2	19:S:61:PHE:HE1	1.85	0.42
22:a:296:U:H2'	22:a:297:G:C8	2.55	0.42
22:a:633:A:O2'	22:a:2404:U:OP1	2.34	0.42
22:a:1295:C:H2'	22:a:1296:G:H8	1.85	0.42
22:a:1412:U:H2'	22:a:1413:A:H8	1.83	0.42
22:a:1538:G:H2'	22:a:1539:U:C6	2.55	0.42
22:a:2271:G:OP1	43:v:18:ALA:HB1	2.20	0.42
22:a:2605:PSU:H2'	22:a:2606:C:C6	2.55	0.42
31:j:52:VAL:C	31:j:53:LYS:HD2	2.45	0.42
41:t:81:ASP:OD1	41:t:98:SER:OG	2.37	0.42
47:z:52:ARG:O	47:z:54:VAL:HG13	2.20	0.42
54:Z:1:C:H2'	54:Z:2:G:H8	1.85	0.42
1:A:421:U:H3'	1:A:422:C:H6	1.84	0.41
1:A:453:G:C4	1:A:454:G:C8	3.08	0.41
1:A:517:G:HO2'	1:A:518:C:P	2.43	0.41
1:A:721:G:H4'	1:A:722:G:O4'	2.20	0.41
1:A:881:G:H2'	1:A:882:C:O4'	2.19	0.41
1:A:1063:C:OP2	1:A:1064:G:O2'	2.34	0.41
1:A:1510:C:H2'	1:A:1511:G:C8	2.55	0.41
4:D:27:ALA:HB3	4:D:30:THR:HG23	2.02	0.41
11:K:47:ALA:HB1	11:K:62:ALA:HB1	2.02	0.41
18:R:11:CYS:HB3	18:R:14:THR:HG22	2.01	0.41
18:R:70:TYR:HB2	18:R:74:HIS:NE2	2.35	0.41
22:a:176:A:O2'	22:a:177:G:H5'	2.20	0.41
22:a:223:A:N1	22:a:407:G:O2'	2.48	0.41
22:a:340:A:H2'	22:a:341:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:861:A:H2'	22:a:862:G:O4'	2.20	0.41
22:a:2331:G:O2'	22:a:2336:A:N1	2.48	0.41
32:k:23:ILE:HG12	38:q:82:HIS:CD2	2.55	0.41
34:m:106:ASP:OD1	34:m:106:ASP:N	2.53	0.41
36:o:7:GLN:O	36:o:11:GLU:HG3	2.20	0.41
54:Z:11:A:H2'	54:Z:12:G:C8	2.54	0.41
1:A:408:A:H2'	1:A:409:U:H6	1.83	0.41
1:A:1524:C:H2'	1:A:1525:G:C8	2.55	0.41
11:K:93:ARG:NH2	11:K:112:ASP:OD2	2.32	0.41
22:a:360:U:H3'	22:a:361:G:C8	2.56	0.41
22:a:857:G:H2'	22:a:858:G:O4'	2.20	0.41
22:a:1473:G:C6	22:a:1519:G:C6	3.08	0.41
22:a:1563:U:H2'	22:a:1564:C:C6	2.55	0.41
22:a:1591:A:H2'	22:a:1592:C:C6	2.56	0.41
22:a:2281:A:O2'	22:a:2282:G:H5'	2.20	0.41
22:a:2295:C:OP1	35:n:10:ARG:NH2	2.53	0.41
22:a:2301:C:H2'	22:a:2302:U:C6	2.55	0.41
50:2:55:LEU:HD23	50:2:55:LEU:HA	1.90	0.41
1:A:620:C:C2	4:D:132:ILE:HD13	2.55	0.41
1:A:747:A:H2'	1:A:748:G:O4'	2.19	0.41
4:D:95:GLU:CD	4:D:104:ARG:HH21	2.27	0.41
9:I:88:MET:HE3	9:I:95:ARG:HG3	2.01	0.41
10:J:10:LEU:CD2	10:J:98:VAL:HG12	2.50	0.41
12:L:46:ASN:ND2	12:L:89:D2T:SB	2.93	0.41
14:N:83:LYS:HA	14:N:83:LYS:HD3	1.79	0.41
22:a:163:C:H2'	22:a:164:C:H6	1.85	0.41
22:a:357:C:H2'	22:a:358:U:H6	1.85	0.41
47:z:12:LYS:HE3	47:z:12:LYS:HB3	1.92	0.41
1:A:539:A:H2'	1:A:540:G:H8	1.84	0.41
1:A:1036:A:H3'	1:A:1037:C:H6	1.84	0.41
1:A:1124:G:N2	1:A:1125:U:O4	2.40	0.41
3:C:178:LEU:HD23	3:C:178:LEU:HA	1.90	0.41
4:D:200:ILE:HD12	4:D:200:ILE:H	1.85	0.41
11:K:31:ILE:HG23	11:K:46:THR:HG22	2.01	0.41
22:a:535:G:C6	22:a:559:G:C6	3.08	0.41
22:a:581:C:H2'	22:a:582:A:C8	2.55	0.41
22:a:1186:G:H2'	22:a:1187:G:O4'	2.20	0.41
22:a:1842:G:H2'	22:a:1843:C:H6	1.85	0.41
22:a:2294:G:P	35:n:94:ARG:HH12	2.44	0.41
28:g:42:GLU:OE2	28:g:42:GLU:HA	2.21	0.41
38:q:34:GLU:OE2	38:q:34:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:49:VAL:O	41:t:54:GLN:HA	2.21	0.41
41:t:97:LYS:O	41:t:98:SER:OG	2.37	0.41
44:w:17:ASN:HB2	44:w:25:THR:OG1	2.20	0.41
52:4:59:ARG:O	52:4:63:ARG:HG2	2.21	0.41
1:A:965:U:H5''	1:A:966:2MG:OP1	2.20	0.41
1:A:981:U:OP1	14:N:9:ARG:NH1	2.53	0.41
1:A:1298:U:H4'	1:A:1299:A:O4'	2.21	0.41
1:A:1315:U:H2'	1:A:1316:G:O4'	2.20	0.41
4:D:62:ARG:HE	4:D:62:ARG:HB3	1.70	0.41
20:T:2:ALA:HB3	20:T:8:LYS:HG2	2.02	0.41
22:a:282:A:H2'	22:a:283:G:H8	1.85	0.41
22:a:649:G:H2'	22:a:650:C:C6	2.55	0.41
22:a:1419:A:O2'	22:a:1421:G:N7	2.45	0.41
22:a:2208:C:H2'	22:a:2209:G:C8	2.55	0.41
54:Z:9:G:N3	54:Z:46:G:H2'	2.35	0.41
1:A:320:A:H2'	1:A:321:A:O4'	2.20	0.41
1:A:1123:U:O2'	1:A:1124:G:H5'	2.20	0.41
6:F:34:GLY:HA2	6:F:65:GLU:O	2.21	0.41
11:K:79:ILE:HB	11:K:105:PHE:HE2	1.84	0.41
13:M:4:ILE:HD12	13:M:9:ILE:HD13	2.01	0.41
22:a:403:U:H5'	22:a:404:A:OP1	2.21	0.41
22:a:822:G:H2'	22:a:823:C:H6	1.85	0.41
22:a:2377:A:H2'	22:a:2378:A:C8	2.56	0.41
29:h:30:LEU:HB3	29:h:36:ALA:HB3	2.02	0.41
1:A:415:A:H62	1:A:428:G:H1	1.69	0.41
1:A:440:C:C2	1:A:441:A:C8	3.08	0.41
1:A:543:U:H2'	1:A:544:G:C8	2.56	0.41
1:A:619:U:H5''	4:D:128:ARG:HH22	1.85	0.41
1:A:985:C:H2'	1:A:986:U:C6	2.55	0.41
12:L:79:VAL:O	12:L:103:ASP:HB2	2.21	0.41
18:R:72:ASP:N	18:R:72:ASP:OD1	2.54	0.41
21:U:21:ARG:HA	21:U:21:ARG:HD2	1.80	0.41
22:a:173:A:H2'	22:a:174:U:C6	2.55	0.41
22:a:322:A:OP2	26:e:163:ASN:HB2	2.21	0.41
22:a:475:C:O2	22:a:479:A:N6	2.51	0.41
22:a:1310:G:N2	22:a:1313:U:C4	2.89	0.41
22:a:1328:A:H2'	22:a:1330:C:C5	2.55	0.41
22:a:2732:G:OP1	25:d:208:LYS:NZ	2.52	0.41
23:b:2:G:H2'	23:b:3:C:H6	1.85	0.41
40:s:5:GLU:O	40:s:9:LYS:HG2	2.20	0.41
40:s:29:THR:HA	40:s:85:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:A:O2'	1:A:572:A:N1	2.51	0.41
1:A:34:C:H2'	1:A:35:G:C8	2.56	0.41
1:A:123:U:OP1	1:A:312:C:H5'	2.21	0.41
1:A:259:G:OP1	20:T:36:TYR:OH	2.28	0.41
1:A:857:C:H2'	1:A:858:G:O4'	2.21	0.41
1:A:1513:A:H2'	1:A:1514:G:C8	2.56	0.41
9:I:84:THR:O	9:I:88:MET:HG3	2.21	0.41
11:K:82:LEU:HD23	11:K:82:LEU:HA	1.93	0.41
22:a:362:A:C4	22:a:363:G:C8	3.08	0.41
22:a:367:G:H2'	22:a:368:A:H8	1.86	0.41
22:a:601:C:H2'	22:a:602:A:O4'	2.21	0.41
22:a:715:A:H2'	22:a:716:A:C8	2.56	0.41
22:a:2014:A:H2'	22:a:2015:A:C8	2.55	0.41
22:a:2347:C:C2	22:a:2348:U:C5	3.08	0.41
22:a:2589:A:H2'	22:a:2590:A:H8	1.85	0.41
22:a:2698:U:H2'	22:a:2699:C:H6	1.86	0.41
23:b:65:U:C4	23:b:108:A:C4	3.09	0.41
24:c:120:VAL:HG12	24:c:131:PRO:HG2	2.02	0.41
32:k:62:PRO:HG2	50:2:25:LYS:HB3	2.03	0.41
35:n:81:ARG:O	35:n:84:GLU:HG2	2.20	0.41
54:Z:70:C:H2'	54:Z:71:G:H8	1.86	0.41
1:A:62:U:OP1	1:A:385:C:O2'	2.36	0.41
1:A:1263:C:H2'	1:A:1264:U:C6	2.56	0.41
3:C:10:ILE:HD12	3:C:10:ILE:HA	1.92	0.41
6:F:74:LEU:HD12	6:F:74:LEU:HA	1.87	0.41
6:F:90:MET:HB3	6:F:90:MET:HE2	1.70	0.41
7:G:103:TRP:CD1	7:G:137:LYS:HZ3	2.39	0.41
15:O:36:ILE:O	15:O:40:GLN:HG2	2.20	0.41
22:a:205:G:O2'	22:a:206:U:OP2	2.39	0.41
22:a:1179:G:H2'	22:a:1180:U:H6	1.86	0.41
22:a:1790:C:H2'	22:a:1791:A:N7	2.36	0.41
22:a:2329:U:H2'	22:a:2330:G:C8	2.55	0.41
22:a:2419:U:H4'	48:0:22:THR:HG21	2.03	0.41
25:d:40:LEU:HD23	25:d:40:LEU:HA	1.89	0.41
25:d:62:LYS:HB3	25:d:63:PRO:HD3	2.03	0.41
36:o:63:LYS:HE2	36:o:65:SER:HB3	2.03	0.41
41:t:14:LEU:O	41:t:19:LYS:HG3	2.21	0.41
54:Z:44:A:H2'	54:Z:45:A:H8	1.86	0.41
1:A:294:U:OP1	1:A:610:U:O2'	2.35	0.41
1:A:521:G:N7	12:L:50:ARG:NH1	2.66	0.41
1:A:1030:U:O2'	1:A:1031:C:P	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:A:OP2	13:M:110:LYS:HE3	2.21	0.41
1:A:1294:G:H2'	1:A:1295:U:C6	2.56	0.41
1:A:1428:A:H2'	1:A:1429:A:O4'	2.21	0.41
4:D:102:VAL:HG11	4:D:117:LEU:HD11	2.02	0.41
5:E:152:MET:HE2	5:E:152:MET:HB3	1.92	0.41
6:F:3:HIS:HB2	6:F:92:THR:O	2.21	0.41
22:a:142:A:O2'	40:s:1:MET:N	2.52	0.41
22:a:169:G:H2'	22:a:170:U:C6	2.56	0.41
22:a:275:C:O2'	22:a:276:U:O4'	2.25	0.41
22:a:319:G:OP2	26:e:132:LYS:HE3	2.21	0.41
22:a:596:U:H2'	22:a:597:G:H8	1.86	0.41
22:a:1044:C:O2'	22:a:1111:A:N1	2.51	0.41
22:a:1349:C:C2	22:a:1350:C:C5	3.09	0.41
22:a:1444:G:C6	22:a:1445:G:C5	3.09	0.41
22:a:1473:G:C6	22:a:1474:U:C4	3.09	0.41
22:a:1614:A:C6	39:r:87:PRO:HB3	2.56	0.41
22:a:2016:U:H2'	22:a:2017:U:C6	2.56	0.41
22:a:2246:G:H2'	22:a:2247:A:H8	1.85	0.41
22:a:2649:C:H2'	22:a:2650:U:C6	2.56	0.41
28:g:44:LYS:O	28:g:50:LEU:HA	2.21	0.41
48:0:11:LEU:HB2	48:0:21:TYR:HB2	2.03	0.41
1:A:224:U:H2'	1:A:225:C:C6	2.57	0.40
1:A:1326:U:H2'	1:A:1327:C:C6	2.56	0.40
4:D:147:GLU:CD	4:D:150:LYS:HD2	2.45	0.40
10:J:25:ILE:HD11	10:J:92:LEU:HD11	2.02	0.40
22:a:359:G:H2'	22:a:360:U:C6	2.55	0.40
22:a:2301:C:H2'	22:a:2302:U:H6	1.85	0.40
26:e:7:ASP:OD1	26:e:7:ASP:N	2.51	0.40
27:f:142:ASP:O	27:f:146:VAL:HG23	2.21	0.40
1:A:607:A:H2'	1:A:608:A:C8	2.57	0.40
1:A:875:U:O2'	8:H:15:ARG:HD2	2.21	0.40
1:A:1318:A:H5''	19:S:3:ARG:NH2	2.36	0.40
1:A:1464:U:H2'	1:A:1465:A:H8	1.87	0.40
7:G:69:VAL:HG21	7:G:134:ALA:HB1	2.03	0.40
11:K:115:PRO:O	11:K:116:ILE:HD13	2.22	0.40
22:a:145:C:H2'	22:a:146:A:C8	2.56	0.40
22:a:242:G:H5''	50:2:64:TYR:CE2	2.56	0.40
22:a:764:A:H5''	24:c:209:GLY:CA	2.51	0.40
22:a:832:U:H2'	22:a:833:A:C8	2.56	0.40
22:a:1020:A:N1	22:a:1141:U:O2'	2.48	0.40
22:a:1808:A:H3'	22:a:1809:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2187:U:H2'	22:a:2188:U:C6	2.56	0.40
22:a:2353:G:H2'	22:a:2354:C:O4'	2.21	0.40
22:a:2638:G:O2'	22:a:2775:G:N2	2.50	0.40
22:a:2803:G:H2'	22:a:2804:U:H6	1.86	0.40
27:f:4:LEU:HD23	27:f:4:LEU:HA	1.80	0.40
54:Z:29:C:H2'	54:Z:30:G:H8	1.86	0.40
1:A:8:A:H4'	1:A:9:G:OP1	2.21	0.40
1:A:335:C:H2'	1:A:336:A:H8	1.87	0.40
1:A:404:G:O6	4:D:2:ALA:N	2.55	0.40
1:A:657:U:H4'	15:O:28:GLN:HG2	2.03	0.40
2:B:101:LEU:HB3	2:B:179:LEU:HD12	2.04	0.40
5:E:14:LYS:HE2	5:E:14:LYS:HB2	1.71	0.40
5:E:44:GLY:O	5:E:74:VAL:N	2.47	0.40
10:J:8:ILE:HB	10:J:74:VAL:HB	2.03	0.40
10:J:27:GLU:HA	10:J:30:LYS:NZ	2.37	0.40
11:K:107:ILE:HG13	21:U:12:PHE:CE1	2.56	0.40
17:Q:26:GLU:OE1	17:Q:39:LYS:HG2	2.22	0.40
22:a:57:C:H2'	22:a:58:G:O4'	2.21	0.40
22:a:57:C:C2	22:a:58:G:C8	3.10	0.40
22:a:274:C:C5	22:a:275:C:N3	2.89	0.40
22:a:1028:A:N6	22:a:1125:G:H2'	2.36	0.40
22:a:1050:A:C2	22:a:2751:G:C4	3.09	0.40
22:a:1386:C:H2'	22:a:1387:A:H8	1.85	0.40
22:a:1883:U:H2'	22:a:1884:G:O4'	2.21	0.40
22:a:2236:U:H2'	22:a:2237:G:O4'	2.20	0.40
26:e:112:LEU:HB3	26:e:118:LEU:HB2	2.02	0.40
1:A:20:U:H2'	1:A:21:G:O4'	2.21	0.40
1:A:745:G:H2'	1:A:746:A:C8	2.56	0.40
1:A:1465:A:H2'	1:A:1466:C:C6	2.56	0.40
2:B:77:SER:HB2	2:B:93:ASN:HB2	2.03	0.40
4:D:172:GLU:CD	4:D:183:LYS:HD3	2.47	0.40
5:E:105:ILE:HD13	5:E:116:GLU:HG3	2.03	0.40
6:F:40:GLU:OE1	6:F:100:SER:OG	2.39	0.40
6:F:59:TYR:CE2	18:R:67:LEU:HD21	2.56	0.40
12:L:7:LEU:HA	12:L:7:LEU:HD23	1.90	0.40
21:U:41:PRO:HA	21:U:44:GLU:HG2	2.03	0.40
22:a:893:C:H2'	22:a:894:U:O4'	2.22	0.40
22:a:1538:G:H2'	22:a:1539:U:H6	1.85	0.40
22:a:2101:A:H2'	22:a:2102:G:C8	2.56	0.40
22:a:2572:A:N7	25:d:150:MEQ:HB3	2.36	0.40
22:a:2605:PSU:C4	22:a:2606:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:132:MET:HG3	24:c:188:CYS:O	2.22	0.40
24:c:245:VAL:HG12	24:c:251:GLN:HA	2.02	0.40
35:n:39:VAL:HB	35:n:49:VAL:HG22	2.04	0.40
41:t:49:VAL:HG13	41:t:52:LEU:O	2.22	0.40
54:Z:65:G:H2'	54:Z:66:C:H6	1.86	0.40
1:A:517:G:O2'	1:A:518:C:O5'	2.36	0.40
2:B:9:MET:HE1	2:B:46:THR:CG2	2.52	0.40
3:C:112:ASP:OD2	3:C:115:LEU:HG	2.22	0.40
9:I:51:PRO:O	9:I:55:VAL:HG22	2.22	0.40
11:K:61:PHE:O	11:K:64:GLN:HG2	2.20	0.40
14:N:89:MET:HE2	14:N:89:MET:HA	2.04	0.40
22:a:263:G:H2'	22:a:264:C:O4'	2.21	0.40
22:a:558:U:H2'	22:a:559:G:H8	1.87	0.40
22:a:710:U:C2	22:a:711:G:C8	3.10	0.40
22:a:889:C:H2'	22:a:890:C:O4'	2.21	0.40
22:a:1328:A:H2'	22:a:1330:C:C4	2.56	0.40
27:f:36:LEU:HD22	27:f:154:ILE:HG12	2.03	0.40
31:j:7:MET:HE3	31:j:7:MET:HB3	1.88	0.40
32:k:82:LEU:HD22	32:k:90:VAL:HG21	2.04	0.40
40:s:74:ILE:HD12	40:s:74:ILE:HA	1.98	0.40
41:t:47:LYS:HD3	41:t:47:LYS:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
10	J	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	12	28
11	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	M	113/118 (96%)	105 (93%)	7 (6%)	1 (1%)	14	31
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	45
26	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
28	g	174/177 (98%)	155 (89%)	19 (11%)	0	100	100
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
30	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
33	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
34	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	94 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	r	108/110 (98%)	108 (100%)	0	0	100	100
40	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
41	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
42	u	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
43	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
44	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	z	54/57 (95%)	54 (100%)	0	0	100	100
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
49	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	18
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
All	All	5481/5913 (93%)	5252 (96%)	225 (4%)	4 (0%)	49	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	d	149	ASN
10	J	57	VAL
13	M	105	ASN
50	2	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	64 (98%)	1 (2%)	57	79
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	59/63 (94%)	59 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4573/4825 (95%)	4572 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	P	63	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	8	ASN
3	C	69	HIS
3	C	102	ASN
4	D	36	GLN
6	F	52	ASN
6	F	68	GLN
7	G	68	ASN
7	G	97	ASN
9	I	5	GLN

