



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:42 PM UTC

PDB ID : 8PV1 / pdb_00008pv1
EMDB ID : EMD-17950
Title : Chaetomium thermophilum pre-60S State 6 - pre-5S rotation - L1 intermediate
- composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

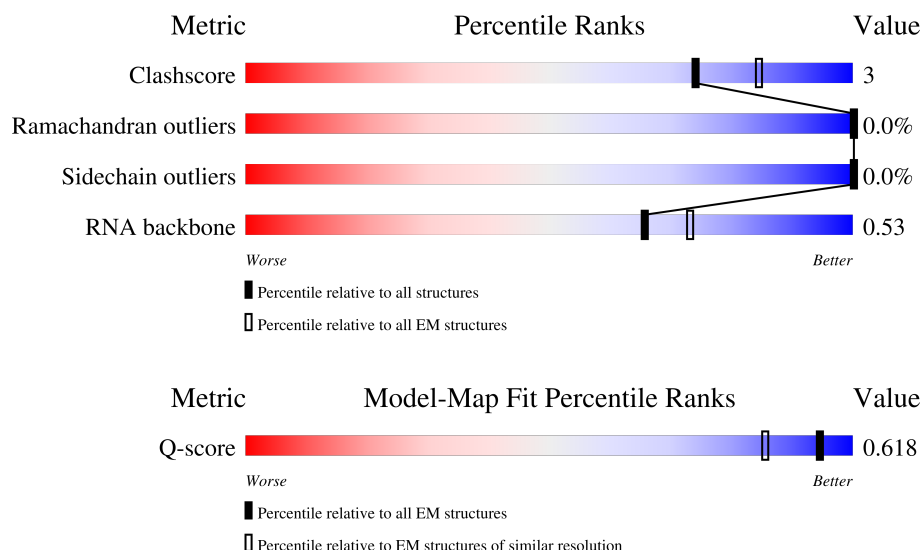
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.56 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	7558 (2.06 - 3.06)

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	C1	3342	
2	C2	156	
3	C3	162	

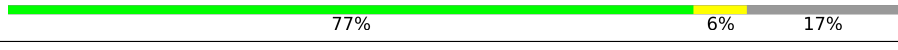
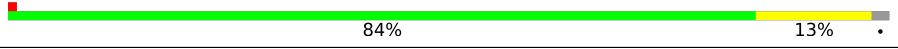
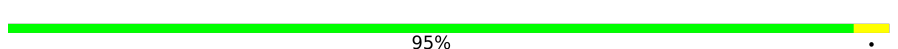
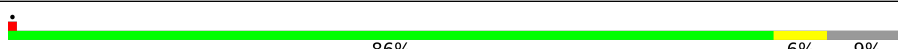
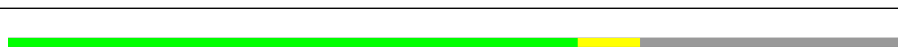
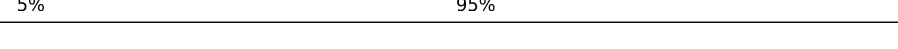
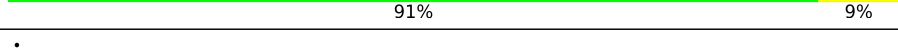
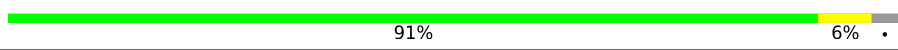
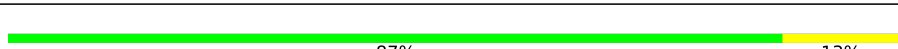
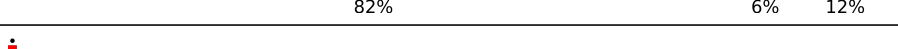
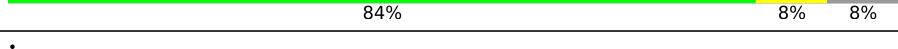
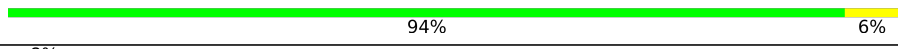
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Mol	Chain	Length	Quality of chain
4	C4	119	
5	CB	391	
6	CF	270	
7	CH	661	
8	CI	414	
9	CJ	679	
10	CK	261	
11	CL	558	
12	CM	249	
12	LF	249	
13	CN	246	
14	CO	120	
15	CQ	225	
16	Cb	117	
17	Cd	627	
18	Ce	443	
19	Cf	350	
20	Cg	202	
21	Ch	517	
22	Cz	123	
23	LA	254	
24	LB	392	
25	LC	365	
26	LD	304	
27	LE	200	

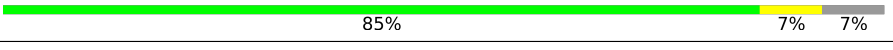
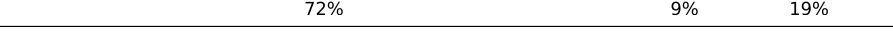
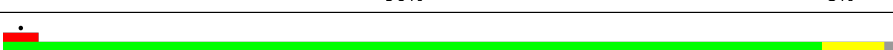
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Mol	Chain	Length	Quality of chain
28	LG	262	
29	LH	229	
30	LJ	173	
31	LK	165	
32	LL	213	
33	LM	142	
34	LN	203	
35	LO	204	
36	LP	187	
37	LQ	213	
38	LR	2898	
39	LS	174	
40	LT	160	
41	LU	127	
42	LV	139	
43	LX	156	
44	LY	138	
45	LZ	135	
46	La	149	
47	Lc	108	
48	Ld	120	
49	Le	131	
50	Lf	109	
51	Lg	119	
52	Lh	935	

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Mol	Chain	Length	Quality of chain
53	Li	110	
54	Lj	95	
55	Lk	94	
56	Ll	51	
57	Lp	92	
58	Lq	147	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 157250 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 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	3078	Total	C	N	O	P	0	0
			65888	29429	11926	21455	3078		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	156	Total	C	N	O	P	0	0
			3319	1484	589	1090	156		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C3	82	Total	C	N	O	P	0	0
			1754	780	316	576	82		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C4	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

- Molecule 5 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CB	265	Total	C	N	O	S	0	0
			2107	1351	371	382	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CF	245	Total	C	N	O	S	0	0
			1934	1215	350	360	9		

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CH	627	Total	C	N	O	S	0	0
			5063	3181	924	939	19		

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CI	152	Total	C	N	O	S	0	0
			1234	791	230	208	5		

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CJ	382	Total	C	N	O	S	0	0
			3116	2008	548	550	10		

- Molecule 10 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CK	237	Total	C	N	O	S	0	0
			1903	1198	368	333	4		

- Molecule 11 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CL	79	Total	C	N	O	S	0	0
			622	389	125	108			

- Molecule 12 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CM	217	Total	C	N	O	S	0	0
			1773	1144	329	297	3		
12	LF	248	Total	C	N	O	S	0	0
			2023	1297	377	346	3		

- Molecule 13 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CN	246	Total	C	N	O	S	0	0
			1853	1156	322	368	7		

- Molecule 14 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 15 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CQ	183	Total	C	N	O	S	0	0
			1480	925	304	241	10		

- Molecule 16 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cb	101	Total	C	N	O	S	0	0
			830	517	161	148	4		

- Molecule 17 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cd	462	Total	C	N	O	S	0	0
			3691	2350	671	659	11		

- Molecule 18 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ce	262	Total	C	N	O	S	0	0
			2148	1337	413	394	4		

- Molecule 19 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Cf	285	Total	C	N	O	S	0	0
			2282	1443	417	401	21		

- Molecule 20 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Cg	188	Total	C	N	O	S	0	0
			1478	924	283	270	1		

- Molecule 21 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ch	485	Total	C	N	O	S	1	0
			3812	2396	696	710	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 22 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Cz	101	Total	C	N	O	S	0	0
			869	541	180	144	4		

- Molecule 23 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LA	191	Total	C	N	O	S	0	0
			1454	917	278	256	3		

- Molecule 24 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LB	389	Total	C	N	O	S	0	0
			3104	1973	579	539	13		

- Molecule 25 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LC	363	Total	C	N	O	S	0	0
			2751	1737	527	478	9		

- Molecule 26 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LD	286	Total	C	N	O	S	0	0
			2266	1434	407	422	3		

- Molecule 27 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LE	191	Total	C	N	O	S	0	0
			1477	944	267	263	3		

- Molecule 28 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LG	235	Total	C	N	O	S	0	0
			1889	1210	350	324	5		

- Molecule 29 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LH	190	Total	C	N	O	S	0	0
			1495	949	268	272	6		

- Molecule 30 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LJ	169	Total	C	N	O	S	0	0
			1357	850	266	235	6		

- Molecule 31 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 32 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 33 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 34 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 35 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 36 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 37 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	150	Total	C	N	O	S	0	0
			1200	759	239	200	2		

- Molecule 38 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LR	155	Total	C	N	O	S	0	0
			1241	772	262	203	4		

- Molecule 39 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LS	174	Total	C	N	O	S	0	0
			1426	917	266	238	5		

- Molecule 40 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LT	129	Total	C	N	O	S	0	0
			1027	651	195	179	2		

- Molecule 41 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LU	105	Total	C	N	O	S	0	0
			846	548	146	151	1		

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	135	Total	C	N	O	S	0	0
			991	630	184	170	7		

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LX	145	Total	C	N	O	S	0	0
			1133	723	211	199			

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LY	133	Total	C	N	O	S	0	0
			1056	658	213	183	2		

- Molecule 45 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 46 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 47 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

- Molecule 48 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 49 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 50 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 51 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lg	118	Total	C	N	O	S	0	0
			914	567	186	157	4		

- Molecule 52 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Lh	122	Total	C	N	O	0	0
			1003	637	198	168		

- Molecule 53 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 54 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 55 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 56 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

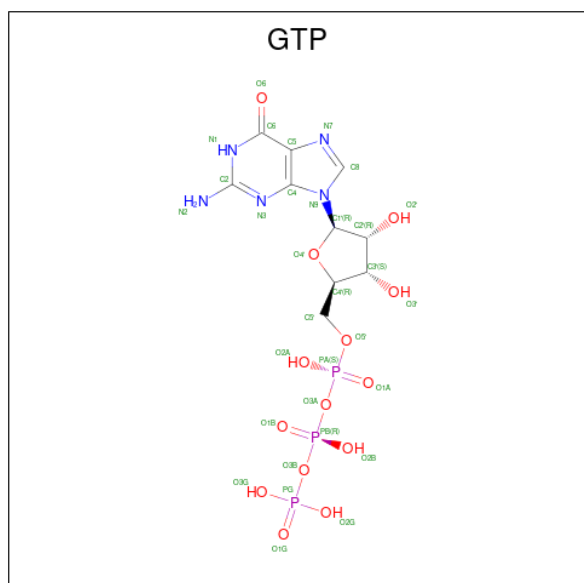
- Molecule 57 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 58 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Lq	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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Mol	Chain	Residues	Atoms					AltConf
59	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	CH	1	Total	Mg	0
			1	1	
60	Cd	2	Total	Mg	0
			2	2	

