



Full wwPDB EM Validation Report ⓘ

Apr 22, 2026 – 03:43 PM JST

PDB ID : 9JPO / pdb_00009jpo
EMDB ID : EMD-61708
Title : Structure of the Bacterial Ribosome with human tRNA Lys(mcm5h2U34) and mRNA(AAA)
Authors : Ishiguro, K.; Mo, Y.; Shirouzu, M.; Suzuki, T.
Deposited on : 2024-09-26
Resolution : 3.18 Å(reported)
Based on initial model : 7y7e

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

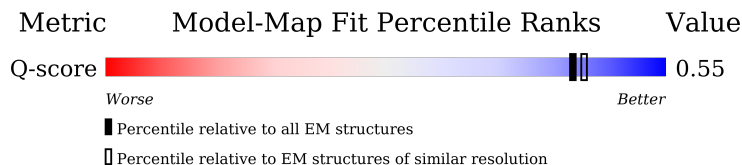
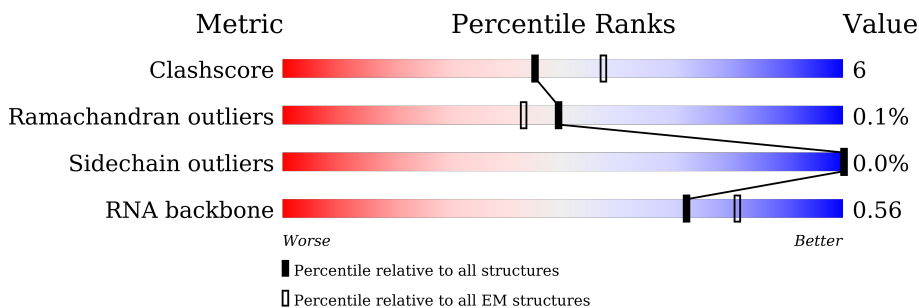
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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	 61% 33%
2	B	241	 91% 63% 30% 7%
3	C	233	 70% 18% 12%

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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	35	

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Mol	Chain	Length	Quality of chain
54	Z	77	<div><div></div><div>5%</div><div>64%</div><div>25%</div><div>12%</div></div>
55	V	76	<div><div></div><div>47%</div><div>39%</div><div>8%</div><div></div></div>

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 142038 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 30S ribosomal protein S2.

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 30S ribosomal protein S3.

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 30S ribosomal protein S4.

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

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

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

- Molecule 6 is a protein called 30S ribosomal protein S6, 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 30S ribosomal protein S7.

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 30S ribosomal protein S8.

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

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

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

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

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

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

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 30S ribosomal protein S12.

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 30S ribosomal protein S13.

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 30S ribosomal protein S14.

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 30S ribosomal protein S15.

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

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

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

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

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 30S ribosomal protein S18.

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 30S ribosomal protein S19.

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 30S ribosomal protein S20.

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 30S ribosomal protein S21.

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
			59301	26460	10925	19155	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 50S ribosomal protein L2.

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 50S ribosomal protein L3.

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 50S ribosomal protein L4.

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 50S ribosomal protein L5.

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 50S ribosomal protein L6.

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 50S ribosomal protein L9.

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 50S ribosomal protein L13.

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 50S ribosomal protein L14.

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 50S ribosomal protein L15.

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 50S ribosomal protein L16.

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 50S ribosomal protein L17.

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 50S ribosomal protein L18.

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 50S ribosomal protein L19.

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 50S ribosomal protein L20.

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 50S ribosomal protein L21.

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 50S ribosomal protein L22.

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 50S ribosomal protein L23.

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 50S ribosomal protein L24.

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 50S ribosomal protein L25.

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 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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 50S ribosomal protein L29.

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 50S ribosomal protein L30.

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 50S ribosomal protein L32.

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 50S ribosomal protein L33.

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 50S ribosomal protein L34.

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 50S ribosomal protein L35.

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 50S ribosomal protein L36.

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 50S ribosomal protein L31.

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	11	Total	C	N	O	P	0	0
			233	105	41	76	11		

- 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 a RNA chain called A-site tRNA-Lys.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	V	73	Total	C	N	O	P	S	0	0
			1578	712	279	514	72	1		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	118	Total	Mg	0
			118	118	
56	a	312	Total	Mg	0
			312	312	
56	b	8	Total	Mg	0
			8	8	
56	d	1	Total	Mg	0
			1	1	
56	m	1	Total	Mg	0
			1	1	
56	p	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	
56	Z	5	Total	Mg	0
			5	5	
56	V	1	Total	Mg	0
			1	1	

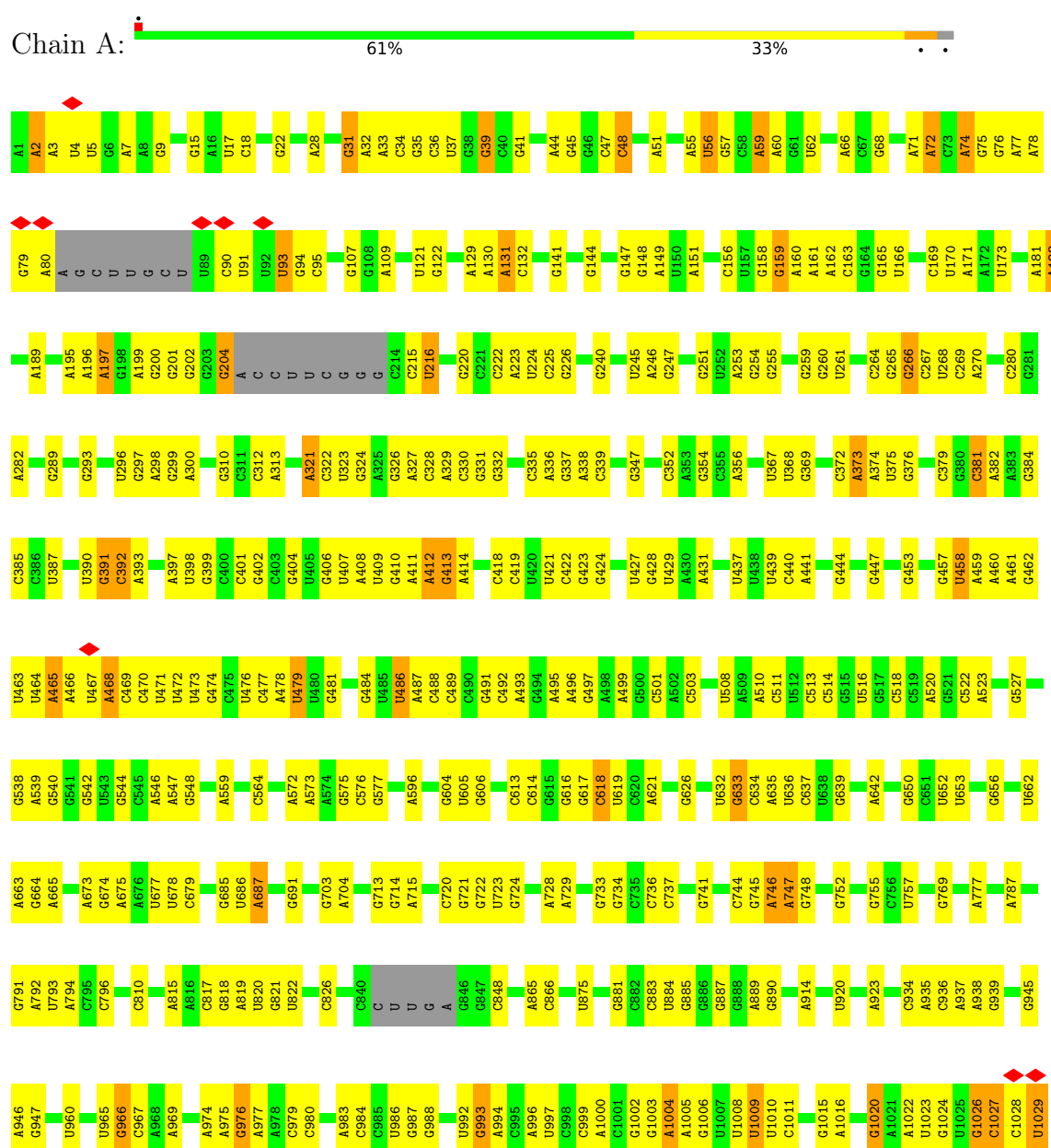
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

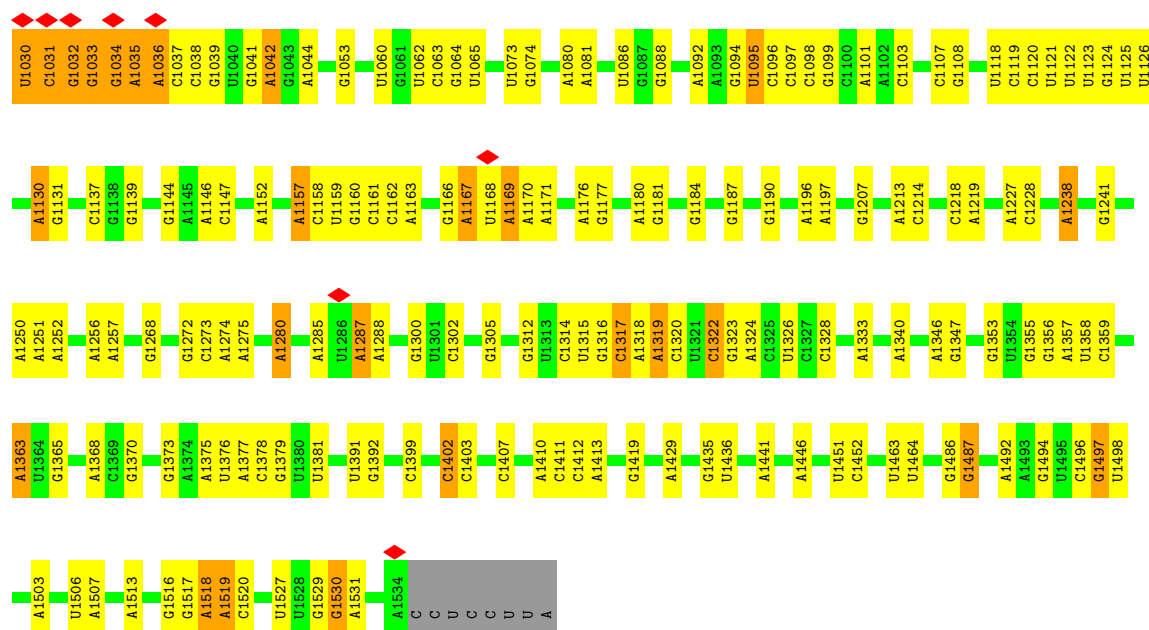
Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

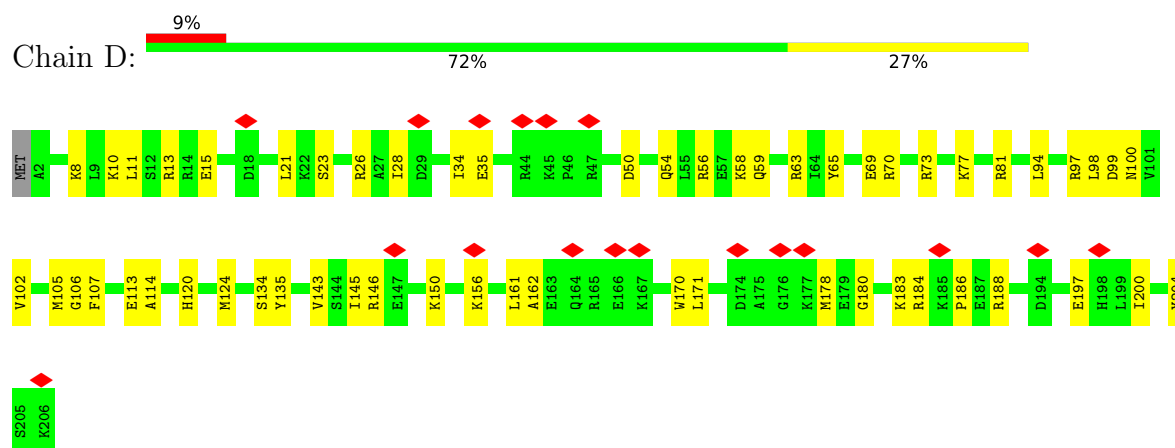
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

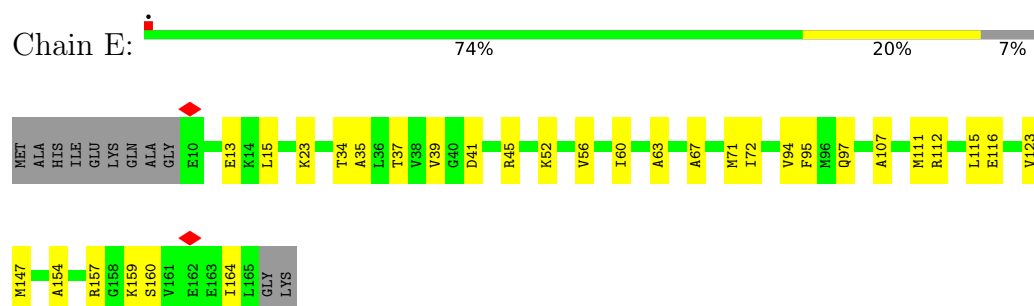




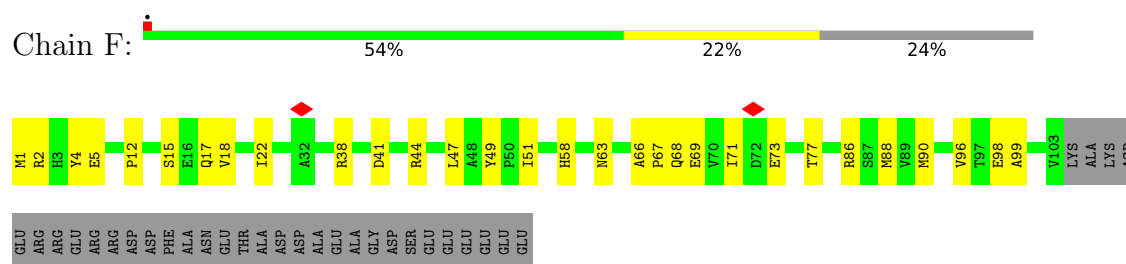
- Molecule 4: 30S ribosomal protein S4



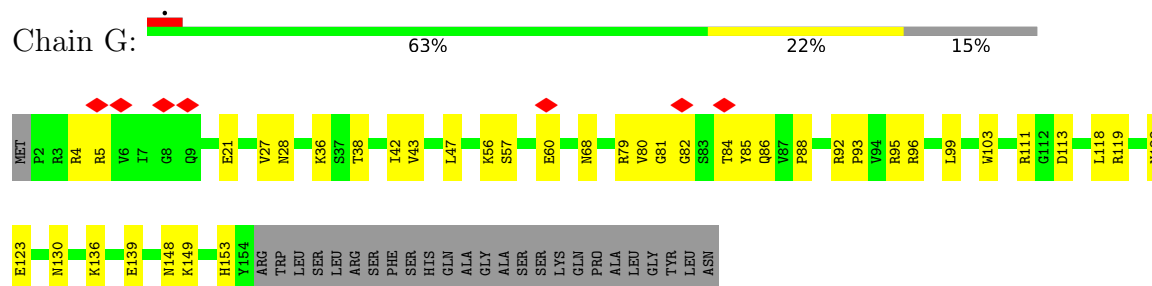
- Molecule 5: 30S ribosomal protein S5



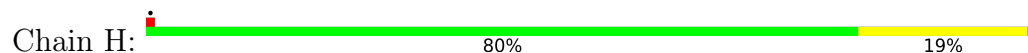
- Molecule 6: 30S ribosomal protein S6, fully modified isoform



- Molecule 7: 30S ribosomal protein S7

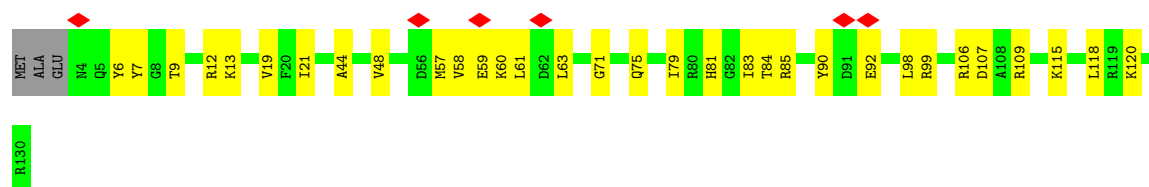


- Molecule 8: 30S ribosomal protein S8

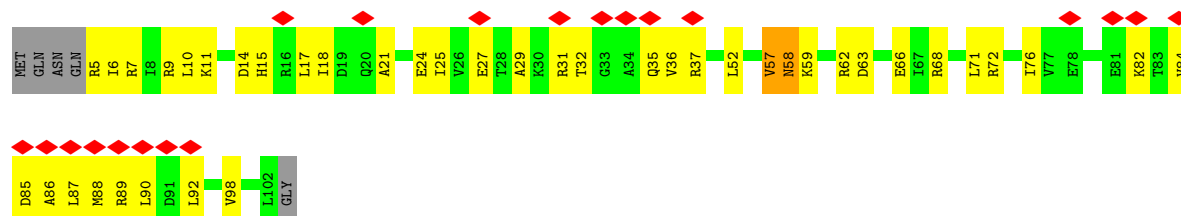




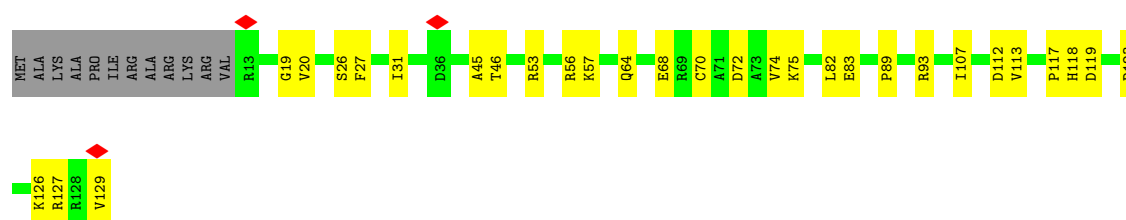
- Molecule 9: 30S ribosomal protein S9



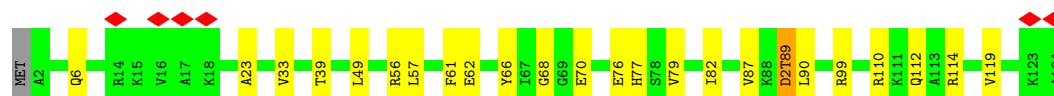
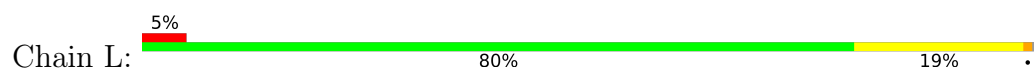
- Molecule 10: 30S ribosomal protein S10



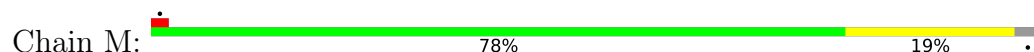
- Molecule 11: 30S ribosomal protein S11

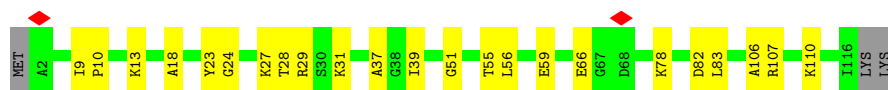


- Molecule 12: 30S ribosomal protein S12

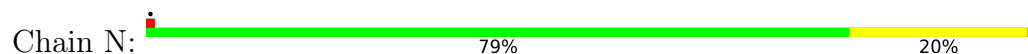


- Molecule 13: 30S ribosomal protein S13





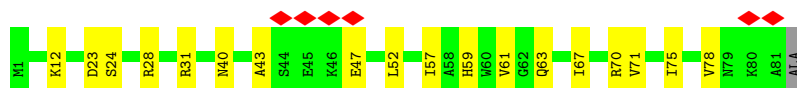
- Molecule 14: 30S ribosomal protein S14



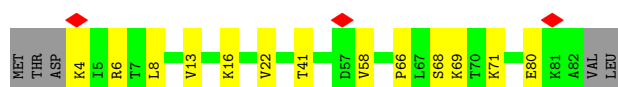
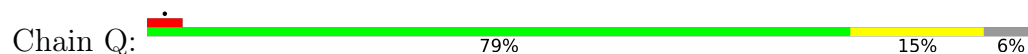
- Molecule 15: 30S ribosomal protein S15



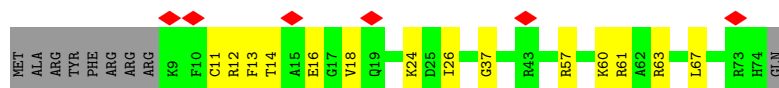
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



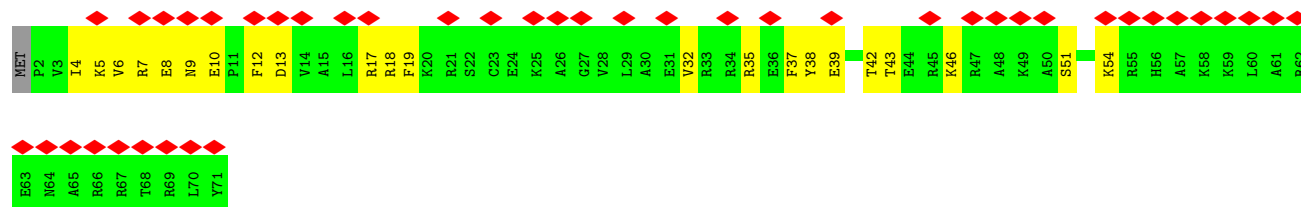
- Molecule 19: 30S ribosomal protein S19



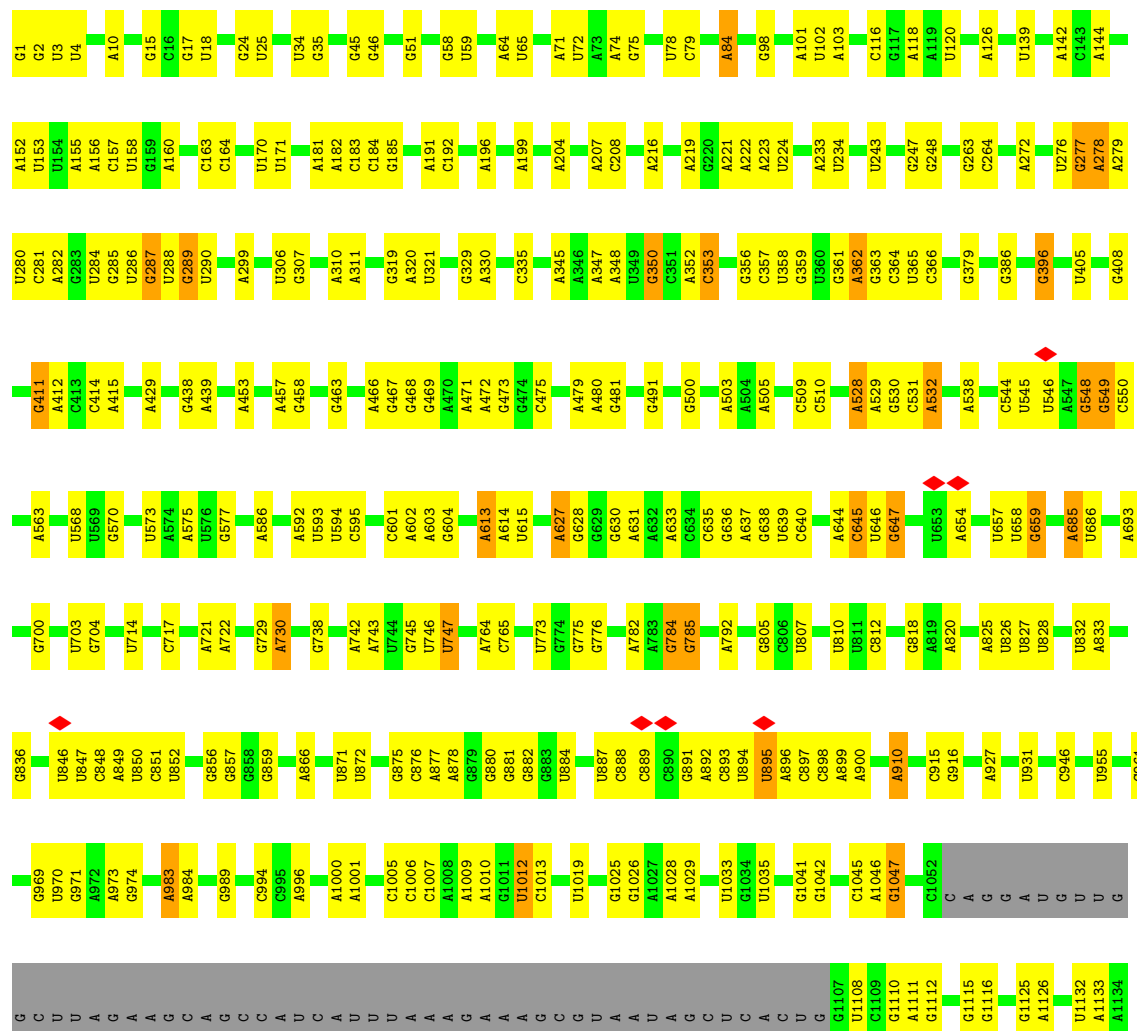
- Molecule 20: 30S ribosomal protein S20



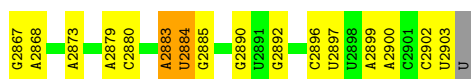
- Chain U:  61% 68% 31%



- Chain a:  67% 25% • 5%



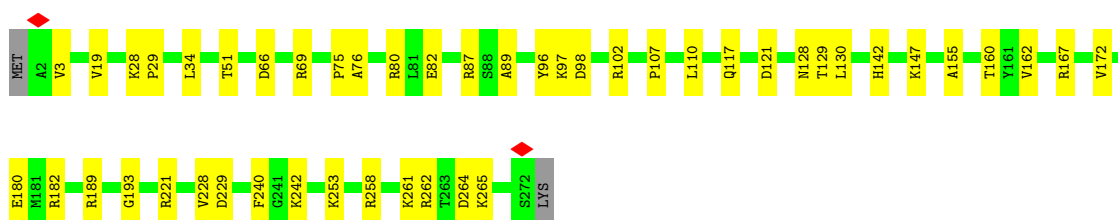
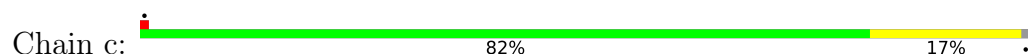
G2732	U2580	U2473	C2350	G2251	C	A2101	G1842	C1675	A1548	G1445	U1281	C1135
A2733	U2585	U2474	G2361	C2258	A	G2102	C1843	G1684	A1549	C1446	U1282	G1138
G2742	U2586	A2476	G2365	C2266	C	C	A1848	C1685	C1550	C1447	G1296	G1139
U2743	A2590	G2481	A2369	A2266	U	U	A1853	A1698	G1560	U1466	G1300	C1140
G2744	C2591	A2482	G2373	G2271	G	A	A1854	G1715	U1563	U1469	A1301	U1141
A2748	G2592	C2483	A2374	U2272	A	U	U1856	U1720	C1565	A1470	G1311	A1142
A2753	A2602	G2484	G2375	U2273	A	G	A1857	G1721	C1566	A1475	C1319	G1149
A2765	U2604	U2491	G2376	G2279	U	G	A1858	U1729	A1566	G1475	C1320	C1150
C2774	U2605	C2498	A2378	G2280	U	U	U1864	C1730	G1567	U1476	U1340	C1153
G2775	U2609	G2502	G2383	A2281	C	A	G1869	G1738	C1568	A1477	U1343	A1156
A2776	A2603	A2504	U2384	G2282	G	G	C1870	U1745	A1569	G1478	G1343	C1172
G2777	U2613	U2505	C2385	C2283	A	G	A1871	A1746	U1570	U1484	G1361	U
A2778	U2614	G2505	G2386	C2284	C	U	A1872	U1747	A1571	G1485	C1362	A
U2796	G2627	U2506	A2392	G2286	C	A	A1889	G1760	U1578	G1482	A1353	U
U2797	C2628	C2515	U2393	A2287	U	G	U1901	C1764	A1583	G1483	G1361	U
U2798	U2629	A2516	G2394	A2288	U	G	G1905	C1764	C1584	U1484	C1362	U
A2799	G2636	G2517	U2402	U2291	A	G	G1906	C1764	C1585	U1485	U1379	U
A2800	U2637	U2518	C2403	U2292	U	G	U1911	A1794	A1586	A1490	U1383	G1177
G2801	G2638	U2519	A2406	A2298	G	A	A1912	C1795	G1587	U1496	U1383	U
G2802	C2646	C2520	G2407	U2302	G	G	A1913	U1796	A1610	U1497	U1386	U
U2804	U2647	C2521	A2408	G2303	U	U	U1914	G1797	A1614	C1498	A1387	G1197
C2805	G2648	U2522	G2410	C2304	U	U	3TD1915	U1782	A1618	U1506	U1394	U1198
C2806	C2649	G2529	G2415	U2305	U	U	A1916	A1786	G1622	C1507	A1395	G1212
U2807	U2650	U2532	G2415	G2306	G	G	U1917	A1801	A1632	A1508	U1405	G1223
G2808	A2657	U2537	U2419	G2308	A	A	A1928	A1791	U1636	A1509	U1406	U
U2812	C2658	C2538	A2425	U2312	G	G	G1929	A1794	A1637	U1513	U1409	G1236
U2813	U2661	U2547	A2426	C2313	U	U	U1930	C1795	U1647	G1514	G1410	G1245
U2818	A2662	U2548	C2427	G2316	G	G	A1936	U1796	U1648	A1515	U1411	U
A2820	G2663	G2428	G2429	A2317	U	U	U1937	U1798	A1815	U1523	A1412	G1250
A2821	U2680	A2430	A2430	G2318	G	G	A1938	G1799	C1816	G1524	A1413	U
G2822	G2682	U2552	G2435	U2321	A	A	U1939	C1800	A1802	A1528	A1414	A1253
A2823	C2683	U2554	A2435	A2322	C	C	U1955	A1801	A1803	G1529	U1415	A1254
G2831	U2689	G2557	U2441	G2325	U	U	C1962	A1808	U1637	U1534	G1416	U1255
G2834	U2690	C2558	G2445	C2326	A	A	A1966	A1808	A1637	A1535	C1417	G1256
A2835	A2564	A2327	A2448	A2328	G	U	C1967	G1814	U1647	A1536	C1428	U
U2698	A2566	U2329	A2449	U2329	U	U	G1968	A1815	U1648	C1536	A1265	U
C2699	G2567	G2330	U2457	G2333	C	C	A1969	C1816	G1649	G1537	A1433	U
G2709	U2571	U2334	G2455	A2333	G	G	U1970	A1819	A1654	G1538	A1434	G1271
G2714	C2572	U2457	U2457	U2334	A	A	G1971	U1827	A1655	U1539	G1435	A1272
U2847	C2573	C2467	C2467	A2340	U	U	G1972	U1827	A1656	G1540	U1273	U
U2849	G2576	A2468	A2468	G2345	G	G	U1991	G1829	C1656	C1541	A1437	A1274
A2850	U2577	A2469	A2469	U2346	U	U	G1992	A1829	U1657	U1542	G1436	A1275
U2861	A2726	G2470	G2470	G2347	A	A	U1993	G1835	G1667	C1544	G1441	U
U2866	A2727	C2579	C2248	C2347	C	C	C2000	G1835	G1674	A1544	U1442	C1278
										A1545	U1443	G1280
										C1547	G1444	



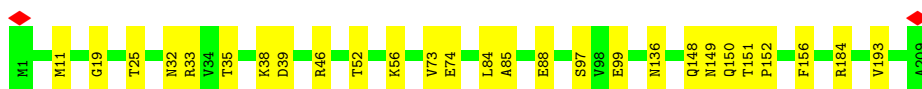
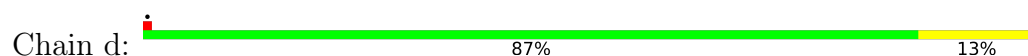
• Molecule 23: 5S rRNA



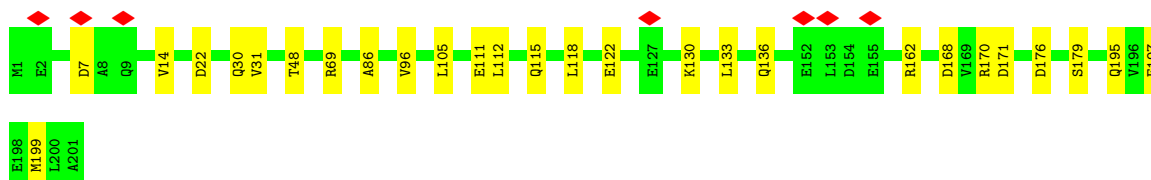
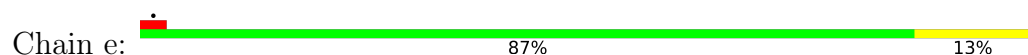
• Molecule 24: 50S ribosomal protein L2