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Mol	Chain	Res	Type
9	I	50	GLN
10	J	58	ASN
11	K	24	HIS
14	N	43	ASN
17	Q	9	GLN
17	Q	45	HIS
17	Q	50	ASN
24	c	90	ASN
24	c	117	GLN
25	d	32	ASN
25	d	42	ASN
25	d	58	ASN
26	e	115	GLN
28	g	22	GLN
28	g	73	ASN
28	g	111	HIS
30	i	58	ASN
30	i	80	HIS
34	m	18	GLN
36	o	3	ASN
36	o	56	HIS
36	o	66	ASN
38	q	43	ASN
39	r	7	HIS
40	s	91	GLN
42	u	87	GLN
45	x	15	ASN
45	x	31	GLN
45	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	200 (13%)	7 (0%)
22	a	2751/2904 (94%)	305 (11%)	0
23	b	118/120 (98%)	10 (8%)	0
53	X	5/66 (7%)	0	0
54	Z	76/77 (98%)	9 (11%)	1 (1%)
All	All	4458/4709 (94%)	524 (11%)	8 (0%)

All (524) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	71	A
1	A	74	A
1	A	91	U
1	A	94	G
1	A	95	C
1	A	116	A
1	A	119	A
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	144	G
1	A	149	A
1	A	160	A
1	A	163	C
1	A	177	G
1	A	181	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	200	G
1	A	204	G
1	A	215	C
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C

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Mol	Chain	Res	Type
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	392	C
1	A	406	G
1	A	413	G
1	A	414	A
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	U
1	A	453	G
1	A	457	G
1	A	458	U
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	479	U
1	A	481	G
1	A	482	A
1	A	484	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	499	A
1	A	505	G
1	A	509	A
1	A	511	C
1	A	513	C
1	A	517	G
1	A	518	C
1	A	521	G

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Mol	Chain	Res	Type
1	A	527	G7M
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	619	U
1	A	620	C
1	A	637	C
1	A	639	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	721	G
1	A	723	U
1	A	734	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	802	A
1	A	815	A
1	A	817	C
1	A	849	G
1	A	884	U
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C

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Mol	Chain	Res	Type
1	A	935	A
1	A	960	U
1	A	965	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1006	G
1	A	1009	U
1	A	1024	G
1	A	1027	C
1	A	1031	C
1	A	1032	G
1	A	1035	A
1	A	1036	A
1	A	1044	A
1	A	1046	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1159	U
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1257	A
1	A	1258	G
1	A	1275	A
1	A	1280	A
1	A	1286	U

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Mol	Chain	Res	Type
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1419	G
1	A	1429	A
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1519	MA6
1	A	1529	G
1	A	1530	G
22	a	10	A
22	a	15	G
22	a	34	U
22	a	42	A
22	a	45	G
22	a	51	G
22	a	61	C
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A

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Mol	Chain	Res	Type
22	a	101	A
22	a	102	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	142	A
22	a	164	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	223	A
22	a	233	A
22	a	248	G
22	a	272	A
22	a	275	C
22	a	277	G
22	a	278	A
22	a	279	A
22	a	281	C
22	a	282	A
22	a	285	G
22	a	289	G
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	356	G
22	a	359	G
22	a	361	G
22	a	362	A
22	a	386	G
22	a	396	G
22	a	405	U
22	a	411	G
22	a	412	A
22	a	481	G
22	a	491	G
22	a	505	A

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Mol	Chain	Res	Type
22	a	509	C
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	544	C
22	a	547	A
22	a	548	G
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	685	A
22	a	686	U
22	a	717	C
22	a	730	A
22	a	738	G
22	a	747	5MU
22	a	775	G
22	a	776	G
22	a	782	A
22	a	783	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	884	U

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Mol	Chain	Res	Type
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	899	A
22	a	907	G
22	a	910	A
22	a	914	G
22	a	931	U
22	a	945	A
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1006	C
22	a	1012	U
22	a	1013	C
22	a	1033	U
22	a	1040	A
22	a	1041	G
22	a	1046	A
22	a	1047	G
22	a	1108	U
22	a	1110	G
22	a	1111	A
22	a	1112	G
22	a	1122	G
22	a	1130	U
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1136	G
22	a	1142	A
22	a	1170	C
22	a	1172	C
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1256	G

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Mol	Chain	Res	Type
22	a	1271	G
22	a	1272	A
22	a	1300	G
22	a	1301	A
22	a	1306	C
22	a	1321	A
22	a	1329	U
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1410	G
22	a	1416	G
22	a	1417	C
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1482	G
22	a	1493	C
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1524	G
22	a	1535	A
22	a	1537	G
22	a	1539	U
22	a	1554	U
22	a	1560	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1607	C
22	a	1608	A
22	a	1610	A
22	a	1626	A
22	a	1647	U
22	a	1648	U

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Mol	Chain	Res	Type
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1730	C
22	a	1731	G
22	a	1738	G
22	a	1764	C
22	a	1773	A
22	a	1779	U
22	a	1786	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1848	A
22	a	1858	A
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1906	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G

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Mol	Chain	Res	Type
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2188	U
22	a	2189	U
22	a	2190	G
22	a	2191	A
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2269	G
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2336	A
22	a	2345	G
22	a	2347	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2475	C
22	a	2476	A

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Mol	Chain	Res	Type
22	a	2478	A
22	a	2491	U
22	a	2492	U
22	a	2494	G
22	a	2505	G
22	a	2518	A
22	a	2525	G
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2582	G
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2630	G
22	a	2661	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2778	A
22	a	2790	U
22	a	2791	G
22	a	2799	A
22	a	2820	A
22	a	2821	A
22	a	2833	U
22	a	2835	A
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2880	C
22	a	2884	U

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Mol	Chain	Res	Type
23	b	13	G
23	b	24	G
23	b	35	C
23	b	42	C
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
54	Z	9	G
54	Z	14	A
54	Z	18	U
54	Z	19	G
54	Z	21	H2U
54	Z	22	A
54	Z	23	G
54	Z	54	G
54	Z	77	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	429	U
1	A	517	G
1	A	532	A
1	A	636	U
1	A	1026	G
1	A	1030	U
1	A	1035	A
54	Z	20	G