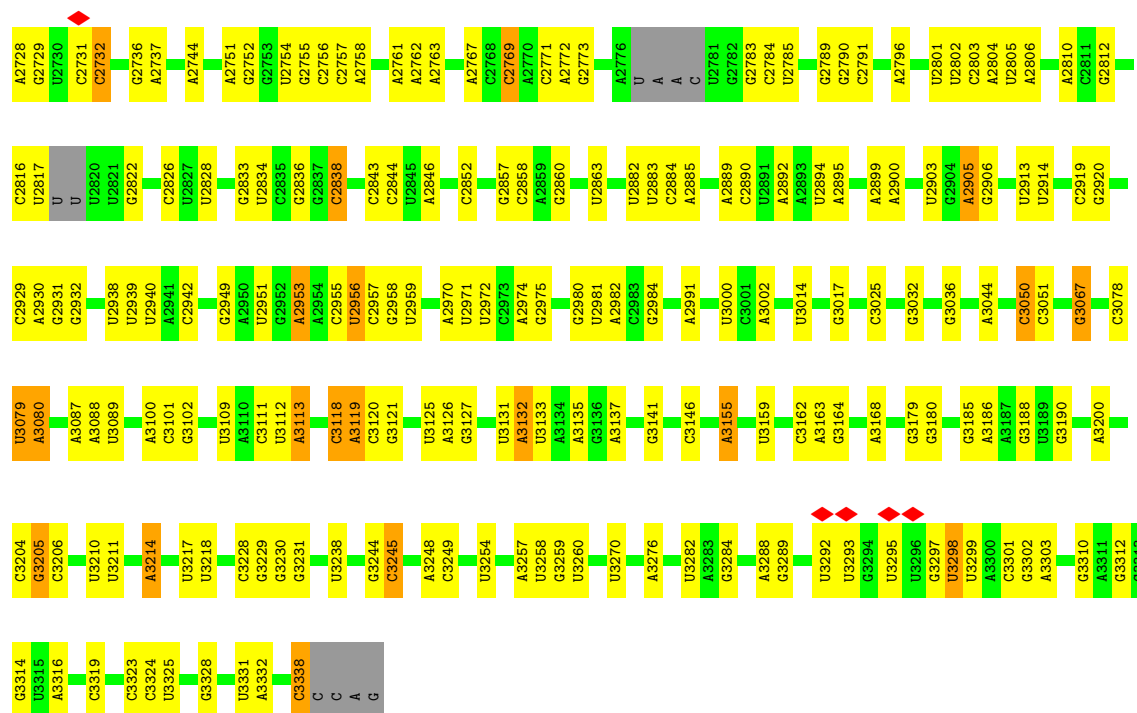
- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total	Zn	0
			1	1	
61	Cb	1	Total	Zn	0
			1	1	
61	Lg	1	Total	Zn	0
			1	1	
61	Lj	1	Total	Zn	0
			1	1	
61	Lp	1	Total	Zn	0
			1	1	

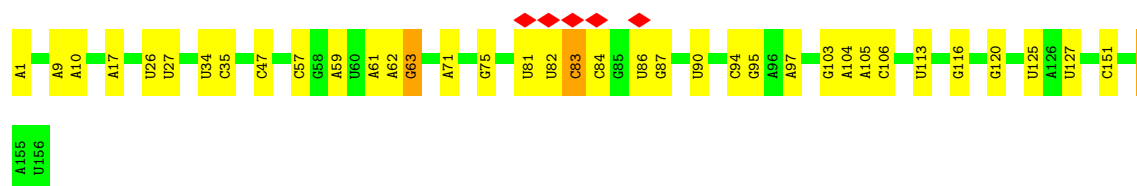
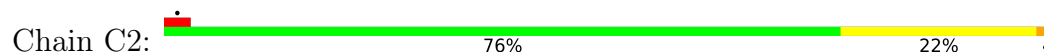
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	CH	1	Total	O	0
			1	1	
62	Cd	2	Total	O	0
			2	2	

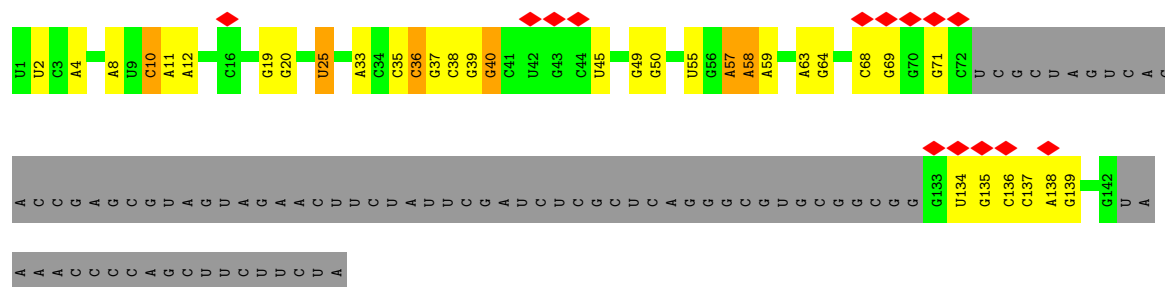
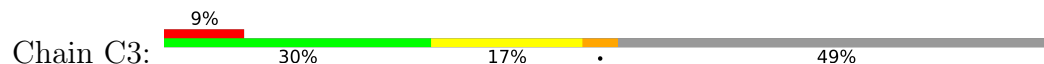
U2614	C2513	A	C2355	G2181	A	G	C1935	C1800	A1683	C1549	A1382	U1248
A2615	U2514	G	G2356	A2182	U	C	A1936	U1801	U1685	U1550	G1383	
G2621	C2515	U	G2359	A2183	A	G	G1937	G1809	C1697	G1554	G1395	U1252
G2622	U	C		A2186	G	C	G1938	U1939	C1698	C1555	C1255	
C2631	C2516	U	A2362	U2187	U	C	U	C1812	U1700	G1559	A1401	C1260
A2632	C2517	C	C2363	U2188	G	U	G	G1813	G1699	U1560	A1261	A1261
A2633	C2518	G	A2364	A2192	A	C	G	C1816	U1701	G1561	G1404	
C2634	C2519	C	C2365	G2197	C	C	U	U1702	U1704	U1562	G1405	U1264
A2635	U2373	C	C2366	A2198	C	C	G	A1822	G1721	G1563	G1417	G1265
G2636	U2374	G		G2203	C	A	U	C1823	U1722	A1567	A1418	C1266
	U2375	C		U2204	A	C	U	G1824	U1723	A1568	C1419	C1267
U2640	A2376	U		A2205	C	C	G	G1825	C1726	A1569	C1420	G1268
U2642	G2377	C		A2206	C	C	U	A1826	U1727	U1421	A1269	A1270
C2643	U2380	A		G2209	G	G	C	C1827	A1730	A1573	A1429	
	C2381	A		G2210	G	G	C	A1828	U1731	C1576	G1430	G1278
U2647	U2382	U		G2211	G	G	C	C1829	U1732	C1577	U1431	
A2648	U2383	C		G2212	G	U	A	A1830	U1733	C1578	A1432	G1283
A2651	U2384	C		G2216	G	U	C	C1836	G1737	U1577	G1433	
A2656	C2392	C		U2217	G	C	C	U1842	U1742	A1583	U1438	A1287
G2657	A2393	C		U2218	A	C	C	G1843	U1743	U1584	U1288	G1289
	U2396	U		A2219	G	A	C	A1844	U1744	A1585	G1449	G1290
U2670	U2397	C		A2220	C	C	U	G1845	U1745	A1586	A1450	A1291
A2664	U2398	C		U2221	C	C	G	A1846	G1746	U1596	A1451	U1292
C2667	U2399	C		U2222	C	C	G	C1847	U1747	C1595	G1468	G1296
	G2400	U		U2223	U	U	A	U1856	G1751	U1597	U1464	U1305
U2671	A2403	C		U2224	A	A	C	G1857	G1758	G1598	A1465	
U2672	A2404	C		G2225	G	C	A	A1858	C1759	A1599	G1466	A1313
G2673	U2405	U		C2226	C	C	G	U1859	G1760	U1609	G1476	C1316
A2674	G2406	U		U2229	G	G	G	A1864	U1761	C1611	U1477	
U2675	C	G		C2230	C	C	G	C1865	C1763	G1614	A1331	
	U2467	U		U2231	U	U	C	A1866	G1766	G1615	G1332	
A2680	U2468	U		U	C	C	C	A1867	A1767	G1638	A1481	
U2683	U2472	A		A	U	U	C	U1868	C1773	A1618	A1333	
U2688	A2474	G		A	C	C	U	A1873	G1776	C1619	A1335	
G2689	U2477	A		G	G	G	U	G1877	A1777	A1623	G1337	
U2690	C2489	C		G2236	C	C	A	G1878	A1778	C1624	A1338	
A2692	U2495	U		U2237	G	C	G	G1879	A1779	U1625	U1339	
A2693	G2496	C		A2243	U	U	C	G1886	A1780	C1637	G1350	
	U2496	C		U	C	C	G	C1887	G1783	G1638	U1351	
A2706	C2499	A		U	G	G	C	A1901	G1784	A1639	U1361	
A2707	U2500	U		C	C	C	C	A1902	C1785	C1640	G1362	
U2711	U2501	A		U	U	U	A	U1917	G1786	G1642	A1369	
G2712	C2502	C		C	C	C	C	G1920	A1793	G1658	U1537	
G2713	C2503	G		U	U	U	C	U1917	A1794	G1639	U1538	
	C2504	U		C	C	C	C	G1929	U1795	A1676	U1370	
A2717	C2505	U		U	C	C	G	U1929	A1796	A1677	U1371	
C2723	U2609	G		U	C	C	C	G1934	U1799	U1683	A1540	
C2724	C2613	G		U	C	C	C				A1541	
				U	C	C	C				G1543	