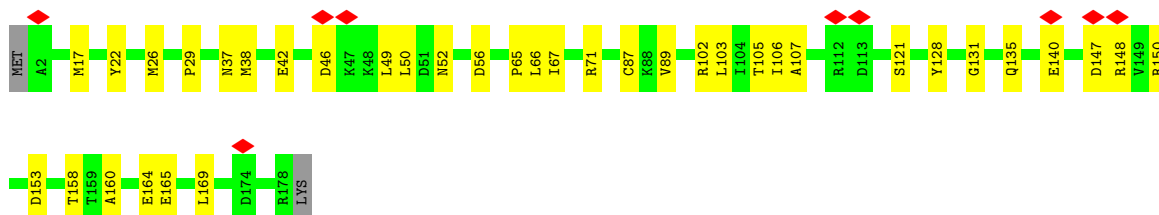
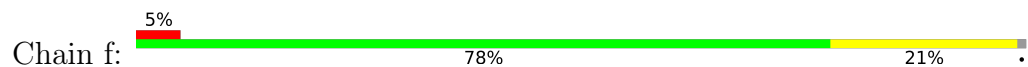
• Molecule 25: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L4



• Molecule 27: 50S ribosomal protein L5





- Molecule 34: 50S ribosomal protein L17

Chain m: 83% 10% 7%



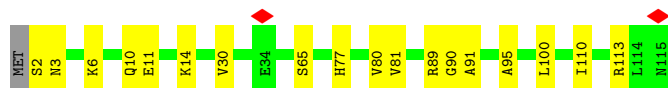
- Molecule 35: 50S ribosomal protein L18

Chain n: 86% 13%



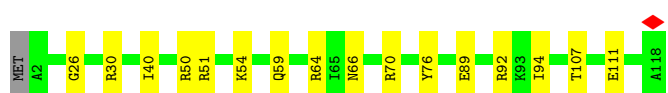
- Molecule 36: 50S ribosomal protein L19

Chain o: 83% 16%



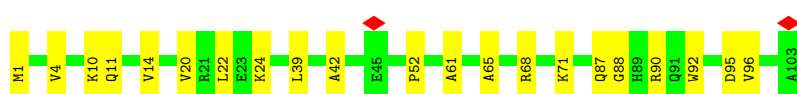
- Molecule 37: 50S ribosomal protein L20

Chain p: 86% 14%



- Molecule 38: 50S ribosomal protein L21

Chain q: 80% 20%



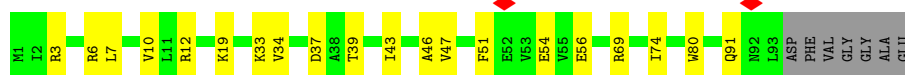
- Molecule 39: 50S ribosomal protein L22

Chain r: 89% 11%




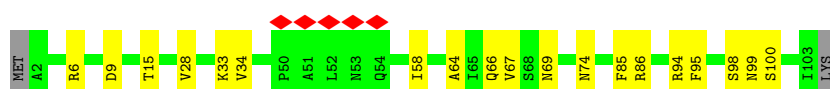
• Molecule 40: 50S ribosomal protein L23

Chain s:  73% 20% 7%




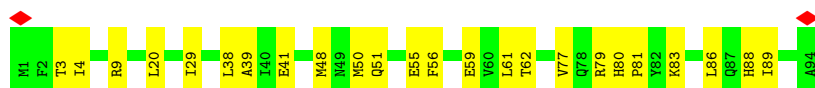
• Molecule 41: 50S ribosomal protein L24

Chain t:  5% 80% 18%




• Molecule 42: 50S ribosomal protein L25

Chain u:  74% 26%



• Molecule 43: 50S ribosomal protein L27

Chain v:  6% 84% 15%




• Molecule 44: 50S ribosomal protein L28

Chain w:  73% 26%




• Molecule 45: 50S ribosomal protein L29

Chain x:  84% 14%

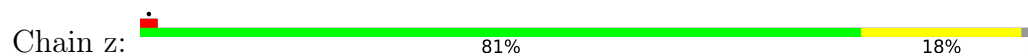


• Molecule 46: 50S ribosomal protein L30

Chain y:  5% 76% 22%



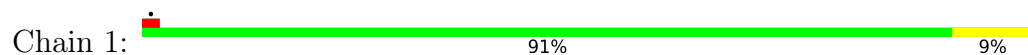
- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



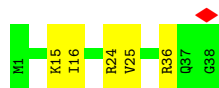
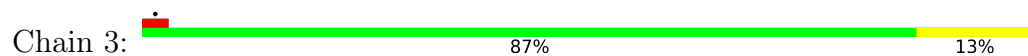
- Molecule 49: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36



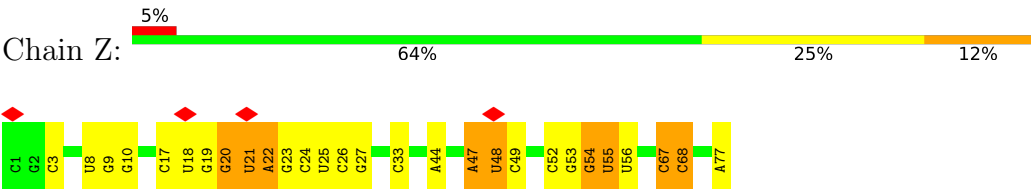
- Molecule 52: 50S ribosomal protein L31



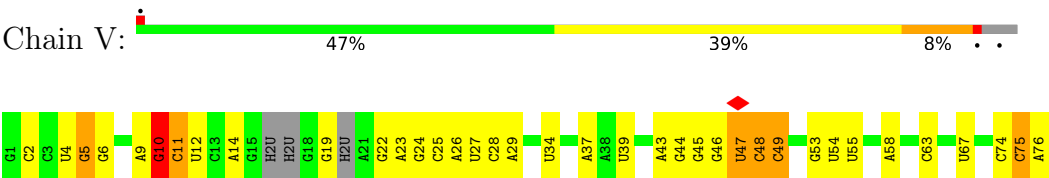
- Molecule 53: mRNA



• Molecule 54: P-site tRNA-fMet



• Molecule 55: A-site tRNA-Lys



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213224	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 ($e^-/\text{\AA}^2$)	50	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	0.077	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, IAS, 3TD, H2U, A1L4U, D2T, 5MC, MG, UR3, 4SU, OMG, 2MU, PSU, 5MU, 6MZ, 4OC, MS6, 12A, 1MA, ZN, OMC, G7M, 4D4, MA6, 2MG, OMU, 1MG, 2MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/36073	0.34	0/56264
2	B	0.20	0/1784	0.45	0/2403
3	C	0.38	0/1651	0.46	0/2225
4	D	0.32	0/1665	0.44	0/2227
5	E	0.42	0/1165	0.48	0/1568
6	F	0.34	0/858	0.45	0/1160
7	G	0.32	0/1219	0.44	0/1635
8	H	0.40	0/989	0.47	0/1326
9	I	0.38	0/1034	0.50	0/1375
10	J	0.38	0/796	0.53	0/1077
11	K	0.38	0/884	0.44	0/1191
12	L	0.42	0/960	0.46	0/1286
13	M	0.37	0/900	0.46	0/1204
14	N	0.41	0/817	0.50	0/1088
15	O	0.38	0/722	0.54	0/964
16	P	0.32	0/653	0.44	0/877
17	Q	0.36	0/650	0.41	0/871
18	R	0.36	0/553	0.49	0/742
19	S	0.35	0/685	0.44	0/922
20	T	0.31	0/676	0.40	0/895
21	U	0.23	0/597	0.41	0/792
22	a	0.51	0/65842	0.35	0/102711
23	b	0.42	0/2850	0.30	0/4444
24	c	0.50	0/2121	0.48	0/2852
25	d	0.48	0/1576	0.43	0/2119
26	e	0.43	0/1571	0.41	0/2113
27	f	0.35	0/1434	0.44	0/1926
28	g	0.33	0/1343	0.46	0/1816
29	h	0.27	0/306	0.51	0/413
30	i	0.46	0/1152	0.41	0/1551
31	j	0.49	0/955	0.44	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.46	0/1062	0.45	0/1413
33	l	0.46	0/1073	0.45	0/1433
34	m	0.50	0/958	0.52	0/1281
35	n	0.39	0/902	0.42	0/1209
36	o	0.45	0/929	0.44	0/1242
37	p	0.55	0/960	0.49	0/1278
38	q	0.45	0/829	0.45	0/1107
39	r	0.48	0/864	0.48	0/1156
40	s	0.39	0/744	0.50	0/994
41	t	0.37	0/787	0.48	0/1051
42	u	0.41	0/766	0.45	0/1025
43	v	0.47	0/642	0.44	0/848
44	w	0.46	0/635	0.48	0/848
45	x	0.32	0/502	0.40	0/667
46	y	0.46	0/453	0.58	0/605
47	z	0.47	0/450	0.45	0/599
48	0	0.43	0/424	0.42	0/565
49	1	0.52	0/380	0.51	0/498
50	2	0.48	0/513	0.49	0/676
51	3	0.50	0/303	0.53	0/397
52	4	0.30	0/488	0.43	0/649
53	X	0.43	0/260	0.26	0/402
54	Z	0.36	0/1725	0.31	0/2687
55	V	0.31	0/1429	0.31	0/2217
All	All	0.46	0/152559	0.38	0/228163