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

46 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
12	D2T	L	89	12	7,9,10	1.20	0	6,11,13	2.26	3 (50%)
1	5MC	A	967	1	18,22,23	3.61	8 (44%)	26,32,35	1.04	1 (3%)
25	MEQ	d	150	25	8,9,10	1.26	1 (12%)	5,10,12	1.38	1 (20%)
22	5MU	a	1939	22	19,22,23	4.41	7 (36%)	28,32,35	3.90	10 (35%)
1	UR3	A	1498	1	19,22,23	2.53	6 (31%)	26,32,35	1.32	1 (3%)
1	5MC	A	1407	1	18,22,23	3.43	7 (38%)	26,32,35	1.06	1 (3%)
22	5MC	a	1962	22	18,22,23	3.35	7 (38%)	26,32,35	1.25	3 (11%)
33	MS6	l	82	33	5,7,8	0.93	0	2,7,9	2.00	1 (50%)
22	PSU	a	746	22,55	18,21,22	1.07	2 (11%)	22,30,33	1.73	3 (13%)
22	PSU	a	2580	22	18,21,22	1.18	2 (11%)	22,30,33	2.11	6 (27%)
22	1MG	a	745	22	22,26,27	2.54	7 (31%)	33,39,42	1.77	8 (24%)
22	PSU	a	2605	22	18,21,22	1.07	1 (5%)	22,30,33	1.86	2 (9%)
22	M5Q	a	2498	22,55	20,23,24	1.30	2 (10%)	27,33,36	2.05	10 (37%)
22	6MZ	a	1618	22	22,25,26	2.65	4 (18%)	30,36,39	2.43	10 (33%)
22	PSU	a	1911	22	18,21,22	1.01	2 (11%)	22,30,33	1.87	3 (13%)
22	PSU	a	2604	22	18,21,22	1.07	2 (11%)	22,30,33	1.84	4 (18%)
22	PSU	a	955	22	18,21,22	1.14	2 (11%)	22,30,33	1.96	5 (22%)
1	2MG	A	966	1	23,26,27	2.55	6 (26%)	32,38,41	2.22	10 (31%)
22	2MG	a	1835	22	23,26,27	2.48	7 (30%)	32,38,41	2.26	10 (31%)
1	2MG	A	1516	1	23,26,27	2.44	7 (30%)	32,38,41	2.20	11 (34%)
22	PSU	a	2504	22	18,21,22	1.10	2 (11%)	22,30,33	1.81	4 (18%)
22	OMG	a	2251	54,22	23,26,27	2.49	8 (34%)	33,38,41	1.96	9 (27%)
22	PSU	a	1917	22	18,21,22	1.01	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	A	516	55,1	18,21,22	1.02	1 (5%)	22,30,33	1.61	5 (22%)
1	4OC	A	1402	55,1	20,23,24	2.83	8 (40%)	26,32,35	1.02	3 (11%)
22	G7M	a	2069	22,55	23,26,27	2.68	9 (39%)	35,39,42	1.73	9 (25%)
22	TKW	a	2501	22	18,22,23	2.46	7 (38%)	28,32,35	1.79	5 (17%)
22	2MA	a	2503	22,55	22,25,26	3.66	10 (45%)	33,37,40	2.89	9 (27%)
22	PSU	a	2457	22	18,21,22	1.13	3 (16%)	22,30,33	2.10	5 (22%)
1	2MG	A	1207	1	23,26,27	2.51	7 (30%)	32,38,41	2.17	10 (31%)
22	3TD	a	1915	22	18,22,23	3.96	7 (38%)	22,32,35	1.81	3 (13%)
22	D5D	a	2449	22	19,22,23	1.47	4 (21%)	22,32,35	2.63	5 (22%)
11	IAS	K	119	11	6,7,8	0.99	0	6,8,10	1.25	0
22	6MZ	a	2030	22	22,25,26	2.64	5 (22%)	30,36,39	2.60	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	H2U	Z	21	54	18,21,22	1.05	2 (11%)	21,30,33	1.01	1 (4%)
54	OMC	Z	33	54	19,22,23	2.79	8 (42%)	26,31,34	0.78	0
1	MA6	A	1518	1	23,26,27	1.55	5 (21%)	34,38,41	2.27	12 (35%)
1	MA6	A	1519	1	23,26,27	1.49	5 (21%)	34,38,41	2.33	12 (35%)
54	5MU	Z	55	54	19,22,23	4.61	7 (36%)	28,32,35	3.75	9 (32%)
54	4SU	Z	8	54	18,21,22	4.08	8 (44%)	26,30,33	2.35	5 (19%)
1	G7M	A	527	1	23,26,27	2.73	8 (34%)	35,39,42	1.71	9 (25%)
22	5MU	a	747	22	19,22,23	4.49	7 (36%)	28,32,35	3.94	10 (35%)
22	2MG	a	2445	22	23,26,27	2.47	7 (30%)	32,38,41	2.30	9 (28%)
54	PSU	Z	56	54	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
22	OMU	a	2552	22	19,22,23	2.61	6 (31%)	26,31,34	1.94	5 (19%)
33	4D4	l	81	33	9,11,12	1.56	2 (22%)	8,13,15	2.08	3 (37%)

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
12	D2T	L	89	12	-	1/7/12/14	-
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
25	MEQ	d	150	25	-	2/8/9/11	-
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
33	MS6	l	82	33	-	1/4/6/8	-
22	PSU	a	746	22,55	-	1/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	M5Q	a	2498	22,55	-	1/11/30/31	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	2504	22	-	1/7/25/26	0/2/2/2
22	OMG	a	2251	54,22	-	1/9/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	55,1	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	55,1	-	1/9/29/30	0/2/2/2
22	G7M	a	2069	22,55	-	2/7/25/26	0/3/3/3
22	TKW	a	2501	22	-	6/7/25/26	0/2/2/2
22	2MA	a	2503	22,55	-	1/7/25/26	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	D5D	a	2449	22	-	1/9/41/42	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
54	H2U	Z	21	54	-	7/7/38/39	0/2/2/2
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
54	5MU	Z	55	54	-	2/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	2/9/27/28	0/3/3/3
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2
33	4D4	l	81	33	-	7/11/12/14	-

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	11.86	1.49	1.35
22	a	2503	2MA	C4-N3	11.13	1.48	1.34
22	a	1618	6MZ	C6-N6	10.82	1.45	1.34
22	a	2030	6MZ	C6-N6	10.55	1.45	1.34
54	Z	55	5MU	C6-N1	10.47	1.55	1.38
54	Z	55	5MU	C2-N1	10.46	1.55	1.38
22	a	747	5MU	C6-N1	10.07	1.55	1.38
22	a	1939	5MU	C6-N1	9.83	1.54	1.38
22	a	747	5MU	C2-N1	9.76	1.54	1.38
22	a	1939	5MU	C2-N1	9.24	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Z	8	4SU	C4-N3	9.17	1.47	1.37
1	A	967	5MC	C6-C5	9.16	1.49	1.34
54	Z	55	5MU	C4-C5	8.89	1.59	1.44
1	A	1407	5MC	C6-C5	8.88	1.49	1.34
22	a	747	5MU	C4-C5	8.53	1.58	1.44
22	a	1915	3TD	C2-N1	8.41	1.48	1.37
22	a	1939	5MU	C4-C5	8.27	1.58	1.44
22	a	1962	5MC	C6-C5	8.23	1.48	1.34
22	a	1939	5MU	C4-N3	-8.23	1.23	1.38
22	a	747	5MU	C4-N3	-7.96	1.24	1.38
54	Z	8	4SU	C2-N1	7.67	1.50	1.38
54	Z	55	5MU	C4-N3	-7.48	1.24	1.38
1	A	966	2MG	C2-N3	7.33	1.45	1.31
1	A	1207	2MG	C2-N3	7.14	1.45	1.31
1	A	967	5MC	C4-N3	6.93	1.45	1.34
22	a	1835	2MG	C2-N3	6.79	1.44	1.31
22	a	2445	2MG	C2-N3	6.79	1.44	1.31
22	a	2503	2MA	C2-N3	6.70	1.46	1.34
22	a	2251	OMG	C4-N3	6.68	1.50	1.34
1	A	1516	2MG	C2-N3	6.68	1.44	1.31
22	a	1962	5MC	C4-N3	6.59	1.45	1.34
54	Z	8	4SU	C2-N3	6.50	1.49	1.38
1	A	1407	5MC	C4-N3	6.31	1.44	1.34
54	Z	55	5MU	C6-C5	6.25	1.44	1.34
1	A	966	2MG	C4-N3	6.23	1.49	1.34
22	a	2501	TKW	C4-N3	-6.21	1.23	1.34
1	A	1207	2MG	C4-N3	6.17	1.48	1.34
1	A	967	5MC	C2-N3	6.16	1.48	1.36
1	A	527	G7M	C2-N2	6.15	1.48	1.34
1	A	1498	UR3	C2-N1	6.13	1.47	1.38
1	A	527	G7M	C4-N3	6.04	1.48	1.34
22	a	2069	G7M	C2-N2	6.02	1.48	1.34
1	A	1516	2MG	C4-N3	5.96	1.48	1.34
22	a	1835	2MG	C4-N3	5.93	1.48	1.34
22	a	747	5MU	C6-C5	5.93	1.44	1.34
1	A	1402	4OC	C4-N3	5.92	1.43	1.32
1	A	1402	4OC	C6-C5	5.90	1.48	1.35
54	Z	33	OMC	C2-N3	5.88	1.48	1.36
22	a	2069	G7M	C4-N3	5.88	1.48	1.34
22	a	2445	2MG	C4-N3	5.84	1.48	1.34
54	Z	8	4SU	C6-C5	5.83	1.48	1.35
22	a	2552	OMU	C2-N1	5.81	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1962	5MC	C2-N3	5.81	1.48	1.36
22	a	1939	5MU	C6-C5	5.80	1.44	1.34
1	A	1498	UR3	C6-C5	5.75	1.48	1.35
22	a	745	1MG	C4-N3	5.73	1.47	1.34
1	A	1407	5MC	C2-N3	5.72	1.48	1.36
22	a	2503	2MA	C2-N1	5.70	1.44	1.34
22	a	745	1MG	C2-N3	5.68	1.44	1.34
54	Z	33	OMC	C6-C5	5.65	1.48	1.35
22	a	1915	3TD	C6-N1	5.63	1.45	1.36
54	Z	8	4SU	C4-S4	-5.55	1.57	1.68
22	a	2552	OMU	C2-N3	5.49	1.47	1.38
22	a	745	1MG	C2-N2	5.49	1.44	1.34
22	a	2552	OMU	C6-C5	5.44	1.47	1.35
1	A	1402	4OC	C2-N3	5.30	1.47	1.36
54	Z	8	4SU	C5-C4	5.30	1.49	1.42
22	a	2069	G7M	C5-N7	-5.28	1.33	1.39
1	A	527	G7M	C2-N3	5.25	1.45	1.33
1	A	527	G7M	C5-N7	-5.21	1.33	1.39
22	a	2503	2MA	C6-N6	-5.11	1.21	1.34
22	a	2501	TKW	C5-C4	5.07	1.48	1.42
22	a	2251	OMG	C2-N3	4.98	1.45	1.33
22	a	2503	2MA	C5-C6	4.88	1.54	1.41
22	a	2069	G7M	C2-N3	4.82	1.44	1.33
1	A	967	5MC	C6-N1	4.72	1.46	1.38
54	Z	33	OMC	C4-N3	4.66	1.43	1.34
54	Z	33	OMC	C4-N4	4.65	1.44	1.33
22	a	2251	OMG	C2-N2	4.59	1.45	1.34
1	A	966	2MG	C2-N1	4.58	1.44	1.36
1	A	1407	5MC	C6-N1	4.48	1.45	1.38
1	A	1207	2MG	C2-N1	4.42	1.43	1.36
1	A	1498	UR3	C2-N3	4.35	1.47	1.39
22	a	1915	3TD	C2-N3	4.26	1.48	1.38
22	a	2501	TKW	C4-N4	4.24	1.45	1.34
22	a	1835	2MG	C2-N1	4.21	1.43	1.36
22	a	1962	5MC	C6-N1	4.16	1.45	1.38
1	A	1516	2MG	C2-N1	4.06	1.43	1.36
1	A	1402	4OC	C4-N4	3.98	1.44	1.35
1	A	967	5MC	C4-N4	3.96	1.44	1.34
22	a	2445	2MG	C2-N1	3.84	1.42	1.36
1	A	1407	5MC	C4-N4	3.82	1.44	1.34
54	Z	33	OMC	C2-N1	3.80	1.48	1.40
22	a	1962	5MC	C4-N4	3.73	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C2-N1	3.71	1.48	1.40
1	A	1519	MA6	C5-C4	-3.70	1.32	1.39
22	a	745	1MG	C5-N7	-3.69	1.31	1.39
22	a	2503	2MA	C5-N7	-3.68	1.32	1.39
22	a	2445	2MG	C5-N7	-3.68	1.31	1.39
22	a	1962	5MC	C2-N1	3.64	1.47	1.40
22	a	2030	6MZ	C5-C4	-3.61	1.32	1.39
1	A	1518	MA6	C5-C4	-3.60	1.32	1.39
22	a	1835	2MG	C5-N7	-3.59	1.32	1.39
22	a	2251	OMG	C5-N7	-3.59	1.32	1.39
22	a	2552	OMU	O2-C2	-3.51	1.16	1.23
1	A	1402	4OC	C2-N1	3.50	1.47	1.40
1	A	1402	4OC	O2-C2	-3.47	1.17	1.23
1	A	1402	4OC	C5-C4	3.42	1.48	1.40
1	A	527	G7M	C5-C6	3.40	1.52	1.43
22	a	2498	M5Q	C2-N1	-3.40	1.32	1.40
1	A	1516	2MG	C5-N7	-3.34	1.32	1.39
22	a	1618	6MZ	C5-C4	-3.32	1.32	1.39
22	a	2552	OMU	O4-C4	-3.31	1.18	1.24
1	A	1407	5MC	C2-N1	3.30	1.47	1.40
22	a	2498	M5Q	O5'-C5'	-3.28	1.41	1.45
22	a	2069	G7M	C5-C6	3.28	1.52	1.43
22	a	2251	OMG	O6-C6	-3.25	1.17	1.23
1	A	966	2MG	C5-N7	-3.24	1.32	1.39
22	a	2449	D5D	C4-N3	-3.19	1.32	1.37
54	Z	8	4SU	O2-C2	-3.17	1.17	1.23
22	a	2449	D5D	C2-N3	-3.16	1.32	1.38
1	A	1207	2MG	C5-N7	-3.14	1.33	1.39
1	A	1518	MA6	C5-N7	-3.14	1.33	1.39
22	a	2069	G7M	O6-C6	-3.10	1.17	1.23
54	Z	56	PSU	C6-C5	3.06	1.38	1.35
54	Z	33	OMC	O2-C2	-3.02	1.18	1.23
54	Z	8	4SU	C6-N1	3.01	1.45	1.38
1	A	1518	MA6	C8-N9	-2.99	1.32	1.37
22	a	2503	2MA	C6-N1	2.97	1.39	1.35
22	a	2445	2MG	O6-C6	-2.95	1.18	1.23
22	a	2501	TKW	C6-N1	-2.90	1.33	1.38
22	a	2449	D5D	O5'-C5'	-2.89	1.42	1.45
1	A	527	G7M	O6-C6	-2.89	1.18	1.23
22	a	1939	5MU	O2-C2	-2.86	1.17	1.23
1	A	1519	MA6	C8-N9	-2.86	1.32	1.37
1	A	1407	5MC	O2-C2	-2.83	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	MA6	C5-N7	-2.83	1.33	1.39
54	Z	21	H2U	C2-N3	-2.80	1.33	1.38
33	l	81	4D4	OB-CB	-2.80	1.37	1.43
22	a	1835	2MG	O6-C6	-2.79	1.18	1.23
22	a	745	1MG	C4-N9	-2.78	1.30	1.38
22	a	1962	5MC	O2-C2	-2.76	1.18	1.23
1	A	1402	4OC	C6-N1	2.75	1.44	1.38
22	a	2030	6MZ	C8-N9	-2.71	1.32	1.37
22	a	745	1MG	O6-C6	-2.71	1.17	1.23
1	A	1516	2MG	O6-C6	-2.68	1.18	1.23
22	a	747	5MU	O2-C2	-2.67	1.18	1.23
1	A	1519	MA6	C6-N6	2.65	1.44	1.36
1	A	516	PSU	C6-C5	2.63	1.38	1.35
1	A	967	5MC	O2-C2	-2.63	1.18	1.23
54	Z	33	OMC	C6-N1	2.62	1.44	1.38
1	A	1498	UR3	O4-C4	-2.61	1.17	1.23
22	a	2030	6MZ	C5-N7	-2.61	1.34	1.39
1	A	1498	UR3	C6-N1	2.61	1.44	1.38
1	A	1518	MA6	C6-N6	2.61	1.44	1.36
54	Z	21	H2U	C4-N3	-2.59	1.33	1.37
1	A	1498	UR3	O2-C2	-2.58	1.17	1.22
1	A	527	G7M	C2-N1	2.57	1.44	1.37
1	A	1207	2MG	O6-C6	-2.55	1.18	1.23
1	A	966	2MG	O6-C6	-2.55	1.18	1.23
1	A	1516	2MG	C4-N9	-2.54	1.31	1.38
22	a	2445	2MG	C4-N9	-2.52	1.31	1.38
22	a	745	1MG	C5-C6	2.51	1.51	1.45
22	a	1618	6MZ	C5-N7	-2.50	1.34	1.39
22	a	1618	6MZ	C8-N9	-2.48	1.33	1.37
1	A	1518	MA6	C4-N9	-2.47	1.32	1.37
22	a	2580	PSU	O4'-C1'	-2.46	1.40	1.43
22	a	2251	OMG	C5-C6	2.45	1.53	1.44
22	a	1835	2MG	C4-N9	-2.44	1.31	1.38
22	a	1939	5MU	O4-C4	-2.44	1.18	1.23
22	a	2449	D5D	C2-N1	-2.41	1.32	1.35
22	a	2069	G7M	C2-N1	2.39	1.43	1.37
22	a	746	PSU	C4-C5	-2.38	1.37	1.44
1	A	527	G7M	C6-N1	2.38	1.43	1.38
1	A	966	2MG	C5-C6	2.38	1.53	1.44
22	a	2552	OMU	C4-N3	2.37	1.42	1.38
22	a	2503	2MA	C8-N9	-2.37	1.33	1.37
22	a	2503	2MA	C5-C4	-2.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2251	OMG	C4-N9	-2.36	1.31	1.38
1	A	1207	2MG	C5-C6	2.33	1.53	1.44
22	a	2251	OMG	C8-N9	-2.32	1.32	1.37
22	a	1915	3TD	C4-N3	2.31	1.45	1.40
22	a	2504	PSU	C6-C5	2.30	1.38	1.35
22	a	955	PSU	C4-C5	-2.30	1.37	1.44
22	a	2501	TKW	C2-N1	-2.29	1.35	1.40
22	a	2604	PSU	C6-C5	2.28	1.38	1.35
1	A	1519	MA6	C4-N9	-2.28	1.32	1.37
22	a	1915	3TD	O4-C4	-2.28	1.18	1.23
22	a	2605	PSU	C4-C5	-2.27	1.37	1.44
22	a	2501	TKW	C2-N3	2.26	1.40	1.36
22	a	747	5MU	O4-C4	-2.26	1.19	1.23
22	a	2580	PSU	C4-C5	-2.25	1.37	1.44
22	a	2457	PSU	C6-C5	2.24	1.37	1.35
1	A	1516	2MG	C5-C6	2.24	1.52	1.44
22	a	1917	PSU	C6-C5	2.23	1.37	1.35
22	a	2504	PSU	C4-C5	-2.23	1.37	1.44
1	A	1207	2MG	C4-N9	-2.20	1.32	1.38
22	a	1911	PSU	C6-C5	2.20	1.37	1.35
22	a	1911	PSU	C4-C5	-2.17	1.38	1.44
22	a	2457	PSU	C4-C5	-2.16	1.38	1.44
22	a	1917	PSU	C4-C5	-2.14	1.38	1.44
22	a	2445	2MG	C5-C6	2.13	1.52	1.44
54	Z	55	5MU	O2-C2	-2.12	1.19	1.23
25	d	150	MEQ	CG-CD	-2.12	1.47	1.51
22	a	2604	PSU	C4-C5	-2.12	1.38	1.44
22	a	1835	2MG	C5-C6	2.12	1.52	1.44
22	a	2069	G7M	C6-N1	2.12	1.42	1.38
22	a	746	PSU	O4'-C1'	-2.11	1.40	1.43
22	a	2457	PSU	O4'-C1'	-2.11	1.40	1.43
33	l	81	4D4	CZ-NE	2.10	1.37	1.33
22	a	1915	3TD	O2-C2	-2.09	1.19	1.23
22	a	955	PSU	O4'-C1'	-2.09	1.40	1.43
54	Z	33	OMC	C5-C4	2.06	1.47	1.42
1	A	967	5MC	CM5-C5	2.05	1.55	1.50
22	a	2069	G7M	C4-N9	-2.03	1.32	1.38
54	Z	55	5MU	O4-C4	-2.02	1.19	1.23
22	a	2501	TKW	O2-C2	-2.02	1.20	1.23
22	a	2503	2MA	CM2-C2	2.01	1.55	1.49
22	a	2030	6MZ	C6-N1	-2.00	1.31	1.35