- Molecule 2: 5.8S rRNA

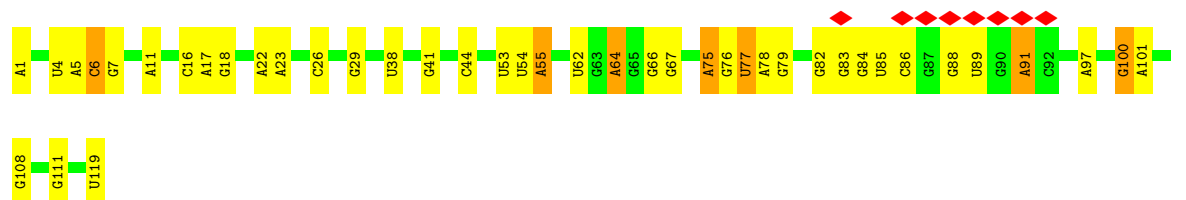


- Molecule 3: ITS2

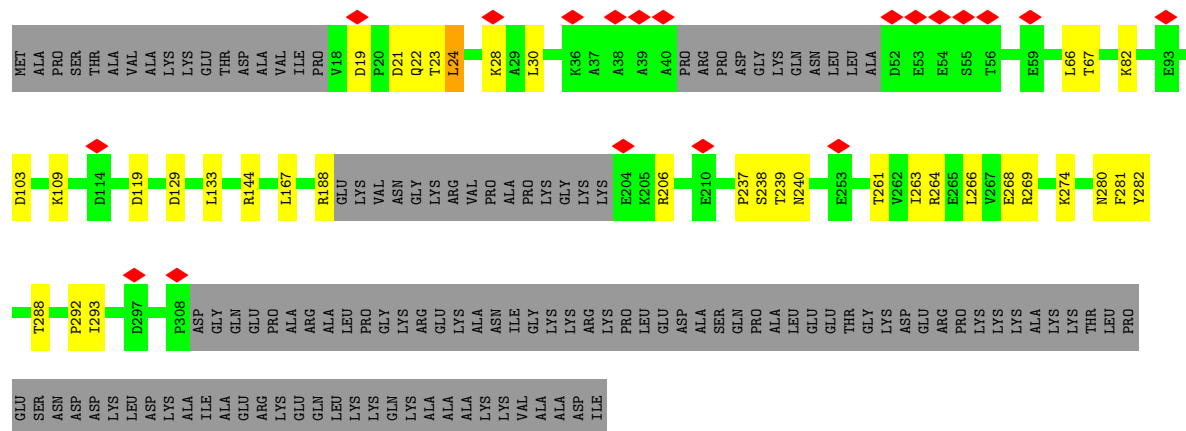


- Molecule 4: 5S rRNA

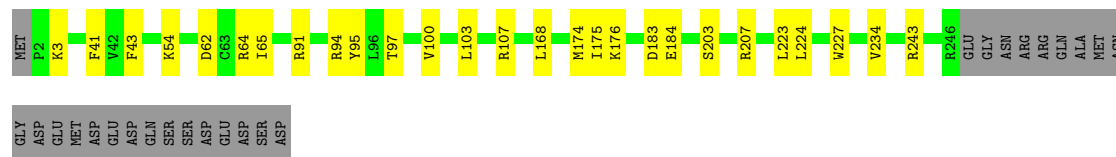
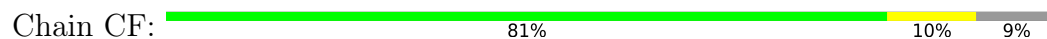




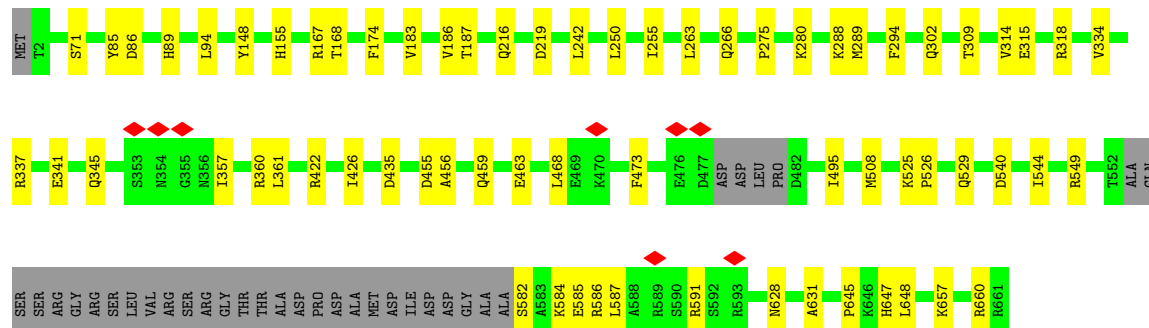
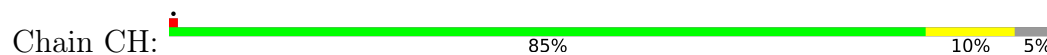
• Molecule 5: Utp30



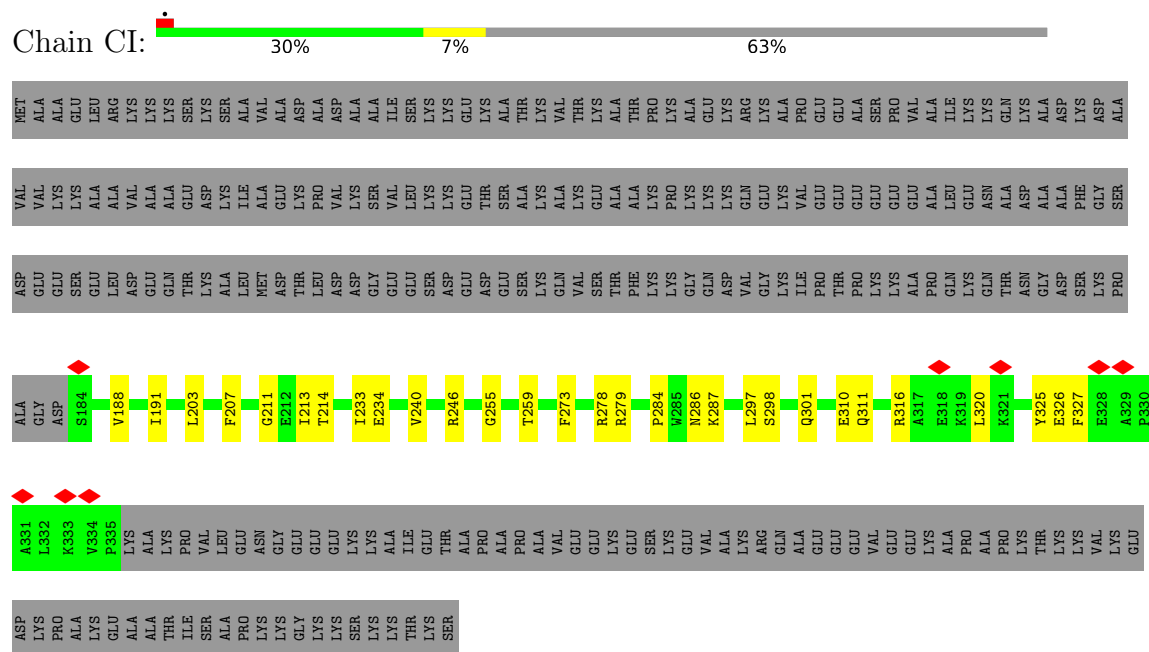
• Molecule 6: Large ribosomal subunit protein uL10



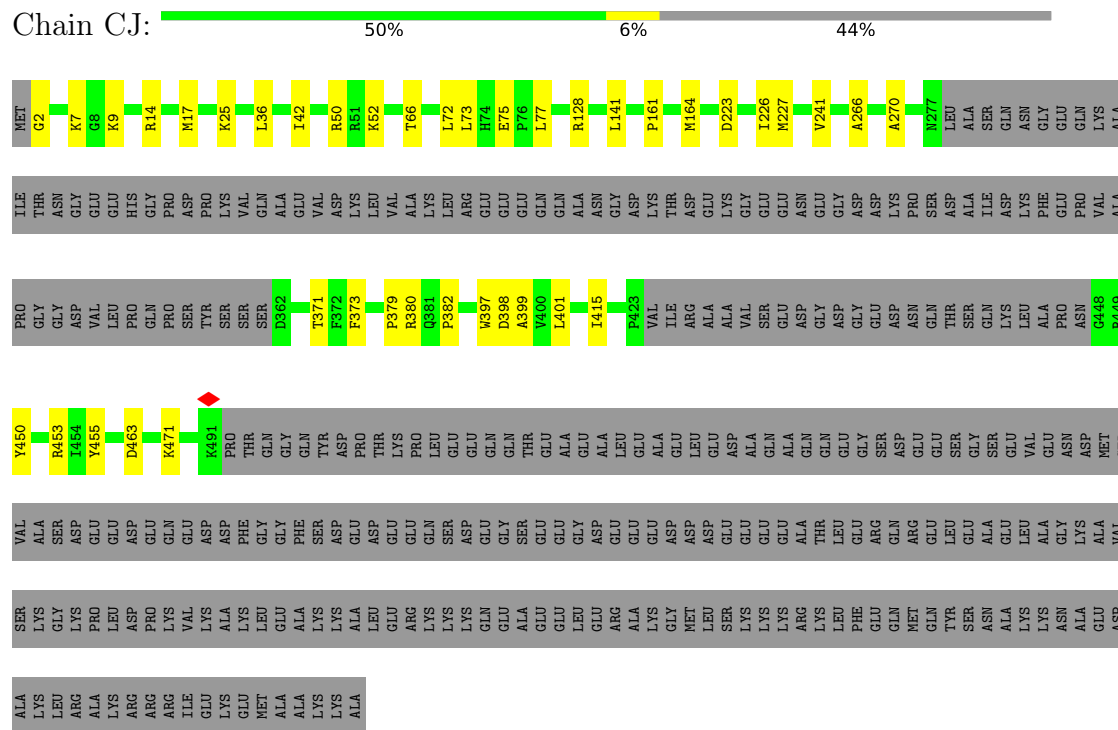
• Molecule 7: Nucleolar GTP-binding protein 1



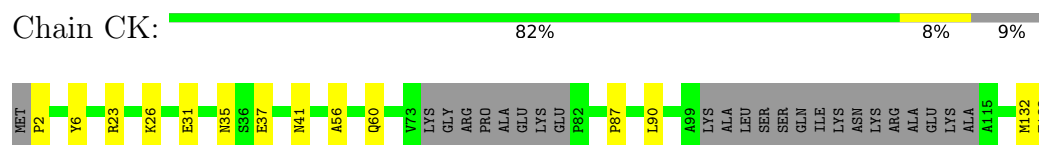
• Molecule 8: Putative RNA-binding protein