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
50	2	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32466	0	16359	346	0
2	B	1753	0	1780	57	0
3	C	1624	0	1696	25	0
4	D	1643	0	1707	50	0
5	E	1152	0	1196	27	0
6	F	839	0	833	23	0
7	G	1203	0	1254	34	0
8	H	979	0	1031	16	0
9	I	1022	0	1070	29	0
10	J	786	0	828	30	0
11	K	877	0	884	28	0
12	L	957	0	1017	17	0
13	M	891	0	952	14	0
14	N	805	0	844	15	0
15	O	714	0	734	6	0
16	P	643	0	661	12	0
17	Q	641	0	682	10	0
18	R	544	0	565	10	0
19	S	668	0	693	17	0
20	T	670	0	719	8	0
21	U	589	0	629	20	0
22	a	59301	0	29849	411	0
23	b	2549	0	1291	21	0
24	c	2082	0	2154	29	0
25	d	1566	0	1618	18	0
26	e	1552	0	1619	17	0
27	f	1410	0	1444	30	0
28	g	1323	0	1371	34	0
29	h	303	0	327	9	0
30	i	1129	0	1162	22	0
31	j	946	0	1023	13	0
32	k	1053	0	1129	11	0
33	l	1075	0	1145	23	0
34	m	945	0	989	10	0
35	n	892	0	923	9	0
36	o	917	0	962	12	0
37	p	947	0	1019	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	q	816	0	839	14	0
39	r	857	0	922	9	0
40	s	738	0	807	16	0
41	t	779	0	831	17	0
42	u	753	0	780	17	0
43	v	634	0	653	8	0
44	w	625	0	652	14	0
45	x	501	0	531	5	0
46	y	449	0	488	11	0
47	z	444	0	458	9	0
48	0	417	0	451	8	0
49	1	377	0	418	3	0
50	2	504	0	572	16	0
51	3	302	0	340	4	0
52	4	480	0	478	13	0
53	X	233	0	118	1	0
54	Z	1645	0	842	10	0
55	V	1578	0	806	19	0
56	A	118	0	0	0	0
56	V	1	0	0	0	0
56	Z	5	0	0	0	0
56	a	312	0	0	0	0
56	b	8	0	0	0	0
56	d	1	0	0	0	0
56	m	1	0	0	0	0
56	p	1	0	0	0	0
56	z	1	0	0	0	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
All	All	142038	0	95145	1478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1478) 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)
1:A:107:G:H1	20:T:6:SER:HG	1.00	0.99
1:A:76:G:H1	1:A:93:U:H3	1.15	0.90
1:A:1028:C:N4	1:A:1033:G:O6	2.06	0.88
14:N:3:LYS:HD3	14:N:6:MET:HE1	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.22	0.87
28:g:42:GLU:OE1	28:g:55:ARG:NE	2.08	0.86
1:A:1009:U:H3	1:A:1020:G:H1	1.23	0.86
22:a:1153:C:OP1	37:p:92:ARG:NH2	2.11	0.83
7:G:68:ASN:ND2	7:G:130:ASN:OD1	2.12	0.83
22:a:2100:G:H1	22:a:2189:U:H3	0.84	0.82
4:D:124:MET:HE2	4:D:146:ARG:HG2	1.62	0.80
1:A:999:C:N3	1:A:1042:A:N6	2.29	0.80
1:A:464:U:O4	1:A:468:A:N7	2.15	0.80
1:A:677:U:H3	1:A:713:G:H22	1.30	0.80
24:c:142:HIS:ND1	24:c:193:GLY:O	2.14	0.79
22:a:602:A:HO2'	22:a:604:G:HO2'	1.31	0.79
1:A:1006:G:N7	1:A:1024:G:N2	2.31	0.79
3:C:11:ARG:NH2	3:C:175:LEU:O	2.16	0.79
19:S:41:PHE:H	19:S:44:MET:HE3	1.47	0.78
1:A:390:U:H4'	16:P:28:ARG:HH22	1.49	0.78
26:e:176:ASP:OD1	26:e:179:SER:OG	2.01	0.78
43:v:26:PHE:N	43:v:29:GLU:OE2	2.16	0.78
22:a:2102:G:H1	22:a:2187:U:H3	1.27	0.78
1:A:673:A:H2'	1:A:674:G:C8	2.20	0.76
7:G:93:PRO:HA	7:G:96:ARG:HD3	1.68	0.76
27:f:56:ASP:OD2	27:f:135:GLN:NE2	2.19	0.75
22:a:2502:G:H5''	22:a:2503:2MA:H5''	1.69	0.75
46:y:16:ARG:HG3	46:y:54:MET:HE1	1.68	0.75
33:l:53:MET:HE3	33:l:117:PHE:HE1	1.52	0.74
22:a:1047:G:HO2'	22:a:1110:G:H1	1.34	0.73
19:S:25:SER:O	19:S:28:LYS:NZ	2.22	0.73
1:A:848:C:OP1	2:B:37:LYS:NZ	2.23	0.72
22:a:2091:C:H4'	44:w:56:MET:HE1	1.69	0.72
38:q:1:MET:HA	38:q:42:ALA:O	1.88	0.72
1:A:427:U:OP1	4:D:13:ARG:NH2	2.23	0.71
50:2:55:LEU:O	50:2:59:ILE:HG12	1.91	0.71
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.23	0.71
22:a:1245:G:OP1	32:k:13:LYS:NZ	2.23	0.71
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.23	0.71
33:l:136:MET:O	42:u:79:ARG:NH2	2.22	0.71
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.22	0.71
1:A:1363:A:O2'	1:A:1365:G:N7	2.22	0.71
3:C:35:SER:OG	3:C:59:ARG:NH2	2.24	0.70
44:w:43:GLU:OE1	44:w:45:ARG:NH1	2.23	0.70
22:a:1010:A:OP1	37:p:66:ASN:ND2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:284:U:H3	22:a:356:G:H1	1.38	0.70
1:A:7:A:N6	5:E:97:GLN:OE1	2.24	0.70
2:B:111:ILE:HD12	2:B:152:LYS:HA	1.73	0.70
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.71	0.70
35:n:15:ARG:NH2	35:n:95:SER:OG	2.25	0.70
9:I:81:HIS:HE1	9:I:85:ARG:HH21	1.39	0.69
22:a:1434:A:H2'	22:a:1435:G:H8	1.57	0.69
54:Z:48:U:H5''	54:Z:49:C:H5'	1.75	0.69
26:e:111:GLU:OE1	26:e:115:GLN:NE2	2.26	0.69
9:I:106:ARG:NH1	9:I:107:ASP:O	2.26	0.69
22:a:1475:G:O2'	22:a:1514:G:O6	2.10	0.69
7:G:86:GLN:HB2	7:G:148:ASN:HD22	1.57	0.69
14:N:90:ARG:NH1	14:N:92:GLU:OE1	2.26	0.69
26:e:168:ASP:OD2	26:e:170:ARG:NH1	2.26	0.69
28:g:99:LYS:NZ	28:g:104:ASN:OD1	2.25	0.69
6:F:2:ARG:NH1	6:F:68:GLN:OE1	2.25	0.68
3:C:164:ARG:NH1	3:C:166:GLU:OE2	2.27	0.68
28:g:104:ASN:ND2	28:g:114:ASP:OD1	2.25	0.68
34:m:32:GLU:HG2	34:m:115:LEU:HD12	1.75	0.68
12:L:68:GLY:O	12:L:99:ARG:NH1	2.26	0.68
22:a:1800:C:OP2	24:c:182:ARG:NH1	2.25	0.68
33:l:14:LYS:O	33:l:71:LYS:NZ	2.23	0.68
44:w:39:TRP:NE1	44:w:41:GLU:OE1	2.25	0.68
1:A:538:G:OP2	12:L:112:GLN:NE2	2.26	0.68
4:D:11:LEU:HB3	4:D:63:ARG:HD3	1.74	0.68
46:y:6:LYS:HB2	46:y:58:GLU:HG2	1.74	0.68
1:A:356:A:N3	1:A:368:U:O2'	2.26	0.68
22:a:247:G:O6	50:2:12:LYS:NZ	2.25	0.68
1:A:501:C:OP1	12:L:114:ARG:NH2	2.24	0.68
1:A:544:G:OP1	4:D:56:ARG:NH2	2.27	0.68
1:A:546:A:O2'	1:A:548:G:O2'	2.09	0.68
1:A:875:U:O2'	8:H:15:ARG:NH1	2.27	0.68
7:G:88:PRO:HG3	7:G:149:LYS:HA	1.76	0.67
24:c:66:ASP:OD2	24:c:102:ARG:NH1	2.27	0.67
24:c:262:ARG:O	24:c:265:LYS:NZ	2.28	0.67
1:A:486:U:H2'	1:A:487:A:H8	1.60	0.67
6:F:90:MET:HE1	18:R:61:ARG:NH1	2.09	0.67
22:a:2285:C:OP2	48:0:6:ARG:NH1	2.27	0.67
1:A:437:U:HO2'	4:D:120:HIS:HD1	1.34	0.67
1:A:408:A:O3'	4:D:23:SER:OG	2.13	0.67
9:I:57:MET:HE2	9:I:61:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2753:A:O2'	51:3:15:LYS:NZ	2.28	0.67
2:B:26:LYS:NZ	2:B:192:ASP:OD1	2.25	0.66
22:a:2303:G:O2'	27:f:121:SER:O	2.13	0.66
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.28	0.66
16:P:61:VAL:HG22	16:P:67:ILE:HD11	1.78	0.66
22:a:1528:A:OP2	22:a:1543:G:N2	2.28	0.66
2:B:67:ILE:HG22	2:B:160:ALA:HB3	1.78	0.66
13:M:78:LYS:NZ	13:M:82:ASP:OD2	2.28	0.66
1:A:974:A:OP1	14:N:69:ARG:NH2	2.29	0.66
1:A:979:C:O2	14:N:59:ARG:NH1	2.28	0.66
1:A:1032:G:N2	1:A:1033:G:N3	2.44	0.66
22:a:639:U:H2'	22:a:640:C:C6	2.30	0.66
55:V:23:A:H2'	55:V:24:G:H8	1.61	0.66
1:A:202:G:H21	1:A:466:A:H61	1.41	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.31	0.65
2:B:18:HIS:ND1	2:B:188:ASP:OD2	2.29	0.65
3:C:142:MET:HG3	3:C:170:GLU:OE2	1.96	0.65
40:s:54:GLU:OE1	40:s:91:GLN:NE2	2.29	0.65
22:a:807:U:OP2	32:k:41:ARG:NH1	2.28	0.65
15:O:74:ASP:OD2	15:O:77:ARG:NH1	2.27	0.65
19:S:45:ILE:HD12	19:S:45:ILE:H	1.62	0.65
1:A:1318:A:OP1	19:S:3:ARG:NH1	2.29	0.65
2:B:100:MET:HA	2:B:107:VAL:HG21	1.79	0.65
4:D:105:MET:HE2	4:D:171:LEU:HD11	1.78	0.65
1:A:410:G:N1	1:A:431:A:OP2	2.21	0.65
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.78	0.65
4:D:58:LYS:HA	4:D:200:ILE:HD11	1.79	0.65
1:A:1530:G:N7	21:U:46:LYS:NZ	2.36	0.64
8:H:22:LYS:O	8:H:65:TYR:OH	2.14	0.64
1:A:4:U:H2'	1:A:5:U:H2'	1.79	0.64
28:g:86:LYS:HB2	28:g:165:ALA:HB2	1.78	0.64
22:a:1607:C:N4	22:a:1622:G:OP2	2.29	0.64
1:A:796:C:O3'	11:K:127:ARG:NH1	2.31	0.64
29:h:30:LEU:HB3	29:h:36:ALA:HB3	1.79	0.64
36:o:90:GLY:O	36:o:113:ARG:NH1	2.31	0.64
41:t:28:VAL:HG22	41:t:34:VAL:HG12	1.78	0.64
36:o:2:SER:OG	36:o:3:ASN:N	2.29	0.64
11:K:20:VAL:HG12	11:K:83:GLU:HB2	1.80	0.64
22:a:2305:U:H5''	27:f:131:GLY:HA3	1.80	0.64
4:D:150:LYS:O	4:D:156:LYS:NZ	2.30	0.64
4:D:183:LYS:HD3	4:D:184:ARG:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:GLU:HB2	3:C:144:LEU:HD12	1.79	0.63
22:a:1417:C:HO2'	22:a:1587:G:HO2'	1.47	0.63
22:a:2328:A:H2'	22:a:2329:U:C6	2.33	0.63
1:A:147:G:H2'	1:A:148:G:C8	2.34	0.63
10:J:63:ASP:OD2	14:N:85:ARG:NH1	2.31	0.63
22:a:1827:U:OP2	24:c:221:ARG:NH1	2.31	0.63
4:D:145:ILE:O	4:D:150:LYS:NZ	2.28	0.63
22:a:639:U:H2'	22:a:640:C:H6	1.62	0.63
25:d:184:ARG:NH2	36:o:11:GLU:OE2	2.29	0.63
18:R:57:ARG:HB3	18:R:61:ARG:HH21	1.63	0.63
27:f:56:ASP:OD2	27:f:150:ARG:NH2	2.29	0.63
1:A:458:U:H2'	1:A:459:A:C8	2.33	0.63
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.79	0.63
37:p:26:GLY:O	37:p:30:ARG:NH1	2.31	0.63
42:u:9:ARG:HG2	42:u:41:GLU:HG3	1.80	0.63
1:A:459:A:H2'	1:A:460:A:C8	2.33	0.62
22:a:1590:A:H2'	22:a:1591:A:H8	1.64	0.62
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.81	0.62
33:l:53:MET:HE3	33:l:117:PHE:CE1	2.33	0.62
1:A:459:A:H2'	1:A:460:A:H8	1.64	0.62
2:B:49:MET:HA	2:B:52:GLU:HG3	1.81	0.62
8:H:10:MET:HG3	8:H:27:MET:HE2	1.80	0.62
22:a:2102:G:N2	22:a:2187:U:O2	2.30	0.62
1:A:202:G:O2'	1:A:468:A:N3	2.28	0.62
25:d:46:ARG:NH1	25:d:85:ALA:O	2.32	0.62
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.82	0.62
22:a:2683:C:O2	31:j:70:ARG:NH1	2.23	0.62
1:A:1356:G:H2'	1:A:1357:A:H8	1.64	0.62
5:E:45:ARG:HG2	5:E:71:MET:HE2	1.81	0.62
22:a:881:G:O6	22:a:895:U:O4	2.18	0.62
22:a:1417:C:O2'	22:a:1587:G:O2'	2.14	0.62
46:y:11:ARG:HG2	46:y:11:ARG:HH21	1.65	0.62
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.81	0.62
1:A:398:U:H2'	1:A:399:G:H8	1.65	0.62
4:D:59:GLN:O	4:D:63:ARG:HG2	1.99	0.62
24:c:261:LYS:HA	24:c:264:ASP:OD2	2.00	0.62
19:S:17:LYS:HB3	19:S:21:LYS:NZ	2.15	0.61
22:a:2522:U:O2'	22:a:2647:U:OP1	2.14	0.61
1:A:542:G:OP1	4:D:10:LYS:NZ	2.33	0.61
28:g:17:VAL:HG12	28:g:26:ILE:HG12	1.82	0.61
41:t:15:THR:OG1	41:t:69:ASN:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1802:A:H2'	22:a:1803:A:C8	2.35	0.61
9:I:12:ARG:HG3	9:I:13:LYS:H	1.65	0.61
22:a:627:A:OP1	32:k:78:ARG:NH2	2.32	0.61
34:m:98:LEU:HD13	47:z:54:VAL:HG11	1.81	0.61
35:n:99:TYR:OH	35:n:111:ARG:NH1	2.34	0.61
1:A:28:A:O2'	1:A:296:U:OP1	2.17	0.61
1:A:1074:G:O2'	2:B:102:THR:OG1	2.17	0.61
49:1:31:LEU:HD22	49:1:42:LEU:HD23	1.82	0.61
28:g:10:VAL:HA	28:g:49:THR:HG22	1.82	0.61
2:B:35:ARG:HB2	2:B:35:ARG:NH1	2.16	0.61
10:J:52:LEU:HD11	10:J:59:LYS:HA	1.82	0.61
22:a:1434:A:H2'	22:a:1435:G:C8	2.36	0.61
22:a:2100:G:H2'	22:a:2101:A:C8	2.36	0.61
24:c:87:ARG:HG3	24:c:89:ALA:H	1.64	0.61
13:M:39:ILE:HD12	13:M:56:LEU:HD11	1.82	0.61
22:a:263:G:O2'	22:a:429:A:N3	2.34	0.61
25:d:35:THR:HG22	25:d:73:VAL:HG21	1.83	0.61
30:i:125:TYR:HH	30:i:132:HIS:CD2	2.18	0.61
1:A:1122:U:H2'	1:A:1123:U:C6	2.36	0.61
2:B:68:LEU:HD13	2:B:158:PRO:HB3	1.83	0.61
8:H:113:ASP:OD1	8:H:114:ARG:N	2.34	0.61
1:A:714:G:H2'	1:A:715:A:C8	2.35	0.60
1:A:1027:C:H2'	1:A:1028:C:C6	2.36	0.60
2:B:41:ILE:HD11	2:B:201:PRO:HB2	1.82	0.60
9:I:19:VAL:HG11	9:I:83:ILE:HD13	1.83	0.60
13:M:27:LYS:O	13:M:31:LYS:HG2	2.00	0.60
22:a:2365:G:N7	50:2:39:LYS:NZ	2.42	0.60
37:p:50:ARG:O	37:p:54:LYS:NZ	2.34	0.60
1:A:938:A:N3	1:A:1376:U:O2'	2.26	0.60
2:B:96:TRP:NE1	2:B:175:GLU:OE2	2.35	0.60
3:C:85:GLU:OE2	3:C:88:ARG:NH2	2.28	0.60
22:a:2100:G:N2	22:a:2189:U:O2	2.27	0.60
1:A:1004:A:C6	1:A:1026:G:H1'	2.37	0.60
2:B:111:ILE:HD13	2:B:148:LEU:HD21	1.83	0.60
2:B:126:PHE:HE1	2:B:137:ARG:HD2	1.65	0.60
7:G:153:HIS:O	7:G:153:HIS:ND1	2.33	0.60
27:f:49:LEU:HD22	27:f:148:ARG:HH12	1.67	0.60
7:G:111:ARG:NH1	7:G:123:GLU:OE1	2.31	0.60
7:G:113:ASP:OD2	7:G:122:ASN:ND2	2.35	0.60
10:J:14:ASP:OD1	10:J:17:LEU:HB3	2.01	0.60
11:K:126:LYS:HZ2	21:U:37:PHE:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:41:GLU:O	44:w:44:LYS:HD2	2.01	0.60
8:H:111:MET:HE3	8:H:116:ALA:HA	1.84	0.60
1:A:1125:U:OP1	10:J:37:ARG:NH1	2.35	0.60
9:I:107:ASP:OD1	9:I:109:ARG:HG2	2.02	0.60
20:T:15:GLU:OE2	20:T:19:LYS:NZ	2.35	0.60
20:T:35:VAL:HG21	20:T:54:MET:HG2	1.82	0.60
1:A:826:C:O2	8:H:16:ASN:ND2	2.35	0.59
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.83	0.59
16:P:52:LEU:HD12	16:P:57:ILE:HD11	1.83	0.59
33:l:30:SER:OG	33:l:106:ASP:OD1	2.19	0.59
1:A:407:U:H2'	1:A:408:A:C8	2.38	0.59
52:4:16:CYS:SG	52:4:17:SER:N	2.75	0.59
22:a:500:G:N1	22:a:503:A:OP2	2.35	0.59
1:A:339:C:OP2	31:j:98:ARG:NH1	2.32	0.59
6:F:1:MET:HE1	6:F:67:PRO:HD3	1.84	0.59
32:k:127:VAL:HG11	32:k:142:ILE:HD13	1.85	0.59
2:B:154:MET:HE1	2:B:158:PRO:HD3	1.84	0.59
22:a:290:U:O2	22:a:350:G:O6	2.19	0.59
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.84	0.59
10:J:85:ASP:OD1	10:J:86:ALA:N	2.35	0.59
13:M:23:TYR:HB3	13:M:66:GLU:HG3	1.84	0.59
2:B:70:VAL:HG11	2:B:96:TRP:HZ3	1.68	0.59
2:B:9:MET:HE1	2:B:47:VAL:HG22	1.85	0.59
31:j:14:SER:OG	31:j:86:LEU:HD12	2.02	0.59
1:A:407:U:H2'	1:A:408:A:H8	1.68	0.59
21:U:4:ILE:HG13	21:U:19:PHE:HA	1.84	0.58
2:B:186:ILE:HD13	2:B:200:ILE:HB	1.85	0.58
1:A:259:G:OP1	20:T:36:TYR:OH	2.20	0.58
1:A:1356:G:H2'	1:A:1357:A:C8	2.38	0.58
1:A:76:G:O6	1:A:93:U:O4	2.21	0.58
1:A:945:G:C2	1:A:946:A:C8	2.92	0.58
1:A:1006:G:O6	1:A:1023:U:O2	2.20	0.58
3:C:57:ILE:HG12	3:C:66:VAL:HG12	1.84	0.58
30:i:114:LEU:HG	30:i:118:MET:HE3	1.85	0.58
55:V:23:A:H2'	55:V:24:G:C8	2.38	0.58
1:A:77:A:H2'	1:A:78:A:C8	2.38	0.58
1:A:269:C:H2'	1:A:270:A:H8	1.68	0.58
22:a:468:G:OP2	49:1:37:LYS:NZ	2.35	0.58
22:a:1466:U:O2'	22:a:1546:G:O2'	2.15	0.58
28:g:22:GLN:OE1	28:g:55:ARG:NH2	2.37	0.58
2:B:101:LEU:HB3	2:B:179:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:243:U:OP2	50:2:8:ARG:NH1	2.37	0.58
1:A:59:A:H5'	1:A:387:U:H5''	1.85	0.58
1:A:77:A:H2'	1:A:78:A:H8	1.67	0.58
1:A:923:A:O2'	1:A:1399:C:OP2	2.20	0.58
5:E:112:ARG:O	5:E:116:GLU:HG2	2.04	0.58
22:a:1870:C:O2'	22:a:1871:A:H8	1.87	0.57
1:A:946:A:H2'	1:A:947:G:H8	1.68	0.57
7:G:38:THR:O	7:G:42:ILE:HD12	2.04	0.57
31:j:24:VAL:HG13	31:j:33:ALA:HB2	1.85	0.57
52:4:58:ASP:O	52:4:62:LYS:HG2	2.05	0.57
27:f:52:ASN:ND2	27:f:147:ASP:OD2	2.38	0.57
1:A:976:G:OP2	1:A:1358:U:O2'	2.22	0.57
1:A:1038:C:H2'	1:A:1039:G:H8	1.69	0.57
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.19	0.57
22:a:848:C:H2'	22:a:849:A:H8	1.69	0.57
43:v:37:ILE:HG22	43:v:38:VAL:HG13	1.85	0.57
1:A:1180:A:OP2	9:I:99:ARG:NH2	2.37	0.57
1:A:1218:C:H2'	1:A:1219:A:C8	2.40	0.57
11:K:56:ARG:HG3	11:K:56:ARG:HH11	1.69	0.57
22:a:2291:U:H2'	22:a:2292:U:C6	2.39	0.57
1:A:1010:U:H2'	1:A:1011:C:C6	2.40	0.57
9:I:21:ILE:HB	9:I:61:LEU:HD23	1.84	0.57
22:a:2:G:H2'	22:a:3:U:C6	2.40	0.57
2:B:70:VAL:HG12	2:B:92:VAL:HB	1.86	0.57
4:D:70:ARG:HH11	4:D:73:ARG:HH21	1.53	0.57
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.86	0.57
24:c:167:ARG:HG3	24:c:172:VAL:HG12	1.86	0.57
26:e:195:GLN:O	26:e:199:MET:HG2	2.05	0.57
27:f:50:LEU:HD21	27:f:67:ILE:HD12	1.87	0.57
42:u:48:MET:SD	42:u:51:GLN:NE2	2.69	0.57
1:A:1328:C:H5''	13:M:28:THR:HG21	1.85	0.57
6:F:18:VAL:O	6:F:22:ILE:HG13	2.05	0.57
22:a:1266:G:O2'	22:a:2012:G:O6	2.21	0.57
28:g:52:PHE:CE1	28:g:72:LEU:HD12	2.40	0.57
22:a:475:C:O2	22:a:479:A:N6	2.37	0.56
40:s:47:VAL:HG23	40:s:51:PHE:HD2	1.70	0.56
47:z:54:VAL:HG12	47:z:55:ILE:HG23	1.88	0.56
3:C:130:PHE:O	3:C:134:MET:HG3	2.06	0.56
7:G:4:ARG:HG3	7:G:4:ARG:HH11	1.70	0.56
22:a:1340:U:OP1	40:s:19:LYS:NZ	2.38	0.56
22:a:2481:G:O2'	22:a:2482:A:O5'	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2850:A:N7	22:a:2868:A:O2'	2.37	0.56
28:g:19:ILE:HG12	28:g:24:ILE:HD12	1.87	0.56
28:g:52:PHE:HE1	28:g:72:LEU:HD12	1.71	0.56
31:j:19:VAL:HB	31:j:41:ILE:HD12	1.87	0.56
1:A:76:G:H2'	1:A:77:A:H8	1.71	0.56
5:E:157:ARG:HH21	5:E:164:ILE:HD12	1.70	0.56
6:F:49:TYR:OH	6:F:86:ARG:NH1	2.37	0.56
22:a:411:G:OP2	22:a:2406:A:O2'	2.23	0.56
22:a:1649:G:O2'	34:m:106:ASP:OD2	2.18	0.56
28:g:95:ARG:HG3	28:g:128:GLN:HG3	1.86	0.56
36:o:30:VAL:HG12	36:o:81:VAL:HA	1.86	0.56
1:A:980:C:O2'	14:N:13:ARG:NH1	2.38	0.56
1:A:1322:C:OP1	19:S:78:ARG:NH2	2.38	0.56
1:A:1027:C:H2'	1:A:1028:C:H6	1.71	0.56
22:a:64:A:H2'	22:a:65:U:C6	2.41	0.56
22:a:729:G:H5''	22:a:730:A:H5''	1.87	0.56
33:l:66:ARG:NH1	33:l:104:GLU:OE1	2.37	0.56
1:A:390:U:H2'	1:A:391:G:H8	1.71	0.56
1:A:1034:G:O2'	1:A:1035:A:O5'	2.23	0.56
22:a:2482:A:HO2'	55:V:63:C:HO2'	1.49	0.56
1:A:744:C:H2'	1:A:745:G:H8	1.71	0.56
22:a:1614:A:C6	39:r:87:PRO:HB3	2.41	0.56
1:A:269:C:H2'	1:A:270:A:C8	2.41	0.56
22:a:1864:U:OP1	22:a:2410:G:O2'	2.18	0.56
4:D:8:LYS:HB3	4:D:21:LEU:HD22	1.88	0.55
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.88	0.55
1:A:720:C:O2	18:R:60:LYS:NZ	2.32	0.55
6:F:15:SER:OG	6:F:44:ARG:NH2	2.35	0.55
1:A:204:G:H1'	1:A:465:A:N1	2.21	0.55
1:A:642:A:C8	8:H:107:SER:HA	2.42	0.55
14:N:27:LEU:O	14:N:31:ILE:HG12	2.07	0.55
22:a:1901:A:OP2	24:c:253:LYS:NZ	2.31	0.55
22:a:2095:A:P	29:h:11:ASN:HD21	2.29	0.55
18:R:13:PHE:HD1	18:R:18:VAL:HG11	1.71	0.55
22:a:1264:A:OP1	47:z:16:ARG:NH1	2.31	0.55
1:A:1038:C:H2'	1:A:1039:G:C8	2.41	0.55
4:D:156:LYS:HZ3	4:D:178:MET:HE1	1.71	0.55
22:a:1794:A:H2'	22:a:1795:C:C6	2.42	0.55
22:a:2473:U:O2'	22:a:2474:U:O2	2.24	0.55
23:b:1:U:H2'	23:b:2:G:H8	1.71	0.55
1:A:324:G:N1	1:A:327:A:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:GLN:OE1	2:B:137:ARG:NH1	2.39	0.55
4:D:102:VAL:HG13	4:D:114:ALA:HB1	1.88	0.55
11:K:107:ILE:HD11	21:U:12:PHE:HD1	1.71	0.55
1:A:401:C:O2'	1:A:621:A:N3	2.33	0.55
1:A:1280:A:OP2	10:J:9:ARG:NH2	2.39	0.55
9:I:79:ILE:O	9:I:83:ILE:HG12	2.07	0.55
22:a:286:U:H2'	22:a:287:G:H8	1.72	0.55
27:f:46:ASP:HB3	27:f:49:LEU:HG	1.88	0.55
1:A:1187:G:H5'	9:I:115:LYS:HE3	1.88	0.55
22:a:880:G:H2'	22:a:881:G:H8	1.72	0.55
22:a:994:C:O2	38:q:10:LYS:NZ	2.39	0.55
22:a:1115:G:O2'	22:a:1116:G:H5''	2.07	0.55
39:r:88:ARG:NH2	39:r:94:ASP:OD2	2.39	0.55
1:A:2:A:HI1'	1:A:613:C:O2'	2.06	0.54
1:A:410:G:OP1	4:D:26:ARG:NH1	2.40	0.54
22:a:856:G:H2'	22:a:857:G:C8	2.42	0.54
1:A:158:G:H2'	1:A:159:G:O4'	2.08	0.54
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.89	0.54
22:a:1149:G:H2'	22:a:1150:C:C6	2.43	0.54
22:a:2848:G:O2'	22:a:2867:G:N2	2.36	0.54
35:n:60:GLU:OE2	35:n:61:GLN:NE2	2.30	0.54
1:A:470:C:H2'	1:A:471:U:C6	2.42	0.54
1:A:1273:C:H2'	1:A:1274:A:O4'	2.07	0.54
5:E:15:LEU:HD21	5:E:60:ILE:HD12	1.88	0.54
22:a:288:U:H2'	22:a:289:G:H8	1.71	0.54
22:a:851:C:H2'	22:a:852:U:C6	2.41	0.54
22:a:1570:A:H2'	22:a:1571:A:C8	2.42	0.54
22:a:2657:A:O3'	28:g:160:LYS:NZ	2.41	0.54
33:l:42:THR:HG22	33:l:93:VAL:HG12	1.89	0.54
42:u:20:LEU:HD21	42:u:41:GLU:HG2	1.88	0.54
1:A:492:C:H2'	1:A:493:A:C8	2.42	0.54
1:A:522:C:OP2	12:L:66:TYR:OH	2.21	0.54
2:B:87:CYS:SG	2:B:221:VAL:HG11	2.47	0.54
12:L:57:LEU:HD21	12:L:82:ILE:HD11	1.89	0.54
22:a:72:U:OP2	45:x:54:LYS:NZ	2.41	0.54
22:a:887:U:O2'	22:a:889:C:OP2	2.17	0.54
31:j:58:LEU:HD11	31:j:86:LEU:HD22	1.88	0.54
4:D:105:MET:SD	4:D:180:GLY:HA3	2.47	0.54
14:N:6:MET:HA	14:N:9:ARG:HD2	1.89	0.54
22:a:851:C:H2'	22:a:852:U:H6	1.73	0.54
22:a:2547:A:H2'	22:a:2548:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2831:G:OP1	25:d:56:LYS:NZ	2.41	0.54
23:b:5:U:OP1	23:b:61:G:O2'	2.22	0.54
28:g:29:LYS:NZ	28:g:80:THR:O	2.34	0.54
48:0:7:GLU:HG2	48:0:27:LYS:HE3	1.88	0.54
22:a:219:A:N3	22:a:234:U:O2'	2.36	0.54
22:a:307:G:N1	22:a:310:A:OP2	2.36	0.54
22:a:630:G:N2	22:a:633:A:OP2	2.35	0.54
34:m:69:ARG:O	34:m:70:THR:OG1	2.25	0.54
40:s:7:LEU:HD12	40:s:46:ALA:HA	1.88	0.54
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.90	0.54
20:T:39:ILE:HG23	20:T:86:LEU:HD22	1.90	0.54
21:U:5:LYS:NZ	21:U:6:VAL:O	2.41	0.54
1:A:76:G:H2'	1:A:77:A:C8	2.43	0.54
1:A:78:A:H2'	1:A:79:G:H8	1.72	0.54
6:F:38:ARG:HB2	6:F:63:ASN:HB2	1.88	0.54
22:a:593:U:H2'	22:a:594:U:C6	2.43	0.54
22:a:818:G:N1	22:a:1188:U:OP2	2.35	0.54
1:A:1064:G:O2'	1:A:1190:G:N2	2.41	0.54
7:G:80:VAL:HG23	7:G:81:GLY:H	1.73	0.54
22:a:458:G:O2'	22:a:469:G:O6	2.25	0.54
22:a:2100:G:O6	22:a:2189:U:O4	2.26	0.54
40:s:12:ARG:HB2	40:s:33:LYS:O	2.08	0.54
2:B:108:ARG:HG2	2:B:108:ARG:HH11	1.73	0.53
11:K:126:LYS:NZ	21:U:37:PHE:HB2	2.22	0.53
22:a:1799:G:H8	24:c:180:GLU:OE1	1.91	0.53
24:c:69:ARG:O	24:c:189:ARG:NH2	2.41	0.53
4:D:8:LYS:HB3	4:D:21:LEU:CD2	2.38	0.53
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.90	0.53
12:L:23:ALA:HA	12:L:61:PHE:HD2	1.74	0.53
23:b:48:U:H2'	23:b:49:C:C6	2.43	0.53
22:a:276:U:O2'	22:a:278:A:N7	2.42	0.53
25:d:25:THR:HG21	25:d:193:VAL:HG22	1.91	0.53
1:A:407:U:O2'	4:D:113:GLU:OE2	2.26	0.53
11:K:93:ARG:NH2	11:K:112:ASP:OD2	2.23	0.53
13:M:37:ALA:HB2	13:M:59:GLU:OE1	2.09	0.53
22:a:644:A:H2'	22:a:645:C:O4'	2.08	0.53
22:a:1405:U:H2'	22:a:1406:U:C6	2.44	0.53
22:a:2079:U:O2'	44:w:23:ASN:OD1	2.23	0.53
22:a:2095:A:O5'	29:h:11:ASN:ND2	2.33	0.53
22:a:2333:A:OP2	43:v:77:ARG:NH2	2.31	0.53
22:a:2483:C:N3	33:l:123:LYS:NZ	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:PHE:CE1	2:B:137:ARG:HD2	2.43	0.53
19:S:11:ILE:HG13	19:S:38:SER:HB3	1.91	0.53
22:a:1009:A:N3	22:a:1153:C:O2'	2.40	0.53
22:a:1853:A:H2'	22:a:1854:A:C8	2.43	0.53
1:A:131:A:H2'	1:A:132:C:C6	2.43	0.53
3:C:12:LEU:HA	3:C:16:LYS:HB2	1.91	0.53
22:a:288:U:H2'	22:a:289:G:C8	2.44	0.53
22:a:2076:U:OP2	22:a:2238:G:N2	2.34	0.53
1:A:486:U:H2'	1:A:487:A:C8	2.42	0.53
1:A:691:G:O6	11:K:57:LYS:NZ	2.37	0.53
11:K:64:GLN:O	11:K:68:GLU:HG3	2.09	0.53
31:j:8:LEU:HD13	31:j:84:CYS:HB3	1.90	0.53
1:A:464:U:O2'	1:A:465:A:O5'	2.18	0.53
11:K:123:PRO:HD2	21:U:38:TYR:HD1	1.73	0.53
1:A:147:G:H2'	1:A:148:G:H8	1.73	0.53
1:A:1037:C:H2'	1:A:1038:C:H6	1.73	0.53
4:D:15:GLU:OE2	4:D:56:ARG:NH1	2.42	0.53
11:K:126:LYS:HZ2	21:U:37:PHE:HD2	1.56	0.53
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.41	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.53
22:a:2:G:H2'	22:a:3:U:H6	1.73	0.53
22:a:989:G:OP2	46:y:12:SER:OG	2.16	0.53
46:y:11:ARG:HG2	46:y:11:ARG:NH2	2.24	0.53
30:i:26:GLY:O	30:i:30:THR:HG23	2.09	0.52
22:a:1590:A:H2'	22:a:1591:A:C8	2.42	0.52
45:x:31:GLN:HG2	45:x:37:LEU:HB2	1.92	0.52
1:A:993:G:O2'	1:A:994:A:N7	2.43	0.52
1:A:1268:G:H1'	1:A:1326:U:O2'	2.09	0.52
22:a:279:A:H61	22:a:361:G:H1'	1.74	0.52
22:a:881:G:H2'	22:a:882:G:H8	1.75	0.52
32:k:91:ASP:OD1	32:k:92:LEU:N	2.41	0.52
1:A:464:U:O2'	1:A:465:A:H3'	2.09	0.52
7:G:80:VAL:HG21	7:G:85:TYR:CE2	2.44	0.52
22:a:1012:U:OP2	37:p:70:ARG:NH2	2.36	0.52
26:e:112:LEU:HD23	26:e:118:LEU:HD12	1.92	0.52
1:A:1166:G:N1	1:A:1169:A:OP2	2.41	0.52
31:j:71:ARG:NH2	31:j:123:LEU:O	2.40	0.52
1:A:337:G:H2'	1:A:338:A:C8	2.44	0.52
22:a:1046:A:H3'	22:a:1047:G:H5'	1.90	0.52
22:a:2469:A:H2'	22:a:2470:G:O4'	2.10	0.52
24:c:76:ALA:HB2	24:c:96:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H2'	1:A:161:A:O4'	2.08	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.52
13:M:10:PRO:HG2	13:M:13:LYS:HE2	1.92	0.52
40:s:56:GLU:N	40:s:56:GLU:OE1	2.42	0.52
1:A:713:G:H2'	1:A:714:G:C8	2.44	0.52
12:L:87:VAL:HG13	12:L:90:LEU:HB2	1.90	0.52
23:b:42:C:C6	27:f:66:LEU:HB2	2.45	0.52
50:2:28:ASN:O	50:2:36:LYS:NZ	2.39	0.52
42:u:77:VAL:HG12	42:u:89:ILE:HG12	1.92	0.52
25:d:33:ARG:NH1	25:d:74:GLU:O	2.34	0.52
34:m:22:ARG:HG3	34:m:70:THR:HA	1.91	0.52
41:t:66:GLN:HB2	41:t:69:ASN:HB2	1.92	0.52
4:D:156:LYS:NZ	4:D:178:MET:HE1	2.25	0.51
22:a:820:A:H4'	22:a:836:G:H22	1.74	0.51
1:A:920:U:O2'	1:A:1081:A:O2'	2.28	0.51
9:I:92:GLU:H	9:I:92:GLU:CD	2.18	0.51
10:J:25:ILE:HD11	10:J:92:LEU:HD21	1.91	0.51
22:a:1140:C:OP2	30:i:68:LYS:NZ	2.29	0.51
22:a:594:U:H2'	22:a:595:C:C6	2.45	0.51
28:g:60:ASP:OD1	28:g:61:GLY:N	2.40	0.51
44:w:72:ARG:HG3	44:w:78:TYR:HE2	1.75	0.51
1:A:202:G:N2	1:A:466:A:H61	2.07	0.51
2:B:70:VAL:HG11	2:B:96:TRP:CZ3	2.45	0.51
22:a:276:U:O2'	22:a:277:G:O4'	2.25	0.51
22:a:1746:A:H2'	22:a:1747:U:C6	2.44	0.51
26:e:130:LYS:HB2	26:e:133:LEU:HD23	1.92	0.51
31:j:121:GLU:OE1	36:o:65:SER:OG	2.24	0.51
1:A:1120:C:H2'	1:A:1121:U:H6	1.75	0.51
19:S:55:ARG:HG3	19:S:56:GLN:HG3	1.91	0.51
33:l:26:VAL:HG13	33:l:104:GLU:HG3	1.92	0.51
4:D:97:ARG:HE	4:D:134:SER:HA	1.76	0.51
7:G:21:GLU:OE1	7:G:21:GLU:N	2.44	0.51
21:U:10:GLU:CD	21:U:18:ARG:HH21	2.18	0.51
22:a:1667:G:O2'	22:a:1991:U:O4	2.26	0.51
22:a:2627:G:N2	22:a:2777:G:OP2	2.42	0.51
27:f:37:ASN:HB3	27:f:153:ASP:OD1	2.10	0.51
40:s:39:THR:O	40:s:43:ILE:HD12	2.10	0.51
8:H:43:GLU:OE1	8:H:112:THR:HG21	2.10	0.51
19:S:30:PRO:HA	19:S:48:THR:HG23	1.92	0.51
22:a:191:A:H2'	22:a:192:C:C6	2.45	0.51
22:a:2902:C:H2'	22:a:2903:U:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:89:LEU:HG	28:g:162:VAL:HG22	1.92	0.51
54:Z:54:G:H3'	54:Z:55:5MU:H73	1.92	0.51
1:A:1162:C:H2'	1:A:1163:A:H8	1.76	0.51
2:B:26:LYS:HZ2	2:B:193:PRO:HD2	1.75	0.51
40:s:34:VAL:HG11	40:s:43:ILE:HG12	1.92	0.51
1:A:56:U:H2'	1:A:57:G:C8	2.46	0.51
1:A:606:G:N2	1:A:632:U:OP1	2.38	0.51
4:D:98:LEU:HB2	4:D:135:TYR:HB3	1.93	0.51
11:K:89:PRO:HG3	21:U:32:VAL:HG11	1.93	0.51
22:a:659:G:N2	26:e:30:GLN:OE1	2.36	0.51
22:a:1469:A:H2'	22:a:1470:A:C8	2.46	0.51
52:4:35:ASP:OD1	52:4:35:ASP:N	2.43	0.51
13:M:83:LEU:HD11	19:S:66:MET:HG2	1.91	0.50
6:F:4:TYR:CE2	6:F:71:ILE:HG13	2.46	0.50
10:J:6:ILE:HB	10:J:76:ILE:HB	1.93	0.50
22:a:2395:C:H2'	22:a:2396:G:O4'	2.12	0.50
22:a:2532:G:N2	22:a:2663:G:O2'	2.43	0.50
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.47	0.50
1:A:215:C:H2'	1:A:216:U:C6	2.46	0.50
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.93	0.50
11:K:45:ALA:HB3	11:K:70:CYS:HB2	1.92	0.50
11:K:117:PRO:O	21:U:35:ARG:NH1	2.38	0.50
19:S:17:LYS:HB3	19:S:21:LYS:HZ1	1.75	0.50
22:a:881:G:O6	22:a:895:U:C4	2.65	0.50
22:a:1311:G:H21	22:a:1603:A:H62	1.57	0.50
42:u:80:HIS:CE1	42:u:83:LYS:HD2	2.45	0.50
48:0:11:LEU:HD21	48:0:34:LEU:HD23	1.93	0.50
22:a:894:U:H2'	22:a:895:U:O4'	2.11	0.50
22:a:1819:A:H5''	24:c:160:THR:HG21	1.93	0.50
33:l:2:LEU:HD23	33:l:68:PHE:CD1	2.46	0.50
1:A:56:U:H2'	1:A:57:G:H8	1.77	0.50
1:A:662:U:H2'	1:A:663:A:C8	2.47	0.50
1:A:722:G:N3	1:A:722:G:H2'	2.27	0.50
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.44	0.50
1:A:1119:C:H2'	1:A:1120:C:H6	1.75	0.50
5:E:41:ASP:HB2	5:E:45:ARG:HB3	1.94	0.50
7:G:5:ARG:HD3	7:G:5:ARG:O	2.12	0.50
22:a:363:G:H2'	22:a:364:C:C6	2.47	0.50
22:a:1794:A:H2'	22:a:1795:C:H6	1.76	0.50
22:a:2571:U:O2'	25:d:151:THR:O	2.30	0.50
16:P:71:VAL:O	16:P:75:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:14:U:OP2	23:b:70:C:O2'	2.30	0.50
33:l:47:GLU:OE2	33:l:51:ARG:NE	2.44	0.50
54:Z:10:G:N2	54:Z:27:G:H1'	2.27	0.50
1:A:90:C:H2'	1:A:91:U:C6	2.47	0.50
1:A:323:U:H2'	1:A:324:G:O4'	2.11	0.50
1:A:1036:A:H2'	1:A:1037:C:O4'	2.12	0.50
1:A:1314:C:H2'	1:A:1315:U:C6	2.46	0.50
8:H:5:ASP:OD1	8:H:77:ARG:NH1	2.45	0.50
22:a:361:G:H8	22:a:361:G:OP2	1.94	0.50
22:a:2484:G:OP1	33:l:44:ARG:HD2	2.11	0.50
22:a:3:U:H2'	22:a:4:U:C6	2.47	0.50
22:a:1856:U:H2'	22:a:1857:G:O4'	2.12	0.50
22:a:2052:A:H4'	25:d:148:GLN:O	2.12	0.50
22:a:2602:A:N6	55:V:76:A:OP2	2.45	0.50
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.93	0.50
32:k:62:PRO:HG2	50:2:25:LYS:HB3	1.94	0.50
33:l:55:ARG:HH22	55:V:53:G:H5''	1.75	0.50
35:n:31:THR:HG23	35:n:34:HIS:H	1.76	0.50
1:A:165:G:H2'	1:A:166:U:C6	2.47	0.50
1:A:1130:A:H2'	1:A:1131:G:H8	1.77	0.50
22:a:279:A:N6	22:a:361:G:H1'	2.27	0.50
22:a:1506:U:H2'	22:a:1507:C:H6	1.77	0.50
22:a:2375:G:N2	22:a:2378:A:OP2	2.37	0.50
22:a:2680:U:O2'	22:a:2681:C:H5'	2.11	0.50
22:a:358:U:H2'	22:a:359:G:H8	1.76	0.49
27:f:158:THR:HG22	27:f:160:ALA:H	1.77	0.49
31:j:69:VAL:HG11	31:j:104:THR:HG21	1.94	0.49
1:A:488:C:H2'	1:A:489:C:H6	1.76	0.49
1:A:636:U:H2'	1:A:637:C:C6	2.47	0.49
1:A:1035:A:C8	1:A:1036:A:H2	2.30	0.49
22:a:1000:A:H2'	22:a:1001:A:C8	2.47	0.49
42:u:29:ILE:HD12	42:u:38:LEU:O	2.12	0.49
3:C:56:VAL:O	3:C:66:VAL:HA	2.12	0.49
13:M:106:ALA:HB3	13:M:110:LYS:HD3	1.94	0.49
22:a:286:U:H2'	22:a:287:G:C8	2.47	0.49
22:a:2808:G:O2'	22:a:2890:G:O6	2.29	0.49
27:f:106:ILE:HD11	52:4:22:MET:CE	2.42	0.49
1:A:1080:A:OP1	5:E:52:LYS:NZ	2.34	0.49
6:F:38:ARG:HD3	6:F:98:GLU:O	2.13	0.49
22:a:1212:G:O2'	22:a:1236:G:N2	2.44	0.49
22:a:1930:G:O2'	22:a:1968:G:O6	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:106:ILE:HD11	52:4:22:MET:HE1	1.92	0.49
30:i:49:ASP:OD1	30:i:118:MET:HG2	2.12	0.49
33:l:69:PRO:HA	33:l:94:ALA:HB2	1.94	0.49
52:4:30:HIS:ND1	52:4:31:ASP:O	2.45	0.49
1:A:634:C:H2'	1:A:635:A:H8	1.78	0.49
1:A:1347:G:O6	9:I:12:ARG:NH2	2.43	0.49
2:B:31:ILE:HD11	2:B:39:HIS:HB3	1.93	0.49
2:B:188:ASP:CG	2:B:189:THR:H	2.21	0.49
22:a:742:A:H2'	22:a:743:A:C8	2.47	0.49
22:a:1432:G:H2'	22:a:1433:A:C8	2.47	0.49
22:a:2316:G:H2'	22:a:2317:A:H8	1.77	0.49
30:i:4:PHE:O	37:p:64:ARG:NH2	2.36	0.49
36:o:14:LYS:HD3	36:o:77:HIS:HA	1.94	0.49
48:0:5:ILE:O	48:0:28:ARG:NH2	2.41	0.49
1:A:1157:A:H5'	1:A:1158:C:C6	2.48	0.49
6:F:98:GLU:CD	6:F:99:ALA:H	2.21	0.49
22:a:881:G:N1	22:a:895:U:N3	2.57	0.49
22:a:2246:G:H2'	22:a:2247:A:C8	2.48	0.49
23:b:28:C:OP1	35:n:31:THR:HG21	2.12	0.49
50:2:24:HIS:ND1	50:2:25:LYS:O	2.42	0.49
1:A:1062:U:H2'	1:A:1063:C:C6	2.47	0.49
13:M:24:GLY:O	13:M:29:ARG:NH1	2.42	0.49
22:a:78:U:H2'	22:a:79:C:C6	2.47	0.49
22:a:347:A:H2'	22:a:348:A:C8	2.47	0.49
22:a:721:A:H2'	22:a:722:A:C8	2.47	0.49
22:a:1156:A:C8	37:p:51:ARG:HG2	2.47	0.49
22:a:2064:C:O2'	22:a:2251:OMG:N2	2.44	0.49
23:b:48:U:H2'	23:b:49:C:H6	1.77	0.49
41:t:98:SER:O	41:t:98:SER:OG	2.29	0.49
1:A:90:C:H2'	1:A:91:U:H6	1.78	0.49
7:G:95:ARG:HG2	7:G:99:LEU:HD23	1.95	0.49
22:a:414:C:H2'	22:a:415:A:C8	2.48	0.49
25:d:38:LYS:O	25:d:46:ARG:HA	2.13	0.49
1:A:323:U:OP1	20:T:25:ARG:NH2	2.45	0.49
1:A:1118:U:H2'	1:A:1119:C:H6	1.77	0.49
1:A:1317:C:H4'	14:N:48:LEU:HD21	1.93	0.49
1:A:1412:C:H2'	1:A:1413:A:C8	2.48	0.49
6:F:69:GLU:O	6:F:73:GLU:HG3	2.13	0.49
6:F:90:MET:HE1	18:R:61:ARG:HH11	1.75	0.49
22:a:1478:G:H1	22:a:1513:U:H3	1.60	0.49
22:a:2445:2MG:OP1	26:e:69:ARG:NH1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2473:U:O2'	22:a:2474:U:O5'	2.31	0.49
1:A:1097:C:H2'	1:A:1098:C:C6	2.48	0.49
22:a:365:U:H2'	22:a:366:C:C6	2.47	0.49
54:Z:67:C:HO2'	54:Z:68:C:P	2.35	0.49
1:A:390:U:H2'	1:A:391:G:C8	2.48	0.48
1:A:1147:C:O2'	9:I:7:TYR:OH	2.23	0.48
11:K:31:ILE:HG12	11:K:46:THR:HG22	1.93	0.48
22:a:1296:G:OP1	22:a:2709:G:O2'	2.28	0.48
22:a:2215:C:H2'	22:a:2216:G:H8	1.78	0.48
1:A:246:A:C2	1:A:282:A:C5	3.01	0.48
1:A:297:G:N2	1:A:300:A:OP2	2.44	0.48
1:A:470:C:H2'	1:A:471:U:H6	1.78	0.48
1:A:745:G:O2'	1:A:746:A:H5'	2.13	0.48
22:a:2482:A:O2'	55:V:63:C:O2'	2.27	0.48
25:d:84:LEU:HD22	25:d:88:GLU:HB2	1.95	0.48
30:i:95:ARG:HG2	30:i:96:ARG:HG2	1.93	0.48
1:A:635:A:H2'	1:A:636:U:C6	2.48	0.48
9:I:81:HIS:CE1	9:I:85:ARG:HH21	2.26	0.48
12:L:56:ARG:NH1	12:L:62:GLU:HB2	2.29	0.48
22:a:1853:A:N3	22:a:2233:U:O2'	2.45	0.48
22:a:2820:A:N3	22:a:2820:A:H2'	2.27	0.48
55:V:44:G:H2'	55:V:45:G:O4'	2.13	0.48
1:A:464:U:N3	1:A:468:A:N6	2.61	0.48
1:A:613:C:H2'	1:A:614:C:C6	2.48	0.48
1:A:1123:U:O2'	1:A:1124:G:H5'	2.14	0.48
2:B:129:LEU:HD21	2:B:137:ARG:HH21	1.78	0.48
4:D:99:ASP:OD1	4:D:100:ASN:N	2.47	0.48
18:R:37:GLY:O	18:R:63:ARG:NH2	2.44	0.48
22:a:155:A:H2'	22:a:156:A:C8	2.49	0.48
22:a:631:A:N3	22:a:2415:G:O2'	2.39	0.48
22:a:2100:G:H2'	22:a:2101:A:H8	1.76	0.48
22:a:2102:G:O6	22:a:2187:U:O4	2.30	0.48
45:x:26:PHE:HD1	45:x:29:ARG:HH11	1.60	0.48
30:i:13:ARG:HG2	30:i:51:GLY:O	2.14	0.48
1:A:78:A:H2'	1:A:79:G:C8	2.49	0.48
1:A:673:A:H2'	1:A:674:G:H8	1.74	0.48
4:D:106:GLY:HA3	4:D:162:ALA:HB2	1.94	0.48
5:E:111:MET:HE3	5:E:125:ALA:HB1	1.95	0.48
22:a:849:A:H2'	22:a:850:U:C6	2.49	0.48
22:a:1009:A:OP2	30:i:39:LYS:NZ	2.47	0.48
22:a:2038:G:H2'	22:a:2039:U:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.49	0.48
27:f:105:THR:HA	52:4:38:SER:HB3	1.95	0.48
52:4:59:ARG:NH1	52:4:63:ARG:HH12	2.11	0.48
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.95	0.48
10:J:35:GLN:N	10:J:35:GLN:OE1	2.47	0.48
17:Q:6:ARG:HH12	17:Q:8:LEU:HD21	1.78	0.48
21:U:51:SER:HA	21:U:54:LYS:HE2	1.96	0.48
22:a:1484:U:H2'	22:a:1485:U:C6	2.49	0.48
1:A:687:A:C2	1:A:704:A:C5	3.02	0.48
1:A:881:G:OP2	12:L:6:GLN:NE2	2.34	0.48
4:D:105:MET:HG3	4:D:171:LEU:HD21	1.96	0.48
7:G:80:VAL:HG23	7:G:81:GLY:N	2.28	0.48
17:Q:58:VAL:HB	17:Q:80:GLU:HG3	1.94	0.48
22:a:1870:C:HO2'	22:a:1871:A:H8	1.61	0.48
27:f:102:ARG:NH2	52:4:25:ARG:O	2.47	0.48
28:g:44:LYS:O	28:g:50:LEU:HA	2.14	0.48
40:s:43:ILE:O	40:s:47:VAL:HG12	2.14	0.48
47:z:46:ASP:OD1	47:z:46:ASP:N	2.40	0.48
1:A:31:G:N1	1:A:48:C:H5''	2.28	0.48
1:A:736:C:H2'	1:A:737:C:H6	1.78	0.48
1:A:939:G:N3	1:A:1375:A:H2	2.12	0.48
1:A:1002:G:H2'	1:A:1003:G:O4'	2.14	0.48
2:B:91:PHE:CE1	2:B:150:GLY:HA3	2.49	0.48
22:a:1447:C:O2'	22:a:1544:A:N3	2.42	0.48
23:b:66:A:N6	23:b:107:G:H2'	2.29	0.48
39:r:73:LYS:HB2	39:r:106:VAL:HB	1.96	0.48
55:V:10:2MG:H2'	55:V:11:C:C6	2.49	0.48
1:A:181:A:N6	1:A:195:A:N7	2.62	0.48
2:B:163:VAL:HG11	2:B:173:ILE:HD11	1.95	0.48
5:E:56:VAL:O	5:E:60:ILE:HG12	2.14	0.48
7:G:56:LYS:HG3	7:G:57:SER:H	1.79	0.48
9:I:120:LYS:HB3	9:I:120:LYS:HE2	1.68	0.48
14:N:47:LYS:O	14:N:50:THR:HG22	2.14	0.48
22:a:279:A:H2'	22:a:280:U:O4'	2.14	0.48
22:a:2328:A:H2'	22:a:2329:U:H6	1.78	0.48
22:a:2430:A:N3	22:a:2430:A:H2'	2.27	0.48
28:g:90:VAL:HG12	28:g:91:GLY:N	2.28	0.48
29:h:3:VAL:CG2	29:h:36:ALA:HB1	2.44	0.48
40:s:69:ARG:HG2	40:s:74:ILE:HD13	1.94	0.48
50:2:9:GLY:O	50:2:13:ARG:HD2	2.13	0.48
55:V:28:C:H2'	55:V:29:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:G:H21	5:E:23:LYS:HA	1.79	0.47
1:A:1319:A:C8	1:A:1323:G:C6	3.02	0.47
10:J:10:LEU:CD2	10:J:98:VAL:HG12	2.44	0.47
11:K:107:ILE:HD11	21:U:12:PHE:CD1	2.48	0.47
22:a:645:C:H2'	22:a:647:G:C8	2.49	0.47
28:g:42:GLU:O	28:g:52:PHE:HA	2.14	0.47
1:A:159:G:H5'	1:A:160:A:OP2	2.15	0.47
5:E:154:ALA:HB2	5:E:164:ILE:HG13	1.95	0.47
9:I:21:ILE:HG22	9:I:63:LEU:HD13	1.95	0.47
9:I:71:GLY:O	9:I:75:GLN:HG3	2.14	0.47
22:a:1490:A:O2'	24:c:98:ASP:OD2	2.31	0.47
22:a:1842:G:H2'	22:a:1843:C:C6	2.49	0.47
38:q:14:VAL:HG12	38:q:20:VAL:HG21	1.96	0.47
1:A:1005:A:H2'	1:A:1006:G:O4'	2.14	0.47
1:A:1316:G:N1	1:A:1319:A:OP2	2.46	0.47
21:U:13:ASP:OD2	21:U:17:ARG:NH1	2.47	0.47
22:a:463:G:N2	22:a:466:A:OP2	2.40	0.47
22:a:1019:U:OP1	22:a:1035:U:O2'	2.26	0.47
22:a:1548:A:H2'	22:a:1549:A:C8	2.48	0.47
24:c:121:ASP:OD1	24:c:121:ASP:N	2.42	0.47
45:x:13:GLU:HA	45:x:16:THR:HG22	1.96	0.47
48:0:17:THR:HG21	48:0:40:ASP:OD1	2.14	0.47
1:A:413:G:O2'	1:A:428:G:N2	2.47	0.47
1:A:464:U:HO2'	1:A:465:A:P	2.37	0.47
1:A:575:G:O2'	1:A:821:G:OP2	2.30	0.47
6:F:47:LEU:HD13	6:F:51:ILE:HD12	1.96	0.47
7:G:4:ARG:HG3	7:G:4:ARG:NH1	2.29	0.47
22:a:321:U:O3'	26:e:162:ARG:NH1	2.44	0.47
22:a:538:A:H5''	30:i:7:LYS:HE3	1.95	0.47
42:u:86:LEU:HD13	42:u:89:ILE:HD11	1.96	0.47
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.47
22:a:1180:U:H2'	22:a:1181:U:O4'	2.14	0.47
22:a:1506:U:H2'	22:a:1507:C:C6	2.48	0.47
22:a:2799:A:O2'	22:a:2800:A:H5''	2.14	0.47
22:a:2812:G:H2'	22:a:2813:A:C8	2.49	0.47
26:e:14:VAL:HA	26:e:197:GLU:OE2	2.14	0.47
26:e:136:GLN:OE1	26:e:136:GLN:HA	2.15	0.47
40:s:6:ARG:O	40:s:10:VAL:HG13	2.14	0.47
43:v:36:ILE:HD12	43:v:58:THR:HG21	1.96	0.47
1:A:736:C:H2'	1:A:737:C:C6	2.50	0.47
26:e:48:THR:HG22	26:e:86:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:m:18:GLN:HE21	34:m:22:ARG:NH1	2.13	0.47
1:A:321:A:H2'	1:A:322:C:C6	2.49	0.47
1:A:1120:C:H2'	1:A:1121:U:C6	2.50	0.47
4:D:58:LYS:NZ	4:D:69:GLU:OE1	2.48	0.47
15:O:79:THR:O	15:O:83:GLU:OE2	2.33	0.47
22:a:1937:A:O2'	22:a:1939:5MU:OP2	2.31	0.47
23:b:2:G:H2'	23:b:3:C:C6	2.49	0.47
27:f:17:MET:SD	27:f:22:TYR:HB2	2.55	0.47
27:f:42:GLU:OE2	27:f:42:GLU:N	2.48	0.47
28:g:43:VAL:C	28:g:44:LYS:HD2	2.39	0.47