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	747	5MU	C5-C4-N3	13.09	126.48	115.31
22	a	1939	5MU	C5-C4-N3	12.82	126.25	115.31
54	Z	55	5MU	C5-C4-N3	12.62	126.08	115.31
22	a	1939	5MU	C5-C6-N1	-11.21	111.81	123.34
22	a	747	5MU	C5-C6-N1	-11.10	111.92	123.34
54	Z	55	5MU	C5-C6-N1	-10.49	112.54	123.34
22	a	2503	2MA	C5-C4-N3	-9.00	117.07	127.19
22	a	2449	D5D	C4-N3-C2	-8.64	118.62	125.79
54	Z	8	4SU	C4-N3-C2	-8.09	119.48	127.34
22	a	2030	6MZ	C9-N6-C6	-7.18	116.69	122.87
22	a	2449	D5D	C34-C5'-C4'	-7.14	97.64	113.34
22	a	1835	2MG	C2-N3-C4	6.60	120.23	112.04
22	a	2503	2MA	C4-N9-C1'	-6.46	111.21	126.59
1	A	966	2MG	C2-N3-C4	6.43	120.01	112.04
22	a	2503	2MA	C1'-N9-C8	6.42	141.64	127.14
22	a	2445	2MG	C2-N3-C4	6.39	119.97	112.04
1	A	1207	2MG	C2-N3-C4	6.20	119.73	112.04
22	a	2552	OMU	C4-N3-C2	-6.15	118.47	126.58
1	A	1519	MA6	N1-C2-N3	-6.08	119.09	128.60
1	A	1516	2MG	C2-N3-C4	6.03	119.52	112.04
22	a	2503	2MA	N3-C4-N9	6.01	135.33	126.99
1	A	1518	MA6	N1-C2-N3	-5.92	119.34	128.60
54	Z	8	4SU	C5-C4-N3	5.83	120.10	114.69
22	a	1915	3TD	N1-C2-N3	5.79	120.70	116.14
22	a	747	5MU	C4-N3-C2	-5.72	119.95	127.35
22	a	2030	6MZ	N1-C2-N3	-5.66	119.75	128.60
22	a	1939	5MU	C4-N3-C2	-5.64	120.05	127.35
22	a	2457	PSU	N1-C2-N3	5.62	121.50	115.13
22	a	2251	OMG	C5-C4-N3	-5.61	119.36	128.46
22	a	2580	PSU	N1-C2-N3	5.52	121.39	115.13
22	a	1618	6MZ	N1-C2-N3	-5.52	119.97	128.60
1	A	966	2MG	C5-C4-N3	-5.48	119.57	128.46
22	a	1618	6MZ	C9-N6-C6	-5.45	118.18	122.87
22	a	1618	6MZ	C5-C4-N3	-5.33	119.80	126.75
22	a	1835	2MG	C5-C4-N3	-5.32	119.82	128.46
22	a	2445	2MG	C5-C4-N3	-5.31	119.85	128.46
22	a	747	5MU	O4-C4-C5	-5.26	118.81	124.90
22	a	2445	2MG	C2-N1-C6	-5.24	118.44	124.48
22	a	1939	5MU	O4-C4-C5	-5.19	118.89	124.90
22	a	955	PSU	C4-N3-C2	-5.18	118.87	126.34
22	a	2605	PSU	C4-N3-C2	-5.18	118.87	126.34
54	Z	55	5MU	O4-C4-C5	-5.18	118.90	124.90
1	A	1498	UR3	C4-N3-C2	-5.15	119.72	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2457	PSU	C4-N3-C2	-5.11	118.97	126.34
22	a	1917	PSU	C4-N3-C2	-5.10	118.99	126.34
54	Z	55	5MU	C4-N3-C2	-5.08	120.77	127.35
22	a	955	PSU	N1-C2-N3	5.01	120.81	115.13
1	A	1207	2MG	C5-C4-N3	-4.99	120.37	128.46
22	a	1911	PSU	C4-N3-C2	-4.97	119.18	126.34
22	a	2030	6MZ	N9-C8-N7	-4.95	107.15	113.91
1	A	966	2MG	C2-N1-C6	-4.94	118.79	124.48
22	a	746	PSU	C4-N3-C2	-4.93	119.24	126.34
1	A	1519	MA6	N9-C8-N7	-4.92	107.18	113.91
22	a	745	1MG	C5-C4-N3	-4.90	120.51	128.46
22	a	2580	PSU	C4-N3-C2	-4.90	119.28	126.34
22	a	2030	6MZ	C5-C4-N3	-4.90	120.36	126.75
22	a	1939	5MU	N3-C2-N1	4.88	121.37	114.89
22	a	1835	2MG	C2-N1-C6	-4.85	118.90	124.48
22	a	1917	PSU	N1-C2-N3	4.83	120.60	115.13
22	a	2498	M5Q	C4-N3-C2	-4.81	112.48	120.25
1	A	1516	2MG	C2-N1-C6	-4.81	118.95	124.48
22	a	747	5MU	N3-C2-N1	4.80	121.26	114.89
22	a	2552	OMU	N3-C2-N1	4.79	121.25	114.89
22	a	2504	PSU	C4-N3-C2	-4.79	119.44	126.34
1	A	1516	2MG	C5-C4-N3	-4.78	120.70	128.46
22	a	2604	PSU	N1-C2-N3	4.74	120.50	115.13
22	a	2604	PSU	C4-N3-C2	-4.73	119.53	126.34
22	a	2504	PSU	N1-C2-N3	4.70	120.45	115.13
54	Z	56	PSU	C4-N3-C2	-4.69	119.58	126.34
22	a	2605	PSU	N1-C2-N3	4.67	120.42	115.13
1	A	1518	MA6	C2-N1-C6	4.64	122.70	111.75
1	A	1518	MA6	N9-C8-N7	-4.62	107.60	113.91
1	A	1207	2MG	C2-N1-C6	-4.59	119.19	124.48
22	a	1911	PSU	N1-C2-N3	4.59	120.33	115.13
54	Z	56	PSU	N1-C2-N3	4.55	120.29	115.13
1	A	1519	MA6	C5-C4-N3	-4.51	120.87	126.75
22	a	2501	TKW	O2-C2-N3	-4.51	115.00	122.33
1	A	1519	MA6	C2-N1-C6	4.48	122.34	111.75
22	a	1618	6MZ	N9-C8-N7	-4.36	107.96	113.91
22	a	2251	OMG	C2-N3-C4	4.32	120.00	112.30
1	A	1518	MA6	C5-C4-N3	-4.32	121.12	126.75
22	a	2501	TKW	C1'-N1-C6	4.30	128.29	121.12
54	Z	55	5MU	N3-C2-N1	4.30	120.59	114.89
22	a	746	PSU	N1-C2-N3	4.28	119.98	115.13
1	A	516	PSU	C4-N3-C2	-4.25	120.22	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2069	G7M	C2-N3-C4	4.24	119.86	112.30
1	A	1518	MA6	C4-C5-C6	4.18	120.56	115.88
22	a	1915	3TD	C4-N3-C2	-4.15	120.10	124.61
22	a	747	5MU	C5M-C5-C6	-4.15	117.31	122.85
1	A	527	G7M	C2-N3-C4	4.07	119.55	112.30
22	a	2069	G7M	C5-C6-N1	4.03	120.21	111.79
54	Z	55	5MU	C5M-C5-C6	-4.03	117.47	122.85
22	a	1939	5MU	C5M-C5-C6	-4.00	117.51	122.85
54	Z	8	4SU	C5-C4-S4	-3.96	119.37	124.47
1	A	516	PSU	N1-C2-N3	3.90	119.55	115.13
1	A	527	G7M	C5-C6-N1	3.89	119.91	111.79
22	a	2498	M5Q	O2-C2-N3	-3.86	116.05	122.33
54	Z	55	5MU	C5M-C5-C4	3.84	122.99	118.77
22	a	747	5MU	C5M-C5-C4	3.78	122.93	118.77
1	A	1519	MA6	C4-C5-C6	3.78	120.11	115.88
1	A	527	G7M	C5-C4-N3	-3.74	120.98	128.15
22	a	2251	OMG	N9-C4-N3	3.70	133.37	125.94
22	a	1618	6MZ	C2-N3-C4	3.67	120.41	111.75
33	l	81	4D4	NE-CZ-NH2	3.66	127.13	120.70
22	a	2030	6MZ	C2-N3-C4	3.66	120.39	111.75
1	A	1519	MA6	C5-N7-C8	3.65	108.70	103.51
54	Z	8	4SU	N3-C2-N1	3.64	119.72	114.89
1	A	1407	5MC	C5-C6-N1	-3.62	119.62	123.34
22	a	1618	6MZ	C4-C5-C6	3.61	119.61	116.81
1	A	966	2MG	N9-C4-N3	3.61	133.18	125.94
22	a	2552	OMU	C5-C4-N3	3.60	120.23	114.84
22	a	2445	2MG	N9-C8-N7	-3.60	106.62	113.39
12	L	89	D2T	OD2-CG-CB	3.56	120.83	113.15
22	a	2503	2MA	N9-C8-N7	-3.53	109.08	113.91
22	a	2251	OMG	C2-N1-C6	-3.52	118.68	125.10
22	a	2069	G7M	O6-C6-C5	-3.50	120.17	128.06
22	a	2069	G7M	C5-C4-N3	-3.49	121.45	128.15
22	a	1939	5MU	C5M-C5-C4	3.49	122.61	118.77
22	a	1962	5MC	C5-C6-N1	-3.49	119.75	123.34
1	A	1207	2MG	N9-C8-N7	-3.48	106.83	113.39
1	A	527	G7M	O6-C6-C5	-3.48	120.21	128.06
22	a	2498	M5Q	C5-C6-N1	-3.48	115.98	121.81
1	A	1518	MA6	C5-N7-C8	3.47	108.44	103.51
1	A	1516	2MG	N9-C8-N7	-3.47	106.86	113.39
22	a	2498	M5Q	C34-C5'-C4'	-3.45	105.75	113.34
22	a	1835	2MG	N9-C4-N3	3.45	132.86	125.94
1	A	1519	MA6	C2-N3-C4	3.42	119.83	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2445	2MG	N9-C4-N3	3.41	132.79	125.94
22	a	2498	M5Q	C5-C4-N3	3.40	127.11	121.33
22	a	2501	TKW	N1-C2-N3	3.40	124.99	118.81
22	a	2030	6MZ	C5-N7-C8	3.37	108.30	103.51
22	a	1618	6MZ	N3-C4-N9	3.37	132.63	127.08
22	a	745	1MG	C2-N3-C4	3.36	119.54	111.98
12	L	89	D2T	OD1-CG-CB	-3.36	115.41	122.44
22	a	745	1MG	C1'-N9-C8	-3.34	117.20	126.70
22	a	1835	2MG	N9-C8-N7	-3.32	107.15	113.39
22	a	2501	TKW	C4-N3-C2	-3.29	116.23	120.69
22	a	745	1MG	N9-C8-N7	-3.26	107.24	113.39
1	A	1207	2MG	N9-C4-N3	3.26	132.48	125.94
1	A	967	5MC	C5-C6-N1	-3.25	119.99	123.34
22	a	2503	2MA	C6-C5-C4	3.25	121.55	117.18
22	a	2580	PSU	O2-C2-N1	-3.20	119.27	122.79
22	a	2251	OMG	N9-C8-N7	-3.17	107.43	113.39
1	A	1518	MA6	C2-N3-C4	3.15	119.19	111.75
22	a	2503	2MA	N3-C2-N1	-3.12	119.98	125.72
22	a	2580	PSU	C6-N1-C2	-3.11	119.50	122.68
22	a	2445	2MG	CM2-N2-C2	-3.10	117.02	123.86
54	Z	21	H2U	C4-N3-C2	-3.06	123.25	125.79
1	A	966	2MG	N9-C8-N7	-3.05	107.64	113.39
1	A	527	G7M	C2-N1-C6	-3.04	119.55	125.10
1	A	527	G7M	N9-C4-N3	2.97	131.90	125.94
22	a	2445	2MG	C5-C6-N1	2.97	120.72	113.19
33	l	81	4D4	CB-CA-C	-2.96	107.04	111.77
22	a	2457	PSU	O2-C2-N1	-2.94	119.56	122.79
22	a	745	1MG	N9-C4-N3	2.93	131.83	125.94
22	a	2457	PSU	C6-N1-C2	-2.91	119.71	122.68
22	a	2498	M5Q	C5-C4-N4	-2.90	116.01	120.57
22	a	1939	5MU	O2-C2-N1	-2.89	118.95	122.79
1	A	1516	2MG	C5-C6-N1	2.88	120.50	113.19
22	a	2251	OMG	C5-C6-N1	2.87	120.48	113.19
22	a	2069	G7M	C2-N1-C6	-2.87	119.87	125.10
22	a	2503	2MA	C5-N7-C8	2.85	107.56	103.51
1	A	1519	MA6	C4-C5-N7	-2.84	107.16	110.62
22	a	1835	2MG	O6-C6-C5	-2.84	119.07	126.60
1	A	1516	2MG	N9-C4-N3	2.84	131.64	125.94
22	a	1835	2MG	C5-C6-N1	2.83	120.38	113.19
22	a	747	5MU	O4-C4-N3	-2.82	114.71	120.12
1	A	966	2MG	C5-C6-N1	2.81	120.33	113.19
22	a	2030	6MZ	C4-C5-C6	2.81	118.98	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	82	MS6	CE-SD-CG	2.81	110.05	100.40
1	A	1207	2MG	C5-C6-N1	2.79	120.28	113.19
22	a	1911	PSU	O2-C2-N1	-2.79	119.72	122.79
1	A	1519	MA6	N1-C6-N6	-2.79	114.04	117.08
1	A	1518	MA6	C4-C5-N7	-2.79	107.22	110.62
22	a	2498	M5Q	C1'-N1-C6	-2.79	114.77	120.84
22	a	1618	6MZ	C5-N7-C8	2.76	107.44	103.51
22	a	2449	D5D	C5-C6-N1	-2.75	102.56	111.61
22	a	2069	G7M	CN7-N7-C5	2.74	130.18	126.77
22	a	1939	5MU	O4-C4-N3	-2.74	114.86	120.12
54	Z	56	PSU	O2-C2-N1	-2.74	119.78	122.79
22	a	745	1MG	C5-C6-N1	2.73	120.18	114.91
22	a	2552	OMU	O4-C4-C5	-2.69	120.43	125.16
1	A	1518	MA6	N1-C6-N6	-2.69	114.14	117.08
22	a	1835	2MG	CM2-N2-C2	-2.67	117.96	123.86
54	Z	55	5MU	O4-C4-N3	-2.66	115.02	120.12
1	A	966	2MG	O6-C6-C5	-2.64	119.59	126.60
1	A	1519	MA6	C4-N9-C8	2.63	108.58	105.73
22	a	1917	PSU	O2-C2-N1	-2.62	119.90	122.79
22	a	1915	3TD	C6-C5-C4	2.62	120.03	118.22
22	a	2457	PSU	C6-C5-C4	2.62	120.03	118.20
22	a	2030	6MZ	C4-N9-C8	2.60	108.55	105.73
22	a	1962	5MC	CM5-C5-C6	-2.60	119.38	122.85
1	A	1516	2MG	CM2-N2-C2	-2.59	118.14	123.86
22	a	2445	2MG	O6-C6-C5	-2.59	119.74	126.60
1	A	527	G7M	CN7-N7-C5	2.58	129.97	126.77
22	a	2030	6MZ	N3-C4-N9	2.54	131.26	127.08
1	A	1516	2MG	O6-C6-C5	-2.52	119.92	126.60
1	A	1207	2MG	O6-C6-C5	-2.51	119.95	126.60
22	a	2449	D5D	O5'-C5'-C4'	2.50	111.48	106.42
22	a	2580	PSU	C6-C5-C4	2.50	119.95	118.20
22	a	2251	OMG	O6-C6-C5	-2.48	120.01	126.60
22	a	1618	6MZ	C4-N9-C8	2.48	108.41	105.73
22	a	2069	G7M	N9-C4-N3	2.47	130.89	125.94
22	a	2498	M5Q	N1-C2-N3	2.45	123.28	118.81
22	a	2580	PSU	O4'-C1'-C2'	2.45	108.60	105.14
22	a	2030	6MZ	C4-C5-N7	-2.45	107.64	110.62
22	a	747	5MU	O2-C2-N1	-2.44	119.55	122.79
22	a	745	1MG	C1'-N9-C4	2.43	133.71	126.50
12	L	89	D2T	O-C-CA	-2.42	118.44	124.78
1	A	516	PSU	O2-C2-N1	-2.41	120.14	122.79
22	a	746	PSU	O2-C2-N1	-2.41	120.14	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2498	M5Q	O5'-C5'-C4'	2.41	111.28	106.42
22	a	1618	6MZ	C5-C6-N1	2.40	120.76	118.20
1	A	1402	4OC	C6-C5-C4	2.40	119.90	116.96
22	a	2604	PSU	O2-C2-N1	-2.40	120.15	122.79
22	a	2552	OMU	O2-C2-N1	-2.39	119.61	122.79
25	d	150	MEQ	OE1-CD-CG	2.37	126.36	122.02
22	a	2445	2MG	C8-N7-C5	2.37	108.53	104.24
1	A	966	2MG	CM2-N2-C2	-2.35	118.67	123.86
22	a	1917	PSU	C6-C5-C4	2.34	119.83	118.20
1	A	1516	2MG	C1'-N9-C4	-2.34	119.55	126.50
22	a	2501	TKW	C1'-N1-C2	-2.34	113.20	118.42
54	Z	8	4SU	C1'-N1-C2	2.33	121.79	117.57
22	a	1962	5MC	C1'-N1-C6	-2.33	117.25	121.12
1	A	1518	MA6	C5-C4-N9	2.32	108.48	105.78
1	A	1518	MA6	C4-N9-C8	2.32	108.24	105.73
22	a	2251	OMG	C1'-N9-C4	-2.31	119.63	126.50
33	l	81	4D4	O-C-CA	-2.30	118.76	124.78
22	a	2030	6MZ	C5-C6-N1	2.29	120.64	118.20
22	a	955	PSU	O2-C2-N1	-2.28	120.28	122.79
22	a	1835	2MG	N1-C2-N3	-2.28	120.43	123.95
22	a	2449	D5D	O4-C4-N3	2.26	123.87	120.28
22	a	2604	PSU	C6-N1-C2	-2.26	120.37	122.68
54	Z	56	PSU	C6-C5-C4	2.24	119.76	118.20
1	A	1207	2MG	C8-N7-C5	2.23	108.28	104.24
1	A	1519	MA6	C5-C4-N9	2.23	108.38	105.78
1	A	1207	2MG	N1-C2-N3	-2.23	120.50	123.95
1	A	1519	MA6	N3-C4-N9	2.23	130.75	127.08
22	a	2030	6MZ	C5-C4-N9	2.22	108.37	105.78
22	a	2504	PSU	O2-C2-N1	-2.22	120.35	122.79
22	a	1939	5MU	C6-C5-C4	2.21	119.88	118.03
1	A	1516	2MG	C8-N7-C5	2.20	108.23	104.24
54	Z	56	PSU	C6-N1-C2	-2.19	120.44	122.68
1	A	527	G7M	N9-C8-N7	-2.19	106.80	112.21
22	a	1835	2MG	C8-N7-C5	2.19	108.20	104.24
22	a	955	PSU	C6-N1-C2	-2.18	120.45	122.68
1	A	1207	2MG	CM2-N2-C2	-2.15	119.11	123.86
1	A	1402	4OC	CM4-N4-C4	-2.15	118.25	122.45
22	a	2504	PSU	C6-N1-C2	-2.15	120.48	122.68
1	A	1402	4OC	O2-C2-N3	-2.12	118.88	122.33
54	Z	55	5MU	O2-C2-N1	-2.11	119.98	122.79
22	a	2069	G7M	N9-C8-N7	-2.10	107.02	112.21
22	a	2498	M5Q	C6-N1-C2	2.09	124.12	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2503	2MA	C2-N3-C4	2.08	122.11	116.99
22	a	745	1MG	C8-N7-C5	2.08	108.00	104.24
22	a	2069	G7M	CN7-N7-C8	-2.07	121.64	124.84
1	A	516	PSU	O4'-C1'-C2'	2.07	108.06	105.14
22	a	747	5MU	C6-C5-C4	2.07	119.76	118.03
1	A	516	PSU	C6-N1-C2	-2.07	120.57	122.68
1	A	966	2MG	C8-N7-C5	2.06	107.98	104.24
22	a	955	PSU	C6-C5-C4	2.06	119.64	118.20
1	A	527	G7M	CN7-N7-C8	-2.06	121.66	124.84
22	a	2251	OMG	C8-N7-C5	2.06	107.97	104.24
1	A	966	2MG	N1-C2-N3	-2.04	120.80	123.95
1	A	1518	MA6	N3-C4-N9	2.01	130.39	127.08
1	A	1516	2MG	N1-C2-N3	-2.01	120.85	123.95