- Molecule 9: Pescadillo homolog

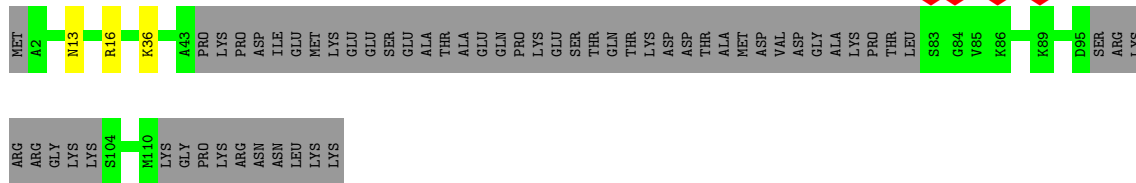


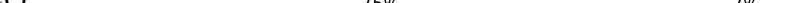
- Molecule 10: Ribosome biogenesis protein NSA2 homolog

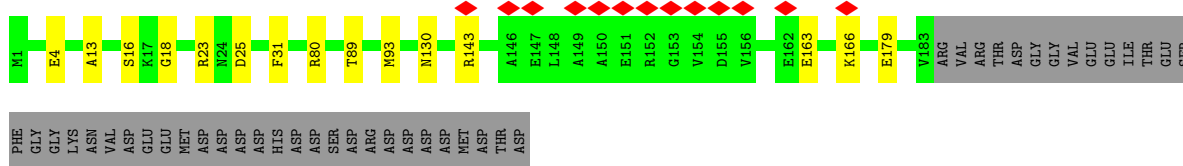


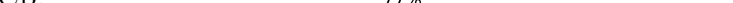
Category	Value (approximate)
M1	1.0
R4	1.0
N1.1	1.0
V1.5	1.0
N2.1	1.0
E3.2	1.0
R5.0	1.0
R6.1	1.0
R6.7	1.0
L1.00	1.0
L1.01	1.0
L1.04	1.0
G1.05	1.0
N1.06	1.0
V1.07	1.0
L1.08	1.0
V1.09	1.0
Q1.40	1.0
T1.41	1.0
T1.42	1.0
V1.48	1.0
G1.49	1.0
H1.62	1.0
P1.63	1.0
K1.64	1.0
L1.73	1.0
V1.86	1.0
D2.09	1.0
T2.10	1.0
L2.18	1.0
E2.19	1.0
L2.24	1.0
E2.43	1.0
Y2.46	1.0

- Chain CO: 49% . 48%

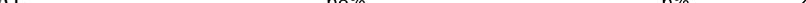


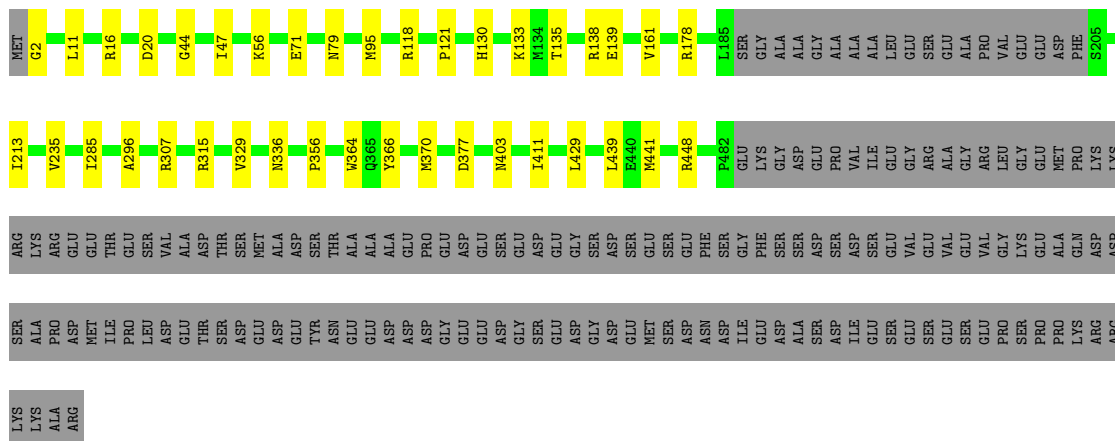
- Chain CQ: 



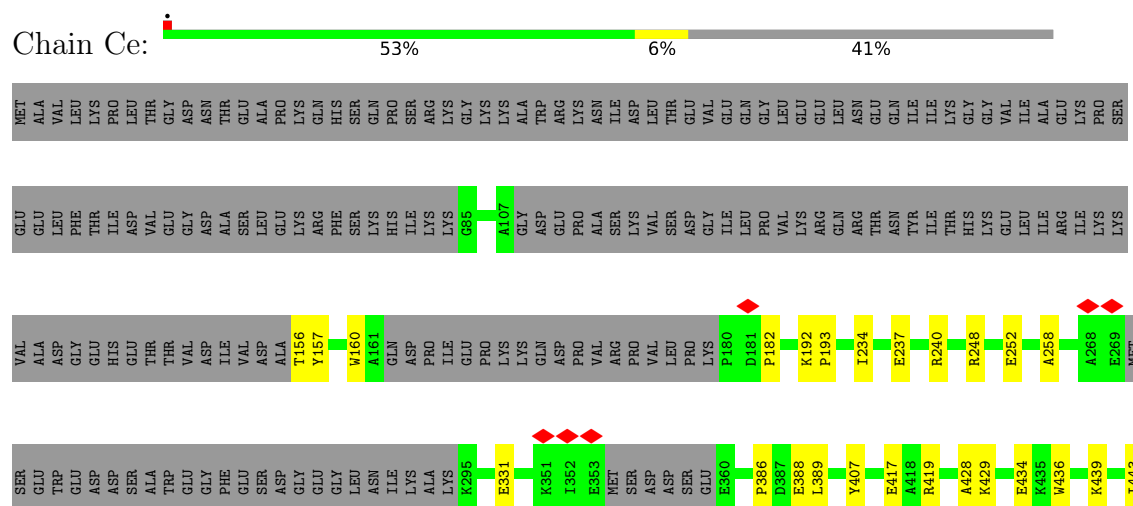
- Chain Cb:  77% 9% 14%



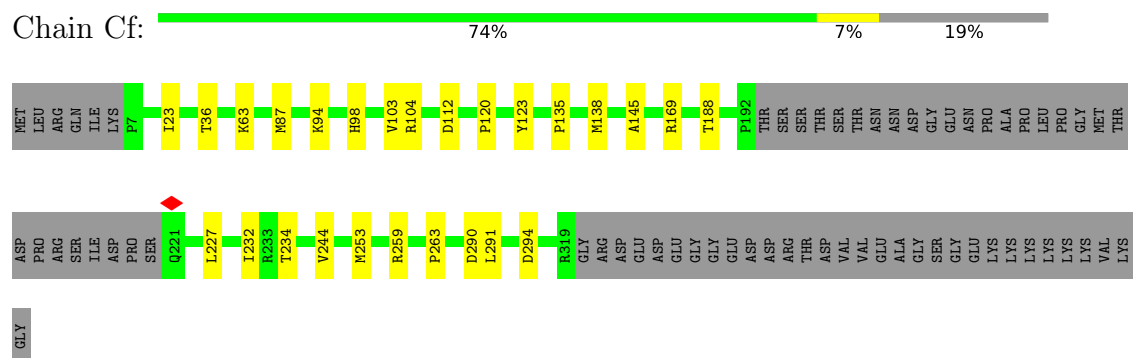
- Chain Cd:  68% 6% 26%



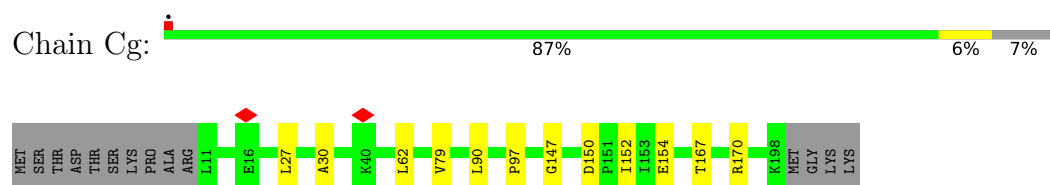
- Molecule 18: Ribosome biogenesis protein NOP53



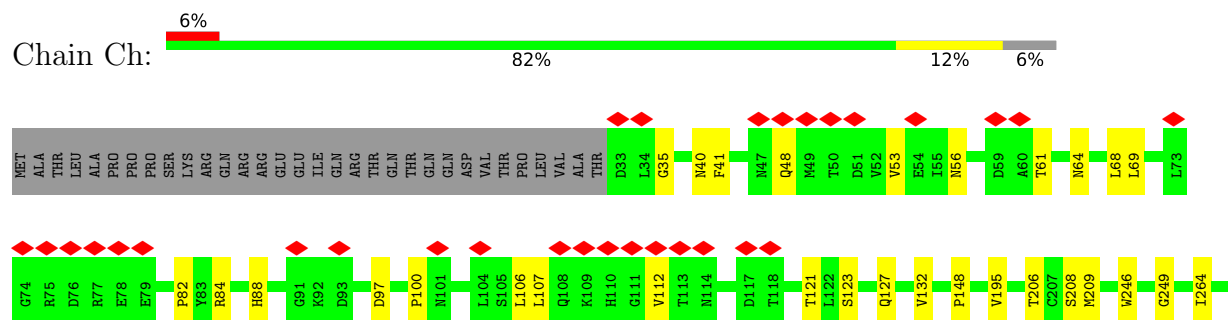
- Molecule 19: Ribosome production factor 2 homolog



- Molecule 20: Ribosome biogenesis regulatory protein



- Molecule 21: Ribosome assembly protein 4

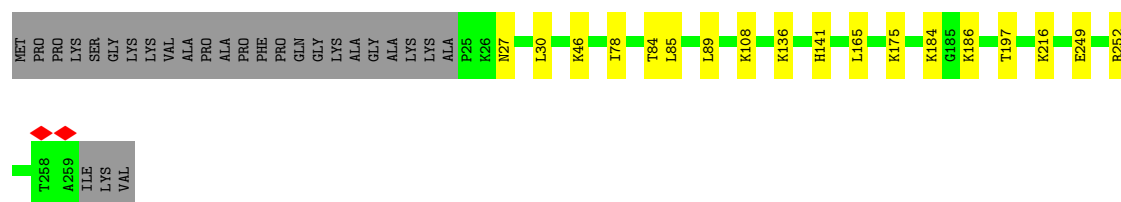


Chain LE:  82% 13% .