38:q:11:GLN:HE21	38:q:39:LEU:HG	1.79	0.47
41:t:6:ARG:N	41:t:9:ASP:OD2	2.36	0.47
45:x:7:ARG:NH1	45:x:59:GLU:OE2	2.48	0.47
46:y:6:LYS:NZ	46:y:37:GLU:OE2	2.29	0.47
54:Z:67:C:O2'	54:Z:68:C:OP1	2.26	0.47
7:G:99:LEU:HD12	7:G:103:TRP:CZ2	2.49	0.47
10:J:21:ALA:O	10:J:25:ILE:HG12	2.15	0.47
12:L:39:THR:HG21	12:L:49:LEU:HB3	1.96	0.47
22:a:784:G:H5'	22:a:785:G:OP1	2.15	0.47
31:j:1:MET:SD	31:j:67:LYS:HE3	2.54	0.47
41:t:58:ILE:HG13	41:t:58:ILE:O	2.15	0.47
1:A:1031:C:O3'	1:A:1032:G:N2	2.47	0.47
4:D:105:MET:HE1	4:D:143:VAL:CG1	2.45	0.47
17:Q:68:SER:OG	17:Q:69:LYS:N	2.48	0.47
22:a:1441:G:H2'	22:a:1442:U:C6	2.50	0.47
30:i:11:VAL:HG21	30:i:50:THR:HG22	1.97	0.47
1:A:222:C:H2'	1:A:223:A:H8	1.79	0.47
1:A:1157:A:C2	1:A:1181:G:C4	3.02	0.47
22:a:2515:C:H2'	22:a:2516:A:H8	1.79	0.47
22:a:2820:A:O2'	22:a:2821:A:OP1	2.28	0.47
1:A:39:G:C4	1:A:404:G:N2	2.83	0.46
22:a:207:A:H2'	22:a:208:C:O4'	2.15	0.46
22:a:532:A:N7	22:a:2021:C:O2'	2.34	0.46
48:O:9:ILE:HD12	48:O:51:GLU:HG3	1.97	0.46
1:A:1359:C:P	14:N:75:ARG:HH21	2.38	0.46
1:A:1496:C:H2'	1:A:1497:G:O4'	2.15	0.46
9:I:58:VAL:HG13	9:I:59:GLU:OE2	2.15	0.46
11:K:72:ASP:O	11:K:75:LYS:HG2	2.15	0.46
13:M:66:GLU:OE2	13:M:66:GLU:N	2.46	0.46
22:a:414:C:H2'	22:a:415:A:H8	1.80	0.46
22:a:2532:G:O2'	22:a:2657:A:N1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2801:G:H2'	22:a:2802:G:H8	1.80	0.46
42:u:56:PHE:O	42:u:61:LEU:HD11	2.16	0.46
1:A:62:U:O2'	1:A:379:C:O2	2.33	0.46
1:A:744:C:H2'	1:A:745:G:C8	2.50	0.46
1:A:1038:C:C2	1:A:1039:G:C8	3.04	0.46
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.49	0.46
5:E:157:ARG:HD3	8:H:45:PHE:CE1	2.51	0.46
9:I:9:THR:H	9:I:85:ARG:HD2	1.80	0.46
11:K:113:VAL:O	11:K:113:VAL:HG12	2.15	0.46
13:M:9:ILE:HD12	13:M:18:ALA:HB1	1.97	0.46
16:P:23:ASP:OD1	16:P:24:SER:N	2.49	0.46
22:a:357:C:H2'	22:a:358:U:C6	2.51	0.46
22:a:363:G:H2'	22:a:364:C:H6	1.79	0.46
22:a:645:C:H2'	22:a:647:G:N7	2.30	0.46
22:a:1796:U:H2'	22:a:1797:G:H8	1.80	0.46
1:A:1026:G:O2'	1:A:1027:C:OP1	2.31	0.46
2:B:15:HIS:HA	2:B:41:ILE:HG22	1.96	0.46
11:K:56:ARG:HG3	11:K:56:ARG:NH1	2.28	0.46
22:a:58:G:H2'	22:a:59:U:C6	2.51	0.46
22:a:479:A:H4'	22:a:480:A:H5'	1.96	0.46
22:a:871:U:H2'	22:a:872:U:C6	2.51	0.46
22:a:2658:C:P	28:g:160:LYS:HZ1	2.39	0.46
22:a:2848:G:C8	36:o:95:ALA:HB2	2.51	0.46
24:c:3:VAL:HG12	24:c:19:VAL:HG22	1.97	0.46
46:y:4:THR:HB	46:y:37:GLU:OE1	2.15	0.46
1:A:1377:A:OP1	7:G:92:ARG:NH2	2.49	0.46
7:G:57:SER:OG	7:G:60:GLU:OE1	2.34	0.46
10:J:27:GLU:HB3	10:J:31:ARG:NH1	2.30	0.46
10:J:32:THR:HA	10:J:82:LYS:NZ	2.30	0.46
16:P:59:HIS:NE2	16:P:63:GLN:OE1	2.49	0.46
22:a:45:G:H5''	22:a:46:G:O5'	2.15	0.46
22:a:613:A:H2'	22:a:614:A:O4'	2.14	0.46
22:a:1197:G:H2'	22:a:1198:U:H6	1.80	0.46
22:a:1684:G:H2'	22:a:1685:C:C6	2.51	0.46
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.98	0.46
40:s:6:ARG:NH2	40:s:37:ASP:OD1	2.41	0.46
1:A:440:C:C2	1:A:441:A:C8	3.03	0.46
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.97	0.46
14:N:29:ALA:O	14:N:33:ASP:HB2	2.15	0.46
22:a:2000:C:OP1	34:m:5:LYS:NZ	2.45	0.46
22:a:2557:G:H2'	22:a:2558:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:103:ILE:HG22	28:g:105:LEU:HD22	1.97	0.46
33:l:27:SER:N	33:l:104:GLU:OE2	2.48	0.46
1:A:1004:A:N6	1:A:1026:G:H1'	2.31	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.15	0.46
6:F:38:ARG:HD3	6:F:98:GLU:H	1.79	0.46
10:J:9:ARG:NH2	10:J:71:LEU:HD21	2.30	0.46
22:a:396:G:OP2	44:w:10:LYS:NZ	2.36	0.46
22:a:881:G:H2'	22:a:882:G:C8	2.49	0.46
22:a:2025:C:H2'	22:a:2026:U:C6	2.50	0.46
1:A:523:A:N6	12:L:89:D2T:OD2	2.38	0.46
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.46
1:A:983:A:H5'	1:A:984:C:OP2	2.15	0.46
1:A:1027:C:C2	1:A:1028:C:C5	3.04	0.46
22:a:84:A:N1	22:a:98:G:O2'	2.47	0.46
22:a:2071:A:H2'	22:a:2072:C:C6	2.50	0.46
22:a:2086:U:H2'	22:a:2087:G:C8	2.51	0.46
22:a:2243:U:H2'	22:a:2244:U:C6	2.51	0.46
24:c:240:PHE:O	24:c:242:LYS:HG3	2.15	0.46
27:f:37:ASN:OD1	27:f:38:MET:N	2.49	0.46
1:A:1121:U:H2'	1:A:1122:U:H6	1.81	0.46
1:A:1410:A:H2'	1:A:1411:C:C6	2.50	0.46
7:G:113:ASP:HB3	7:G:118:LEU:HD23	1.98	0.46
18:R:26:ILE:HD11	18:R:67:LEU:HD23	1.98	0.46
22:a:1656:C:H2'	22:a:1657:U:H6	1.81	0.46
22:a:1715:G:O2'	22:a:1743:G:O6	2.30	0.46
22:a:2281:A:O2'	22:a:2282:G:H5'	2.15	0.46
22:a:2896:C:H2'	22:a:2897:U:C6	2.51	0.46
23:b:2:G:H2'	23:b:3:C:H6	1.81	0.46
44:w:12:PRO:HB3	44:w:30:LEU:HD23	1.98	0.46
55:V:11:C:H2'	55:V:12:U:C6	2.51	0.46
1:A:1037:C:H2'	1:A:1038:C:C6	2.51	0.46
1:A:1314:C:H2'	1:A:1315:U:H6	1.81	0.46
1:A:1373:G:N7	9:I:13:LYS:NZ	2.64	0.46
1:A:1530:G:H2'	1:A:1531:A:C8	2.51	0.46
5:E:13:GLU:HG3	5:E:39:VAL:HG23	1.97	0.46
10:J:66:GLU:OE2	10:J:68:ARG:NH2	2.34	0.46
11:K:26:SER:OG	11:K:27:PHE:N	2.49	0.46
22:a:306:U:H2'	22:a:307:G:O4'	2.15	0.46
29:h:24:GLY:O	29:h:28:ASN:HB2	2.16	0.46
38:q:71:LYS:HE3	38:q:90:ARG:HD2	1.98	0.46
1:A:398:U:H2'	1:A:399:G:C8	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.51	0.45
9:I:60:LYS:C	9:I:61:LEU:HD12	2.40	0.45
22:a:969:G:H2'	22:a:970:U:C6	2.51	0.45
22:a:2402:U:O2'	22:a:2403:C:O5'	2.34	0.45
24:c:117:GLN:N	24:c:128:ASN:OD1	2.49	0.45
3:C:120:ILE:HD11	3:C:137:ALA:HB2	1.98	0.45
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.99	0.45
7:G:47:LEU:HD23	7:G:47:LEU:HA	1.79	0.45
22:a:1182:G:H2'	22:a:1183:U:O4'	2.17	0.45
22:a:1443:U:H2'	22:a:1444:G:H8	1.82	0.45
22:a:2246:G:H2'	22:a:2247:A:H8	1.81	0.45
24:c:28:LYS:HA	24:c:28:LYS:HD3	1.84	0.45
28:g:43:VAL:HG12	28:g:52:PHE:CD1	2.51	0.45
44:w:59:ILE:HG12	44:w:67:VAL:HG21	1.98	0.45
54:Z:22:A:H61	54:Z:47:A:H2'	1.81	0.45
1:A:418:C:H2'	1:A:419:C:C6	2.52	0.45
1:A:1008:U:H2'	1:A:1009:U:O4'	2.16	0.45
1:A:1086:U:H3	1:A:1099:G:H22	1.64	0.45
1:A:1238:A:H2	1:A:1241:G:N3	2.15	0.45
22:a:876:C:H2'	22:a:877:A:O4'	2.16	0.45
22:a:2481:G:O2'	22:a:2482:A:H8	1.99	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.52	0.45
1:A:412:A:O2'	1:A:413:G:H4'	2.16	0.45
1:A:632:U:H5''	1:A:633:G:C8	2.52	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.16	0.45
22:a:1278:C:H2'	22:a:1279:G:H8	1.81	0.45
22:a:2698:U:H2'	22:a:2699:C:C6	2.52	0.45
25:d:19:GLY:HA3	36:o:80:VAL:HG23	1.98	0.45
44:w:64:ILE:HG13	44:w:68:LEU:HD13	1.97	0.45
1:A:460:A:H2'	1:A:461:A:H8	1.82	0.45
1:A:476:U:H2'	1:A:477:C:C6	2.52	0.45
1:A:546:A:OP1	4:D:69:GLU:HB3	2.16	0.45
1:A:613:C:OP1	4:D:81:ARG:NH2	2.41	0.45
1:A:999:C:H2'	1:A:1000:A:H8	1.82	0.45
2:B:64:LYS:O	2:B:64:LYS:HD3	2.17	0.45
13:M:107:ARG:NH2	13:M:110:LYS:HE2	2.32	0.45
22:a:64:A:H2'	22:a:65:U:H6	1.82	0.45
22:a:528:A:H5''	30:i:113:PRO:HG3	1.99	0.45
22:a:2726:A:O2'	22:a:2727:A:O5'	2.26	0.45
42:u:77:VAL:HG12	42:u:89:ILE:HG23	1.99	0.45
54:Z:20:G:H4'	54:Z:21:H2U:OP2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:G:P	17:Q:71:LYS:HZ1	2.38	0.45
1:A:513:C:H2'	1:A:514:C:H6	1.81	0.45
1:A:1120:C:C2	1:A:1121:U:C5	3.05	0.45
9:I:44:ALA:O	9:I:48:VAL:HG23	2.16	0.45
11:K:117:PRO:HD2	21:U:35:ARG:HH11	1.81	0.45
22:a:170:U:H2'	22:a:171:U:C6	2.52	0.45
22:a:224:U:OP2	22:a:408:G:N2	2.46	0.45
22:a:638:G:H2'	22:a:639:U:C6	2.52	0.45
22:a:2481:G:O2'	22:a:2482:A:P	2.74	0.45
22:a:2552:OMU:HM23	22:a:2554:U:C6	2.51	0.45
22:a:2591:C:H2'	22:a:2592:G:H8	1.80	0.45
4:D:102:VAL:HG23	4:D:107:PHE:HD2	1.82	0.45
6:F:96:VAL:HG12	6:F:96:VAL:O	2.16	0.45
7:G:80:VAL:HG21	7:G:85:TYR:CZ	2.51	0.45
17:Q:4:LYS:HE3	17:Q:4:LYS:HB3	1.82	0.45
22:a:2271:G:OP1	43:v:18:ALA:HB1	2.17	0.45
22:a:2579:C:O2'	25:d:136:ASN:ND2	2.50	0.45
22:a:2638:G:O2'	22:a:2775:G:N2	2.44	0.45
52:4:20:ASN:ND2	52:4:39:LYS:HE2	2.31	0.45
1:A:165:G:H2'	1:A:166:U:H6	1.80	0.45
1:A:202:G:H1'	1:A:468:A:H2	1.81	0.45
1:A:264:C:O2'	17:Q:66:PRO:O	2.34	0.45
1:A:513:C:H2'	1:A:514:C:C6	2.51	0.45
1:A:539:A:H2'	1:A:540:G:C8	2.52	0.45
1:A:988:G:H1'	1:A:1015:G:H22	1.81	0.45
1:A:1167:A:O2'	1:A:1169:A:N7	2.44	0.45
4:D:170:TRP:CD2	4:D:186:PRO:HB3	2.52	0.45
10:J:57:VAL:O	10:J:58:ASN:HB2	2.16	0.45
22:a:299:A:N3	22:a:319:G:O2'	2.42	0.45
22:a:1428:C:C5	22:a:1569:A:H5''	2.52	0.45
22:a:2394:C:H5''	32:k:63:LYS:HE2	1.99	0.45
41:t:67:VAL:C	41:t:69:ASN:H	2.25	0.45
50:2:32:ILE:O	50:2:32:ILE:HG13	2.16	0.45
1:A:618:C:H5'	1:A:619:U:H5''	1.98	0.45
1:A:1092:A:H4'	7:G:4:ARG:HH22	1.82	0.45
1:A:1095:U:H2'	1:A:1096:C:C6	2.52	0.45
2:B:35:ARG:O	2:B:38:VAL:HG12	2.16	0.45
5:E:131:THR:HG22	5:E:131:THR:O	2.17	0.45
5:E:160:SER:O	5:E:164:ILE:HG12	2.17	0.45
10:J:11:LYS:HG2	10:J:71:LEU:HD13	1.98	0.45
12:L:76:GLU:HG3	12:L:77:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:89:D2T:OD2	12:L:89:D2T:N	2.50	0.45
22:a:24:G:O2'	39:r:78:GLU:O	2.34	0.45
22:a:693:A:O2'	22:a:1353:A:N3	2.41	0.45
22:a:880:G:H2'	22:a:881:G:C8	2.51	0.45
41:t:95:PHE:HD2	41:t:100:SER:HA	1.81	0.45
1:A:674:G:H21	11:K:118:HIS:HB2	1.82	0.45
2:B:27:MET:HE1	2:B:193:PRO:HG3	1.98	0.45
2:B:133:GLU:HA	2:B:136:MET:HG2	1.99	0.45
22:a:182:A:H2'	22:a:183:C:H6	1.81	0.45
22:a:549:G:H2'	22:a:550:C:C6	2.53	0.45
25:d:46:ARG:NH2	25:d:88:GLU:O	2.50	0.45
39:r:1:MET:HE3	39:r:1:MET:HB2	1.89	0.45
1:A:635:A:H2'	1:A:636:U:H6	1.82	0.44
1:A:1144:G:N2	1:A:1146:A:H62	2.16	0.44
2:B:117:LEU:HB3	2:B:141:LEU:HD12	1.98	0.44
4:D:21:LEU:HD23	4:D:21:LEU:O	2.17	0.44
7:G:27:VAL:HG22	7:G:43:VAL:HG21	1.99	0.44
16:P:70:ARG:HA	16:P:70:ARG:HD2	1.75	0.44
22:a:1637:A:H5'	22:a:1760:C:O2'	2.17	0.44
22:a:2718:G:O2'	22:a:2847:U:OP1	2.35	0.44
28:g:155:GLU:OE1	28:g:158:LYS:N	2.50	0.44
1:A:299:G:H2'	1:A:300:A:C8	2.52	0.44
1:A:373:A:C2	1:A:374:A:C8	3.05	0.44
1:A:478:A:H2'	1:A:479:U:O4'	2.17	0.44
7:G:111:ARG:NH2	7:G:122:ASN:HB3	2.33	0.44
22:a:635:C:OP2	32:k:109:LYS:NZ	2.48	0.44
22:a:1047:G:O2'	22:a:1110:G:N1	2.42	0.44
22:a:1386:C:H2'	22:a:1387:A:H8	1.82	0.44
22:a:2006:C:O2'	22:a:2823:A:N3	2.49	0.44
22:a:2591:C:H2'	22:a:2592:G:C8	2.52	0.44
36:o:89:ARG:HE	36:o:113:ARG:NH2	2.15	0.44
38:q:61:ALA:HB1	38:q:96:VAL:HG22	1.99	0.44
52:4:59:ARG:CZ	52:4:63:ARG:HH22	2.30	0.44
10:J:27:GLU:HB3	10:J:31:ARG:HH12	1.82	0.44
22:a:1028:A:H2'	22:a:1029:A:C8	2.52	0.44
22:a:2636:C:H2'	22:a:2637:U:H6	1.83	0.44
22:a:2803:G:H2'	22:a:2804:U:H6	1.82	0.44
28:g:40:ALA:HA	28:g:55:ARG:HG3	1.99	0.44
2:B:208:ARG:O	2:B:212:LEU:HD23	2.16	0.44
15:O:72:ARG:HH11	15:O:72:ARG:HG3	1.83	0.44
25:d:32:ASN:HD22	25:d:52:THR:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:C:H2'	1:A:35:G:H8	1.82	0.44
1:A:634:C:H2'	1:A:635:A:C8	2.53	0.44
1:A:757:U:OP1	1:A:822:U:O2'	2.32	0.44
1:A:1107:C:C4	1:A:1108:G:C8	3.06	0.44
5:E:107:ALA:HB1	5:E:111:MET:HB2	1.99	0.44
22:a:358:U:H2'	22:a:359:G:C8	2.52	0.44
22:a:1281:G:H2'	22:a:1282:U:C6	2.53	0.44
22:a:2064:C:H2'	22:a:2065:C:C6	2.52	0.44
22:a:2258:C:O2'	22:a:2427:C:OP2	2.32	0.44
22:a:2537:U:H2'	22:a:2538:C:C6	2.52	0.44
27:f:38:MET:HB2	27:f:87:CYS:SG	2.58	0.44
55:V:25:C:C2	55:V:26:A:C8	3.06	0.44
55:V:47:H2U:H2'	55:V:47:H2U:H61	1.65	0.44
11:K:53:ARG:HH21	11:K:57:LYS:NZ	2.15	0.44
22:a:157:C:H2'	22:a:158:U:O4'	2.18	0.44
22:a:1141:U:H4'	22:a:1142:A:O4'	2.18	0.44
22:a:2402:U:O2'	22:a:2403:C:H6	2.01	0.44
33:l:21:ALA:HB2	33:l:97:GLN:HB2	1.99	0.44
1:A:35:G:H2'	1:A:36:C:C6	2.53	0.44
1:A:411:A:P	4:D:26:ARG:HH12	2.39	0.44
1:A:685:G:O2'	1:A:686:U:H5'	2.18	0.44
2:B:214:LEU:HA	2:B:217:VAL:HG12	2.00	0.44
22:a:1444:G:C4	22:a:1445:G:C8	3.06	0.44
30:i:114:LEU:O	30:i:118:MET:HG3	2.17	0.44
35:n:2:ASP:HB3	35:n:5:SER:OG	2.18	0.44
55:V:14:A:C5	55:V:22:G:C2	3.06	0.44
1:A:310:G:H5''	16:P:31:ARG:HG2	1.99	0.44
1:A:652:U:O4	1:A:752:G:O2'	2.27	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	2.00	0.44
6:F:66:ALA:HB3	6:F:71:ILE:HD11	2.00	0.44
22:a:742:A:H2'	22:a:743:A:H8	1.82	0.44
22:a:2327:A:H2'	22:a:2328:A:C8	2.53	0.44
22:a:2585:U:O2'	22:a:2586:U:O5'	2.34	0.44
22:a:2803:G:H2'	22:a:2804:U:C6	2.52	0.44
24:c:75:PRO:HG2	24:c:97:LYS:HG3	2.00	0.44
27:f:29:PRO:HB2	27:f:169:LEU:HD22	1.98	0.44
51:3:24:ARG:NH1	51:3:36:ARG:HD2	2.33	0.44
2:B:46:THR:HA	2:B:49:MET:HE2	2.00	0.44
19:S:36:ARG:HD2	19:S:52:HIS:O	2.17	0.44
24:c:129:THR:C	24:c:130:LEU:HD12	2.43	0.44
30:i:32:LEU:HD22	30:i:54:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:i:36:LEU:HD11	30:i:122:LEU:HB2	2.00	0.44
41:t:33:LYS:HB3	41:t:64:ALA:HB1	1.99	0.44
1:A:674:G:H2'	1:A:675:A:H8	1.83	0.43
1:A:1035:A:C8	1:A:1036:A:C2	3.06	0.43
2:B:167:ASP:HB3	2:B:191:SER:HA	2.00	0.43
5:E:94:VAL:HB	5:E:111:MET:HE1	2.00	0.43
9:I:6:TYR:HB2	9:I:21:ILE:CG1	2.48	0.43
9:I:57:MET:HE1	9:I:90:TYR:CE2	2.53	0.43
12:L:114:ARG:HB3	12:L:119:VAL:HB	2.00	0.43
22:a:1496:A:H2'	22:a:1498:C:C5	2.53	0.43
22:a:2839:G:O2'	34:m:49:GLU:OE1	2.21	0.43
23:b:75:G:H21	42:u:88:HIS:CE1	2.35	0.43
25:d:11:MET:HE2	25:d:11:MET:HB3	1.88	0.43
33:l:17:ASN:CG	33:l:95:LEU:HD12	2.42	0.43
35:n:53:THR:HB	35:n:65:THR:HB	2.00	0.43
38:q:20:VAL:HG12	38:q:22:LEU:HD12	2.00	0.43
41:t:100:SER:O	41:t:100:SER:OG	2.33	0.43
1:A:44:A:H2'	1:A:45:G:H8	1.83	0.43
1:A:946:A:O2'	1:A:1333:A:N3	2.46	0.43
1:A:1218:C:H2'	1:A:1219:A:H8	1.82	0.43
1:A:1272:G:H2'	1:A:1273:C:C6	2.53	0.43
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.43
2:B:35:ARG:HB2	2:B:35:ARG:CZ	2.47	0.43
10:J:5:ARG:O	10:J:6:ILE:HD13	2.17	0.43
11:K:19:GLY:O	11:K:82:LEU:HA	2.19	0.43
17:Q:16:LYS:HB2	17:Q:16:LYS:HE2	1.88	0.43
22:a:356:G:C6	22:a:357:C:C4	3.06	0.43
30:i:99:ARG:HD2	30:i:99:ARG:HA	1.80	0.43
1:A:464:U:HO2'	1:A:465:A:C5'	2.28	0.43
1:A:1355:G:H2'	1:A:1356:G:C8	2.52	0.43
3:C:64:ILE:O	3:C:99:ALA:HA	2.18	0.43
6:F:12:PRO:O	6:F:44:ARG:NH2	2.51	0.43
9:I:60:LYS:HB2	9:I:61:LEU:HD12	2.00	0.43
9:I:60:LYS:HD3	9:I:60:LYS:N	2.33	0.43
22:a:570:G:H2'	22:a:2030:6MZ:N7	2.33	0.43
1:A:224:U:H2'	1:A:225:C:C6	2.54	0.43
1:A:253:A:H2'	1:A:254:G:H8	1.83	0.43
1:A:268:U:H2'	1:A:269:C:H6	1.83	0.43
1:A:746:A:H2'	1:A:747:A:C8	2.53	0.43
1:A:1176:A:H3'	1:A:1177:G:H8	1.83	0.43
8:H:13:ARG:HD2	8:H:27:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:51:GLY:O	13:M:55:THR:HG23	2.18	0.43
22:a:155:A:H2'	22:a:156:A:H8	1.84	0.43
22:a:848:C:H2'	22:a:849:A:C8	2.51	0.43
22:a:1636:U:H2'	22:a:1637:A:C8	2.54	0.43
43:v:23:VAL:HG22	43:v:38:VAL:HG12	2.00	0.43
1:A:72:A:H2'	1:A:72:A:N3	2.33	0.43
1:A:1157:A:N7	1:A:1180:A:N6	2.67	0.43
2:B:45:LYS:HB2	2:B:45:LYS:HE2	1.67	0.43
22:a:636:G:N2	32:k:76:GLU:OE1	2.50	0.43
22:a:832:U:H2'	22:a:833:A:H8	1.83	0.43
28:g:94:TYR:HA	28:g:106:SER:O	2.18	0.43
1:A:195:A:H2'	1:A:196:A:C8	2.53	0.43
3:C:153:VAL:HG12	3:C:157:LEU:HD21	1.99	0.43
22:a:1814:G:H4'	24:c:51:THR:HG21	2.01	0.43
22:a:1915:3TD:H6	22:a:1915:3TD:O5'	2.18	0.43
22:a:2097:A:H2'	22:a:2098:U:C6	2.54	0.43
22:a:2801:G:H2'	22:a:2802:G:C8	2.53	0.43
22:a:2834:G:H2'	22:a:2879:A:H61	1.83	0.43
23:b:36:C:N4	23:b:49:C:O2'	2.42	0.43
36:o:91:ALA:HB2	36:o:113:ARG:HB2	2.00	0.43
48:0:10:LYS:O	48:0:52:ALA:N	2.49	0.43
50:2:26:HIS:HB3	50:2:44:LEU:HD22	2.00	0.43
54:Z:24:C:H2'	54:Z:25:U:C6	2.54	0.43
5:E:95:PHE:CE2	5:E:97:GLN:HG3	2.53	0.43
6:F:15:SER:HA	6:F:18:VAL:HG23	2.00	0.43
9:I:12:ARG:O	9:I:13:LYS:C	2.62	0.43
10:J:59:LYS:HE2	10:J:62:ARG:NH2	2.33	0.43
22:a:3:U:H2'	22:a:4:U:H6	1.84	0.43
22:a:144:A:H4'	40:s:3:ARG:HH12	1.84	0.43
22:a:471:A:H2'	22:a:472:A:O4'	2.19	0.43
22:a:1541:C:H2'	22:a:1542:U:C6	2.54	0.43
22:a:1799:G:OP1	24:c:258:ARG:NH1	2.47	0.43
27:f:103:LEU:HA	27:f:107:ALA:HB3	1.99	0.43
28:g:80:THR:OG1	28:g:81:GLU:OE1	2.26	0.43
33:l:22:GLN:HA	33:l:22:GLN:OE1	2.19	0.43
35:n:115:LEU:HD23	35:n:115:LEU:HA	1.88	0.43
1:A:1463:U:H2'	1:A:1464:U:H6	1.83	0.43
22:a:352:A:H2'	22:a:353:C:O4'	2.18	0.43
22:a:2419:U:H4'	48:0:22:THR:HG21	2.00	0.43
24:c:228:VAL:HG13	24:c:229:ASP:OD1	2.19	0.43
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:G:H21	1:A:1167:A:H61	1.66	0.43
1:A:1527:U:H5	21:U:42:THR:HG21	1.82	0.43
1:A:1530:G:H2'	1:A:1531:A:H8	1.83	0.43
10:J:84:VAL:O	10:J:88:MET:HG3	2.18	0.43
21:U:7:ARG:HG2	21:U:10:GLU:OE2	2.19	0.43
22:a:17:G:H2'	22:a:18:U:C6	2.53	0.43
22:a:645:C:O2'	22:a:646:U:H5''	2.19	0.43
22:a:1007:C:OP1	30:i:37:ARG:NH2	2.52	0.43
22:a:1041:G:C2	22:a:1042:G:C8	3.06	0.43
22:a:1583:A:O2'	22:a:1585:C:N4	2.52	0.43
22:a:1928:A:H2'	22:a:1929:G:O4'	2.19	0.43
22:a:2577:A:H2'	22:a:2614:A:N6	2.34	0.43
23:b:54:G:N2	27:f:26:MET:SD	2.91	0.43
26:e:31:VAL:HG22	26:e:96:VAL:HG11	2.00	0.43
33:l:20:LEU:HD13	42:u:81:PRO:HG3	2.01	0.43
35:n:4:LYS:O	35:n:8:ILE:HG12	2.19	0.43
38:q:65:ALA:HB3	38:q:95:ASP:HB2	2.00	0.43
42:u:55:GLU:O	42:u:59:GLU:HG2	2.18	0.43
44:w:77:LYS:HA	44:w:77:LYS:HD2	1.75	0.43
1:A:1026:G:HO2'	1:A:1027:C:P	2.42	0.43
1:A:1152:A:OP1	10:J:72:ARG:NH2	2.37	0.43
2:B:68:LEU:HD21	2:B:151:ILE:HD11	2.01	0.43
2:B:107:VAL:O	2:B:111:ILE:HG12	2.19	0.43
5:E:35:ALA:HB1	5:E:60:ILE:HD13	2.01	0.43
5:E:147:MET:HE2	5:E:147:MET:HB3	1.78	0.43
5:E:159:LYS:HB2	5:E:164:ILE:HD11	2.00	0.43
22:a:191:A:H2'	22:a:192:C:H6	1.83	0.43
28:g:96:ALA:HB1	28:g:131:ILE:HD11	1.99	0.43
32:k:81:ASP:HB3	32:k:100:ILE:HD12	1.99	0.43
46:y:45:ARG:HH12	46:y:59:GLU:CD	2.27	0.43
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.42
1:A:264:C:H2'	1:A:265:G:O4'	2.19	0.42
1:A:1005:A:O5'	1:A:1005:A:H8	2.02	0.42
10:J:24:GLU:OE2	10:J:90:LEU:HD11	2.19	0.42
16:P:52:LEU:HD23	16:P:78:VAL:HG21	2.00	0.42
18:R:11:CYS:HB3	18:R:14:THR:HG22	2.00	0.42
19:S:50:ALA:HB1	19:S:57:HIS:HB3	2.01	0.42
22:a:1:G:H2'	22:a:2:G:H8	1.83	0.42
22:a:276:U:O2'	22:a:277:G:O5'	2.35	0.42
22:a:1386:C:H2'	22:a:1387:A:C8	2.54	0.42
22:a:1539:U:H2'	22:a:1540:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2313:C:O4'	27:f:37:ASN:ND2	2.52	0.42
22:a:2373:G:H2'	22:a:2374:C:C6	2.54	0.42
26:e:171:ASP:OD1	26:e:171:ASP:N	2.52	0.42
30:i:36:LEU:O	30:i:51:GLY:HA3	2.18	0.42
33:l:41:LEU:HG	33:l:96:ILE:HG13	2.00	0.42
50:2:54:ASP:O	50:2:58:VAL:HG23	2.19	0.42
1:A:182:A:H2'	1:A:182:A:OP2	2.19	0.42
1:A:392:C:C2	1:A:393:A:C8	3.07	0.42
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.52	0.42
6:F:88:MET:HE3	6:F:90:MET:SD	2.59	0.42
22:a:379:G:N1	22:a:396:G:C6	2.87	0.42
22:a:577:G:O2'	22:a:1254:A:OP1	2.37	0.42
22:a:1405:U:H2'	22:a:1406:U:H6	1.83	0.42
22:a:2883:A:OP2	47:z:50:ARG:NH1	2.52	0.42
23:b:46:A:C5	23:b:47:C:C5	3.06	0.42
27:f:140:GLU:OE2	27:f:140:GLU:N	2.52	0.42
33:l:105:MET:HE3	33:l:108:VAL:HG21	2.00	0.42
47:z:43:ILE:HG22	47:z:49:TYR:HB2	2.01	0.42
1:A:129:A:H1'	1:A:130:A:C8	2.54	0.42
1:A:329:A:C6	1:A:332:G:C2	3.07	0.42
3:C:85:GLU:O	3:C:89:LYS:HG2	2.20	0.42
11:K:83:GLU:OE1	11:K:83:GLU:N	2.53	0.42
21:U:8:GLU:OE1	21:U:9:ASN:ND2	2.52	0.42
22:a:2329:U:H2'	22:a:2330:G:C8	2.54	0.42
23:b:1:U:H2'	23:b:2:G:C8	2.52	0.42
23:b:18:G:H2'	23:b:19:C:H6	1.84	0.42
25:d:97:SER:OG	25:d:99:GLU:OE1	2.29	0.42
31:j:107:LEU:O	31:j:109:SER:N	2.45	0.42
55:V:10:2MG:HO2'	55:V:11:C:P	2.42	0.42
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.42
1:A:678:U:H2'	1:A:679:C:C6	2.54	0.42
1:A:883:C:O2'	1:A:884:U:H5'	2.20	0.42
1:A:1041:G:H2'	1:A:1042:A:C8	2.55	0.42
22:a:545:U:HO2'	22:a:548:G:H1	1.67	0.42
22:a:1636:U:H2'	22:a:1637:A:H8	1.84	0.42
22:a:1684:G:H2'	22:a:1685:C:H6	1.83	0.42
22:a:2726:A:HO2'	22:a:2727:A:P	2.39	0.42
23:b:29:A:H2'	23:b:30:C:C6	2.54	0.42
30:i:13:ARG:HD2	30:i:53:TYR:CE1	2.55	0.42
37:p:107:THR:O	37:p:111:GLU:HG2	2.19	0.42
1:A:33:A:H2'	1:A:34:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:C:O2'	1:A:170:U:H5'	2.18	0.42
1:A:444:G:C6	1:A:491:G:C6	3.08	0.42
1:A:1010:U:H2'	1:A:1011:C:H6	1.80	0.42
1:A:1287:A:H2'	1:A:1288:A:C8	2.54	0.42
2:B:148:LEU:HD23	2:B:148:LEU:O	2.19	0.42
3:C:150:LYS:HG2	3:C:201:TRP:CE3	2.54	0.42
4:D:73:ARG:HH12	4:D:77:LYS:NZ	2.17	0.42
8:H:64:LYS:HG3	8:H:71:VAL:HG21	2.02	0.42
22:a:184:C:H2'	22:a:185:G:H8	1.84	0.42
22:a:438:G:H2'	22:a:439:A:C8	2.55	0.42
22:a:657:U:H2'	22:a:658:U:C6	2.55	0.42
22:a:878:A:C6	22:a:900:A:C8	3.08	0.42
22:a:1591:A:H2'	22:a:1592:C:C6	2.54	0.42
22:a:2804:U:H2'	22:a:2805:C:H6	1.84	0.42
23:b:45:A:C4	23:b:46:A:C8	3.08	0.42
25:d:39:ASP:N	25:d:39:ASP:OD1	2.52	0.42
29:h:12:LEU:HD13	29:h:19:VAL:HG11	2.00	0.42
39:r:31:GLN:O	39:r:35:ILE:HG13	2.19	0.42
1:A:260:G:H2'	1:A:261:U:C6	2.54	0.42
4:D:188:ARG:HE	4:D:197:GLU:CD	2.28	0.42
20:T:75:HIS:O	20:T:79:LEU:HD23	2.20	0.42
22:a:592:A:H2	50:2:4:ILE:HD11	1.83	0.42
22:a:832:U:H2'	22:a:833:A:C8	2.55	0.42
27:f:147:ASP:OD1	27:f:148:ARG:N	2.50	0.42
37:p:89:GLU:HG3	38:q:52:PRO:HB3	2.02	0.42
42:u:4:ILE:HG12	42:u:50:MET:HE1	2.01	0.42
52:4:56:ARG:HA	52:4:56:ARG:HD2	1.66	0.42
1:A:41:G:C6	1:A:402:G:C6	3.07	0.42
1:A:1029:U:H5''	1:A:1030:U:H5	1.84	0.42
3:C:114:LYS:HD2	3:C:114:LYS:HA	1.75	0.42
4:D:65:TYR:CD2	4:D:94:LEU:HB3	2.55	0.42
7:G:95:ARG:O	7:G:99:LEU:HD23	2.20	0.42
15:O:88:ARG:NH1	22:a:714:U:OP2	2.44	0.42
22:a:544:C:H2'	22:a:545:U:O4'	2.20	0.42
22:a:851:C:C2	22:a:852:U:C5	3.08	0.42
22:a:2318:G:O2'	22:a:2321:U:O4	2.35	0.42
22:a:2838:G:C4	22:a:2839:G:C8	3.08	0.42
26:e:105:LEU:HD23	26:e:105:LEU:HA	1.75	0.42
52:4:32:LEU:HD12	52:4:32:LEU:HA	1.86	0.42
1:A:312:C:H2'	1:A:313:A:C8	2.55	0.42
1:A:1073:U:O2	2:B:103:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:VAL:HG12	5:E:67:ALA:HB1	2.02	0.42
6:F:5:GLU:OE1	18:R:24:LYS:NZ	2.52	0.42
14:N:82:ILE:O	14:N:86:GLU:HG3	2.19	0.42
22:a:116:C:O2'	22:a:126:A:N3	2.47	0.42
22:a:152:A:H2'	22:a:153:U:C6	2.55	0.42
22:a:984:A:N3	22:a:984:A:H2'	2.34	0.42
22:a:2251:OMG:HM23	22:a:2251:OMG:H1'	1.59	0.42
28:g:37:LEU:HD23	28:g:37:LEU:HA	1.88	0.42
28:g:90:VAL:HG12	28:g:91:GLY:H	1.85	0.42
40:s:3:ARG:O	40:s:7:LEU:HD23	2.20	0.42
1:A:616:G:O2'	16:P:47:GLU:OE2	2.35	0.42
22:a:278:A:N6	22:a:362:A:N7	2.68	0.42
22:a:1720:U:H2'	22:a:1721:G:O4'	2.20	0.42
22:a:2096:C:H2'	22:a:2097:A:C8	2.55	0.42
22:a:2576:G:O2'	22:a:2579:C:OP2	2.35	0.42
23:b:39:A:C2	23:b:44:G:C2	3.08	0.42
34:m:54:LEU:HD22	34:m:66:ALA:HB2	2.01	0.42
36:o:6:LYS:O	36:o:10:GLN:HG2	2.20	0.42
39:r:41:LYS:HE3	47:z:22:LEU:HD11	2.02	0.42
46:y:19:LYS:HE2	46:y:19:LYS:HB2	1.83	0.42
1:A:195:A:H1'	1:A:222:C:O2'	2.20	0.42
1:A:335:C:H2'	1:A:336:A:H8	1.85	0.42
1:A:604:G:H2'	1:A:605:U:O4'	2.20	0.42
1:A:791:G:O6	1:A:792:A:N6	2.52	0.42
1:A:1319:A:C8	1:A:1323:G:C5	3.07	0.42
5:E:37:THR:HG22	5:E:63:ALA:HB1	2.02	0.42
7:G:79:ARG:HG2	7:G:84:THR:HG22	2.01	0.42
10:J:87:LEU:HD23	10:J:87:LEU:HA	1.85	0.42
16:P:40:ASN:HB3	16:P:43:ALA:HB2	2.02	0.42
21:U:39:GLU:HG2	21:U:43:THR:HB	2.01	0.42
22:a:78:U:H2'	22:a:79:C:H6	1.85	0.42
22:a:1361:G:H2'	22:a:1362:C:C6	2.55	0.42
38:q:22:LEU:HD13	38:q:96:VAL:HG12	2.02	0.42
40:s:33:LYS:HG2	40:s:80:TRP:CZ3	2.55	0.42
42:u:3:THR:HA	42:u:62:THR:O	2.20	0.42
44:w:19:SER:OG	44:w:20:HIS:N	2.53	0.42
1:A:411:A:OP1	4:D:26:ARG:NH1	2.45	0.41
1:A:678:U:H2'	1:A:679:C:H6	1.84	0.41
4:D:69:GLU:OE2	4:D:204:TYR:OH	2.26	0.41
7:G:136:LYS:O	7:G:139:GLU:HG3	2.19	0.41
10:J:86:ALA:HA	10:J:89:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:160:A:N3	22:a:2208:C:O2'	2.50	0.41
22:a:347:A:H2'	22:a:348:A:H8	1.84	0.41
22:a:1115:G:N3	22:a:1116:G:C8	2.87	0.41
22:a:2247:A:H2'	22:a:2248:C:H6	1.85	0.41
22:a:2649:C:H2'	22:a:2650:U:H6	1.84	0.41
22:a:2807:U:H1'	22:a:2892:G:N2	2.35	0.41
28:g:9:VAL:CG1	28:g:50:LEU:HB2	2.50	0.41
28:g:127:THR:HG22	28:g:128:GLN:H	1.85	0.41
55:V:43:A:H2'	55:V:44:G:C8	2.54	0.41
1:A:253:A:H2'	1:A:254:G:C8	2.55	0.41
1:A:280:C:N3	17:Q:41:THR:HG22	2.35	0.41
1:A:1062:U:O4	3:C:2:GLY:HA2	2.20	0.41
1:A:1169:A:H2'	1:A:1170:A:C8	2.55	0.41
4:D:8:LYS:HD2	4:D:21:LEU:HD21	2.02	0.41
4:D:50:ASP:O	4:D:54:GLN:HG3	2.20	0.41
4:D:161:LEU:HD23	4:D:161:LEU:HA	1.87	0.41
22:a:700:G:O2'	22:a:1632:A:N3	2.48	0.41
22:a:1138:G:N2	30:i:108:MET:HE2	2.35	0.41
22:a:2884:U:H5	47:z:41:HIS:CD2	2.38	0.41
42:u:9:ARG:HD3	42:u:39:ALA:HB1	2.02	0.41
46:y:6:LYS:HZ3	46:y:37:GLU:CD	2.19	0.41
1:A:503:C:O2'	1:A:510:A:N1	2.51	0.41
1:A:520:A:O2'	12:L:70:GLU:OE1	2.23	0.41
1:A:1130:A:C8	1:A:1146:A:N1	2.88	0.41
2:B:96:TRP:CZ2	2:B:101:LEU:HD23	2.55	0.41
19:S:38:SER:O	19:S:71:LEU:HD12	2.20	0.41
22:a:453:A:N3	22:a:457:A:O2'	2.54	0.41
28:g:98:VAL:HG22	28:g:103:ILE:HG13	2.01	0.41
1:A:460:A:H2'	1:A:461:A:C8	2.55	0.41
1:A:865:A:H2'	1:A:866:C:C6	2.55	0.41
1:A:1009:U:O4	1:A:1020:G:O6	2.39	0.41
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.41
2:B:81:LYS:O	2:B:85:LEU:HD23	2.21	0.41
6:F:73:GLU:O	6:F:77:THR:HG23	2.21	0.41
18:R:12:ARG:O	18:R:16:GLU:HG3	2.19	0.41
22:a:319:G:H2'	22:a:320:A:O4'	2.20	0.41
22:a:910:A:C5	33:l:13:HIS:CD2	3.08	0.41
22:a:1125:G:OP2	22:a:1126:A:O2'	2.35	0.41
22:a:1563:U:H2'	22:a:1564:C:C6	2.56	0.41
22:a:2074:U:H2'	22:a:2075:U:C6	2.56	0.41
24:c:80:ARG:NE	24:c:82:GLU:OE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:24:ILE:HD13	39:r:36:LEU:HD11	2.02	0.41
41:t:74:ASN:HD22	41:t:74:ASN:C	2.26	0.41
1:A:392:C:OP2	16:P:12:LYS:HG3	2.20	0.41
5:E:45:ARG:HG3	5:E:72:ILE:O	2.19	0.41
7:G:82:GLY:HA3	53:X:14:A:C8	2.55	0.41
15:O:79:THR:O	15:O:80:GLN:C	2.63	0.41
22:a:278:A:H2	22:a:361:G:N2	2.19	0.41
22:a:1009:A:O4'	37:p:59:GLN:HG3	2.20	0.41
22:a:1551:A:H2'	22:a:1552:A:O4'	2.21	0.41
26:e:7:ASP:CG	26:e:122:GLU:H	2.29	0.41
37:p:94:ILE:HG21	38:q:4:VAL:HG11	2.02	0.41
1:A:447:G:N1	1:A:486:U:OP2	2.40	0.41
1:A:728:A:H2'	1:A:729:A:C8	2.56	0.41
1:A:936:C:C2	1:A:937:A:C8	3.09	0.41
1:A:1152:A:P	10:J:72:ARG:HH22	2.42	0.41
1:A:1250:A:H2'	1:A:1251:A:C8	2.55	0.41
4:D:188:ARG:HD2	4:D:188:ARG:HA	1.86	0.41
5:E:97:GLN:HE21	5:E:97:GLN:HB3	1.74	0.41
11:K:127:ARG:NH2	11:K:129:VAL:HG11	2.36	0.41
22:a:593:U:H2'	22:a:594:U:H6	1.86	0.41
22:a:810:U:C4	32:k:29:LYS:O	2.73	0.41
22:a:1394:U:H2'	22:a:1395:A:O4'	2.20	0.41
22:a:1842:G:H2'	22:a:1843:C:H6	1.84	0.41
28:g:2:SER:OG	28:g:3:ARG:N	2.53	0.41
41:t:99:ASN:OD1	41:t:99:ASN:C	2.63	0.41
55:V:25:C:N3	55:V:26:A:C8	2.88	0.41
1:A:1015:G:H2'	1:A:1016:A:C8	2.56	0.41
1:A:1103:C:H4'	2:B:97:LEU:HD13	2.03	0.41
1:A:1119:C:H2'	1:A:1120:C:C6	2.55	0.41
1:A:1160:G:C2	1:A:1161:C:C6	3.09	0.41
11:K:123:PRO:HD2	21:U:38:TYR:CD1	2.54	0.41
22:a:1871:A:H2'	22:a:1872:A:C8	2.55	0.41
36:o:100:LEU:HD11	36:o:110:ILE:HD11	2.03	0.41
38:q:24:LYS:HD3	38:q:92:TRP:HB3	2.02	0.41
49:1:35:ARG:HG3	49:1:42:LEU:HD21	2.02	0.41
1:A:59:A:H3'	1:A:331:G:H22	1.85	0.41
1:A:374:A:C4	1:A:375:U:C5	3.09	0.41
1:A:471:U:H2'	1:A:472:U:C6	2.56	0.41
1:A:996:A:H2'	1:A:997:U:C6	2.56	0.41
4:D:105:MET:HE1	4:D:143:VAL:HG11	2.03	0.41
15:O:7:ALA:O	15:O:11:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2455:G:H2'	22:a:2456:C:C6	2.55	0.41
22:a:2646:C:H6	22:a:2646:C:O5'	2.03	0.41
31:j:63:VAL:HG12	31:j:107:LEU:HD11	2.03	0.41
41:t:86:ARG:NH2	41:t:100:SER:OG	2.53	0.41
50:2:23:LYS:HA	50:2:48:ALA:O	2.20	0.41
1:A:36:C:H2'	1:A:37:U:O4'	2.21	0.41
1:A:74:A:H2'	1:A:75:G:O4'	2.21	0.41
1:A:109:A:C6	1:A:326:G:C6	3.09	0.41
1:A:408:A:H2'	1:A:409:U:H6	1.85	0.41
1:A:473:U:C2	1:A:474:G:C8	3.09	0.41
1:A:745:G:H2'	1:A:746:A:C8	2.56	0.41
1:A:986:U:H2'	1:A:987:G:C8	2.55	0.41
1:A:1391:U:H2'	1:A:1392:G:C8	2.56	0.41
2:B:60:ILE:O	2:B:65:GLY:N	2.54	0.41
2:B:208:ARG:O	2:B:211:THR:HG22	2.21	0.41
4:D:35:GLU:OE1	4:D:35:GLU:N	2.54	0.41
10:J:29:ALA:O	10:J:32:THR:HG22	2.21	0.41
20:T:35:VAL:HG22	20:T:50:ALA:HB1	2.02	0.41
22:a:601:C:H2'	22:a:602:A:O4'	2.21	0.41
22:a:628:G:C6	22:a:636:G:C2	3.09	0.41
22:a:1223:G:OP1	38:q:68:ARG:NH2	2.54	0.41
22:a:1319:C:O2'	22:a:1320:C:H5'	2.21	0.41
22:a:2020:A:H5'	47:z:9:THR:HG21	2.03	0.41
22:a:2193:G:H2'	22:a:2194:U:C6	2.56	0.41
22:a:2298:A:OP1	27:f:71:ARG:NH2	2.52	0.41
22:a:2340:A:H5'	23:b:41:G:H21	1.86	0.41
22:a:2467:C:H2'	22:a:2468:A:O4'	2.20	0.41
22:a:2742:G:OP1	51:3:24:ARG:NH1	2.54	0.41
22:a:2796:U:H3	22:a:2799:A:N6	2.18	0.41
30:i:114:LEU:HA	30:i:114:LEU:HD12	1.78	0.41
33:l:39:GLY:HA3	33:l:126:ILE:HD11	2.03	0.41
37:p:40:ILE:HD13	37:p:40:ILE:HA	1.93	0.41
37:p:66:ASN:HA	37:p:76:TYR:HB2	2.02	0.41
38:q:87:GLN:HG2	38:q:88:GLY:N	2.36	0.41
42:u:80:HIS:CG	42:u:81:PRO:HD2	2.56	0.41
43:v:53:CYS:SG	43:v:57:HIS:HA	2.61	0.41
46:y:8:THR:OG1	46:y:35:THR:HG22	2.20	0.41
54:Z:26:C:C2	54:Z:27:G:C8	3.09	0.41
55:V:28:C:C2	55:V:29:A:C8	3.09	0.41
1:A:461:A:C4	1:A:462:G:C8	3.09	0.41
1:A:674:G:H2'	1:A:675:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:A:C6	1:A:1023:U:C4	3.08	0.41
3:C:87:LEU:HD23	3:C:87:LEU:HA	1.93	0.41
22:a:592:A:C2	50:2:4:ILE:HD11	2.56	0.41
22:a:685:A:C8	22:a:773:U:O4	2.74	0.41
22:a:2521:C:O2'	22:a:2564:A:N3	2.43	0.41
24:c:155:ALA:HB2	24:c:162:VAL:HG23	2.03	0.41
41:t:95:PHE:CD2	41:t:100:SER:HA	2.55	0.41
1:A:946:A:C2	1:A:947:G:C5	3.09	0.40
2:B:129:LEU:HD21	2:B:137:ARG:NH2	2.36	0.40
3:C:135:LYS:HE3	3:C:135:LYS:HB2	1.92	0.40
3:C:149:ILE:CD1	3:C:202:ILE:HG12	2.50	0.40
6:F:17:GLN:OE1	6:F:17:GLN:N	2.54	0.40
17:Q:13:VAL:HG23	17:Q:22:VAL:HG13	2.03	0.40
22:a:644:A:C2	22:a:2369:A:H1'	2.56	0.40
22:a:1410:G:H2'	22:a:1411:U:C6	2.56	0.40
22:a:1853:A:N7	22:a:1889:A:N6	2.69	0.40
22:a:2804:U:H2'	22:a:2805:C:C6	2.56	0.40
23:b:18:G:H2'	23:b:19:C:C6	2.56	0.40
29:h:5:LEU:HD21	29:h:12:LEU:HD11	2.02	0.40
41:t:6:ARG:HG2	41:t:6:ARG:HH21	1.86	0.40
50:2:50:VAL:HG23	50:2:55:LEU:HD22	2.03	0.40
1:A:266:G:H3'	17:Q:69:LYS:HB2	2.04	0.40
1:A:375:U:C2	1:A:376:G:C8	3.09	0.40
1:A:463:U:O2'	1:A:464:U:H5'	2.21	0.40
1:A:875:U:O2'	8:H:15:ARG:HD2	2.21	0.40
2:B:174:LYS:HB2	2:B:174:LYS:HE2	1.90	0.40
4:D:102:VAL:HG22	4:D:107:PHE:HB2	2.03	0.40
10:J:29:ALA:HB1	10:J:36:VAL:HG11	2.03	0.40
22:a:1433:A:H2'	22:a:1434:A:C8	2.56	0.40
22:a:2302:U:N3	22:a:2303:G:N7	2.69	0.40
22:a:2820:A:HO2'	22:a:2821:A:P	2.44	0.40
26:e:22:ASP:OD1	26:e:22:ASP:N	2.51	0.40
27:f:103:LEU:HD12	27:f:107:ALA:HB3	2.03	0.40
27:f:164:GLU:HG2	27:f:165:GLU:N	2.35	0.40
1:A:34:C:H2'	1:A:35:G:C8	2.56	0.40
1:A:268:U:H2'	1:A:269:C:C6	2.54	0.40
1:A:488:C:H2'	1:A:489:C:C6	2.56	0.40
2:B:49:MET:HE3	2:B:201:PRO:CD	2.51	0.40
2:B:158:PRO:HG2	2:B:181:ILE:HD13	2.02	0.40
3:C:79:LYS:O	3:C:80:LYS:HG2	2.21	0.40
3:C:131:ARG:NH2	3:C:168:TYR:OH	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:57:SER:OG	7:G:60:GLU:HB2	2.20	0.40
14:N:46:LEU:HD12	19:S:13:LEU:HD12	2.04	0.40
19:S:71:LEU:HD12	19:S:71:LEU:H	1.86	0.40
22:a:24:G:H2'	22:a:25:U:H6	1.85	0.40
22:a:703:U:H2'	22:a:704:G:O4'	2.21	0.40
22:a:1413:A:H2'	22:a:1414:C:H6	1.86	0.40
22:a:2215:C:H2'	22:a:2216:G:C8	2.56	0.40
22:a:2304:G:H22	22:a:2312:U:H3	1.70	0.40
22:a:2308:G:H2'	22:a:2308:G:N3	2.36	0.40
1:A:1034:G:O2'	1:A:1035:A:H2'	2.21	0.40
8:H:85:ILE:HG23	8:H:87:LYS:HE3	2.03	0.40
22:a:263:G:H2'	22:a:264:C:O4'	2.21	0.40
22:a:594:U:H2'	22:a:595:C:H6	1.87	0.40
22:a:892:A:H2'	22:a:893:C:C6	2.56	0.40
22:a:2590:A:H2'	22:a:2591:C:H6	1.87	0.40
22:a:2649:C:H2'	22:a:2650:U:C6	2.56	0.40
22:a:2774:C:H2'	22:a:2775:G:O4'	2.21	0.40
27:f:65:PRO:HA	27:f:89:VAL:HG12	2.03	0.40
29:h:32:PRO:HA	44:w:39:TRP:CD1	2.56	0.40
34:m:1:MET:HE3	34:m:1:MET:HB2	1.98	0.40
39:r:88:ARG:HG3	39:r:94:ASP:OD2	2.22	0.40
41:t:74:ASN:O	41:t:74:ASN:ND2	2.53	0.40
55:V:4:U:O2'	55:V:5:G:H8	2.03	0.40
1:A:68:G:H5'	1:A:171:A:O2'	2.21	0.40
1:A:201:G:H2'	1:A:202:G:O4'	2.21	0.40
1:A:268:U:C2	1:A:269:C:C5	3.09	0.40
1:A:471:U:H2'	1:A:472:U:H6	1.86	0.40
1:A:818:G:O2'	1:A:819:A:H5'	2.21	0.40
2:B:70:VAL:HG23	2:B:163:VAL:HG13	2.04	0.40
4:D:146:ARG:O	4:D:150:LYS:HG3	2.22	0.40
11:K:74:VAL:O	11:K:74:VAL:HG22	2.21	0.40
22:a:825:A:H2'	22:a:826:U:O4'	2.22	0.40
22:a:875:G:H2'	22:a:876:C:C6	2.56	0.40
22:a:971:G:O2'	22:a:983:A:N3	2.49	0.40
22:a:2092:U:OP2	29:h:27:ARG:NH2	2.53	0.40
22:a:2481:G:HO2'	22:a:2482:A:P	2.41	0.40
40:s:69:ARG:NH1	40:s:69:ARG:HB3	2.37	0.40
54:Z:52:C:C2	54:Z:53:G:C8	3.09	0.40
55:V:75:C:H2'	55:V:76:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	202 (91%)	20 (9%)	0	100	100
3	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	D	203/206 (98%)	193 (95%)	10 (5%)	0	100	100
5	E	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
6	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
7	G	151/179 (84%)	138 (91%)	13 (9%)	0	100	100
8	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
9	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	J	96/103 (93%)	89 (93%)	5 (5%)	2 (2%)	5	27
11	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	M	113/118 (96%)	103 (91%)	10 (9%)	0	100	100
14	N	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
17	Q	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
18	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
19	S	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
20	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	253 (94%)	16 (6%)	0	100	100
25	d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	57
26	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	g	174/177 (98%)	158 (91%)	16 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
30	i	140/142 (99%)	137 (98%)	3 (2%)	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%)	125 (95%)	7 (5%)	0	100	100
34	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
35	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
36	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
37	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
38	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
39	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
40	s	91/100 (91%)	83 (91%)	8 (9%)	0	100	100
41	t	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
42	u	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
43	v	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
44	w	75/78 (96%)	75 (100%)	0	0	100	100
45	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
46	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
47	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	34
51	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5487/5913 (93%)	5189 (95%)	294 (5%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	d	149	ASN
10	J	57	VAL
10	J	58	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
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%)	65 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	62/63 (98%)	62 (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%)	54 (98%)	1 (2%)	51	71
All	All	4576/4825 (95%)	4575 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
52	4	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	HIS
3	C	190	HIS
4	D	152	GLN
5	E	122	ASN
10	J	15	HIS
11	K	109	ASN
13	M	105	ASN
14	N	4	GLN
16	P	26	ASN
18	R	31	ASN
20	T	52	ASN
21	U	56	HIS
24	c	143	ASN
26	e	115	GLN
27	f	5	HIS
27	f	27	GLN
28	g	116	GLN
30	i	136	GLN
30	i	138	GLN
31	j	9	ASN
33	l	13	HIS
34	m	18	GLN
35	n	29	HIS
35	n	100	HIS
37	p	44	GLN
38	q	11	GLN
41	t	54	GLN
52	4	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	221 (14%)	4 (0%)
22	a	2757/2904 (94%)	329 (11%)	0
23	b	118/120 (98%)	11 (9%)	0
53	X	10/35 (28%)	0	0
54	Z	76/77 (98%)	14 (18%)	1 (1%)
55	V	68/76 (89%)	11 (16%)	1 (1%)
All	All	4537/4754 (95%)	586 (12%)	6 (0%)