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
33	l	81	4D4	C-CA-CB-OB
33	l	81	4D4	C-CA-CB-CG
33	l	81	4D4	N-CA-CB-OB
33	l	81	4D4	N-CA-CB-CG
33	l	81	4D4	CA-CB-CG-CD
33	l	81	4D4	OB-CB-CG-CD
54	Z	21	H2U	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	O4'-C1'-N1-C6
22	a	2251	OMG	C1'-C2'-O2'-CM2
22	a	2449	D5D	C34-C5'-O5'-P
1	A	1519	MA6	C3'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2501	TKW	O4'-C4'-C5'-O5'
54	Z	21	H2U	C2'-C1'-N1-C6
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
1	A	516	PSU	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	2501	TKW	C2'-C1'-N1-C6
1	A	516	PSU	O4'-C4'-C5'-O5'
22	a	2445	2MG	O4'-C4'-C5'-O5'
22	a	2498	M5Q	O4'-C4'-C5'-C34
54	Z	21	H2U	C2'-C1'-N1-C2
1	A	527	G7M	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
22	a	2552	OMU	C3'-C2'-O2'-CM2
22	a	2501	TKW	O4'-C1'-N1-C6
33	l	82	MS6	CB-CG-SD-CE
1	A	1402	4OC	O4'-C4'-C5'-O5'
22	a	2501	TKW	C3'-C4'-C5'-O5'
22	a	2501	TKW	C2'-C1'-N1-C2
22	a	2501	TKW	O4'-C1'-N1-C2
1	A	527	G7M	C4'-C5'-O5'-P
54	Z	21	H2U	C4'-C5'-O5'-P
54	Z	55	5MU	C3'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
54	Z	55	5MU	O4'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB
22	a	2069	G7M	C4'-C5'-O5'-P

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	89	D2T	1	0
1	A	967	5MC	1	0
25	d	150	MEQ	1	0
22	a	2605	PSU	2	0
22	a	955	PSU	1	0
1	A	966	2MG	1	0
1	A	1516	2MG	1	0
22	a	2251	OMG	1	0
22	a	2503	2MA	1	0
1	A	1207	2MG	1	0
22	a	1915	3TD	1	0
22	a	2030	6MZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 471 ligands modelled in this entry, 471 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

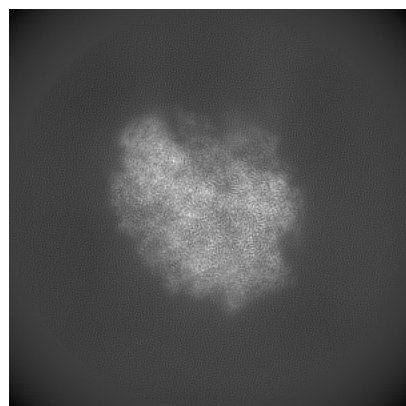
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60060. These allow visual inspection of the internal detail of the map and identification of artifacts.