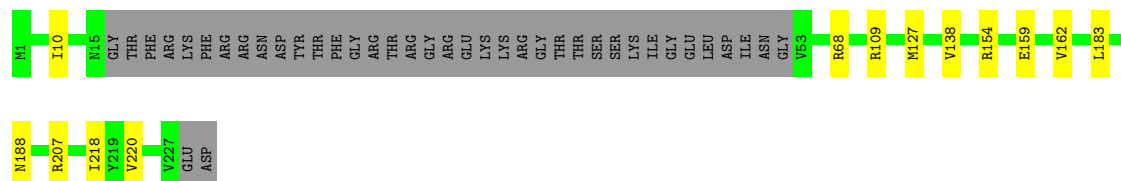
- Molecule 28: 60S ribosomal protein L8

Chain LG:  83% 7% 10%



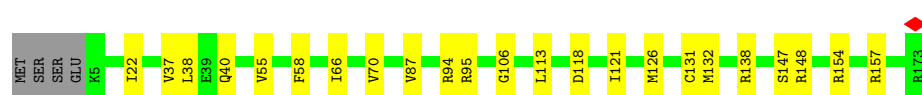
- Molecule 29: 60S ribosomal protein I9-like protein

Chain LH:  77% 6% 17%



- Molecule 30: Putative ribosomal protein

Chain LJ:  84% 13% .



- Molecule 31: 60S ribosomal protein L12-like protein

Chain LK:  90% 5% .

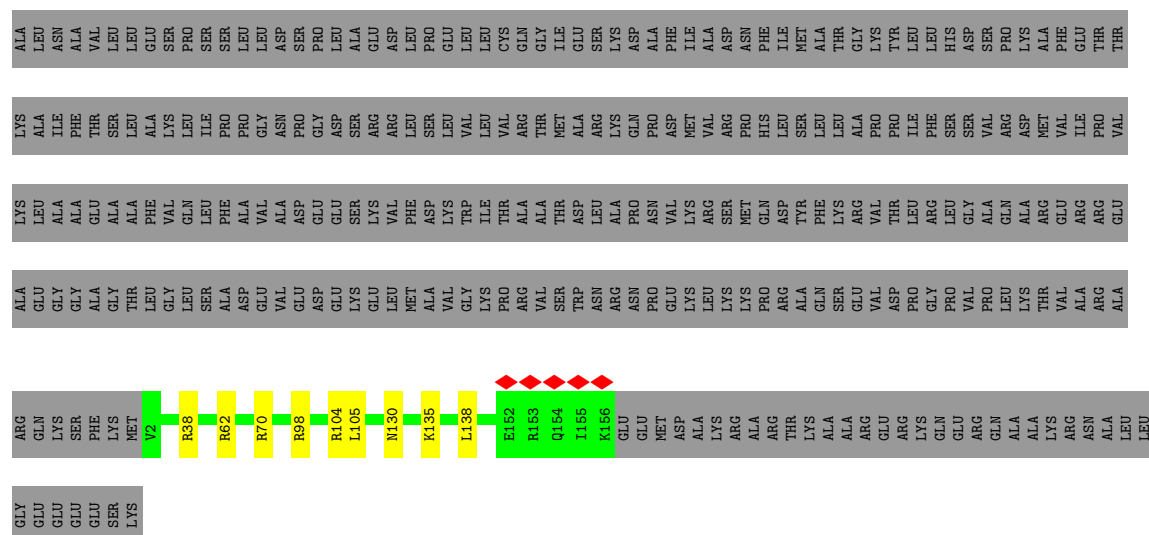


- Molecule 32: 60S ribosomal protein L13

Chain LL:  91% 5% 5%







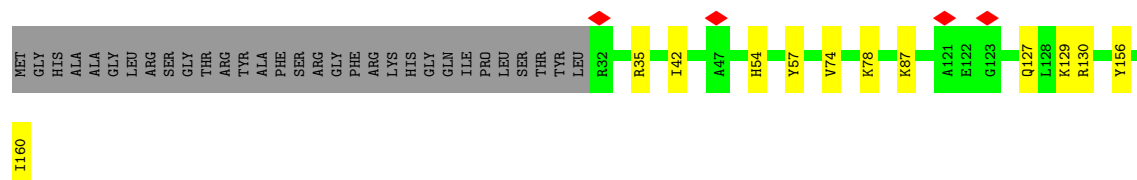
- Molecule 39: 60S ribosomal protein L20

Chain LS: 91% 9%



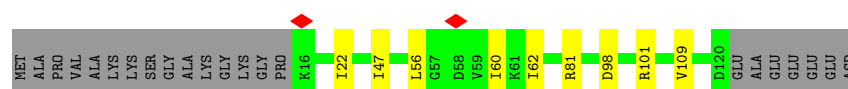
- Molecule 40: 60S ribosomal protein l21-like protein

Chain LT: 73% 8% 19%



- Molecule 41: 60S ribosomal protein L22-like protein

Chain LU: 76% 7% 17%



- Molecule 42: 60S ribosomal protein l23-like protein

Chain LV: 91% 6%



- Molecule 43: 60S ribosomal protein L25-like protein

Chain LX:  88% 5% 7%



- Molecule 44: 60S ribosomal protein L26-like protein

Chain LY:  83% 13% . .



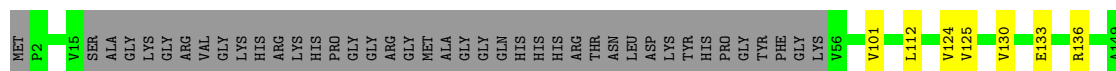
- Molecule 45: 60S ribosomal protein L27

Chain LZ:  87% 13%



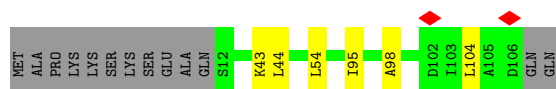
- Molecule 46: 60S ribosomal protein L28-like protein

Chain La:  68% 5% 28%



- Molecule 47: 60S ribosomal protein l30-like protein

Chain Lc:  82% 6% 12%



- Molecule 48: Putative 60S ribosomal protein

Chain Ld:  84% 8% 8%

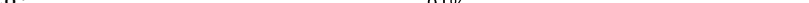


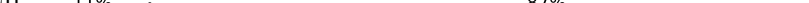
- Molecule 49: 60S ribosomal protein L32-like protein

Chain Le:  89% 7% .

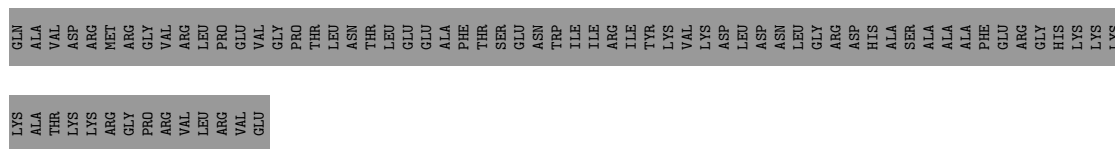


- Molecule 50: 60S ribosomal protein l33-like protein

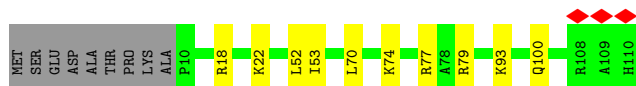
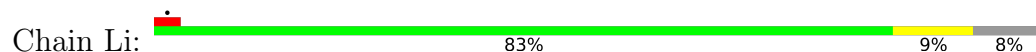
- Chain Lg:  8% 91% 1%

- Chain Lh:  11% 87%

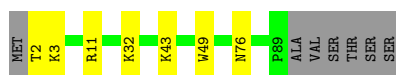
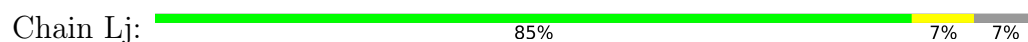
[illegible]



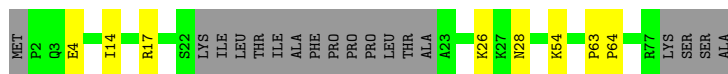
- Molecule 53: 60S ribosomal protein L36



- Molecule 54: Ribosomal protein L37



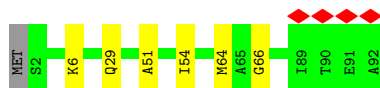
- Molecule 55: 60S ribosomal protein L38-like protein



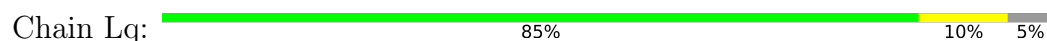
- Molecule 56: Ribosomal protein eL39



- Molecule 57: 60S ribosomal protein L43-like protein



- Molecule 58: Putative 60S ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74642	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 ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.056	Depositor
Minimum map value	0.000	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.169	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, MG, GTP, OMG, OMC, ZN, A2M

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	C1	0.18	1/72882 (0.0%)	0.33	0/113631
2	C2	0.16	0/3710	0.31	0/5778
3	C3	0.13	0/1958	0.30	0/3050
4	C4	0.16	0/2833	0.32	0/4414
5	CB	0.17	0/2153	0.45	1/2926 (0.0%)
6	CF	0.16	0/1972	0.39	0/2660
7	CH	0.17	0/5147	0.40	0/6926
8	CI	0.23	0/1265	0.64	2/1702 (0.1%)
9	CJ	0.17	0/3196	0.38	0/4319
10	CK	0.17	0/1939	0.38	0/2608
11	CL	0.19	0/631	0.45	0/843
12	CM	0.18	0/1805	0.43	0/2417
12	LF	0.20	0/2061	0.43	0/2765
13	CN	0.17	0/1878	0.44	0/2555
14	CO	0.17	0/470	0.37	0/619
15	CQ	0.23	0/1504	0.44	0/2000
16	Cb	0.18	0/845	0.46	0/1128
17	Cd	0.17	0/3770	0.37	0/5082
18	Ce	0.16	0/2173	0.37	0/2890
19	Cf	0.15	0/2326	0.37	0/3113
20	Cg	0.16	0/1508	0.39	0/2051
21	Ch	0.17	0/3914	0.44	0/5319
22	Cz	0.21	0/877	0.48	0/1148
23	LA	0.17	0/1488	0.45	0/2009
24	LB	0.19	0/3172	0.45	0/4260
25	LC	0.17	0/2808	0.38	0/3785
26	LD	0.16	0/2308	0.36	0/3105
27	LE	0.16	0/1504	0.40	0/2027
28	LG	0.17	0/1918	0.38	0/2565
29	LH	0.16	0/1515	0.40	0/2037
30	LJ	0.16	0/1379	0.46	0/1844
31	LK	0.18	0/1198	0.47	0/1611