All (586) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	55	A
1	A	56	U
1	A	59	A
1	A	60	A
1	A	66	A
1	A	71	A
1	A	72	A
1	A	74	A
1	A	80	A
1	A	93	U
1	A	94	G
1	A	95	C
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	149	A
1	A	151	A
1	A	156	C
1	A	159	G
1	A	162	A
1	A	163	C
1	A	173	U
1	A	182	A
1	A	189	A
1	A	197	A
1	A	199	A
1	A	200	G
1	A	204	G
1	A	216	U
1	A	226	G
1	A	240	G

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Mol	Chain	Res	Type
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	293	G
1	A	298	A
1	A	321	A
1	A	328	C
1	A	330	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	369	G
1	A	372	C
1	A	373	A
1	A	381	C
1	A	391	G
1	A	392	C
1	A	397	A
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	439	U
1	A	453	G
1	A	457	G
1	A	458	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	479	U
1	A	481	G
1	A	484	G

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Mol	Chain	Res	Type
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	G
1	A	499	A
1	A	508	U
1	A	511	C
1	A	518	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	596	A
1	A	617	G
1	A	618	C
1	A	626	G
1	A	633	G
1	A	639	G
1	A	650	G
1	A	653	U
1	A	656	G
1	A	665	A
1	A	687	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	733	G
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	787	A
1	A	793	U
1	A	794	A
1	A	810	C
1	A	815	A

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Mol	Chain	Res	Type
1	A	817	C
1	A	885	G
1	A	887	G
1	A	889	A
1	A	890	G
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	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	1004	A
1	A	1009	U
1	A	1020	G
1	A	1027	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1044	A
1	A	1053	G
1	A	1065	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1130	A
1	A	1137	C
1	A	1139	G
1	A	1157	A
1	A	1159	U
1	A	1167	A
1	A	1168	U

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Mol	Chain	Res	Type
1	A	1169	A
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1256	A
1	A	1257	A
1	A	1275	A
1	A	1280	A
1	A	1285	A
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1340	A
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	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1487	G
1	A	1492	A
1	A	1494	G

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Mol	Chain	Res	Type
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1518	MA6
1	A	1519	MA6
1	A	1520	C
1	A	1529	G
1	A	1530	G
22	a	10	A
22	a	15	G
22	a	34	U
22	a	35	G
22	a	51	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	101	A
22	a	102	U
22	a	103	A
22	a	118	A
22	a	120	U
22	a	139	U
22	a	142	A
22	a	163	C
22	a	164	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	204	A
22	a	216	A
22	a	221	A
22	a	222	A
22	a	223	A
22	a	233	A
22	a	248	G
22	a	272	A
22	a	277	G
22	a	278	A
22	a	281	C

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Mol	Chain	Res	Type
22	a	282	A
22	a	285	G
22	a	287	G
22	a	289	G
22	a	311	A
22	a	329	G
22	a	330	A
22	a	335	C
22	a	345	A
22	a	350	G
22	a	353	C
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	467	G
22	a	473	G
22	a	481	G
22	a	491	G
22	a	505	A
22	a	509	C
22	a	510	C
22	a	528	A
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	546	U
22	a	548	G
22	a	549	G
22	a	563	A
22	a	568	U
22	a	573	U
22	a	575	A
22	a	586	A
22	a	603	A
22	a	613	A
22	a	615	U
22	a	627	A
22	a	637	A

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Mol	Chain	Res	Type
22	a	645	C
22	a	647	G
22	a	654	A
22	a	659	G
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	764	A
22	a	765	C
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	792	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	847	U
22	a	859	G
22	a	866	A
22	a	884	U
22	a	888	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	910	A
22	a	915	C
22	a	916	G
22	a	927	A
22	a	931	U
22	a	946	C
22	a	961	C
22	a	973	A

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Mol	Chain	Res	Type
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1005	C
22	a	1006	C
22	a	1012	U
22	a	1013	C
22	a	1025	G
22	a	1026	G
22	a	1033	U
22	a	1045	C
22	a	1047	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1212	G
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1265	A
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1275	A
22	a	1300	G
22	a	1301	A
22	a	1343	G
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1386	C
22	a	1409	U
22	a	1416	G
22	a	1417	C
22	a	1428	C
22	a	1437	C
22	a	1452	G

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Mol	Chain	Res	Type
22	a	1453	A
22	a	1476	U
22	a	1482	G
22	a	1493	C
22	a	1508	A
22	a	1510	G
22	a	1515	A
22	a	1523	U
22	a	1524	G
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1538	G
22	a	1539	U
22	a	1560	G
22	a	1566	A
22	a	1567	G
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1608	A
22	a	1610	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1654	A
22	a	1674	G
22	a	1675	C
22	a	1698	A
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1738	G
22	a	1744	A
22	a	1764	C
22	a	1773	A
22	a	1782	U
22	a	1786	A