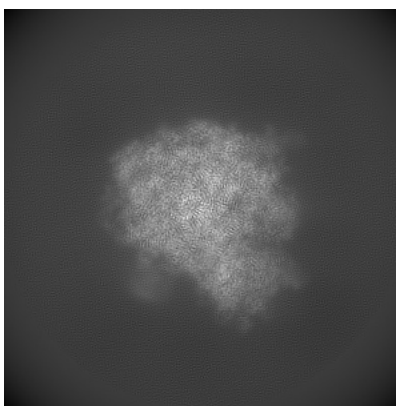
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

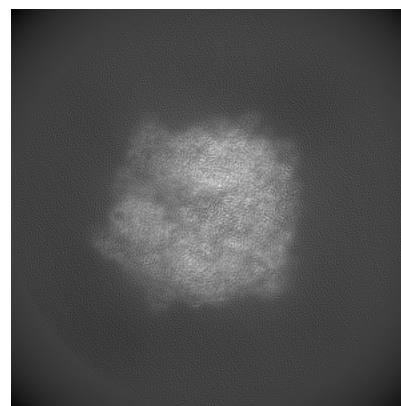
6.1.1 Primary map



X

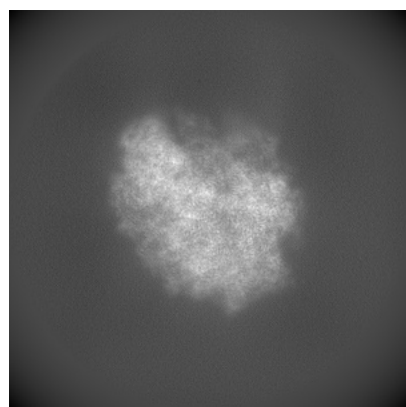


Y

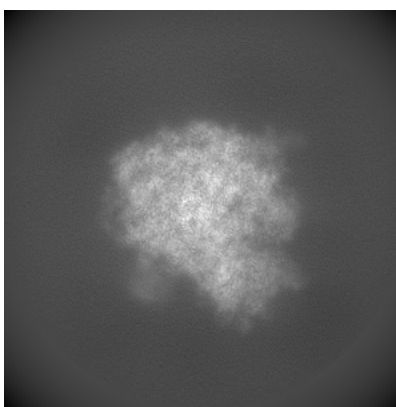


Z

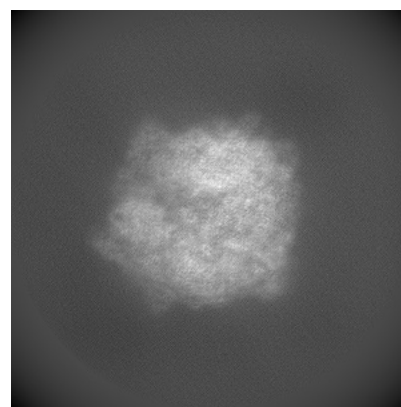
6.1.2 Raw map



X



Y

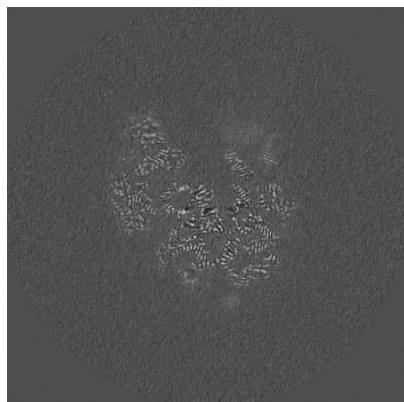


Z

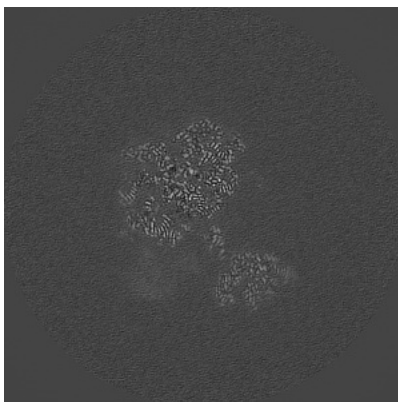
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

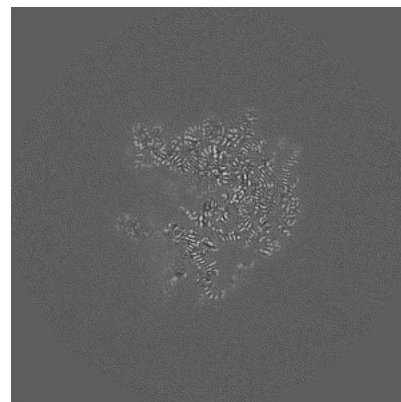
6.2.1 Primary map



X Index: 265

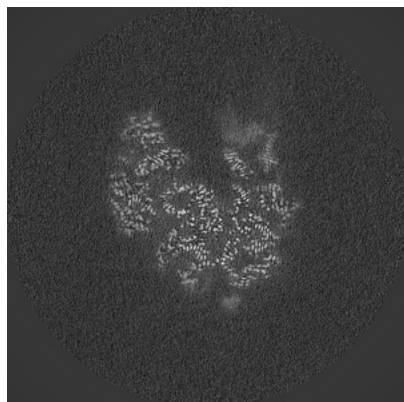


Y Index: 265

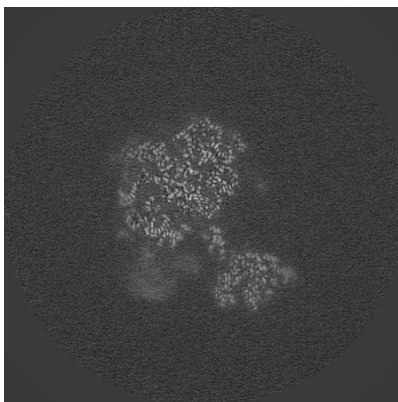


Z Index: 265

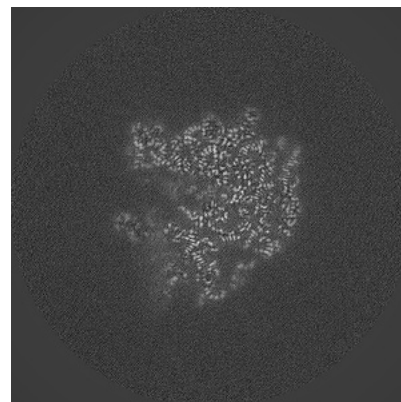
6.2.2 Raw map



X Index: 265



Y Index: 265

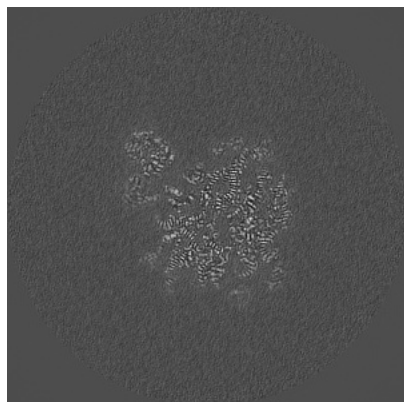


Z Index: 265

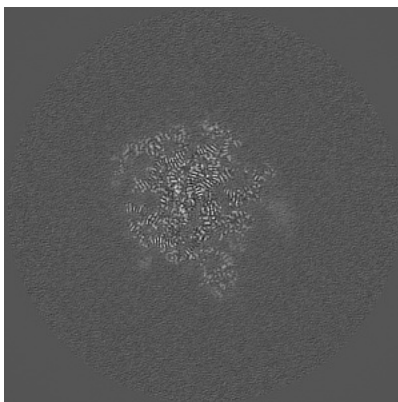
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

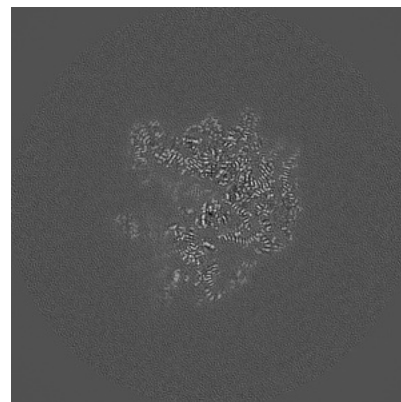
6.3.1 Primary map



X Index: 298

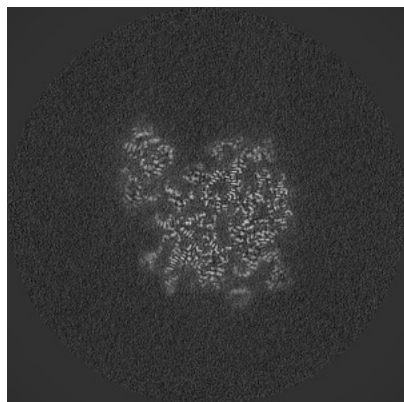


Y Index: 320

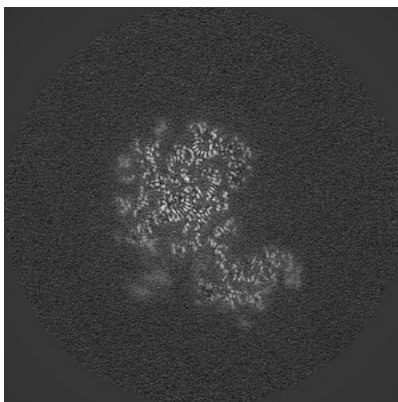


Z Index: 268

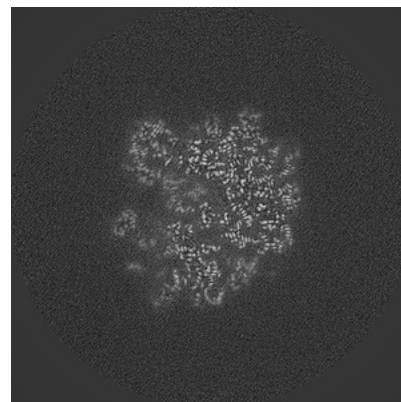
6.3.2 Raw map



X Index: 297



Y Index: 244

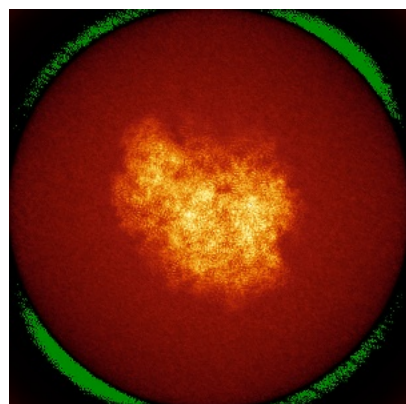


Z Index: 272

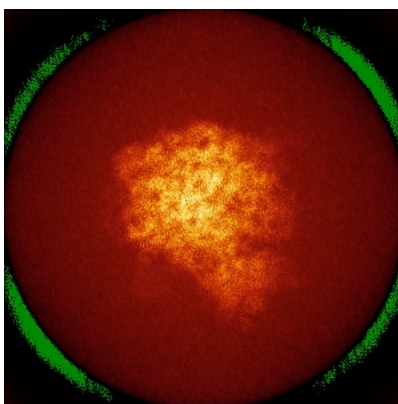
The images above show the largest variance slices of the map in three orthogonal directions.