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LL	0.16	0/1614	0.35	0/2168
33	LM	0.18	0/1145	0.37	0/1539
34	LN	0.17	0/1741	0.38	0/2332
35	LO	0.21	0/1645	0.45	0/2205
36	LP	0.18	0/1364	0.40	0/1835
37	LQ	0.16	0/1218	0.38	0/1639
38	LR	0.16	0/1260	0.36	0/1683
39	LS	0.16	0/1461	0.39	0/1966
40	LT	0.19	0/1046	0.48	0/1409
41	LU	0.17	0/859	0.42	0/1151
42	LV	0.18	0/1009	0.40	0/1357
43	LX	0.18	0/1151	0.41	0/1547
44	LY	0.17	0/1070	0.44	0/1432
45	LZ	0.17	0/1135	0.37	0/1519
46	La	0.14	0/892	0.35	0/1200
47	Lc	0.16	0/714	0.39	0/960
48	Ld	0.18	0/889	0.37	0/1192
49	Le	0.17	0/1035	0.40	0/1379
50	Lf	0.17	0/883	0.38	0/1187
51	Lg	0.18	0/927	0.41	0/1244
52	Lh	0.21	0/1014	0.48	0/1349
53	Li	0.18	0/834	0.41	0/1099
54	Lj	0.19	0/712	0.46	0/944
55	Lk	0.20	0/640	0.47	0/850
56	Ll	0.18	0/446	0.35	0/593
57	Lp	0.17	0/706	0.46	0/940
58	Lq	0.17	0/1091	0.37	0/1468
All	All	0.18	1/166608 (0.0%)	0.37	3/241374 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O3'-P	5.07	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	CI	310	GLU	N-CA-CB	6.24	119.40	110.16
5	CB	24	LEU	CA-CB-CG	5.90	136.96	116.30
8	CI	311	GLN	N-CA-CB	5.11	118.87	110.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	65888	0	33241	340	0
2	C2	3319	0	1678	17	0
3	C3	1754	0	890	16	0
4	C4	2536	0	1286	20	0
5	CB	2107	0	2161	29	0
6	CF	1934	0	1945	17	0
7	CH	5063	0	5157	44	0
8	CI	1234	0	1245	20	0
9	CJ	3116	0	3122	29	0
10	CK	1903	0	1990	16	0
11	CL	622	0	641	11	0
12	CM	1773	0	1879	9	0
12	LF	2023	0	2132	9	0
13	CN	1853	0	1852	19	0
14	CO	468	0	503	2	0
15	CQ	1480	0	1523	10	0
16	Cb	830	0	838	7	0
17	Cd	3691	0	3818	26	0
18	Ce	2148	0	2250	18	0
19	Cf	2282	0	2347	18	0
20	Cg	1478	0	1517	10	0
21	Ch	3812	0	3715	33	0
22	Cz	869	0	956	7	0
23	LA	1454	0	1490	10	0
24	LB	3104	0	3221	26	0
25	LC	2751	0	2875	11	0
26	LD	2266	0	2219	24	0
27	LE	1477	0	1567	19	0
28	LG	1889	0	2043	13	0
29	LH	1495	0	1573	8	0
30	LJ	1357	0	1385	15	0
31	LK	1184	0	1249	5	0
32	LL	1587	0	1655	7	0
33	LM	1126	0	1198	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	LN	1704	0	1767	14	0
35	LO	1611	0	1702	8	0
36	LP	1343	0	1369	11	0
37	LQ	1200	0	1296	10	0
38	LR	1241	0	1298	7	0
39	LS	1426	0	1481	13	0
40	LT	1027	0	1076	11	0
41	LU	846	0	883	6	0
42	LV	991	0	1044	7	0
43	LX	1133	0	1234	7	0
44	LY	1056	0	1143	14	0
45	LZ	1112	0	1181	12	0
46	La	872	0	903	4	0
47	Lc	705	0	751	4	0
48	Ld	875	0	918	7	0
49	Le	1017	0	1092	6	0
50	Lf	862	0	891	4	0
51	Lg	914	0	960	9	0
52	Lh	1003	0	1116	13	0
53	Li	827	0	906	8	0
54	Lj	698	0	726	7	0
55	Lk	632	0	693	6	0
56	Ll	436	0	473	3	0
57	Lp	698	0	737	5	0
58	Lq	1073	0	1130	9	0
59	CH	32	0	12	1	0
59	Cd	32	0	12	0	0
60	CH	1	0	0	0	0
60	Cd	2	0	0	0	0
61	CQ	1	0	0	0	0
61	Cb	1	0	0	0	0
61	Lg	1	0	0	0	0
61	Lj	1	0	0	0	0
61	Lp	1	0	0	0	0
62	CH	1	0	0	0	0
62	Cd	2	0	0	0	0
All	All	157250	0	123955	870	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 3.