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Mol	Chain	Res	Type
22	a	1791	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	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	1905	C
22	a	1906	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1936	A
22	a	1937	A
22	a	1955	U
22	a	1966	A
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	2021	C
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2080	A
22	a	2093	G
22	a	2190	G

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Mol	Chain	Res	Type
22	a	2191	A
22	a	2198	A
22	a	2203	U
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2266	A
22	a	2273	A
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	2333	A
22	a	2334	U
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2410	G
22	a	2425	A
22	a	2426	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2445	2MG
22	a	2448	A
22	a	2474	U
22	a	2475	C
22	a	2476	A
22	a	2482	A
22	a	2491	U

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Mol	Chain	Res	Type
22	a	2505	G
22	a	2507	C
22	a	2518	A
22	a	2520	C
22	a	2529	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2661	G
22	a	2663	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2726	A
22	a	2727	A
22	a	2732	G
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2765	A
22	a	2778	A
22	a	2798	U
22	a	2799	A
22	a	2818	U
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2849	U
22	a	2861	U
22	a	2866	U
22	a	2873	A
22	a	2880	C
22	a	2883	A
22	a	2884	U

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Mol	Chain	Res	Type
22	a	2885	G
22	a	2899	A
22	a	2900	A
23	b	9	G
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	3	C
54	Z	9	G
54	Z	17	C
54	Z	18	U
54	Z	19	G
54	Z	20	G
54	Z	22	A
54	Z	23	G
54	Z	44	A
54	Z	47	A
54	Z	48	U
54	Z	54	G
54	Z	68	C
54	Z	77	A
55	V	2	C
55	V	5	G
55	V	9	A
55	V	10	2MG
55	V	11	C
55	V	19	G
55	V	48	5MC
55	V	49	5MC
55	V	67	U
55	V	74	C
55	V	75	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	965	U
1	A	1026	G
1	A	1034	G
1	A	1035	A
54	Z	67	C
55	V	10	2MG

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

58 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	$\# Z > 2$
1	5MC	A	967	1	18,22,23	3.63	8 (44%)	26,32,35	1.01	1 (3%)
1	MA6	A	1518	1	23,26,27	1.47	5 (21%)	34,38,41	2.20	11 (32%)
22	PSU	a	746	56,22	18,21,22	1.07	3 (16%)	22,30,33	1.74	3 (13%)
22	5MU	a	1939	22	19,22,23	4.42	7 (36%)	28,32,35	3.89	9 (32%)
55	12A	V	37	56,55	33,36,37	1.62	6 (18%)	47,52,55	1.29	6 (12%)
55	A1L4U	V	34	53,55	20,25,26	0.86	0	30,35,38	1.38	5 (16%)
55	5MC	V	48	55	18,22,23	3.63	8 (44%)	26,32,35	1.05	1 (3%)
22	OMU	a	2552	22	19,22,23	2.67	6 (31%)	26,31,34	1.77	5 (19%)
12	D2T	L	89	12	7,9,10	1.04	0	6,11,13	1.10	1 (16%)
55	PSU	V	39	55	18,21,22	1.01	1 (5%)	22,30,33	1.77	4 (18%)
1	5MC	A	1407	1	18,22,23	3.47	7 (38%)	26,32,35	1.03	1 (3%)
1	UR3	A	1498	1	19,22,23	2.45	6 (31%)	26,32,35	1.28	1 (3%)
54	OMC	Z	33	54	19,22,23	2.86	8 (42%)	26,31,34	0.74	0
22	G7M	a	2069	22	23,26,27	2.73	9 (39%)	35,39,42	1.72	8 (22%)
22	PSU	a	2504	22	18,21,22	1.05	2 (11%)	22,30,33	1.88	4 (18%)
1	PSU	A	516	56,1	18,21,22	0.98	2 (11%)	22,30,33	1.71	5 (22%)
22	2MG	a	2445	22	23,26,27	2.50	7 (30%)	32,38,41	2.13	10 (31%)
22	2MG	a	1835	22	23,26,27	2.56	7 (30%)	32,38,41	2.27	10 (31%)
55	G7M	V	46	55	23,26,27	2.80	8 (34%)	35,39,42	1.75	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1516	1	23,26,27	2.49	8 (34%)	32,38,41	2.18	11 (34%)
33	4D4	l	81	33	9,11,12	1.59	1 (11%)	8,13,15	1.97	3 (37%)
54	4SU	Z	8	54	18,21,22	4.02	8 (44%)	26,30,33	2.40	5 (19%)
22	PSU	a	955	22	18,21,22	1.09	3 (16%)	22,30,33	1.82	4 (18%)
22	H2U	a	2449	22	18,21,22	1.43	3 (16%)	21,30,33	1.10	3 (14%)
22	5MU	a	747	22	19,22,23	4.40	7 (36%)	28,32,35	3.87	9 (32%)
1	2MG	A	966	1	23,26,27	2.56	8 (34%)	32,38,41	2.21	10 (31%)
22	3TD	a	1915	22	18,22,23	3.88	7 (38%)	22,32,35	1.70	2 (9%)
22	1MG	a	745	22	22,26,27	2.58	7 (31%)	33,39,42	1.85	7 (21%)
22	PSU	a	2604	22	18,21,22	1.13	2 (11%)	22,30,33	1.85	4 (18%)
11	IAS	K	119	11	6,7,8	1.03	0	6,8,10	1.38	2 (33%)
22	6MZ	a	2030	22	23,25,26	2.63	5 (21%)	29,36,39	2.62	12 (41%)
55	H2U	V	47	55	18,21,22	1.04	3 (16%)	21,30,33	0.96	1 (4%)
55	PSU	V	55	55	18,21,22	1.04	2 (11%)	22,30,33	1.97	5 (22%)
22	OMG	a	2251	54,22	23,26,27	2.53	9 (39%)	33,38,41	1.95	9 (27%)
55	2MG	V	10	55	23,26,27	2.62	8 (34%)	32,38,41	2.21	9 (28%)
54	5MU	Z	55	54	19,22,23	4.54	6 (31%)	28,32,35	3.75	9 (32%)
1	2MG	A	1207	1	23,26,27	2.58	8 (34%)	32,38,41	2.18	10 (31%)
1	G7M	A	527	1	23,26,27	2.78	8 (34%)	35,39,42	1.81	9 (25%)
55	5MC	V	49	55	18,22,23	3.67	8 (44%)	26,32,35	1.02	1 (3%)
22	6MZ	a	1618	22	23,25,26	2.61	4 (17%)	29,36,39	2.55	11 (37%)
25	MEQ	d	150	25	8,9,10	1.56	2 (25%)	5,10,12	1.83	2 (40%)
54	PSU	Z	56	54	18,21,22	1.03	1 (5%)	22,30,33	1.80	3 (13%)
22	5MC	a	1962	22	18,22,23	3.47	7 (38%)	26,32,35	1.22	3 (11%)
1	MA6	A	1519	1	23,26,27	1.54	5 (21%)	34,38,41	2.30	12 (35%)
54	H2U	Z	21	54	18,21,22	1.08	2 (11%)	21,30,33	1.03	1 (4%)
55	2MG	V	6	55	23,26,27	2.65	7 (30%)	32,38,41	2.21	9 (28%)
22	PSU	a	1917	22	18,21,22	1.03	3 (16%)	22,30,33	1.82	4 (18%)
22	PSU	a	2605	22	18,21,22	1.09	2 (11%)	22,30,33	1.84	4 (18%)
22	PSU	a	2580	22	18,21,22	1.13	3 (16%)	22,30,33	2.00	6 (27%)
55	2MU	V	54	55	20,23,24	1.41	5 (25%)	28,33,36	2.02	8 (28%)
22	2MA	a	2503	56,22	22,25,26	3.78	8 (36%)	33,37,40	2.86	9 (27%)
55	1MA	V	58	55	21,25,26	0.65	0	31,37,40	0.77	1 (3%)
22	PSU	a	1911	22	18,21,22	1.01	2 (11%)	22,30,33	1.81	4 (18%)
33	MS6	l	82	33	5,7,8	1.04	0	2,7,9	1.97	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	V	27	55	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
1	4OC	A	1402	56,1	20,23,24	2.87	8 (40%)	26,32,35	0.98	2 (7%)
22	PSU	a	2457	22	18,21,22	1.10	3 (16%)	22,30,33	2.08	6 (27%)
22	OMC	a	2498	56,22	19,22,23	2.62	7 (36%)	26,31,34	0.85	1 (3%)

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
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	3/11/29/30	0/3/3/3
22	PSU	a	746	56,22	-	1/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
55	12A	V	37	56,55	-	0/25/43/44	0/3/3/3
55	A1L4U	V	34	53,55	-	5/13/31/32	0/2/2/2
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2
12	D2T	L	89	12	-	1/7/12/14	-
55	PSU	V	39	55	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
22	G7M	a	2069	22	-	2/7/25/26	0/3/3/3
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	56,1	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	2/9/27/28	0/3/3/3
22	2MG	a	1835	22	-	2/9/27/28	0/3/3/3
55	G7M	V	46	55	-	0/7/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
33	4D4	l	81	33	-	4/11/12/14	-
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
22	3TD	a	1915	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	2604	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	IAS	K	119	11	-	1/7/7/8	-
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
55	H2U	V	47	55	-	5/7/38/39	0/2/2/2
55	PSU	V	55	55	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	54,22	-	1/9/27/28	0/3/3/3
55	2MG	V	10	55	-	0/9/27/28	0/3/3/3
54	5MU	Z	55	54	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	G7M	A	527	1	-	1/7/25/26	0/3/3/3
55	5MC	V	49	55	-	2/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
25	MEQ	d	150	25	-	3/8/9/11	-
54	PSU	Z	56	54	-	2/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	3/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/11/29/30	0/3/3/3
54	H2U	Z	21	54	-	4/7/38/39	0/2/2/2
55	2MG	V	6	55	-	2/9/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
55	2MU	V	54	55	-	0/9/27/28	0/2/2/2
22	2MA	a	2503	56,22	-	1/7/25/26	0/3/3/3
55	1MA	V	58	55	-	1/7/25/26	0/3/3/3
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
33	MS6	l	82	33	-	2/4/6/8	-
55	PSU	V	27	55	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	56,1	-	2/9/29/30	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	56,22	-	0/9/27/28	0/2/2/2

All (281) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2503	2MA	C4-N3	11.70	1.49	1.34
22	a	1915	3TD	C6-C5	11.63	1.48	1.35
22	a	1618	6MZ	C6-N6	10.90	1.46	1.34
22	a	2030	6MZ	C6-N6	10.64	1.45	1.34
54	Z	55	5MU	C6-N1	10.45	1.55	1.38
54	Z	55	5MU	C2-N1	10.07	1.54	1.38
22	a	1939	5MU	C6-N1	10.04	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	747	5MU	C6-N1	10.04	1.55	1.38
22	a	747	5MU	C2-N1	9.54	1.53	1.38
22	a	1939	5MU	C2-N1	9.33	1.53	1.38
55	V	49	5MC	C6-C5	9.28	1.49	1.34
1	A	967	5MC	C6-C5	9.19	1.49	1.34
55	V	48	5MC	C6-C5	9.14	1.49	1.34
54	Z	8	4SU	C4-N3	8.96	1.47	1.37
1	A	1407	5MC	C6-C5	8.82	1.49	1.34
54	Z	55	5MU	C4-C5	8.75	1.59	1.44
22	a	1962	5MC	C6-C5	8.44	1.48	1.34
22	a	1939	5MU	C4-C5	8.25	1.58	1.44
22	a	747	5MU	C4-C5	8.12	1.58	1.44
22	a	1939	5MU	C4-N3	-8.01	1.24	1.38
22	a	1915	3TD	C2-N1	8.01	1.47	1.37
22	a	747	5MU	C4-N3	-7.83	1.24	1.38
55	V	6	2MG	C2-N3	7.70	1.46	1.31
55	V	10	2MG	C2-N3	7.67	1.46	1.31
54	Z	55	5MU	C4-N3	-7.52	1.24	1.38
1	A	1207	2MG	C2-N3	7.34	1.46	1.31
1	A	966	2MG	C2-N3	7.28	1.45	1.31
22	a	1835	2MG	C2-N3	7.25	1.45	1.31
54	Z	8	4SU	C2-N1	7.25	1.50	1.38
22	a	2503	2MA	C2-N3	7.23	1.46	1.34
55	V	48	5MC	C4-N3	7.08	1.46	1.34
55	V	49	5MC	C4-N3	7.04	1.46	1.34
22	a	1962	5MC	C4-N3	6.95	1.45	1.34
1	A	967	5MC	C4-N3	6.92	1.45	1.34
1	A	1516	2MG	C2-N3	6.88	1.45	1.31
22	a	2445	2MG	C2-N3	6.83	1.45	1.31
22	a	2251	OMG	C4-N3	6.80	1.50	1.34
1	A	1407	5MC	C4-N3	6.66	1.45	1.34
55	V	6	2MG	C4-N3	6.50	1.49	1.34
55	V	46	G7M	C4-N3	6.45	1.49	1.34
55	V	46	G7M	C2-N2	6.39	1.49	1.34
55	V	10	2MG	C4-N3	6.36	1.49	1.34
1	A	1207	2MG	C4-N3	6.35	1.49	1.34
54	Z	8	4SU	C2-N3	6.32	1.49	1.38
1	A	527	G7M	C2-N2	6.31	1.49	1.34
1	A	966	2MG	C4-N3	6.24	1.49	1.34
1	A	527	G7M	C4-N3	6.23	1.49	1.34
1	A	967	5MC	C2-N3	6.22	1.49	1.36
22	a	1835	2MG	C4-N3	6.20	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	49	5MC	C2-N3	6.19	1.48	1.36
1	A	1402	4OC	C4-N3	6.17	1.43	1.32
55	V	48	5MC	C2-N3	6.15	1.48	1.36
54	Z	55	5MU	C6-C5	6.15	1.44	1.34
22	a	2069	G7M	C2-N2	6.10	1.48	1.34
22	a	1962	5MC	C2-N3	6.09	1.48	1.36
1	A	1402	4OC	C6-C5	6.05	1.49	1.35
54	Z	33	OMC	C2-N3	6.04	1.48	1.36
22	a	2552	OMU	C2-N3	6.00	1.48	1.38
1	A	1498	UR3	C2-N1	5.99	1.47	1.38
1	A	1516	2MG	C4-N3	5.98	1.48	1.34
22	a	2552	OMU	C2-N1	5.95	1.48	1.38
22	a	2445	2MG	C4-N3	5.94	1.48	1.34
22	a	745	1MG	C2-N3	5.92	1.45	1.34
22	a	2069	G7M	C4-N3	5.91	1.48	1.34
22	a	1939	5MU	C6-C5	5.90	1.44	1.34
54	Z	8	4SU	C6-C5	5.90	1.48	1.35
22	a	2503	2MA	C2-N1	5.90	1.44	1.34
22	a	745	1MG	C4-N3	5.88	1.48	1.34
22	a	747	5MU	C6-C5	5.88	1.44	1.34
1	A	1407	5MC	C2-N3	5.83	1.48	1.36
22	a	745	1MG	C2-N2	5.78	1.44	1.34
54	Z	33	OMC	C6-C5	5.76	1.48	1.35
1	A	1498	UR3	C6-C5	5.71	1.48	1.35
22	a	2069	G7M	C5-N7	-5.66	1.32	1.39
54	Z	8	4SU	C4-S4	-5.65	1.57	1.68
22	a	1915	3TD	C6-N1	5.65	1.45	1.36
55	V	46	G7M	C2-N3	5.62	1.46	1.33
22	a	2552	OMU	C6-C5	5.47	1.47	1.35
22	a	2498	OMC	C6-C5	5.44	1.47	1.35
1	A	1402	4OC	C2-N3	5.42	1.47	1.36
1	A	527	G7M	C2-N3	5.40	1.46	1.33
22	a	2498	OMC	C2-N3	5.36	1.47	1.36
54	Z	8	4SU	C5-C4	5.31	1.49	1.42
1	A	527	G7M	C5-N7	-5.25	1.33	1.39
22	a	2503	2MA	C5-C6	5.08	1.55	1.41
22	a	2503	2MA	C6-N6	-5.07	1.21	1.34
22	a	2251	OMG	C2-N3	5.04	1.45	1.33
55	V	6	2MG	C2-N1	5.03	1.44	1.36
22	a	2069	G7M	C2-N3	5.01	1.45	1.33
55	V	10	2MG	C2-N1	4.94	1.44	1.36
55	V	49	5MC	C6-N1	4.94	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Z	33	OMC	C4-N3	4.84	1.44	1.34
54	Z	33	OMC	C4-N4	4.82	1.45	1.33
1	A	967	5MC	C6-N1	4.81	1.46	1.38
55	V	48	5MC	C6-N1	4.80	1.46	1.38
22	a	2251	OMG	C2-N2	4.77	1.45	1.34
55	V	46	G7M	C5-N7	-4.73	1.33	1.39
1	A	966	2MG	C2-N1	4.72	1.44	1.36
1	A	1516	2MG	C2-N1	4.56	1.44	1.36
1	A	1407	5MC	C6-N1	4.53	1.45	1.38
1	A	1207	2MG	C2-N1	4.51	1.43	1.36
22	a	1835	2MG	C2-N1	4.44	1.43	1.36
22	a	2498	OMC	C4-N4	4.40	1.44	1.33
22	a	2445	2MG	C2-N1	4.34	1.43	1.36
22	a	1962	5MC	C6-N1	4.29	1.45	1.38
1	A	1402	4OC	C4-N4	4.19	1.44	1.35
22	a	1915	3TD	C2-N3	4.15	1.47	1.38
22	a	2498	OMC	C4-N3	4.07	1.42	1.34
1	A	1498	UR3	C2-N3	4.04	1.46	1.39
55	V	49	5MC	C4-N4	4.02	1.44	1.34
55	V	48	5MC	C4-N4	4.00	1.44	1.34
55	V	49	5MC	C2-N1	3.99	1.48	1.40
55	V	37	12A	O5'-C5'	-3.94	1.35	1.44
1	A	1407	5MC	C4-N4	3.94	1.44	1.34
1	A	967	5MC	C4-N4	3.92	1.44	1.34
22	a	1962	5MC	C4-N4	3.92	1.44	1.34
54	Z	33	OMC	C2-N1	3.92	1.48	1.40
55	V	48	5MC	C2-N1	3.84	1.48	1.40
1	A	967	5MC	C2-N1	3.82	1.48	1.40
55	V	37	12A	CA-C	3.81	1.58	1.52
22	a	1962	5MC	C2-N1	3.71	1.48	1.40
22	a	1835	2MG	C5-N7	-3.61	1.32	1.39
1	A	1519	MA6	C5-C4	-3.60	1.32	1.39
22	a	2498	OMC	C2-N1	3.60	1.47	1.40
22	a	745	1MG	C5-N7	-3.60	1.32	1.39
55	V	46	G7M	C5-C6	3.59	1.53	1.43
22	a	2251	OMG	C5-N7	-3.59	1.32	1.39
22	a	2445	2MG	C5-N7	-3.55	1.32	1.39
22	a	2449	H2U	C4-N3	-3.52	1.31	1.37
55	V	37	12A	CC-N6	3.50	1.44	1.37
54	Z	8	4SU	O2-C2	-3.42	1.16	1.23
1	A	1402	4OC	C5-C4	3.39	1.48	1.40
22	a	2498	OMC	O2-C2	-3.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2030	6MZ	C5-C4	-3.36	1.32	1.39
1	A	1402	4OC	O2-C2	-3.35	1.17	1.23
22	a	2449	H2U	C2-N3	-3.33	1.32	1.38
1	A	1207	2MG	C5-N7	-3.33	1.32	1.39
1	A	527	G7M	C5-C6	3.25	1.52	1.43
22	a	2503	2MA	C6-N1	3.24	1.39	1.35
22	a	2503	2MA	C5-N7	-3.23	1.32	1.39
1	A	1402	4OC	C2-N1	3.21	1.47	1.40
55	V	6	2MG	C5-N7	-3.21	1.32	1.39
1	A	1407	5MC	C2-N1	3.18	1.46	1.40
1	A	966	2MG	C5-N7	-3.17	1.32	1.39
22	a	2069	G7M	C5-C6	3.17	1.52	1.43
1	A	1518	MA6	C5-C4	-3.15	1.33	1.39
54	Z	56	PSU	C6-C5	3.13	1.39	1.35
1	A	1519	MA6	C5-N7	-3.11	1.33	1.39
1	A	1519	MA6	C8-N9	-3.09	1.32	1.37
1	A	1516	2MG	C5-N7	-3.09	1.33	1.39
22	a	1618	6MZ	C5-C4	-3.07	1.33	1.39
22	a	2251	OMG	O6-C6	-3.04	1.17	1.23
22	a	2552	OMU	O2-C2	-3.04	1.17	1.23
55	V	27	PSU	C6-C5	3.03	1.38	1.35
22	a	2552	OMU	O4-C4	-3.01	1.18	1.24
1	A	1518	MA6	C5-N7	-3.00	1.33	1.39
55	V	10	2MG	C5-N7	-2.99	1.33	1.39
33	l	81	4D4	OB-CB	-2.98	1.37	1.43
54	Z	33	OMC	O2-C2	-2.96	1.18	1.23
54	Z	8	4SU	C6-N1	2.91	1.45	1.38
1	A	527	G7M	O6-C6	-2.90	1.18	1.23
55	V	37	12A	C4-N3	2.89	1.37	1.34
55	V	39	PSU	C6-C5	2.89	1.38	1.35
22	a	2030	6MZ	C8-N9	-2.88	1.32	1.37
1	A	1518	MA6	C8-N9	-2.87	1.32	1.37
55	V	46	G7M	C6-N1	2.87	1.44	1.38
22	a	2552	OMU	C4-N3	2.85	1.43	1.38
54	Z	21	H2U	C2-N3	-2.83	1.32	1.38
55	V	46	G7M	C2-N1	2.83	1.44	1.37
1	A	1518	MA6	C6-N6	2.80	1.45	1.36
55	V	54	2MU	C4-N3	-2.79	1.33	1.38
22	a	1835	2MG	O6-C6	-2.77	1.18	1.23
55	V	55	PSU	C6-C5	2.75	1.38	1.35
54	Z	21	H2U	C4-N3	-2.74	1.32	1.37
22	a	2069	G7M	O6-C6	-2.74	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2449	H2U	C2-N1	-2.73	1.31	1.35
1	A	1407	5MC	O2-C2	-2.73	1.18	1.23
1	A	1402	4OC	C6-N1	2.70	1.44	1.38
54	Z	33	OMC	C6-N1	2.69	1.44	1.38
1	A	1519	MA6	C6-N6	2.69	1.44	1.36
1	A	1498	UR3	O4-C4	-2.69	1.17	1.23
22	a	2445	2MG	O6-C6	-2.68	1.18	1.23
22	a	2030	6MZ	C5-N7	-2.64	1.34	1.39
22	a	1939	5MU	O2-C2	-2.64	1.18	1.23
55	V	54	2MU	C2-N1	2.64	1.42	1.38
55	V	47	H2U	C2-N3	-2.62	1.33	1.38
22	a	745	1MG	C5-C6	2.60	1.52	1.45
22	a	2445	2MG	C4-N9	-2.59	1.31	1.38
22	a	745	1MG	O6-C6	-2.58	1.17	1.23
22	a	2580	PSU	O4'-C1'	-2.58	1.40	1.43
22	a	1962	5MC	O2-C2	-2.55	1.19	1.23
1	A	527	G7M	C6-N1	2.55	1.43	1.38
25	d	150	MEQ	CG-CD	-2.55	1.46	1.51
1	A	1498	UR3	O2-C2	-2.54	1.17	1.22
22	a	2604	PSU	C6-C5	2.54	1.38	1.35
22	a	2504	PSU	C6-C5	2.53	1.38	1.35
55	V	6	2MG	C5-C6	2.52	1.53	1.44
1	A	1516	2MG	C4-N9	-2.52	1.31	1.38
55	V	10	2MG	C5-C6	2.52	1.53	1.44
55	V	46	G7M	O6-C6	-2.51	1.18	1.23
22	a	747	5MU	O2-C2	-2.49	1.18	1.23
1	A	967	5MC	O2-C2	-2.49	1.19	1.23
1	A	527	G7M	C2-N1	2.49	1.43	1.37
1	A	1516	2MG	O6-C6	-2.49	1.18	1.23
22	a	2069	G7M	C2-N1	2.46	1.43	1.37
22	a	2605	PSU	C4-C5	-2.46	1.37	1.44
22	a	1618	6MZ	C8-N9	-2.45	1.33	1.37
22	a	1618	6MZ	C5-N7	-2.44	1.34	1.39
22	a	2604	PSU	C4-C5	-2.44	1.37	1.44
1	A	1207	2MG	O6-C6	-2.43	1.19	1.23
22	a	2251	OMG	C5-C6	2.43	1.53	1.44
22	a	745	1MG	C4-N9	-2.43	1.31	1.38
22	a	1915	3TD	O4-C4	-2.43	1.18	1.23
1	A	966	2MG	O6-C6	-2.41	1.19	1.23
22	a	2069	G7M	C6-N1	2.41	1.43	1.38
22	a	2580	PSU	C4-C5	-2.40	1.37	1.44
55	V	48	5MC	O2-C2	-2.40	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C6-N1	2.39	1.43	1.38
55	V	37	12A	C8-N9	2.39	1.41	1.37
1	A	966	2MG	C5-C6	2.39	1.53	1.44
22	a	2498	OMC	C6-N1	2.37	1.43	1.38
55	V	49	5MC	O2-C2	-2.37	1.19	1.23
22	a	1939	5MU	O4-C4	-2.37	1.19	1.23
1	A	1516	2MG	C5-C6	2.36	1.53	1.44
22	a	2251	OMG	C4-N9	-2.36	1.31	1.38
55	V	10	2MG	O6-C6	-2.36	1.19	1.23
1	A	1207	2MG	C5-C6	2.33	1.53	1.44
22	a	746	PSU	C4-C5	-2.29	1.37	1.44
1	A	516	PSU	C6-C5	2.29	1.38	1.35
1	A	1519	MA6	C4-N9	-2.28	1.32	1.37
55	V	54	2MU	C6-C5	2.27	1.38	1.34
22	a	955	PSU	C6-C5	2.27	1.38	1.35
22	a	1917	PSU	C6-C5	2.27	1.38	1.35
22	a	747	5MU	O4-C4	-2.26	1.19	1.23
22	a	1915	3TD	C4-N3	2.25	1.45	1.40
22	a	1911	PSU	C6-C5	2.25	1.37	1.35
22	a	2457	PSU	C4-C5	-2.24	1.37	1.44
55	V	47	H2U	C4-N3	-2.24	1.33	1.37
22	a	746	PSU	C6-C5	2.23	1.37	1.35
55	V	6	2MG	C6-N1	2.22	1.43	1.38
22	a	2457	PSU	O4'-C1'	-2.21	1.40	1.43
22	a	2457	PSU	C6-C5	2.21	1.37	1.35
22	a	2251	OMG	C8-N9	-2.21	1.32	1.37
22	a	2605	PSU	C6-C5	2.21	1.37	1.35
22	a	1835	2MG	C5-C6	2.20	1.52	1.44
1	A	1518	MA6	C4-N9	-2.20	1.32	1.37
22	a	1911	PSU	C4-C5	-2.20	1.37	1.44
55	V	54	2MU	C4-C5	2.20	1.48	1.44
54	Z	33	OMC	C5-C4	2.19	1.47	1.42
55	V	6	2MG	O6-C6	-2.19	1.19	1.23
22	a	1835	2MG	C4-N9	-2.19	1.32	1.38
22	a	2251	OMG	C6-N1	2.18	1.42	1.38
55	V	48	5MC	CM5-C5	2.18	1.56	1.50
22	a	1917	PSU	C4-C5	-2.18	1.38	1.44
22	a	2503	2MA	CM2-C2	2.16	1.55	1.49
1	A	966	2MG	C6-N1	2.16	1.42	1.38
55	V	49	5MC	CM5-C5	2.16	1.56	1.50
55	V	55	PSU	C4-C5	-2.15	1.38	1.44
22	a	1915	3TD	O2-C2	-2.15	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C4-C5	-2.15	1.38	1.44
55	V	10	2MG	C6-N1	2.14	1.42	1.38
54	Z	55	5MU	O2-C2	-2.14	1.19	1.23
22	a	955	PSU	O4'-C1'	-2.13	1.40	1.43
1	A	1207	2MG	C6-N1	2.13	1.42	1.38
1	A	1207	2MG	C4-N9	-2.13	1.32	1.38
25	d	150	MEQ	CB-CA	-2.13	1.50	1.53
1	A	966	2MG	C4-N9	-2.12	1.32	1.38
55	V	54	2MU	C2-N3	-2.12	1.34	1.38
22	a	955	PSU	C4-C5	-2.11	1.38	1.44
22	a	2504	PSU	C4-C5	-2.11	1.38	1.44
22	a	2445	2MG	C5-C6	2.10	1.52	1.44
22	a	2580	PSU	C6-C5	2.09	1.37	1.35
22	a	746	PSU	O4'-C1'	-2.08	1.41	1.43
22	a	2069	G7M	C4-N9	-2.08	1.32	1.38
1	A	967	5MC	CM5-C5	2.07	1.55	1.50
22	a	1917	PSU	O4'-C1'	-2.04	1.41	1.43
55	V	37	12A	C2-N1	2.03	1.37	1.34
55	V	47	H2U	C2-N1	-2.03	1.32	1.35
55	V	10	2MG	C4-N9	-2.02	1.32	1.38
22	a	2030	6MZ	C6-N1	-2.02	1.31	1.35
1	A	1516	2MG	C6-N1	2.02	1.42	1.38