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

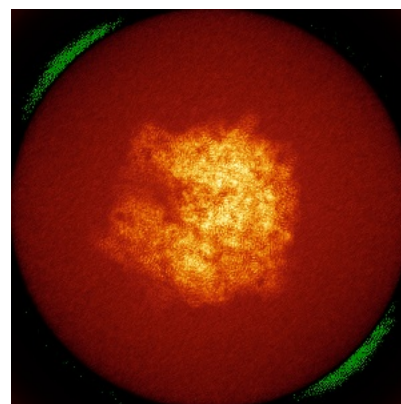
6.4.1 Primary map



X

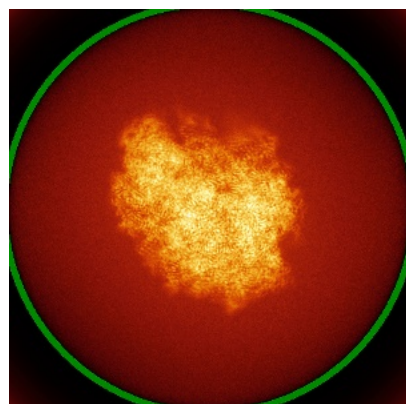


Y

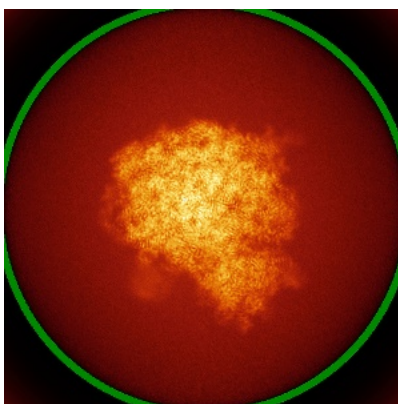


Z

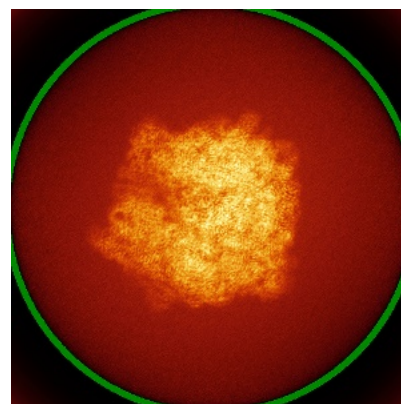
6.4.2 Raw map



X



Y

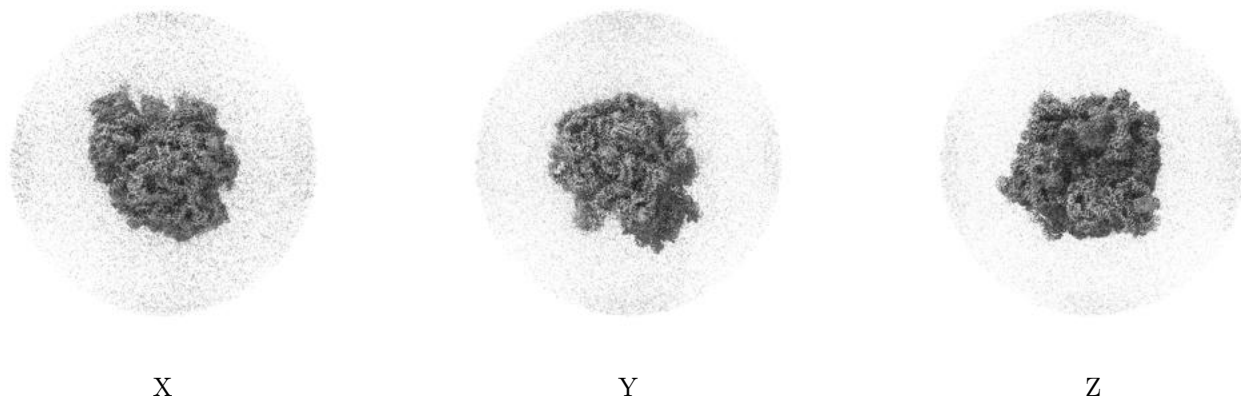


Z

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

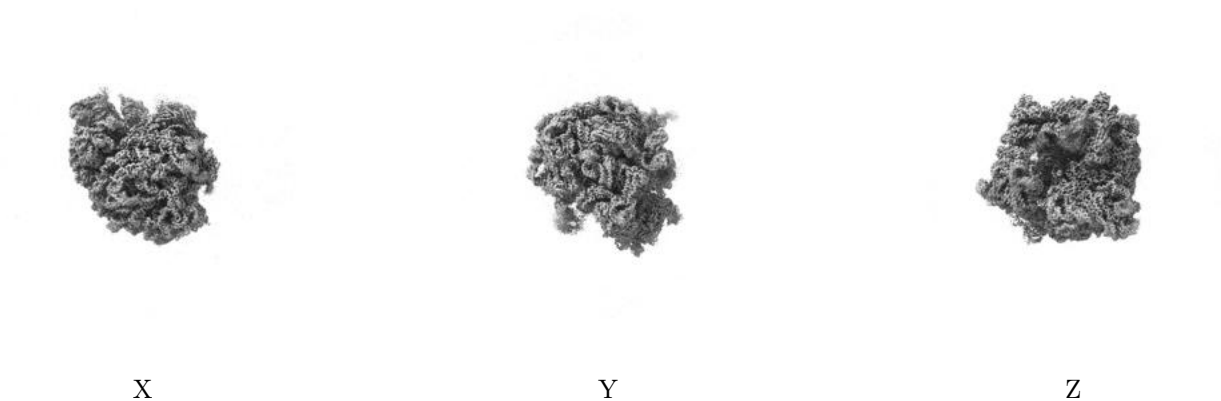
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0244. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

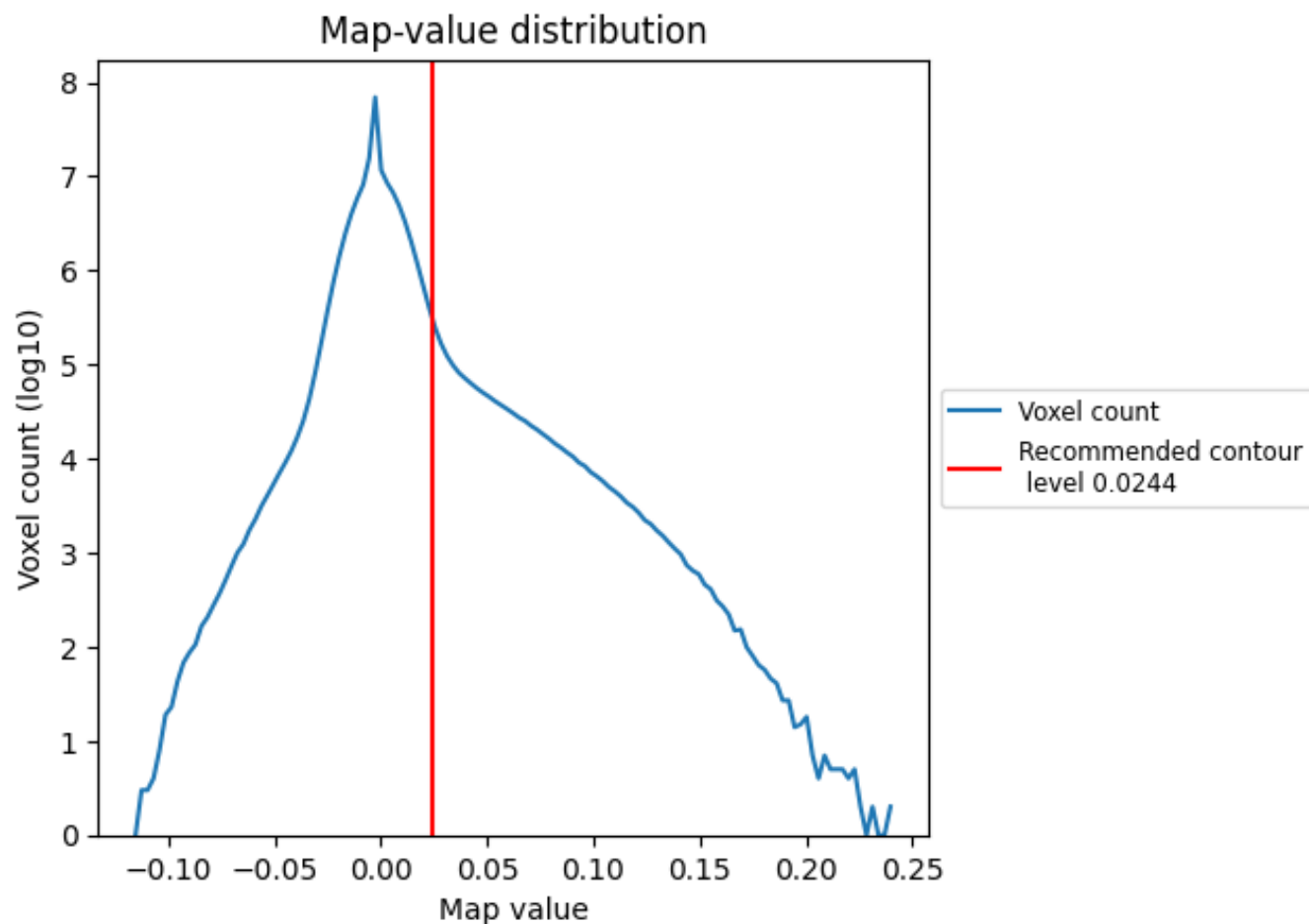
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

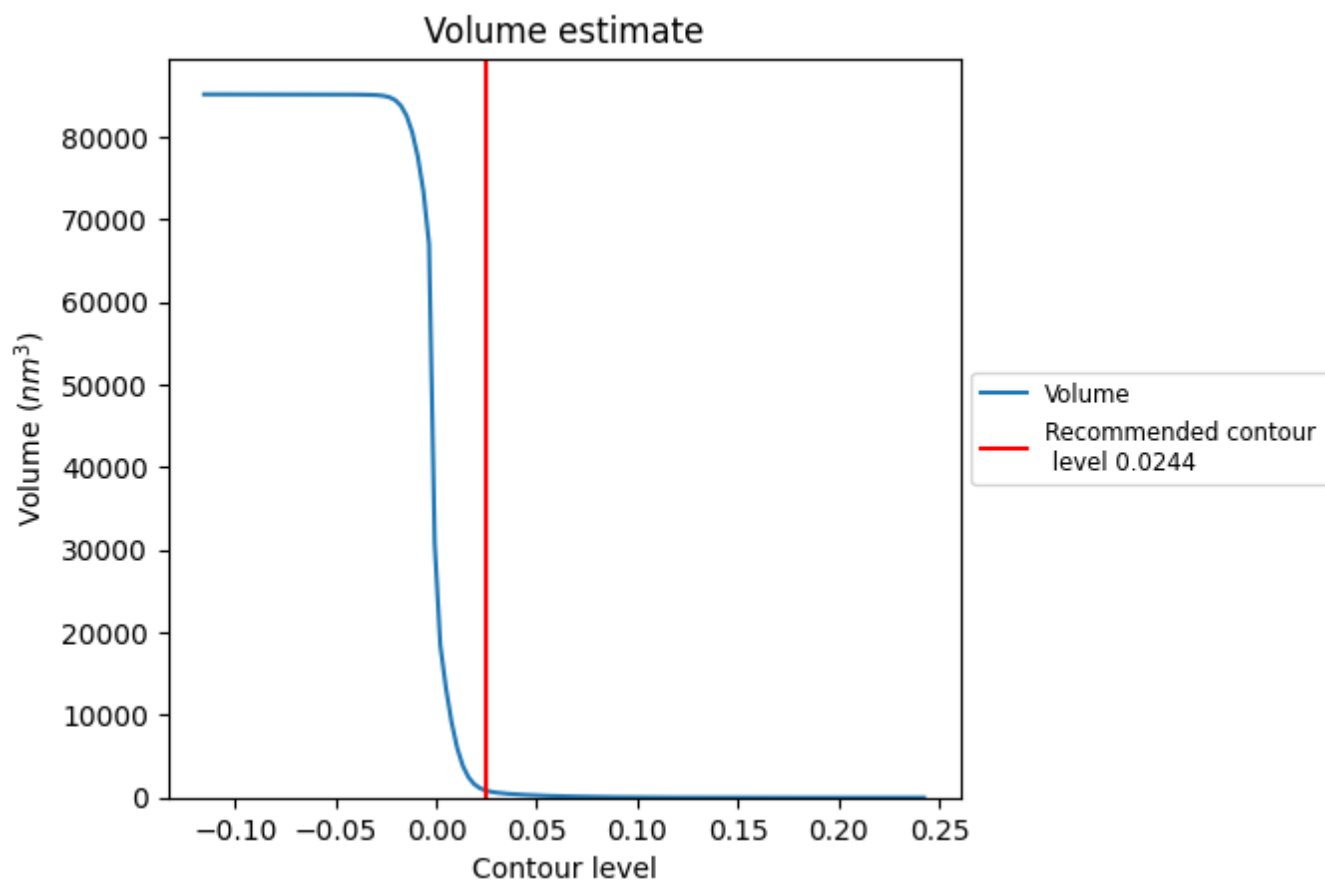
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

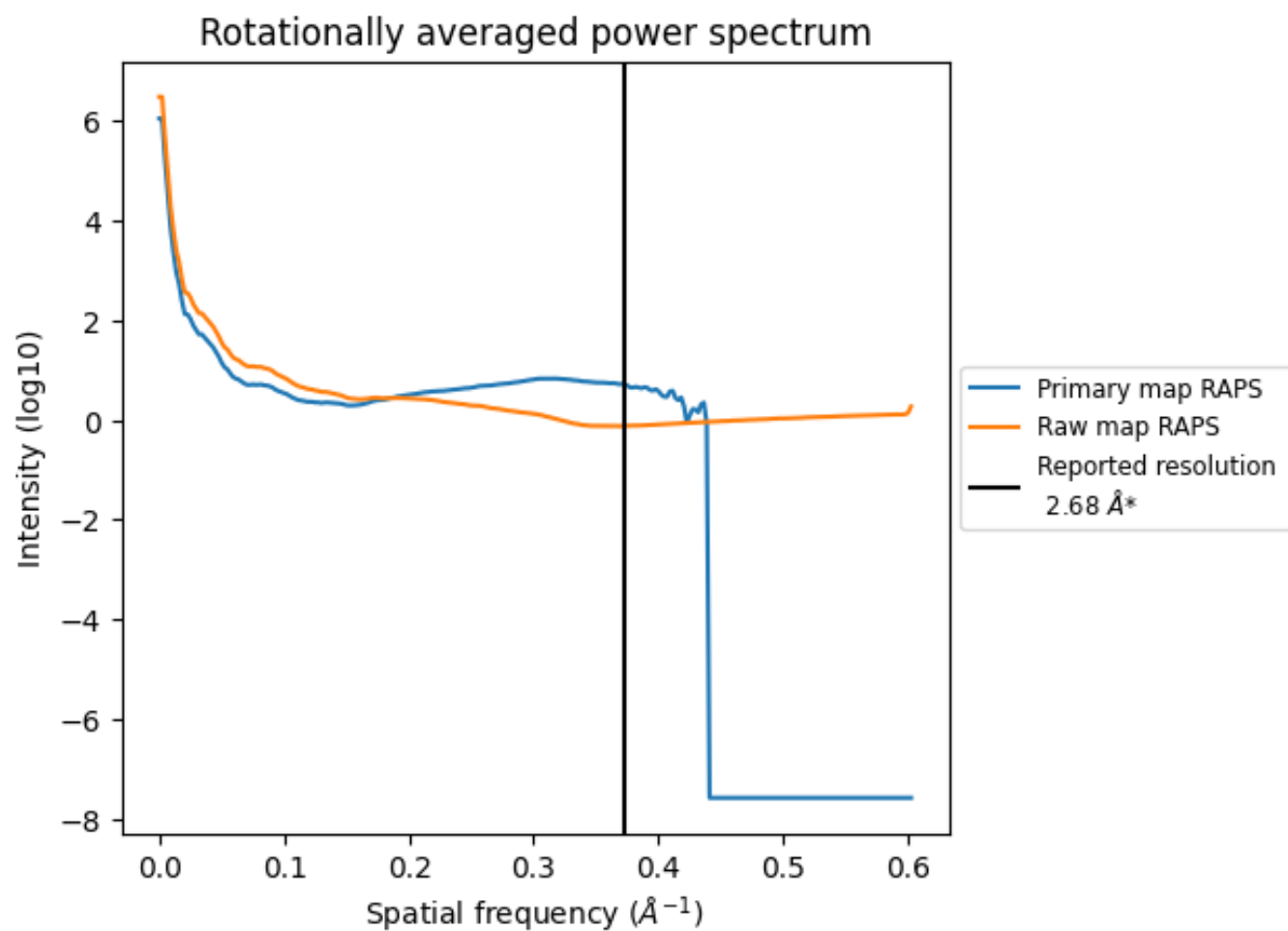
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 875 nm³; this corresponds to an approximate mass of 790 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 ⓘ