All (870) 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:C1:2400:G:H1	1:C1:2473:U:H3	0.96	0.92
1:C1:1054:U:H3	1:C1:1070:G:H1	0.89	0.89
1:C1:1809:G:HO2'	9:CJ:2:GLY:N	1.77	0.83
1:C1:3289:G:H1	1:C1:3298:U:H3	1.26	0.82
3:C3:40:G:H1	3:C3:45:U:H3	1.32	0.79
28:LG:84:THR:HG21	28:LG:184:LYS:HG3	1.67	0.76
1:C1:2101:A:HO2'	54:Lj:2:THR:N	1.87	0.73
1:C1:2899:A:H2'	24:LB:256:TRP:HB3	1.74	0.70
26:LD:132:THR:HG21	26:LD:143:ARG:HH12	1.57	0.69
5:CB:237:PRO:HB2	8:CI:286:ASN:HD21	1.56	0.69
27:LE:162:GLN:NE2	27:LE:166:ASP:OD2	2.24	0.69
1:C1:448:C:H41	27:LE:15:ARG:HH21	1.42	0.68
26:LD:85:ALA:HB2	26:LD:258:TYR:HB2	1.77	0.67
1:C1:2932:G:N7	10:CK:140:LYS:NZ	2.43	0.66
13:CN:162:HIS:HD1	13:CN:164:LYS:H	1.42	0.66
40:LT:127:GLN:NE2	40:LT:129:LYS:O	2.28	0.65
26:LD:37:ILE:HG13	26:LD:38:THR:HG23	1.78	0.64
1:C1:949:A:H62	1:C1:1098:G:H8	1.46	0.64
44:LY:47:ILE:HD13	44:LY:114:ARG:HH21	1.62	0.64
17:Cd:285:ILE:HD11	17:Cd:296:ALA:HB2	1.79	0.63
24:LB:136:LYS:HA	24:LB:139:GLU:HG2	1.80	0.63
3:C3:71:G:H1	3:C3:134:U:H3	1.44	0.63
26:LD:35:ARG:HA	26:LD:39:GLN:HG3	1.81	0.63
10:CK:56:ALA:O	10:CK:60:GLN:NE2	2.32	0.62
1:C1:1182:C:O2'	11:CL:27:ARG:NH1	2.33	0.62
17:Cd:95:MET:HE1	17:Cd:118:ARG:HG2	1.81	0.62
21:Ch:470:LEU:HB2	21:Ch:484:LEU:HB2	1.81	0.62
5:CB:66:LEU:HD22	5:CB:266:LEU:HD21	1.81	0.62
8:CI:246:ARG:NH2	18:Ce:443:ILE:OXT	2.33	0.62
23:LA:80:GLU:HG3	57:Lp:66:GLY:HA2	1.82	0.62
24:LB:84:MET:O	24:LB:203:PRO:HA	1.99	0.62
14:CO:13:ASN:OD1	14:CO:16:ARG:NH2	2.32	0.62
18:Ce:248:ARG:NH1	18:Ce:252:GLU:OE2	2.32	0.61
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.66	0.61
3:C3:49:G:H21	5:CB:240:ASN:HD22	1.48	0.61
9:CJ:373:PHE:HB2	9:CJ:415:ILE:HG21	1.82	0.61
36:LP:125:GLN:HB3	36:LP:141:SER:HB2	1.83	0.61
16:Cb:15:ARG:NH2	16:Cb:18:ASP:OD2	2.33	0.61
26:LD:245:GLU:HG3	26:LD:249:GLN:HE21	1.66	0.61
31:LK:16:ARG:HB3	31:LK:57:ARG:HD2	1.83	0.61
1:C1:984:A:N1	1:C1:1033:U:O2'	2.34	0.61
27:LE:86:PRO:HG3	27:LE:169:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CI:214:THR:OG1	8:CI:234:GLU:OE1	2.18	0.60
1:C1:3204:C:H2'	1:C1:3205:G:H8	1.65	0.60
1:C1:958:G:OP2	37:LQ:78:ARG:NH1	2.32	0.60
1:C1:1420:OMC:HM22	1:C1:1421:U:H5'	1.83	0.60
25:LC:287:LEU:HD11	37:LQ:60:LEU:HB2	1.84	0.60
1:C1:1812:OMC:H2'	1:C1:1813:G:H8	1.67	0.60
7:CH:86:ASP:OD2	7:CH:89:HIS:ND1	2.35	0.60
18:Ce:331:GLU:OE1	55:Lk:54:LYS:NZ	2.32	0.59
1:C1:2087:G:O2'	17:Cd:448:ARG:NH1	2.35	0.59
1:C1:2803:C:OP1	22:Cz:76:ARG:NH2	2.35	0.59
1:C1:1305:U:O2'	39:LS:1:MET:SD	2.59	0.59
13:CN:109:VAL:HB	13:CN:149:GLY:HA2	1.83	0.59
17:Cd:364:TRP:HA	17:Cd:377:ASP:O	2.02	0.59
1:C1:3270:U:H5''	24:LB:309:MET:HE2	1.83	0.59
21:Ch:264:ILE:HD12	21:Ch:274:HIS:HB2	1.84	0.59
30:LJ:94:ARG:O	30:LJ:157:ARG:NH2	2.36	0.59
31:LK:11:LYS:HB2	31:LK:64:ILE:HB	1.84	0.59
24:LB:307:THR:HG21	24:LB:317:GLU:HG2	1.84	0.59
1:C1:277:A:N1	1:C1:2744:A:O2'	2.36	0.59
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.38	0.59
1:C1:2197:G:HO2'	17:Cd:2:GLY:N	2.01	0.59
1:C1:3025:C:H3'	38:LR:62:ARG:HH22	1.68	0.59
1:C1:1611:C:OP2	45:LZ:47:ARG:NH2	2.35	0.58
8:CI:203:LEU:HD22	8:CI:233:ILE:HD11	1.84	0.58
52:Lh:15:LYS:O	52:Lh:66:LYS:NZ	2.34	0.58
30:LJ:118:ASP:HB3	30:LJ:121:ILE:HG12	1.83	0.58
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.31	0.58
21:Ch:417:THR:HG23	21:Ch:418:LEU:HG	1.86	0.58
19:Cf:290:ASP:OD1	19:Cf:294:ASP:N	2.37	0.58
26:LD:83:LEU:HB3	26:LD:88:ILE:HB	1.85	0.58
1:C1:1067:A:O2'	40:LT:35:ARG:NH2	2.37	0.58
7:CH:186:VAL:HG23	7:CH:187:THR:HG23	1.86	0.58
9:CJ:397:TRP:HB2	9:CJ:401:LEU:HD12	1.86	0.58
1:C1:42:G:H21	1:C1:2571:U:H4'	1.69	0.58
1:C1:2892:A:OP2	42:LV:6:ARG:NH1	2.37	0.58
2:C2:71:A:O2'	2:C2:83:C:N4	2.37	0.58
21:Ch:509:ASP:OD2	21:Ch:513:ARG:NH1	2.36	0.58
45:LZ:49:PRO:HD3	45:LZ:67:ILE:HG12	1.86	0.57
1:C1:643:C:H2'	1:C1:644:A:H8	1.69	0.57
21:Ch:84:ARG:NH1	21:Ch:97:ASP:OD1	2.37	0.57
16:Cb:25:ASP:OD1	16:Cb:31:HIS:ND1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Ch:195:VAL:HG12	21:Ch:206:THR:HG22	1.83	0.57
1:C1:1842:U:OP1	38:LR:70:ARG:NH2	2.38	0.57
27:LE:24:ALA:O	58:Lq:88:ARG:NH1	2.38	0.57
21:Ch:40:ASN:OD1	21:Ch:48:GLN:NE2	2.38	0.57
25:LC:185:VAL:HG11	25:LC:231:GLY:HA3	1.87	0.57
33:LM:135:LEU:HG	33:LM:139:LYS:HE2	1.86	0.57
1:C1:1081:A:OP2	40:LT:130:ARG:NH1	2.38	0.56
12:LF:245:ILE:O	12:LF:249:ASN:HB2	2.05	0.56
5:CB:103:ASP:O	5:CB:206:ARG:NH1	2.38	0.56
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.87	0.56
1:C1:2544:G:H5'	18:Ce:436:TRP:HE1	1.71	0.56
1:C1:2398:G:OP1	34:LN:20:ARG:NH2	2.38	0.56
9:CJ:128:ARG:HD3	18:Ce:160:TRP:H	1.70	0.56
9:CJ:380:ARG:NH1	9:CJ:401:LEU:O	2.39	0.56
10:CK:31:GLU:OE2	10:CK:35:ASN:ND2	2.37	0.56
17:Cd:130:HIS:HB3	17:Cd:133:LYS:HE3	1.86	0.56
35:LO:13:LYS:O	39:LS:169:ARG:NH2	2.39	0.56
1:C1:2405:G:H1	1:C1:2468:U:H3	1.53	0.56
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.24	0.56
9:CJ:25:LYS:HE3	9:CJ:73:LEU:HD11	1.86	0.56
44:LY:1:MET:HE3	44:LY:2:LYS:HG3	1.87	0.55
53:Li:79:ARG:HH12	53:Li:93:LYS:HG3	1.71	0.55
1:C1:2079:G:OP1	1:C1:2081:C:N4	2.38	0.55
41:LU:47:ILE:HD12	41:LU:62:ILE:HD11	1.88	0.55
1:C1:890:G:N2	34:LN:76:PRO:O	2.40	0.55
2:C2:63:G:O2'	52:Lh:54:LYS:NZ	2.39	0.55
10:CK:202:LYS:NZ	17:Cd:71:GLU:OE1	2.40	0.55
18:Ce:417:GLU:OE2	18:Ce:419:ARG:NH1	2.39	0.55
1:C1:1877:G:OP2	16:Cb:11:LYS:NZ	2.32	0.55
2:C2:63:G:H22	2:C2:97:A:H2	1.54	0.55
7:CH:294:PHE:O	7:CH:302:GLN:NE2	2.39	0.55
7:CH:242:LEU:O	7:CH:280:LYS:NZ	2.39	0.55
1:C1:1685:U:O2	1:C1:1766:G:O2'	2.25	0.55
3:C3:57:A:OP2	5:CB:144:ARG:NH2	2.40	0.55
9:CJ:379:PRO:HB2	9:CJ:382:PRO:HG2	1.88	0.55
28:LG:165:LEU:HA	34:LN:7:LEU:HD11	1.88	0.55
55:Lk:14:ILE:HA	55:Lk:17:ARG:HD3	1.86	0.55
7:CH:174:PHE:HE2	7:CH:266:GLN:HA	1.71	0.55
7:CH:591:ARG:NH1	43:LX:90:GLU:OE2	2.38	0.55
13:CN:32:GLU:OE1	13:CN:50:ARG:NH1	2.39	0.55
44:LY:86:ARG:HB3	44:LY:96:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:948:U:H2'	1:C1:949:A:H8	1.70	0.55
7:CH:315:GLU:OE2	7:CH:337:ARG:NH1	2.39	0.55
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.25	0.55
7:CH:586:ARG:HE	43:LX:156:VAL:HB	1.72	0.55
33:LM:44:PRO:HG3	33:LM:81:VAL:HG12	1.89	0.55
7:CH:508:MET:HE1	48:Ld:66:LYS:HB2	1.89	0.54
21:Ch:41:PHE:HD2	21:Ch:69:LEU:HD13	1.72	0.54
3:C3:55:U:O2'	3:C3:58:A:N7	2.38	0.54
11:CL:6:ASN:OD1	35:LO:52:LYS:NZ	2.34	0.54
15:CQ:179:GLU:OE1	48:Ld:86:ARG:NH1	2.40	0.54
25:LC:236:PRO:HG2	25:LC:239:ALA:HB3	1.89	0.54
53:Li:70:LEU:HD13	53:Li:100:GLN:HG2	1.88	0.54
9:CJ:42:ILE:HG13	9:CJ:72:LEU:HD11	1.88	0.54
1:C1:1614:G:N7	45:LZ:16:ARG:NH1	2.56	0.54
4:C4:88:G:O2'	4:C4:91:A:N6	2.41	0.54
7:CH:255:ILE:HA	7:CH:263:LEU:HD12	1.89	0.54
20:Cg:150:ASP:O	20:Cg:170:ARG:NH1	2.40	0.54
1:C1:489:A:O2'	1:C1:3214:A:N1	2.40	0.54
1:C1:1619:C:OP2	51:Lg:75:ARG:NH1	2.35	0.54
1:C1:2591:G:H21	1:C1:2605:C:H41	1.56	0.54
9:CJ:450:TYR:HB2	9:CJ:453:ARG:HE	1.73	0.54
17:Cd:213:ILE:HD12	17:Cd:403:ASN:HB2	1.89	0.54
20:Cg:30:ALA:HB2	20:Cg:62:LEU:HD13	1.87	0.54
1:C1:877:A:O2'	1:C1:879:U:OP2	2.26	0.54
1:C1:1372:G:H5''	49:Le:102:SER:HB3	1.90	0.54
13:CN:61:ARG:HD3	42:LV:133:SER:HA	1.90	0.54
18:Ce:434:GLU:HB3	18:Ce:439:LYS:HE3	1.89	0.54
21:Ch:35:GLY:O	21:Ch:56:ASN:ND2	2.41	0.54
44:LY:73:TYR:HE2	44:LY:76:LYS:HG3	1.73	0.54
1:C1:2796:A:O2'	1:C1:2810:A:N6	2.41	0.53
1:C1:1240:C:O2	6:CF:54:LYS:NZ	2.41	0.53
20:Cg:154:GLU:OE2	40:LT:54:HIS:ND1	2.41	0.53
21:Ch:88:HIS:NE2	21:Ch:123:SER:OG	2.42	0.53
21:Ch:379:SER:OG	21:Ch:381:ASP:OD1	2.26	0.53
1:C1:1929:G:OP2	38:LR:135:LYS:NZ	2.34	0.53