All (309) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1939	5MU	C5-C4-N3	13.18	126.56	115.31
22	a	747	5MU	C5-C4-N3	13.03	126.43	115.31
54	Z	55	5MU	C5-C4-N3	12.76	126.20	115.31
22	a	747	5MU	C5-C6-N1	-10.82	112.21	123.34
22	a	1939	5MU	C5-C6-N1	-10.74	112.29	123.34
54	Z	55	5MU	C5-C6-N1	-10.53	112.51	123.34
22	a	2503	2MA	C5-C4-N3	-8.49	117.64	127.19
54	Z	8	4SU	C4-N3-C2	-8.43	119.15	127.34
22	a	2503	2MA	C4-N9-C1'	-6.94	110.05	126.59
22	a	2503	2MA	C1'-N9-C8	6.88	142.67	127.14
55	V	6	2MG	C2-N3-C4	6.60	120.22	112.04
22	a	1835	2MG	C2-N3-C4	6.59	120.20	112.04
1	A	966	2MG	C2-N3-C4	6.49	120.09	112.04
1	A	1207	2MG	C2-N3-C4	6.48	120.08	112.04
22	a	1618	6MZ	C9-N6-C6	-6.44	117.33	122.87
1	A	1516	2MG	C2-N3-C4	6.21	119.75	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	10	2MG	C2-N3-C4	6.19	119.71	112.04
22	a	2030	6MZ	C9-N6-C6	-6.05	117.66	122.87
22	a	2445	2MG	C2-N3-C4	5.99	119.47	112.04
22	a	747	5MU	O4-C4-C5	-5.93	118.02	124.90
54	Z	8	4SU	C5-C4-N3	5.81	120.08	114.69
22	a	1939	5MU	O4-C4-C5	-5.67	118.33	124.90
22	a	2503	2MA	N3-C4-N9	5.65	134.83	126.99
54	Z	55	5MU	O4-C4-C5	-5.63	118.37	124.90
55	V	6	2MG	C5-C4-N3	-5.60	119.38	128.46
22	a	1915	3TD	N1-C2-N3	5.59	120.55	116.14
22	a	2552	OMU	C4-N3-C2	-5.54	119.27	126.58
22	a	1835	2MG	C5-C4-N3	-5.54	119.48	128.46
22	a	1939	5MU	C4-N3-C2	-5.50	120.23	127.35
22	a	747	5MU	C4-N3-C2	-5.44	120.31	127.35
22	a	1618	6MZ	N1-C2-N3	-5.42	120.13	128.60
22	a	1618	6MZ	C5-C4-N3	-5.41	119.69	126.75
1	A	1519	MA6	N1-C2-N3	-5.41	120.14	128.60
22	a	2251	OMG	C5-C4-N3	-5.37	119.76	128.46
22	a	2030	6MZ	N1-C2-N3	-5.30	120.32	128.60
22	a	2030	6MZ	C5-C4-N3	-5.27	119.88	126.75
22	a	745	1MG	C5-C4-N3	-5.27	119.92	128.46
1	A	1518	MA6	N1-C2-N3	-5.24	120.40	128.60
1	A	966	2MG	C5-C4-N3	-5.23	119.97	128.46
22	a	2457	PSU	N1-C2-N3	5.20	121.02	115.13
1	A	1207	2MG	C5-C4-N3	-5.18	120.06	128.46
55	V	10	2MG	C5-C4-N3	-5.12	120.16	128.46
22	a	2580	PSU	N1-C2-N3	5.10	120.90	115.13
22	a	2030	6MZ	N9-C8-N7	-5.08	106.97	113.91
22	a	1835	2MG	C2-N1-C6	-5.07	118.65	124.48
1	A	1519	MA6	C5-C4-N3	-5.05	120.16	126.75
54	Z	55	5MU	C4-N3-C2	-5.02	120.86	127.35
22	a	746	PSU	C4-N3-C2	-5.01	119.12	126.34
22	a	2457	PSU	C4-N3-C2	-4.99	119.15	126.34
55	V	55	PSU	N1-C2-N3	4.92	120.70	115.13
22	a	2605	PSU	C4-N3-C2	-4.91	119.26	126.34
1	A	1519	MA6	C4-C5-C6	4.86	121.32	115.88
55	V	54	2MU	N3-C2-N1	4.85	121.33	114.89
55	V	55	PSU	C4-N3-C2	-4.83	119.38	126.34
22	a	2504	PSU	C4-N3-C2	-4.82	119.39	126.34
22	a	2504	PSU	N1-C2-N3	4.82	120.59	115.13
1	A	1518	MA6	C5-C4-N3	-4.82	120.46	126.75
1	A	1518	MA6	C4-C5-C6	4.79	121.24	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	2MG	C2-N1-C6	-4.79	118.97	124.48
22	a	2580	PSU	C4-N3-C2	-4.78	119.44	126.34
1	A	1498	UR3	C4-N3-C2	-4.78	120.07	124.56
22	a	2445	2MG	C5-C4-N3	-4.77	120.72	128.46
22	a	1911	PSU	C4-N3-C2	-4.71	119.55	126.34
55	V	27	PSU	C4-N3-C2	-4.71	119.56	126.34
22	a	955	PSU	C4-N3-C2	-4.69	119.58	126.34
54	Z	56	PSU	C4-N3-C2	-4.69	119.58	126.34
55	V	34	A1L4U	O9-C8-C5M	4.69	119.95	111.27
55	V	39	PSU	N1-C2-N3	4.67	120.43	115.13
22	a	2604	PSU	C4-N3-C2	-4.67	119.62	126.34
22	a	1917	PSU	C4-N3-C2	-4.65	119.64	126.34
22	a	1939	5MU	N3-C2-N1	4.65	121.06	114.89
22	a	955	PSU	N1-C2-N3	4.65	120.39	115.13
22	a	2604	PSU	N1-C2-N3	4.61	120.35	115.13
1	A	1516	2MG	C5-C4-N3	-4.60	121.01	128.46
55	V	10	2MG	C2-N1-C6	-4.59	119.20	124.48
1	A	1519	MA6	N9-C8-N7	-4.57	107.66	113.91
22	a	1917	PSU	N1-C2-N3	4.55	120.28	115.13
55	V	6	2MG	C2-N1-C6	-4.53	119.27	124.48
22	a	2445	2MG	C2-N1-C6	-4.53	119.27	124.48
55	V	27	PSU	N1-C2-N3	4.52	120.25	115.13
1	A	516	PSU	C4-N3-C2	-4.48	119.88	126.34
22	a	1911	PSU	N1-C2-N3	4.48	120.20	115.13
22	a	2605	PSU	N1-C2-N3	4.45	120.17	115.13
1	A	1207	2MG	C2-N1-C6	-4.45	119.36	124.48
1	A	527	G7M	C2-N3-C4	4.43	120.20	112.30
22	a	747	5MU	N3-C2-N1	4.43	120.77	114.89
1	A	1516	2MG	C2-N1-C6	-4.41	119.40	124.48
22	a	2251	OMG	C2-N3-C4	4.41	120.15	112.30
54	Z	56	PSU	N1-C2-N3	4.38	120.09	115.13
55	V	39	PSU	C4-N3-C2	-4.36	120.06	126.34
22	a	1618	6MZ	N9-C8-N7	-4.33	107.99	113.91
1	A	1518	MA6	C2-N1-C6	4.29	121.89	111.75
55	V	46	G7M	C2-N3-C4	4.29	119.94	112.30
55	V	54	2MU	C4-N3-C2	-4.25	121.85	127.35
22	a	746	PSU	N1-C2-N3	4.16	119.84	115.13
22	a	2069	G7M	C2-N3-C4	4.16	119.70	112.30
1	A	527	G7M	C5-C6-N1	4.15	120.46	111.79
54	Z	55	5MU	N3-C2-N1	4.12	120.36	114.89
54	Z	8	4SU	N3-C2-N1	4.10	120.33	114.89
1	A	1518	MA6	N9-C8-N7	-4.08	108.34	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	C2-N1-C6	4.07	121.37	111.75
22	a	2552	OMU	N3-C2-N1	4.03	120.25	114.89
22	a	1915	3TD	C4-N3-C2	-4.01	120.26	124.61
1	A	516	PSU	N1-C2-N3	3.99	119.66	115.13
55	V	46	G7M	C5-C6-N1	3.99	120.12	111.79
55	V	46	G7M	C5-C4-N3	-3.93	120.61	128.15
1	A	527	G7M	C5-C4-N3	-3.92	120.62	128.15
22	a	2030	6MZ	C4-C5-C6	3.92	119.85	116.81
22	a	2069	G7M	C5-C6-N1	3.92	119.97	111.79
1	A	527	G7M	O6-C6-C5	-3.83	119.41	128.06
55	V	6	2MG	N9-C4-N3	3.83	133.63	125.94
55	V	54	2MU	C5-C4-N3	3.78	118.54	115.31
54	Z	8	4SU	C5-C4-S4	-3.72	119.67	124.47
22	a	1939	5MU	C5M-C5-C6	-3.72	117.88	122.85
22	a	1939	5MU	C5M-C5-C4	3.69	122.83	118.77
22	a	1835	2MG	N9-C4-N3	3.68	133.32	125.94
22	a	1618	6MZ	C2-N3-C4	3.67	120.41	111.75
22	a	747	5MU	C5M-C5-C6	-3.65	117.97	122.85
22	a	745	1MG	C1'-N9-C8	-3.64	116.32	126.70
22	a	2069	G7M	C5-C4-N3	-3.63	121.18	128.15
22	a	2251	OMG	N9-C4-N3	3.63	133.22	125.94
22	a	2030	6MZ	C5-N7-C8	3.63	108.66	103.51
54	Z	55	5MU	C5M-C5-C6	-3.61	118.02	122.85
22	a	1618	6MZ	C4-C5-C6	3.60	119.59	116.81
1	A	1519	MA6	C5-N7-C8	3.59	108.60	103.51
55	V	46	G7M	O6-C6-C5	-3.58	119.98	128.06
22	a	2457	PSU	O2-C2-N1	-3.57	118.86	122.79
22	a	745	1MG	C2-N3-C4	3.57	119.99	111.98
22	a	2069	G7M	O6-C6-C5	-3.56	120.02	128.06
54	Z	55	5MU	C5M-C5-C4	3.54	122.67	118.77
22	a	2030	6MZ	C2-N3-C4	3.52	120.06	111.75
54	Z	21	H2U	C4-N3-C2	-3.50	122.89	125.79
22	a	2503	2MA	N9-C8-N7	-3.50	109.13	113.91
55	V	49	5MC	C5-C6-N1	-3.47	119.77	123.34
22	a	2552	OMU	C5-C4-N3	3.45	120.00	114.84
1	A	1207	2MG	N9-C4-N3	3.42	132.81	125.94
22	a	2251	OMG	C2-N1-C6	-3.41	118.88	125.10
1	A	527	G7M	N9-C4-N3	3.41	132.78	125.94
55	V	54	2MU	O4-C4-C5	-3.40	120.96	124.90
1	A	1407	5MC	C5-C6-N1	-3.38	119.86	123.34
22	a	2445	2MG	N9-C8-N7	-3.37	107.04	113.39
22	a	747	5MU	C5M-C5-C4	3.37	122.47	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	48	5MC	C5-C6-N1	-3.37	119.88	123.34
1	A	1516	2MG	N9-C8-N7	-3.35	107.08	113.39
55	V	10	2MG	N9-C8-N7	-3.33	107.13	113.39
55	V	10	2MG	N9-C4-N3	3.31	132.59	125.94
22	a	2251	OMG	N9-C8-N7	-3.29	107.19	113.39
22	a	745	1MG	N9-C4-N3	3.28	132.52	125.94
33	l	81	4D4	NE-CZ-NH2	3.28	126.46	120.70
1	A	1518	MA6	C5-N7-C8	3.26	108.13	103.51
1	A	966	2MG	N9-C4-N3	3.25	132.47	125.94
1	A	1519	MA6	C2-N3-C4	3.24	119.41	111.75
55	V	46	G7M	N9-C4-N3	3.20	132.36	125.94
22	a	2503	2MA	N3-C2-N1	-3.19	119.84	125.72
22	a	1962	5MC	C5-C6-N1	-3.19	120.05	123.34
22	a	1618	6MZ	N3-C4-N9	3.19	132.34	127.08
1	A	966	2MG	N9-C8-N7	-3.19	107.38	113.39
55	V	55	PSU	O2-C2-N1	-3.15	119.33	122.79
1	A	1207	2MG	N9-C8-N7	-3.13	107.49	113.39
55	V	46	G7M	C2-N1-C6	-3.08	119.48	125.10
22	a	745	1MG	N9-C8-N7	-3.06	107.62	113.39
22	a	1835	2MG	N9-C8-N7	-3.06	107.62	113.39
1	A	527	G7M	C2-N1-C6	-3.02	119.59	125.10
22	a	2069	G7M	C2-N1-C6	-3.02	119.60	125.10
1	A	1518	MA6	C2-N3-C4	3.01	118.87	111.75
33	l	81	4D4	CB-CA-C	-3.01	106.96	111.77
1	A	967	5MC	C5-C6-N1	-3.00	120.25	123.34
22	a	955	PSU	O2-C2-N1	-3.00	119.49	122.79
55	V	6	2MG	N9-C8-N7	-3.00	107.75	113.39
22	a	1917	PSU	O2-C2-N1	-2.99	119.50	122.79
22	a	1835	2MG	C5-C6-N1	2.98	120.76	113.19
22	a	2580	PSU	C6-N1-C2	-2.95	119.66	122.68
22	a	1939	5MU	O2-C2-N1	-2.95	118.86	122.79
54	Z	56	PSU	O2-C2-N1	-2.94	119.55	122.79
22	a	2445	2MG	N9-C4-N3	2.94	131.84	125.94
1	A	1519	MA6	C4-C5-N7	-2.94	107.04	110.62
55	V	39	PSU	O2-C2-N1	-2.93	119.56	122.79
22	a	1618	6MZ	C5-N7-C8	2.93	107.67	103.51
1	A	516	PSU	O2-C2-N1	-2.92	119.57	122.79
22	a	2552	OMU	O4-C4-C5	-2.91	120.04	125.16
22	a	2251	OMG	C5-C6-N1	2.89	120.53	113.19
22	a	2503	2MA	C6-C5-C4	2.86	121.02	117.18
22	a	2030	6MZ	N3-C4-N9	2.85	131.78	127.08
1	A	1518	MA6	C4-C5-N7	-2.85	107.15	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	54	2MU	C5M-C5-C4	2.83	121.89	118.77
22	a	1835	2MG	CM2-N2-C2	-2.83	117.60	123.86
22	a	2580	PSU	O2-C2-N1	-2.83	119.68	122.79
22	a	2457	PSU	C6-C5-C4	2.82	120.17	118.20
22	a	1911	PSU	O2-C2-N1	-2.82	119.68	122.79
1	A	966	2MG	C5-C6-N1	2.82	120.34	113.19
1	A	1207	2MG	C5-C6-N1	2.81	120.32	113.19
22	a	2030	6MZ	C4-N9-C8	2.80	108.77	105.73
22	a	745	1MG	C1'-N9-C4	2.80	134.83	126.50
1	A	1516	2MG	CM2-N2-C2	-2.80	117.69	123.86
22	a	745	1MG	C5-C6-N1	2.79	120.30	114.91
22	a	2445	2MG	CM2-N2-C2	-2.78	117.71	123.86
25	d	150	MEQ	OE1-CD-CG	2.78	127.10	122.02
55	V	47	H2U	C5-C6-N1	-2.78	102.45	111.61
22	a	2030	6MZ	C4-C5-N7	-2.76	107.26	110.62
22	a	2457	PSU	C6-N1-C2	-2.76	119.86	122.68
55	V	10	2MG	C5-C6-N1	2.75	120.19	113.19
1	A	1516	2MG	C5-C6-N1	2.75	120.18	113.19
22	a	2251	OMG	O6-C6-C5	-2.74	119.33	126.60
33	l	82	MS6	CE-SD-CG	2.74	109.81	100.40
1	A	1402	4OC	CM4-N4-C4	-2.73	117.12	122.45
22	a	1835	2MG	O6-C6-C5	-2.72	119.37	126.60
22	a	2503	2MA	C5-N7-C8	2.71	107.36	103.51
22	a	2445	2MG	C5-C6-N1	2.70	120.06	113.19
55	V	6	2MG	C5-C6-N1	2.69	120.01	113.19
55	V	37	12A	CA-N-CC	-2.68	117.48	121.94
22	a	2069	G7M	N9-C4-N3	2.68	131.31	125.94
55	V	27	PSU	O2-C2-N1	-2.68	119.84	122.79
55	V	39	PSU	C6-N1-C2	-2.66	119.96	122.68
55	V	37	12A	N6-CC-N	2.65	117.47	113.76
1	A	1207	2MG	O6-C6-C5	-2.65	119.58	126.60
22	a	2604	PSU	O2-C2-N1	-2.63	119.89	122.79
33	l	81	4D4	O-C-CA	-2.62	117.91	124.78
22	a	1939	5MU	O4-C4-N3	-2.61	115.11	120.12
55	V	55	PSU	C6-C5-C4	2.61	120.02	118.20
1	A	966	2MG	O6-C6-C5	-2.60	119.70	126.60
1	A	1516	2MG	N9-C4-N3	2.60	131.16	125.94
55	V	34	A1L4U	C5M-C5-C6	2.58	128.33	122.42
22	a	747	5MU	O2-C2-N1	-2.58	119.35	122.79
22	a	2605	PSU	O2-C2-N1	-2.58	119.95	122.79
55	V	54	2MU	C6-N1-C2	-2.57	118.69	121.30
1	A	527	G7M	CN7-N7-C5	2.55	129.94	126.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2504	PSU	O2-C2-N1	-2.54	119.99	122.79
22	a	2445	2MG	O6-C6-C5	-2.54	119.86	126.60
1	A	1518	MA6	C5-C4-N9	2.54	108.74	105.78
1	A	1519	MA6	N3-C4-N9	2.53	131.26	127.08
1	A	1516	2MG	O6-C6-C5	-2.52	119.91	126.60
22	a	2604	PSU	C6-N1-C2	-2.52	120.11	122.68
22	a	1618	6MZ	C5-C6-N1	2.51	120.87	118.20
55	V	6	2MG	O6-C6-C5	-2.50	119.95	126.60
22	a	1962	5MC	C1'-N1-C6	-2.50	116.95	121.12
22	a	2580	PSU	O4'-C1'-C2'	2.49	108.66	105.14
55	V	55	PSU	C6-N1-C2	-2.49	120.14	122.68
22	a	2069	G7M	CN7-N7-C5	2.49	129.86	126.77
22	a	955	PSU	C6-N1-C2	-2.46	120.17	122.68
25	d	150	MEQ	CG-CD-NE2	-2.46	112.88	116.29
1	A	1207	2MG	N1-C2-N3	-2.45	120.16	123.95
54	Z	55	5MU	O4-C4-N3	-2.45	115.43	120.12
55	V	10	2MG	O6-C6-C5	-2.44	120.11	126.60
22	a	2504	PSU	C6-N1-C2	-2.44	120.19	122.68
22	a	2552	OMU	O2-C2-N1	-2.43	119.55	122.79
22	a	2449	H2U	C4-N3-C2	-2.42	123.79	125.79
55	V	37	12A	OG1-CB-CA	2.41	113.97	109.13
1	A	1519	MA6	C5-C4-N9	2.41	108.58	105.78
1	A	1516	2MG	C1'-N9-C4	-2.40	119.37	126.50
22	a	747	5MU	O4-C4-N3	-2.39	115.54	120.12
55	V	46	G7M	CN7-N7-C5	2.38	129.73	126.77
22	a	746	PSU	O2-C2-N1	-2.38	120.17	122.79
1	A	1516	2MG	N1-C2-N3	-2.38	120.27	123.95
22	a	2503	2MA	CM2-C2-N3	2.36	120.83	117.15
55	V	54	2MU	O2-C2-N3	-2.35	117.12	121.50
55	V	34	A1L4U	O4-C4-C5	-2.35	119.53	121.67
22	a	1917	PSU	C6-N1-C2	-2.35	120.28	122.68
1	A	966	2MG	CM2-N2-C2	-2.34	118.69	123.86
55	V	6	2MG	N1-C2-N3	-2.31	120.38	123.95
22	a	2449	H2U	O4-C4-N3	2.31	123.94	120.28
54	Z	8	4SU	O2-C2-N1	-2.31	119.72	122.79
22	a	2251	OMG	C1'-N9-C4	-2.29	119.69	126.50
55	V	34	A1L4U	C5M-C5-C4	-2.29	113.89	120.45
55	V	34	A1L4U	C6-N1-C2	-2.29	116.63	119.20
22	a	1618	6MZ	C4-N9-C8	2.27	108.19	105.73
12	L	89	D2T	O-C-CA	-2.26	118.84	124.78
1	A	966	2MG	N1-C2-N3	-2.26	120.46	123.95
1	A	1518	MA6	N3-C4-N9	2.25	130.80	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	N1-C6-N6	-2.25	114.62	117.08
55	V	10	2MG	C8-N7-C5	2.25	108.31	104.24
22	a	1911	PSU	C6-N1-C2	-2.24	120.39	122.68
22	a	2445	2MG	N1-C2-N3	-2.23	120.50	123.95
55	V	37	12A	N3-C4-N9	2.22	130.07	126.99
54	Z	55	5MU	O2-C2-N1	-2.21	119.84	122.79
22	a	1835	2MG	N1-C2-N3	-2.21	120.54	123.95
55	V	54	2MU	O4'-C1'-N1	2.20	113.40	108.36
22	a	2030	6MZ	C5-C4-N9	2.20	108.35	105.78
22	a	2069	G7M	N9-C8-N7	-2.20	106.76	112.21
55	V	37	12A	OO-CC-N6	-2.20	119.90	123.62
1	A	1519	MA6	C4-N9-C8	2.20	108.11	105.73
55	V	37	12A	N6-C6-N1	2.20	125.81	118.44
55	V	10	2MG	N1-C2-N3	-2.19	120.56	123.95
22	a	1962	5MC	CM5-C5-C6	-2.18	119.93	122.85
11	K	119	IAS	OXT-C-CA	2.16	120.75	113.38
55	V	46	G7M	N9-C8-N7	-2.16	106.86	112.21
1	A	1402	4OC	C6-C5-C4	2.16	119.61	116.96
1	A	516	PSU	O4'-C1'-C2'	2.16	108.19	105.14
11	K	119	IAS	OXT-C-O	-2.15	119.20	124.09
1	A	966	2MG	C8-N7-C5	2.14	108.12	104.24
1	A	527	G7M	N9-C8-N7	-2.14	106.92	112.21
1	A	1207	2MG	CM2-N2-C2	-2.14	119.14	123.86
55	V	6	2MG	C8-N7-C5	2.12	108.08	104.24
22	a	2498	OMC	O2-C2-N3	-2.11	118.90	122.33
22	a	2030	6MZ	C5-C6-N1	2.11	120.45	118.20
22	a	2445	2MG	C8-N7-C5	2.11	108.06	104.24
1	A	516	PSU	C6-N1-C2	-2.10	120.53	122.68
22	a	2449	H2U	C5-C6-N1	-2.10	104.68	111.61
55	V	27	PSU	C6-N1-C2	-2.10	120.54	122.68
22	a	2605	PSU	C6-N1-C2	-2.08	120.56	122.68
22	a	2580	PSU	C6-C5-C4	2.07	119.64	118.20
1	A	1516	2MG	C8-N7-C5	2.06	107.96	104.24
1	A	1207	2MG	C8-N7-C5	2.05	107.96	104.24
22	a	2457	PSU	O4'-C1'-C2'	2.05	108.03	105.14
55	V	58	1MA	C6-C5-N7	-2.04	128.48	132.20
22	a	1835	2MG	C8-N7-C5	2.04	107.94	104.24
1	A	1519	MA6	N1-C6-N6	-2.03	114.86	117.08
22	a	1618	6MZ	C4-C5-N7	-2.01	108.17	110.62
22	a	2251	OMG	C8-N7-C5	2.01	107.88	104.24
1	A	527	G7M	N1-C2-N3	-2.00	119.58	123.32

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
33	l	81	4D4	N-CA-CB-CG
33	l	81	4D4	NE-CD-CG-CB
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	2445	2MG	C3'-C4'-C5'-O5'
55	V	34	A1L4U	C5M-C8-O9-C9
55	V	34	A1L4U	C6-C5-C5M-C8
55	V	34	A1L4U	C4-C5-C5M-C8
55	V	47	H2U	O4'-C1'-N1-C6
55	V	47	H2U	C2'-C1'-N1-C2
55	V	47	H2U	C2'-C1'-N1-C6
55	V	48	5MC	O4'-C4'-C5'-O5'
55	V	49	5MC	O4'-C4'-C5'-O5'
55	V	49	5MC	C3'-C4'-C5'-O5'
55	V	34	A1L4U	O8-C8-O9-C9
55	V	34	A1L4U	O4'-C1'-N1-C2
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
55	V	6	2MG	C3'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
25	d	150	MEQ	CA-CB-CG-CD
54	Z	21	H2U	C2'-C1'-N1-C6
33	l	82	MS6	CB-CG-SD-CE
22	a	2445	2MG	O4'-C4'-C5'-O5'
55	V	6	2MG	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C10
1	A	1519	MA6	C5-C6-N6-C10
33	l	82	MS6	CA-CB-CG-SD
22	a	1835	2MG	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
22	a	2503	2MA	O4'-C4'-C5'-O5'
54	Z	21	H2U	C2'-C1'-N1-C2
22	a	1835	2MG	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
11	K	119	IAS	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
25	d	150	MEQ	OE1-CD-CG-CB
1	A	1519	MA6	C4'-C5'-O5'-P
55	V	47	H2U	C4'-C5'-O5'-P
25	d	150	MEQ	NE2-CD-CG-CB
54	Z	56	PSU	O4'-C1'-C5-C4
22	a	2552	OMU	C3'-C2'-O2'-CM2
22	a	1962	5MC	C2'-C1'-N1-C6
22	a	1962	5MC	O4'-C1'-N1-C6
55	V	47	H2U	O4'-C1'-N1-C2
55	V	58	1MA	O4'-C4'-C5'-O5'
54	Z	56	PSU	O4'-C1'-C5-C6
22	a	746	PSU	O4'-C1'-C5-C6
1	A	1402	4OC	C3'-C4'-C5'-O5'
22	a	2069	G7M	C3'-C4'-C5'-O5'
33	l	81	4D4	C-CA-CB-CG
33	l	81	4D4	O-C-CA-CB
22	a	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	1939	5MU	1	0
22	a	2552	OMU	1	0
12	L	89	D2T	2	0
22	a	2445	2MG	1	0
22	a	1915	3TD	1	0
22	a	2030	6MZ	1	0
55	V	47	H2U	1	0
22	a	2251	OMG	2	0
55	V	10	2MG	2	0
54	Z	55	5MU	1	0
54	Z	21	H2U	1	0
22	a	2503	2MA	1	0
1	A	1402	4OC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 450 ligands modelled in this entry, 450 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

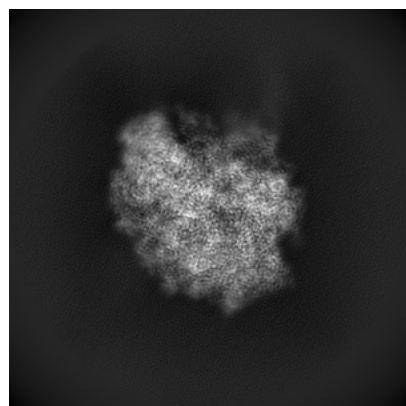
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61708. These allow visual inspection of the internal detail of the map and identification of artifacts.

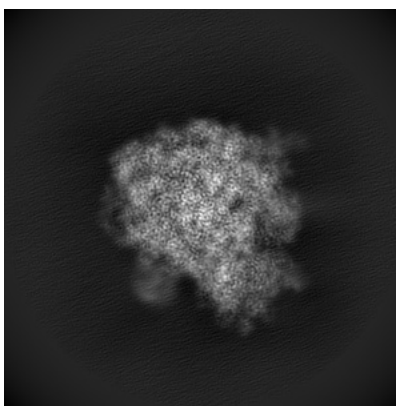
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

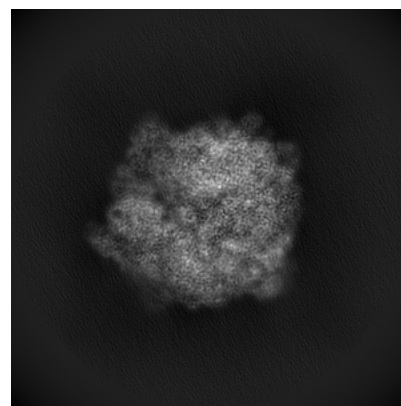
6.1.1 Primary map



X

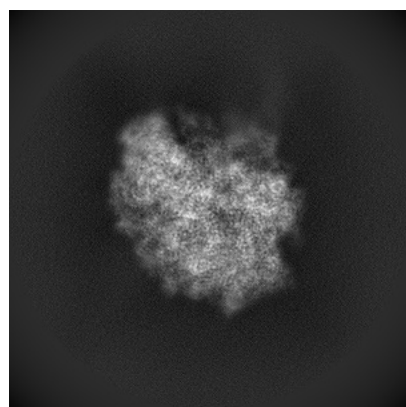


Y

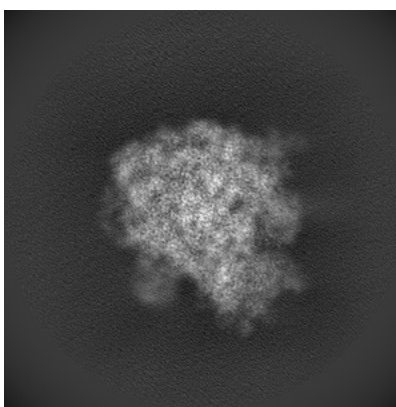


Z

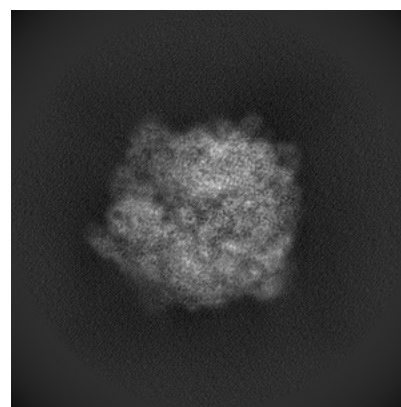
6.1.2 Raw map



X



Y

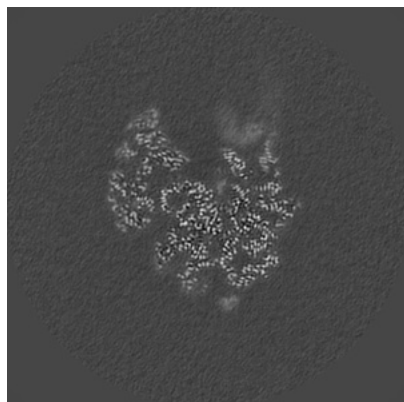


Z

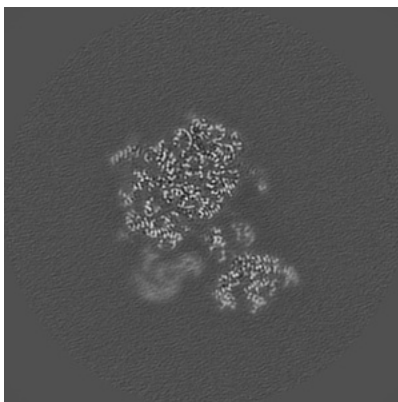
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

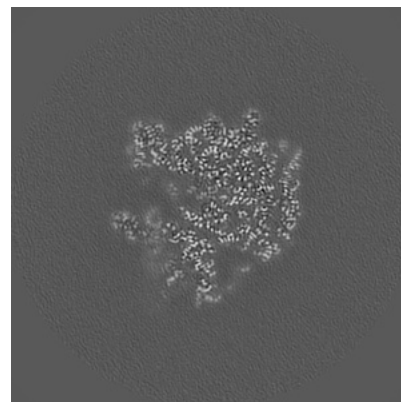
6.2.1 Primary map



X Index: 265

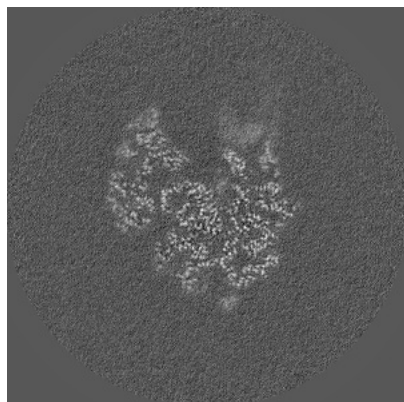


Y Index: 265

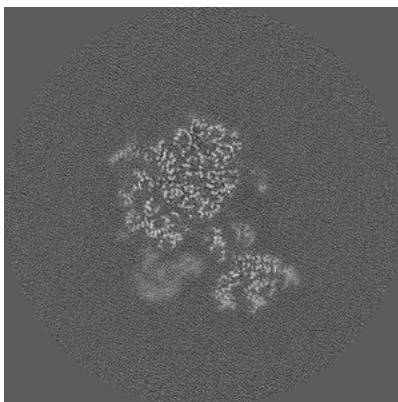


Z Index: 265

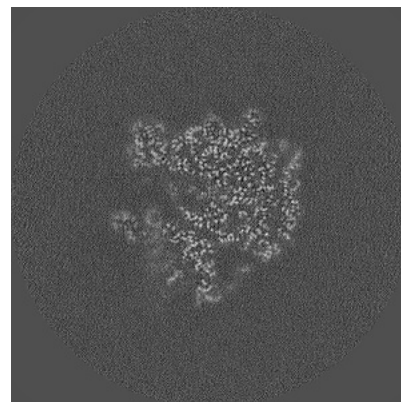
6.2.2 Raw map



X Index: 265



Y Index: 265

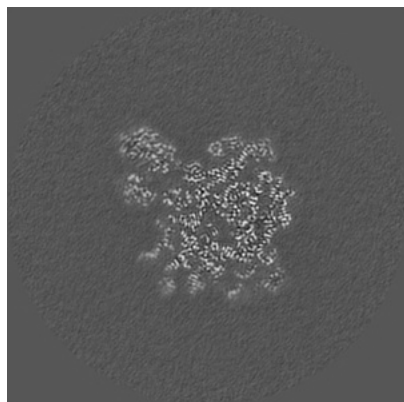


Z Index: 265

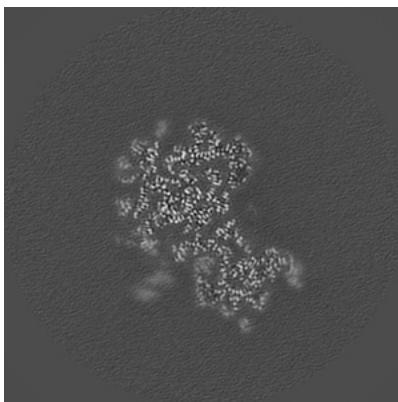
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