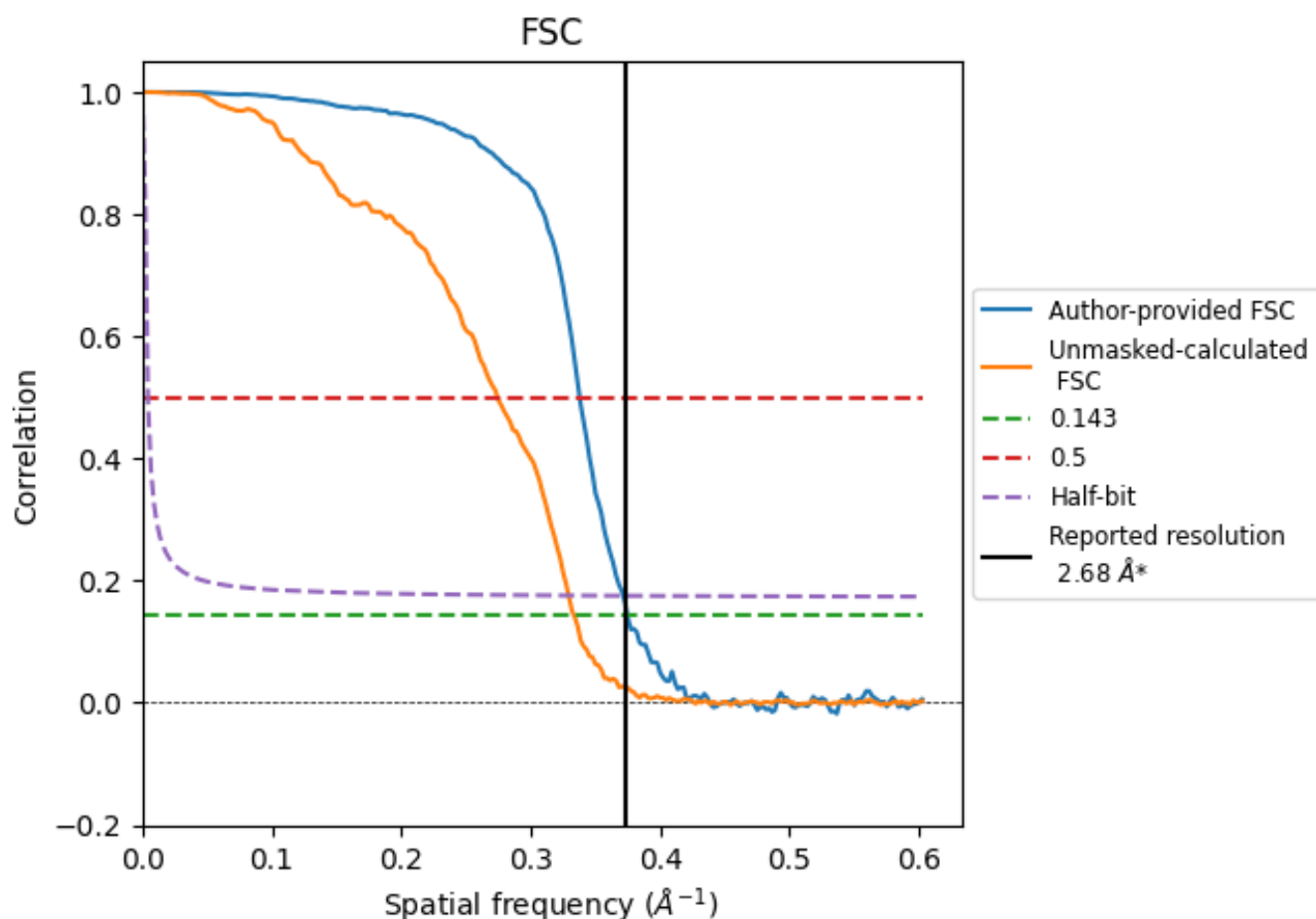


*Reported resolution corresponds to spatial frequency of 0.373 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 \AA^{-1}

8.2 Resolution estimates [i](#)

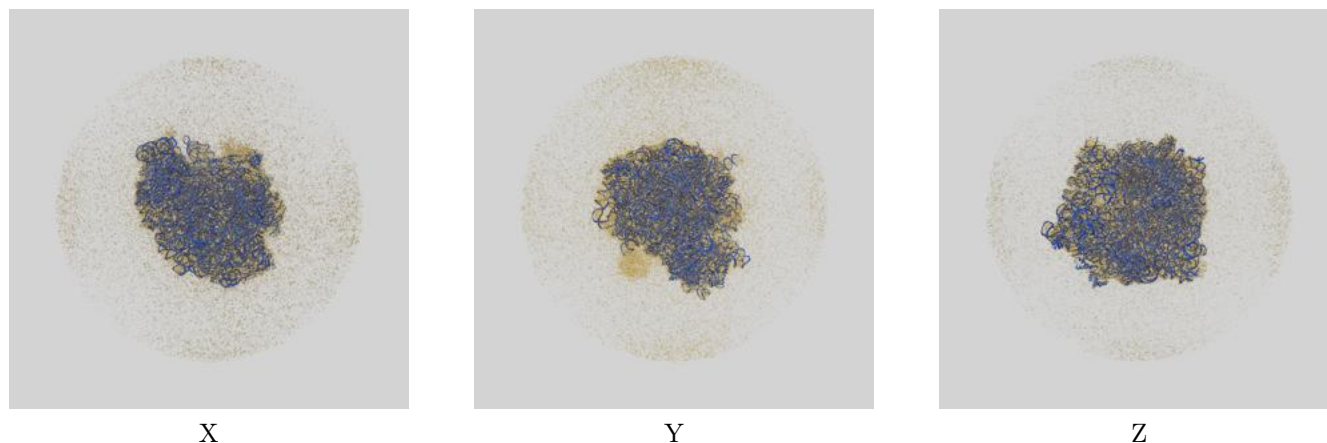
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.67	2.96	2.69
Unmasked-calculated*	3.00	3.64	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

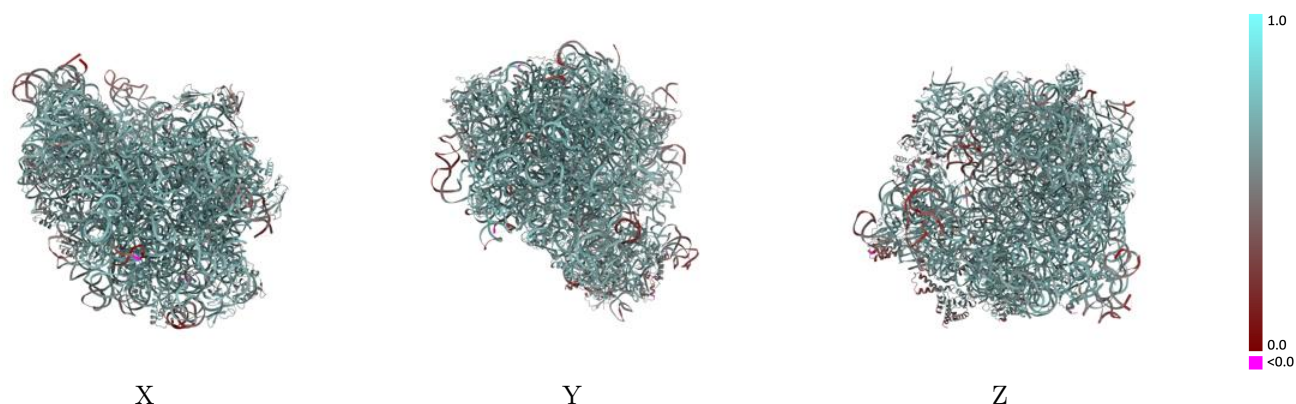
This section contains information regarding the fit between EMDB map EMD-60060 and PDB model 8ZFG. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



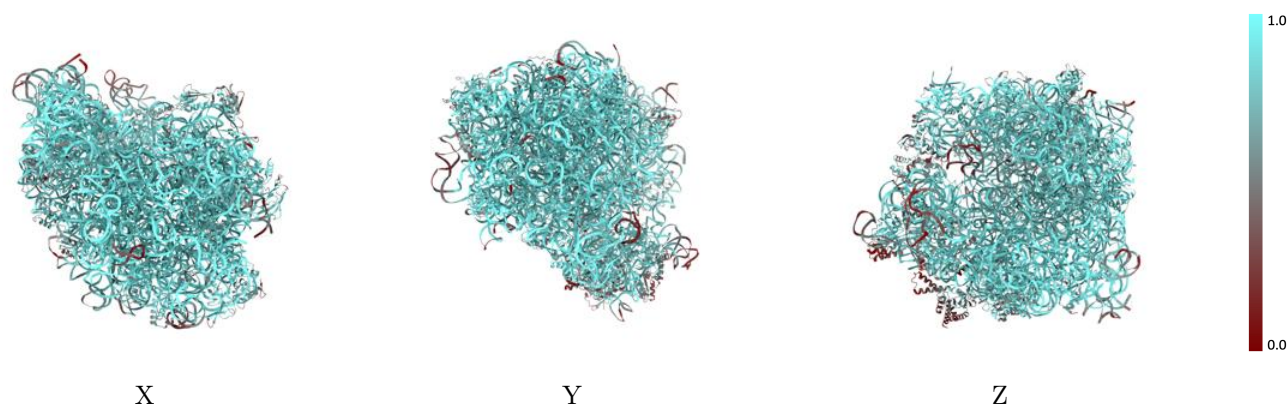
The images above show the 3D surface view of the map at the recommended contour level 0.0244 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



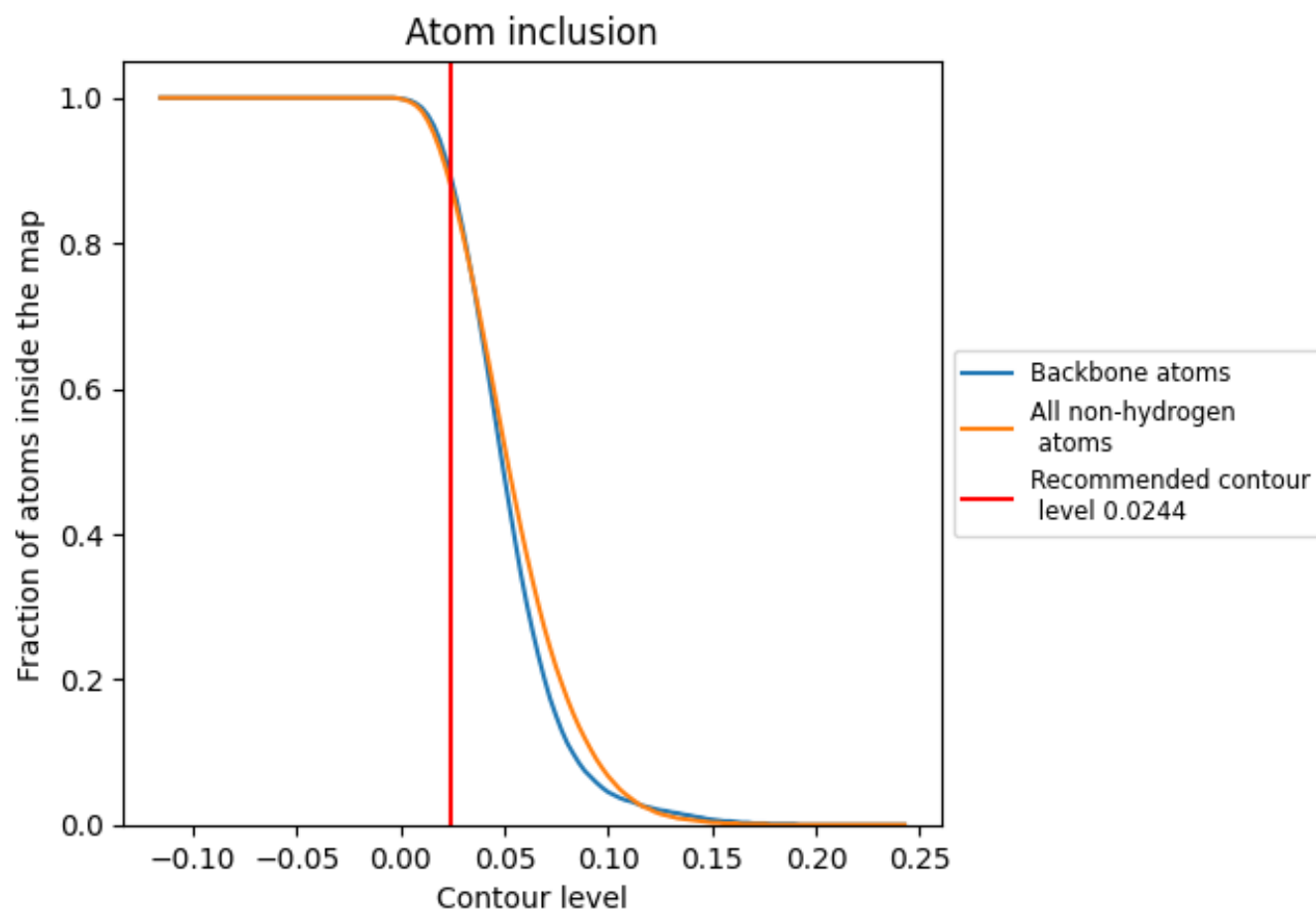
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0244).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.0244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.6140
0	 0.8220	 0.6100
1	 0.9580	 0.6690
2	 0.9590	 0.6650
3	 0.9140	 0.6290
4	 0.5100	 0.4380
A	 0.9030	 0.6190
B	 0.4440	 0.4730
C	 0.7640	 0.5860
D	 0.7470	 0.5780
E	 0.8740	 0.6290
F	 0.7080	 0.5360
G	 0.5640	 0.5000
H	 0.8640	 0.6220
I	 0.7020	 0.5600
J	 0.5330	 0.4700
K	 0.7940	 0.5740
L	 0.8710	 0.6210
M	 0.7330	 0.5590
N	 0.7970	 0.5850
O	 0.8420	 0.5880
P	 0.8410	 0.5910
Q	 0.7980	 0.5920
R	 0.8030	 0.5690
S	 0.7180	 0.5570
T	 0.8380	 0.6060
U	 0.4720	 0.4620
X	 0.7690	 0.5320
Z	 0.7330	 0.5230
a	 0.9280	 0.6320
b	 0.9000	 0.6090
c	 0.9520	 0.6660
d	 0.9060	 0.6460
e	 0.7950	 0.5960
f	 0.7220	 0.5550



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Chain	Atom inclusion	Q-score
g	 0.6490	 0.5160
h	 0.5900	 0.4930
i	 0.9100	 0.6380
j	 0.9110	 0.6520
k	 0.8770	 0.6250
l	 0.8980	 0.6340
m	 0.9410	 0.6580
n	 0.8400	 0.6020
o	 0.8910	 0.6410
p	 0.9310	 0.6520
q	 0.8090	 0.6000
r	 0.8680	 0.6230
s	 0.8030	 0.5750
t	 0.7070	 0.5390
u	 0.7860	 0.5890
v	 0.9100	 0.6490
w	 0.9030	 0.6270
x	 0.7240	 0.5450
y	 0.8560	 0.6020
z	 0.8810	 0.6300