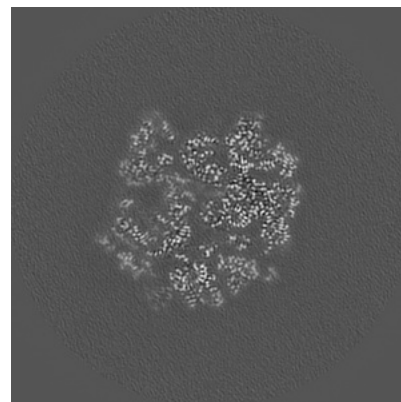
6.3.1 Primary map



X Index: 302

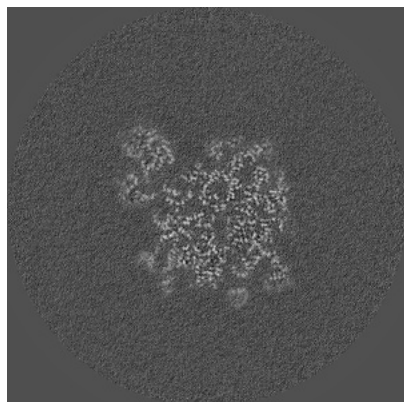


Y Index: 242

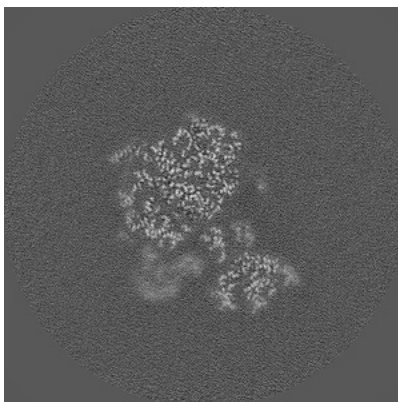


Z Index: 280

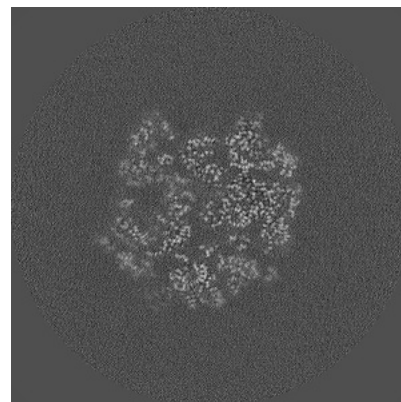
6.3.2 Raw map



X Index: 296



Y Index: 264

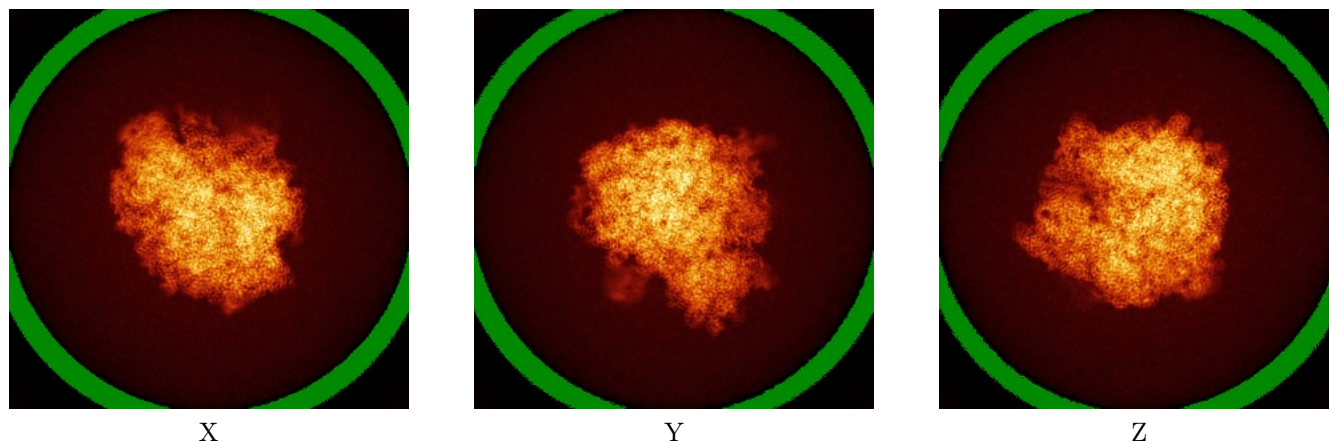


Z Index: 280

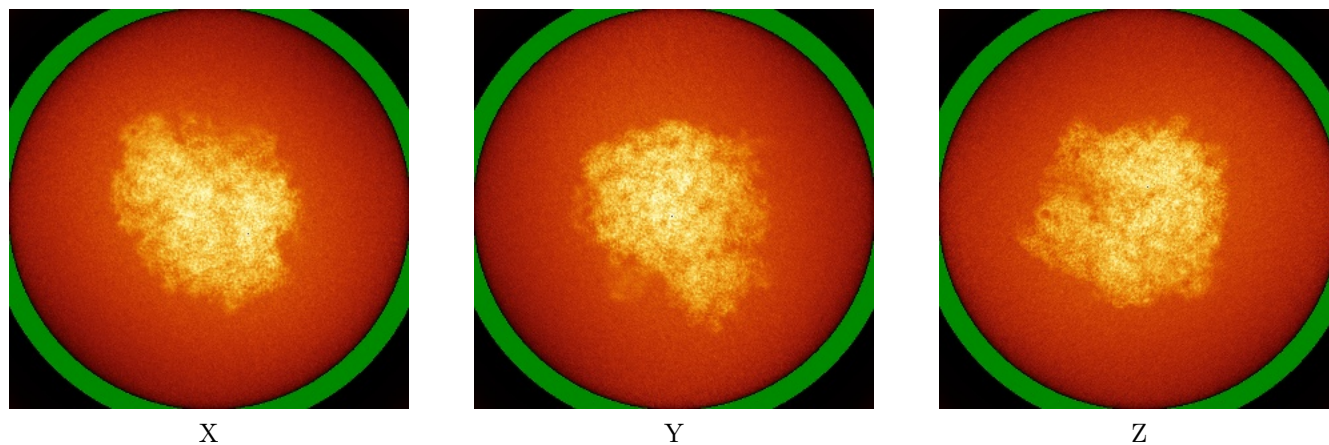
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



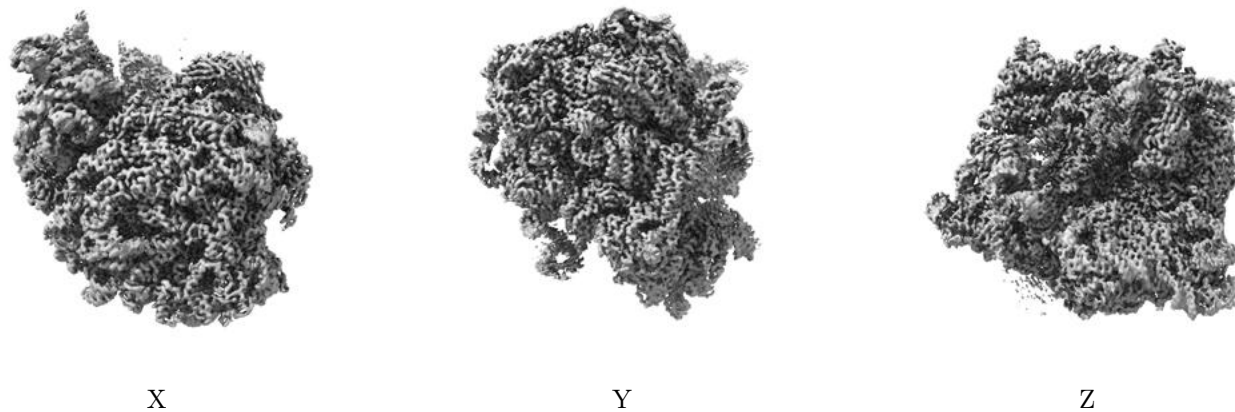
6.4.2 Raw map



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

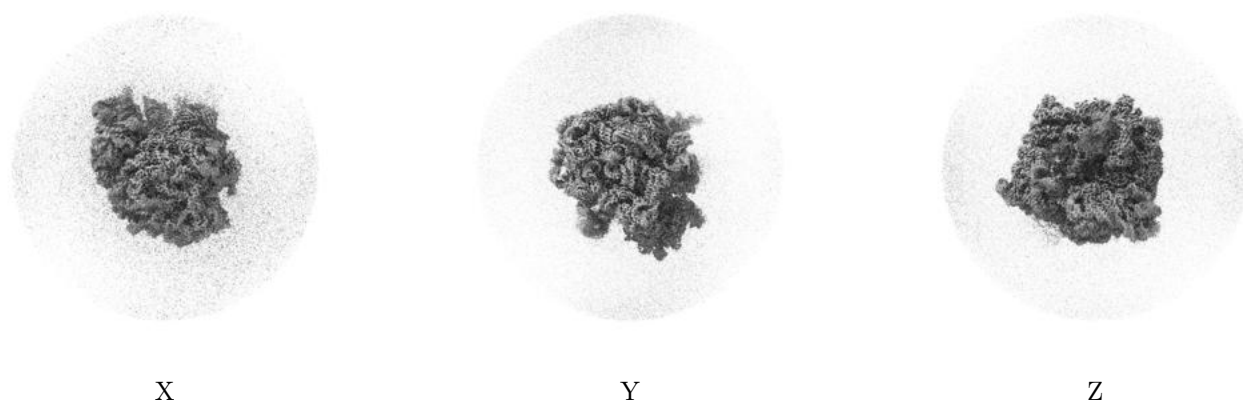
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

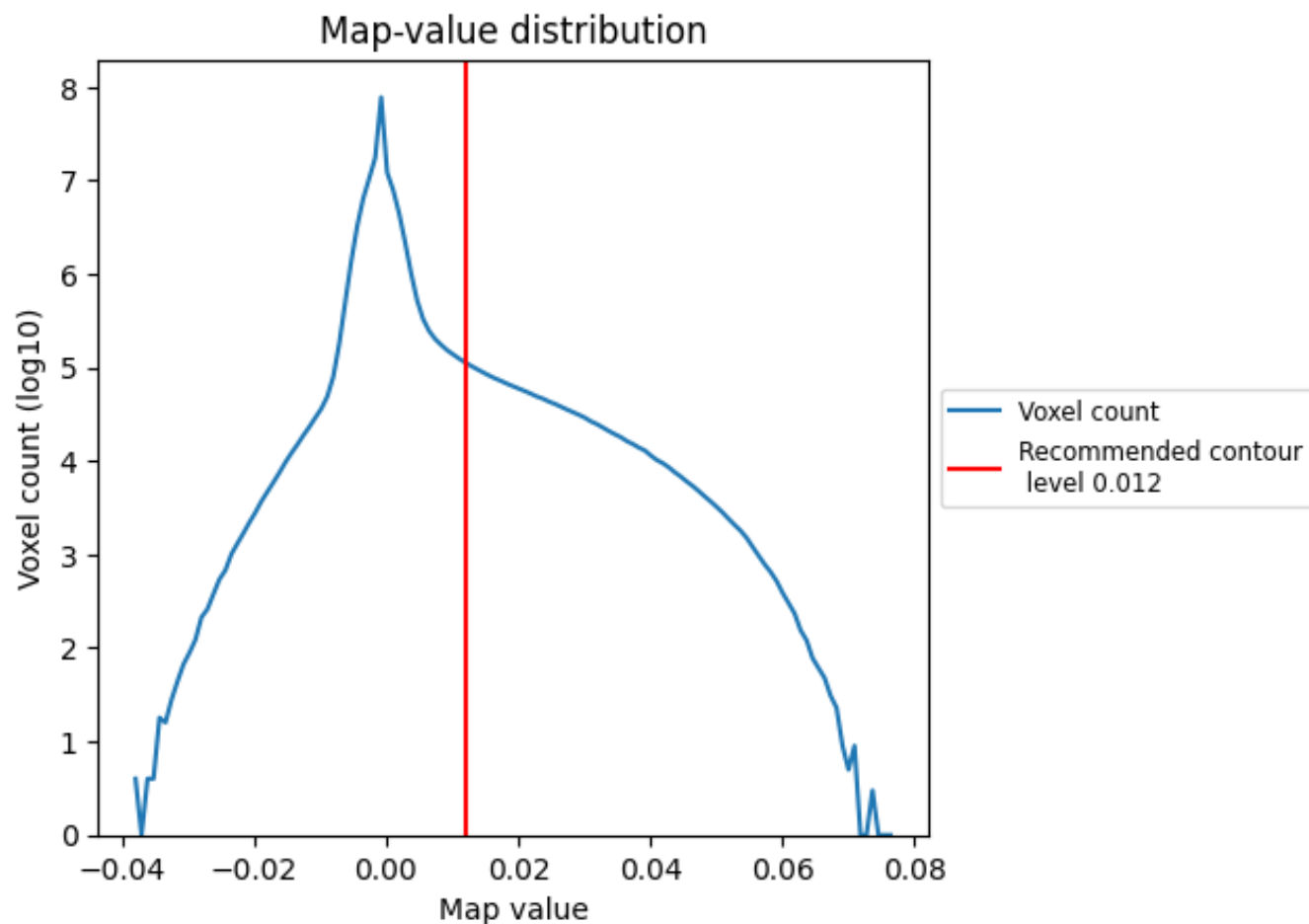
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

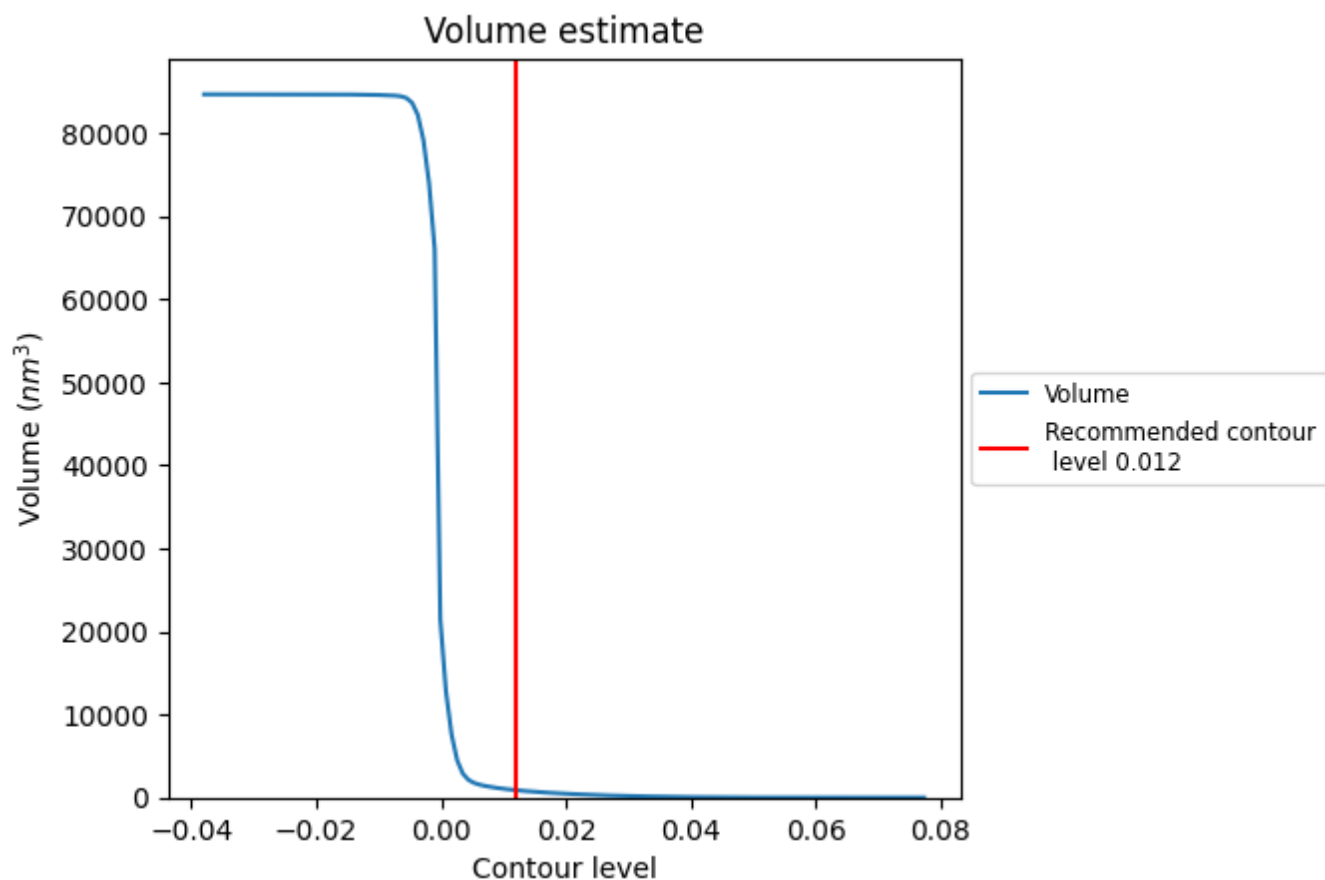
This section contains the results of statistical analysis of the map.

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.

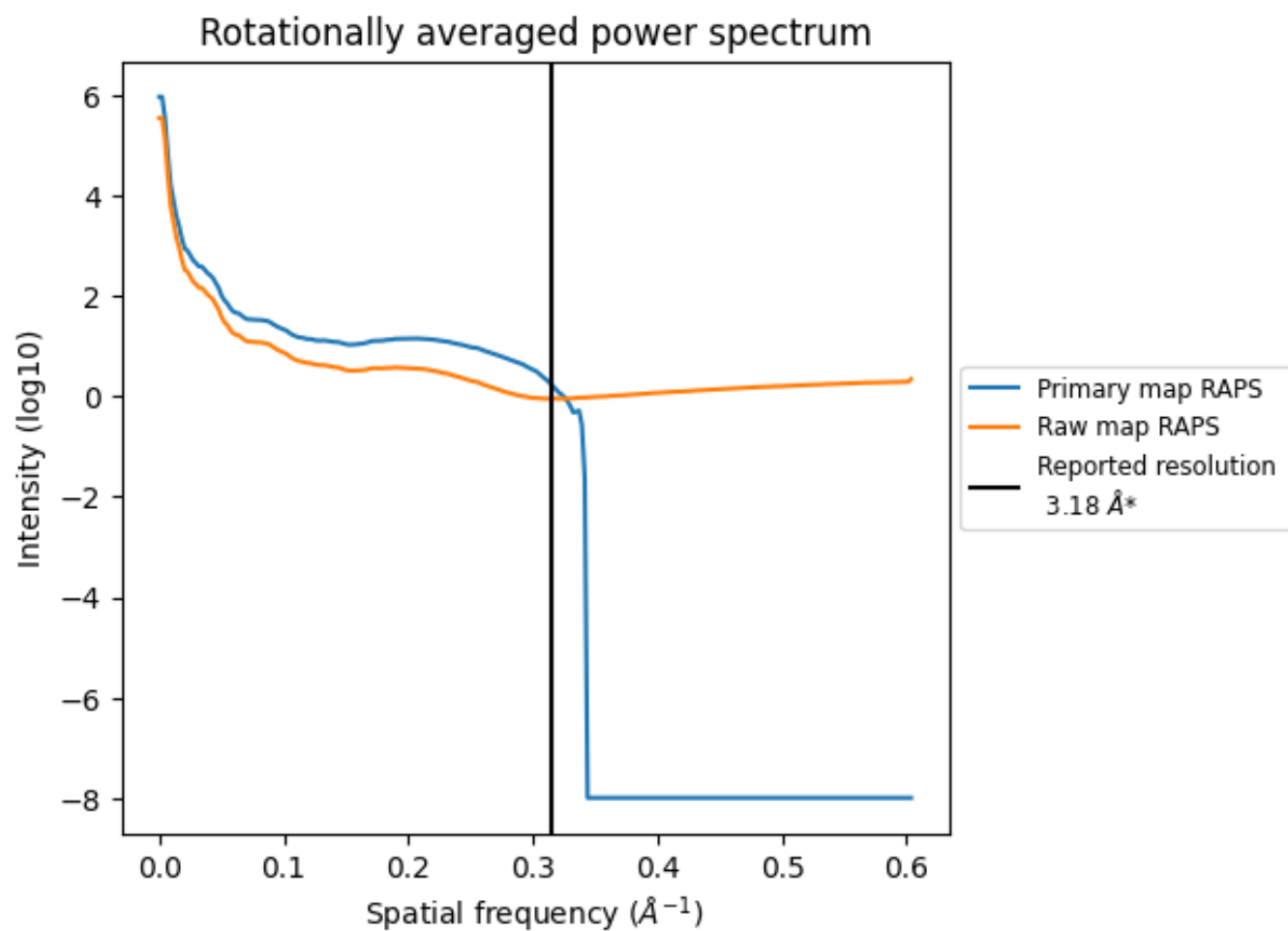
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 890 nm³; this corresponds to an approximate mass of 804 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 ⓘ

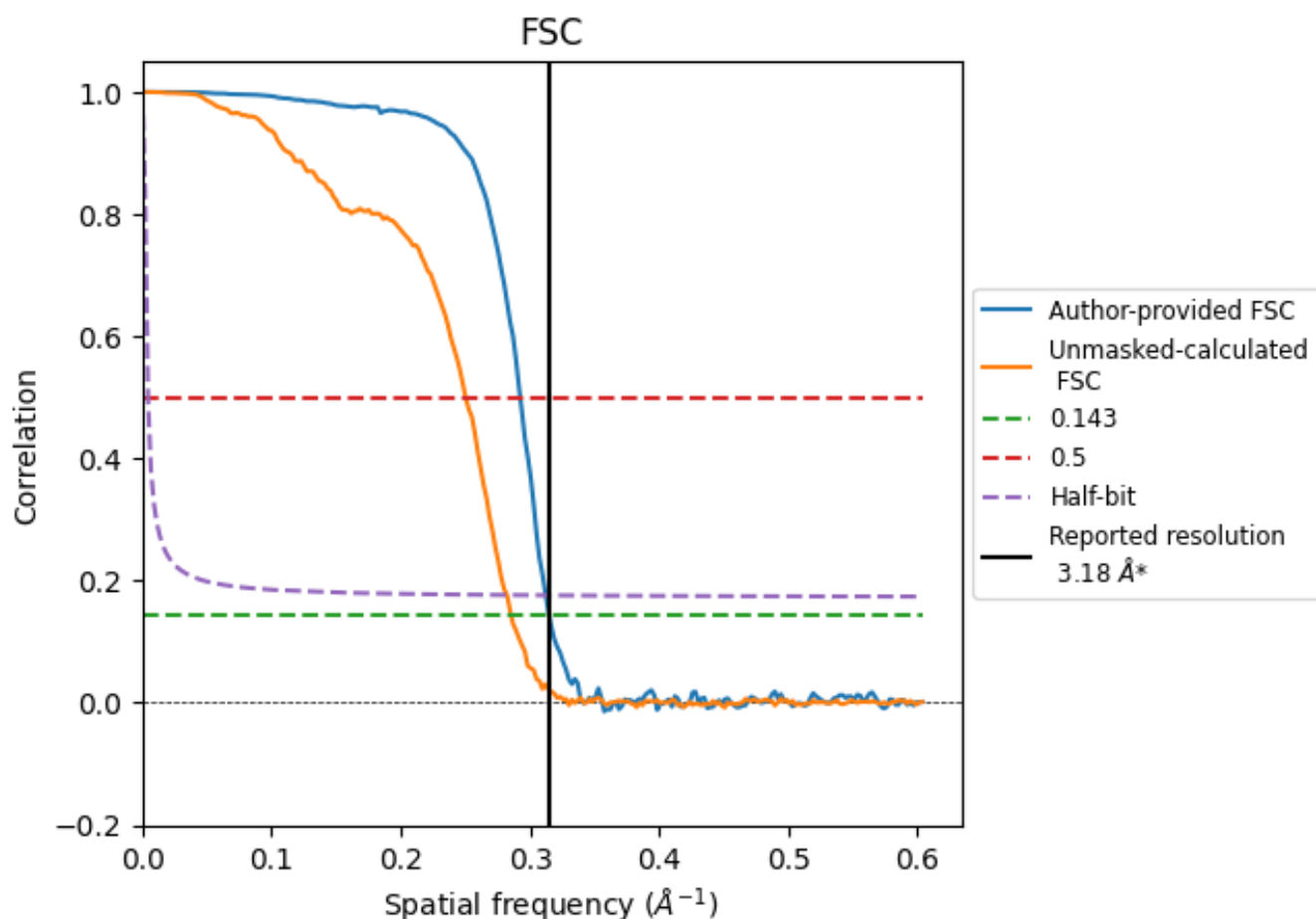


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8.2 Resolution estimates [i](#)

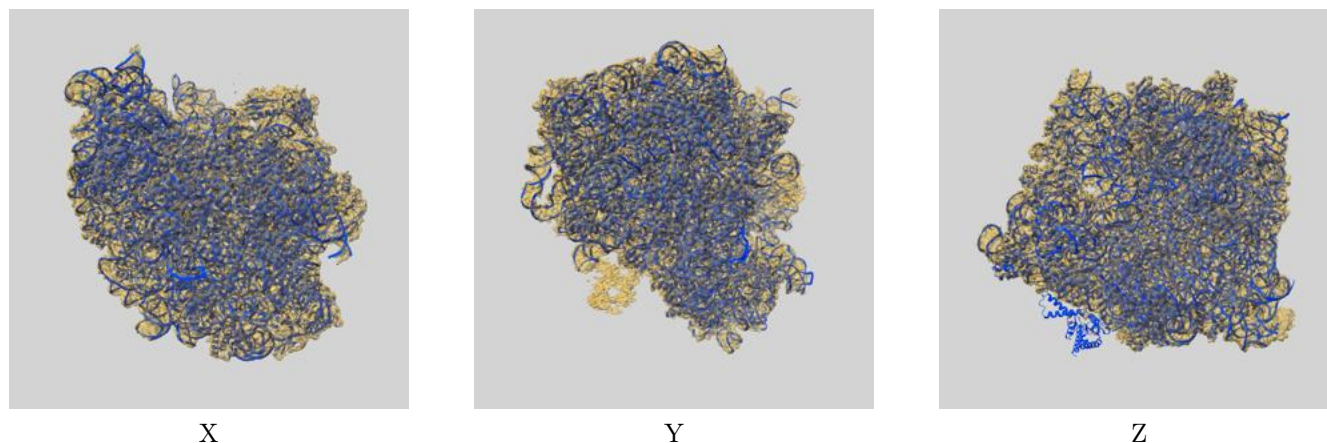
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.42	3.20
Unmasked-calculated*	3.50	4.00	3.54

*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 3.50 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

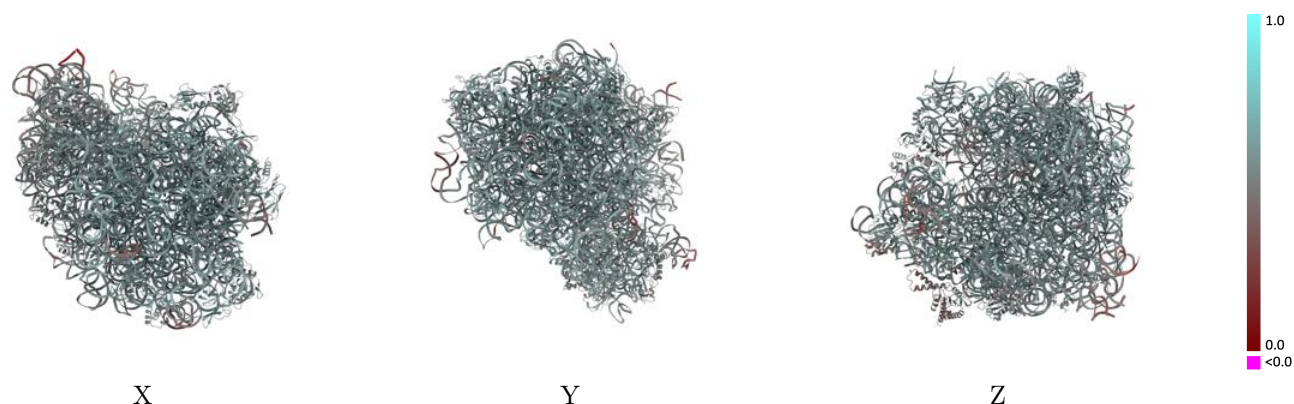
This section contains information regarding the fit between EMDB map EMD-61708 and PDB model 9JPO. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



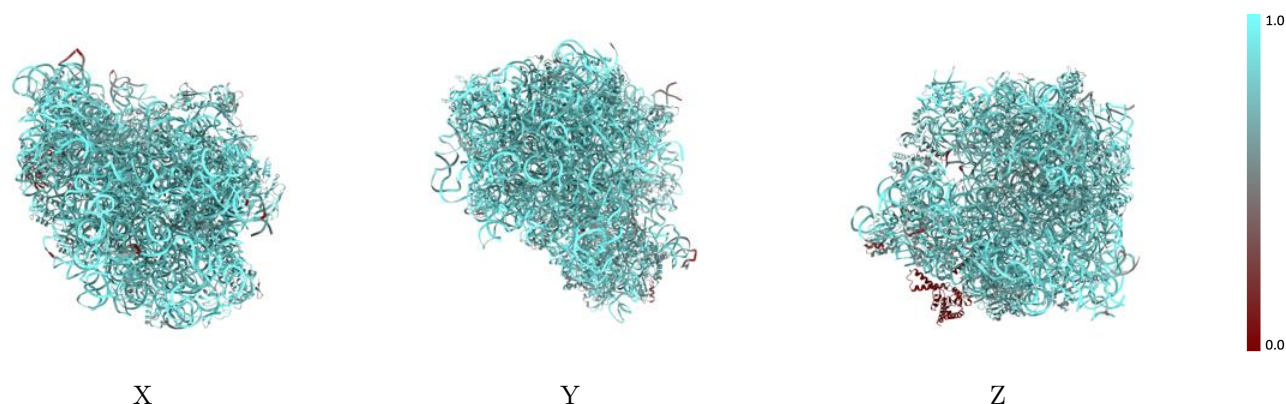
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



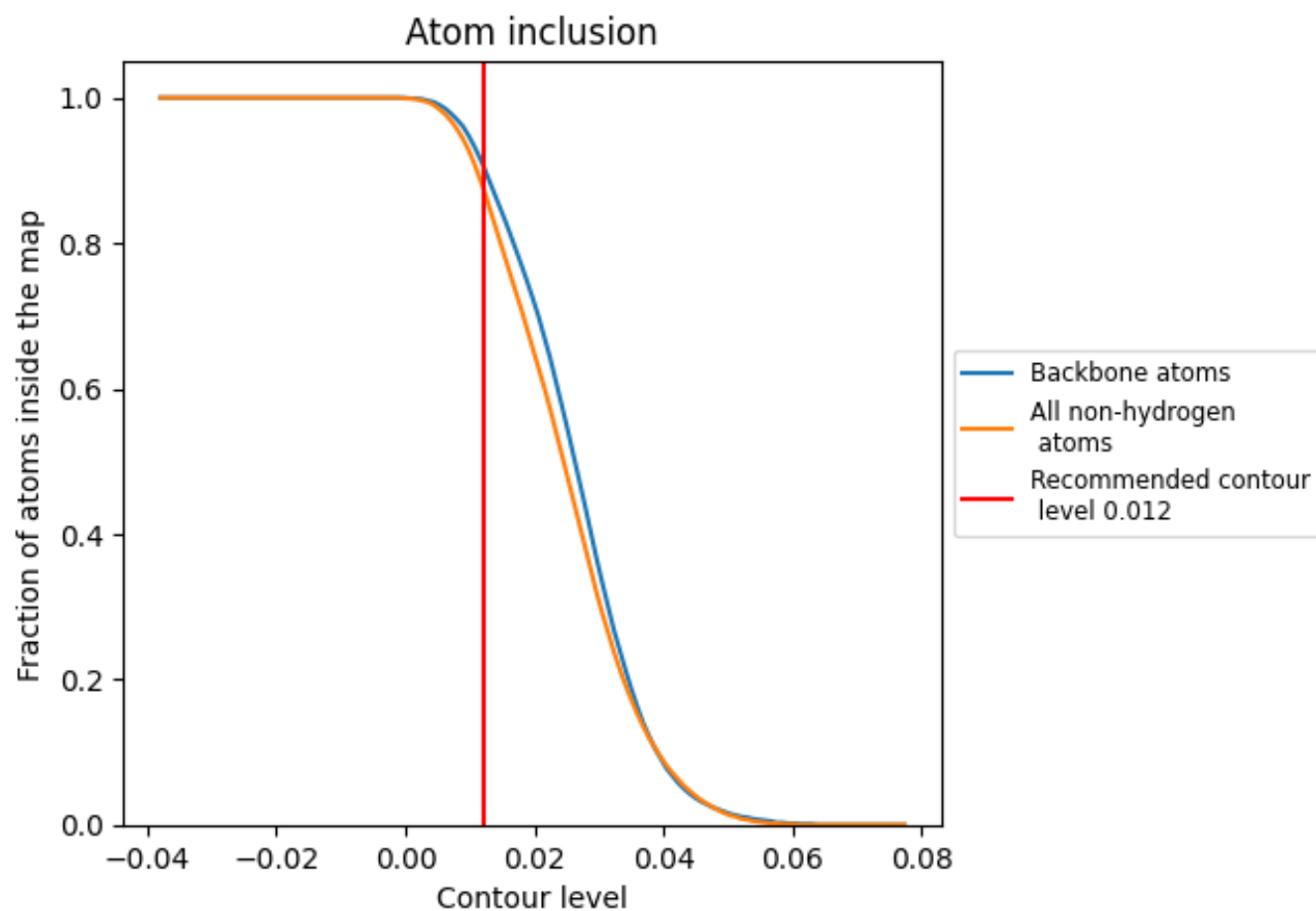
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5500
0	 0.8090	 0.5790
1	 0.8510	 0.5910
2	 0.8860	 0.5920
3	 0.8640	 0.5800
4	 0.7230	 0.5260
A	 0.9170	 0.5360
B	 0.0460	 0.4380
C	 0.7510	 0.5500
D	 0.7110	 0.5200
E	 0.7920	 0.5570
F	 0.7570	 0.5290
G	 0.7180	 0.5190
H	 0.7840	 0.5560
I	 0.7710	 0.5420
J	 0.6250	 0.4980
K	 0.7570	 0.5440
L	 0.7970	 0.5650
M	 0.7620	 0.5420
N	 0.7970	 0.5490
O	 0.7970	 0.5410
P	 0.7600	 0.5340
Q	 0.7570	 0.5470
R	 0.7510	 0.5410
S	 0.7960	 0.5440
T	 0.7540	 0.5190
U	 0.3510	 0.4490
V	 0.8110	 0.5040
X	 0.8800	 0.5510
Z	 0.8380	 0.5190
a	 0.9410	 0.5610
b	 0.9370	 0.5490
c	 0.8880	 0.5850
d	 0.8570	 0.5810
e	 0.7980	 0.5560



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Chain	Atom inclusion	Q-score
f	 0.7490	 0.5440
g	 0.7130	 0.5230
h	 0.5200	 0.5050
i	 0.8720	 0.5740
j	 0.8310	 0.5780
k	 0.8380	 0.5710
l	 0.8390	 0.5730
m	 0.8820	 0.5860
n	 0.8400	 0.5560
o	 0.8160	 0.5770
p	 0.8700	 0.5770
q	 0.8330	 0.5660
r	 0.8120	 0.5670
s	 0.7730	 0.5480
t	 0.7870	 0.5370
u	 0.8090	 0.5600
v	 0.8400	 0.5910
w	 0.8500	 0.5660
x	 0.7460	 0.5240
y	 0.8150	 0.5620
z	 0.8350	 0.5730