1:C1:1095:A:H2'	1:C1:1096:G:C8	2.43	0.53
4:C4:53:U:O2'	4:C4:55:A:N7	2.39	0.53
34:LN:177:GLY:O	34:LN:184:ARG:NH1	2.41	0.53
39:LS:1:MET:HG3	39:LS:118:PHE:HB2	1.91	0.53
1:C1:716:G:H5''	37:LQ:71:PRO:HB2	1.90	0.53
13:CN:106:ASN:ND2	42:LV:135:ALA:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2368:C:H4'	10:CK:142:THR:HG21	1.91	0.53
1:C1:3155:A:OP1	33:LM:109:ARG:NH1	2.42	0.53
13:CN:219:GLU:HA	13:CN:224:LEU:HD12	1.91	0.53
17:Cd:411:ILE:HG13	17:Cd:439:LEU:HD11	1.90	0.53
1:C1:1824:C:O2'	54:Lj:11:ARG:NH1	2.42	0.53
1:C1:2147:U:OP1	23:LA:209:HIS:NE2	2.35	0.53
47:Lc:43:LYS:HB3	47:Lc:104:LEU:HD21	1.90	0.53
56:Ll:44:TRP:CZ3	56:Ll:45:ARG:HD3	2.44	0.53
1:C1:3289:G:O6	1:C1:3298:U:O4	2.26	0.53
33:LM:94:TRP:O	33:LM:97:THR:OG1	2.27	0.53
43:LX:66:HIS:ND1	43:LX:67:GLU:O	2.42	0.53
1:C1:64:A:H5''	34:LN:174:LEU:HD13	1.90	0.53
1:C1:300:A:H2'	1:C1:301:A:C8	2.43	0.53
1:C1:1252:U:H1'	1:C1:1255:C:H5	1.74	0.53
7:CH:183:VAL:HG21	7:CH:219:ASP:HB2	1.91	0.53
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.44	0.52
3:C3:36:C:H2'	3:C3:37:G:H8	1.74	0.52
5:CB:282:TYR:OH	8:CI:316:ARG:NH1	2.42	0.52
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.40	0.52
1:C1:3000:U:OP2	1:C1:3050:C:N4	2.42	0.52
9:CJ:75:GLU:HG3	9:CJ:77:LEU:H	1.73	0.52
11:CL:5:ILE:HD13	35:LO:49:PHE:HB2	1.91	0.52
33:LM:54:ARG:HG2	39:LS:70:LEU:HD22	1.90	0.52
53:Li:74:LYS:HD3	53:Li:77:ARG:HE	1.74	0.52
1:C1:282:U:H2'	1:C1:283:G:H8	1.74	0.52
1:C1:1816:C:O2'	1:C1:1822:A:N1	2.39	0.52
1:C1:3002:A:H4'	24:LB:13:SER:HB2	1.90	0.52
4:C4:11:A:N1	4:C4:67:G:O2'	2.42	0.52
29:LH:10:ILE:HG12	29:LH:109:ARG:HG2	1.90	0.52
1:C1:1658:G:O6	41:LU:81:ARG:NH2	2.42	0.52
1:C1:1737:G:OP1	41:LU:101:ARG:NH2	2.36	0.52
1:C1:2516:G:O6	51:Lg:100:LYS:NZ	2.43	0.52
7:CH:540:ASP:OD2	15:CQ:143:ARG:NH1	2.43	0.52
15:CQ:18:GLY:HA3	15:CQ:31:PHE:O	2.09	0.52
1:C1:967:U:H2'	1:C1:968:U:H6	1.75	0.52
28:LG:175:LYS:HD2	53:Li:52:LEU:HD13	1.91	0.52
1:C1:643:C:H2'	1:C1:644:A:C8	2.43	0.52
25:LC:36:VAL:HG21	25:LC:251:LEU:HD21	1.91	0.52
2:C2:75:G:OP2	44:LY:73:TYR:OH	2.28	0.52
13:CN:186:VAL:HG12	13:CN:218:ILE:HD11	1.92	0.52
18:Ce:386:PRO:HA	18:Ce:389:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2308:A:H5''	48:Ld:32:THR:HG23	1.91	0.52
8:CI:211:GLY:HA3	8:CI:240:VAL:HG11	1.91	0.52
1:C1:3137:A:OP1	35:LO:38:ARG:NH2	2.43	0.52
9:CJ:17:MET:HE3	9:CJ:66:THR:HA	1.91	0.52
21:Ch:384:MET:HB2	21:Ch:400:LEU:HB2	1.92	0.51
33:LM:54:ARG:NH2	33:LM:76:ALA:O	2.41	0.51
52:Lh:17:LYS:NZ	52:Lh:70:GLN:OE1	2.43	0.51
6:CF:64:ARG:NH1	6:CF:65:ILE:O	2.43	0.51
58:Lq:7:ASP:OD1	58:Lq:41:ARG:NH1	2.39	0.51
3:C3:40:G:O6	3:C3:45:U:O4	2.28	0.51
13:CN:142:ILE:HG13	13:CN:148:VAL:HG12	1.92	0.51
17:Cd:16:ARG:HH11	17:Cd:20:ASP:HB2	1.74	0.51
1:C1:1067:A:H2'	1:C1:1068:A:C8	2.46	0.51
1:C1:979:A:N6	1:C1:1033:U:O4	2.44	0.51
4:C4:100:G:OP1	19:Cf:259:ARG:NH2	2.41	0.51
15:CQ:16:SER:HB3	24:LB:73:VAL:HG11	1.92	0.51
10:CK:241:ARG:NH1	17:Cd:79:ASN:OD1	2.43	0.51
1:C1:2100:U:OP2	1:C1:2105:A:N6	2.38	0.51
37:LQ:98:ASN:HB3	37:LQ:165:LEU:HD21	1.93	0.51
38:LR:98:ARG:NH1	38:LR:130:ASN:OD1	2.44	0.51
49:Le:120:VAL:HB	49:Le:123:ALA:HB2	1.92	0.51
34:LN:36:ILE:HG12	34:LN:64:VAL:HG23	1.93	0.51
4:C4:23:A:N3	4:C4:119:U:O2'	2.39	0.51
21:Ch:53:VAL:HG21	21:Ch:68:LEU:HD21	1.92	0.51
33:LM:20:LEU:HD21	33:LM:30:ILE:HD11	1.93	0.51
1:C1:388:A:H2'	1:C1:389:A2M:H8	1.92	0.51
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.46	0.51
7:CH:525:LYS:NZ	41:LU:98:ASP:O	2.41	0.51
21:Ch:61:THR:OG1	21:Ch:64:ASN:OD1	2.28	0.51
1:C1:1677:A:OP1	51:Lg:22:ARG:NH2	2.44	0.50
52:Lh:29:THR:O	52:Lh:33:GLN:OE1	2.29	0.50
1:C1:1077:U:O2'	1:C1:1078:U:O2	2.25	0.50
1:C1:1260:C:H2'	1:C1:1261:A:H8	1.76	0.50
1:C1:2489:C:OP1	23:LA:37:ARG:NH1	2.39	0.50
2:C2:26:U:O2'	25:LC:52:ALA:O	2.29	0.50
33:LM:59:LEU:O	39:LS:155:ARG:NH2	2.43	0.50
21:Ch:338:ALA:O	21:Ch:360:ARG:NH1	2.40	0.50
21:Ch:374:ARG:HH21	21:Ch:386:LEU:HD21	1.75	0.50
2:C2:120:G:H5'	18:Ce:182:PRO:HB3	1.92	0.50
7:CH:631:ALA:HB2	36:LP:125:GLN:HE21	1.77	0.50
19:Cf:145:ALA:HB3	19:Cf:188:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:341:C:O2	1:C1:345:A:O2'	2.30	0.50
11:CL:52:ASP:OD2	39:LS:80:ARG:NH1	2.41	0.50
28:LG:27:ASN:HB3	28:LG:30:LEU:HG	1.94	0.50
9:CJ:36:LEU:HD11	9:CJ:75:GLU:HG2	1.93	0.50
1:C1:2767:A:N6	1:C1:2913:U:O2'	2.43	0.50
28:LG:136:LYS:HD2	28:LG:141:HIS:HE1	1.76	0.50
1:C1:1599:A:OP2	9:CJ:52:LYS:NZ	2.39	0.50
19:Cf:169:ARG:HD2	20:Cg:90:LEU:HD13	1.94	0.50
1:C1:976:G:H4'	1:C1:977:U:H5'	1.93	0.50
1:C1:2396:U:H1'	34:LN:125:SER:HB3	1.92	0.50
1:C1:2640:U:H5'	30:LJ:66:ILE:HD11	1.93	0.50
13:CN:11:ASN:ND2	13:CN:209:ASP:OD2	2.44	0.50
1:C1:457:U:H5'	58:Lq:67:LYS:HD3	1.93	0.49
1:C1:464:C:H2'	1:C1:465:G:H8	1.76	0.49
1:C1:1193:U:H5	6:CF:3:LYS:HB2	1.77	0.49
5:CB:23:THR:HG22	5:CB:293:ILE:HB	1.92	0.49
7:CH:85:TYR:O	7:CH:148:TYR:OH	2.30	0.49
21:Ch:489:ASP:HB3	21:Ch:508:LYS:HB3	1.94	0.49
43:LX:78:HIS:HB2	52:Lh:39:ILE:HD13	1.94	0.49
1:C1:3078:C:OP2	10:CK:26:LYS:NZ	2.45	0.49
7:CH:495:ILE:HD13	15:CQ:130:ASN:HB2	1.93	0.49
26:LD:208:ALA:HB2	26:LD:239:LEU:HD12	1.93	0.49
1:C1:1920:G:H21	1:C1:3303:A:H8	1.59	0.49
1:C1:2073:G:OP2	16:Cb:79:LYS:NZ	2.45	0.49
1:C1:3284:G:H21	1:C1:3303:A:H2	1.60	0.49
3:C3:64:G:O6	8:CI:278:ARG:NH1	2.41	0.49
7:CH:85:TYR:OH	7:CH:155:HIS:ND1	2.37	0.49
41:LU:22:ILE:HB	41:LU:109:VAL:HG22	1.93	0.49
1:C1:2919:C:H2'	1:C1:2920:G:H8	1.77	0.49
8:CI:207:PHE:HB2	8:CI:213:ILE:HD11	1.94	0.49
28:LG:186:LYS:HB2	28:LG:197:THR:HG23	1.94	0.49
21:Ch:88:HIS:HB2	21:Ch:121:THR:HB	1.94	0.49
21:Ch:132:VAL:O	21:Ch:459:ARG:NH1	2.46	0.49
21:Ch:148:PRO:HB3	21:Ch:508:LYS:HA	1.92	0.49
26:LD:223:LYS:O	26:LD:227:VAL:HB	2.12	0.49
28:LG:249:GLU:OE1	28:LG:252:ARG:NH2	2.45	0.49
33:LM:114:ASP:OD1	33:LM:117:ARG:NH1	2.45	0.49
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.48	0.49
27:LE:139:GLU:HG3	27:LE:152:LYS:HG2	1.94	0.49
42:LV:25:MET:HE1	42:LV:80:ILE:HG12	1.93	0.49
1:C1:1186:A:H62	1:C1:1283:G:H21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.28	0.49
4:C4:77:U:H2'	4:C4:78:A:H8	1.77	0.49
10:CK:132:MET:HG2	10:CK:209:TYR:CE1	2.48	0.49
24:LB:90:VAL:HG22	24:LB:104:THR:HG23	1.94	0.49
25:LC:211:ILE:HG13	25:LC:256:VAL:HB	1.94	0.49
44:LY:54:GLU:HB2	44:LY:107:LYS:HB3	1.95	0.49
57:Lp:51:ALA:HB3	57:Lp:54:ILE:HD12	1.93	0.49
1:C1:1045:A:N3	40:LT:130:ARG:NH2	2.61	0.49
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.48	0.49
21:Ch:378:ALA:HA	21:Ch:384:MET:HG2	1.94	0.49
37:LQ:90:VAL:HG13	37:LQ:94:ARG:HD2	1.93	0.49
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.77	0.49
1:C1:967:U:H2'	1:C1:968:U:C6	2.48	0.49
1:C1:1812:OMC:HM23	56:Ll:7:PHE:HB2	1.95	0.49
1:C1:2981:U:H2'	1:C1:2982:A:H8	1.78	0.49
3:C3:49:G:H4'	5:CB:238:SER:HB3	1.95	0.49
24:LB:313:VAL:HG23	24:LB:365:GLU:HG3	1.95	0.49
12:CM:21:LYS:HG3	12:CM:25:GLN:HE22	1.78	0.48
30:LJ:55:VAL:HG12	30:LJ:58:PHE:H	1.77	0.48
49:Le:97:ILE:HG21	49:Le:106:ARG:HG2	1.95	0.48
1:C1:586:G:H1	1:C1:597:G:H5'	1.78	0.48
5:CB:22:GLN:NE2	8:CI:326:GLU:O	2.43	0.48
28:LG:46:LYS:HB3	43:LX:41:LYS:HD2	1.93	0.48
34:LN:9:GLU:HB2	53:Li:53:ILE:HG13	1.95	0.48
6:CF:227:TRP:HB2	6:CF:234:VAL:HG22	1.96	0.48
34:LN:159:ARG:HB3	34:LN:164:LEU:HB2	1.94	0.48
50:Lf:16:LEU:HD11	50:Lf:33:LYS:HB2	1.94	0.48
58:Lq:54:ILE:HG12	58:Lq:63:VAL:HG22	1.96	0.48
1:C1:696:G:N2	1:C1:699:A:OP2	2.42	0.48
1:C1:782:G:H22	25:LC:102:ALA:HA	1.77	0.48
2:C2:9:A:H2'	2:C2:10:A:C8	2.49	0.48
8:CI:298:SER:H	8:CI:301:GLN:NE2	2.11	0.48
9:CJ:9:LYS:O	9:CJ:14:ARG:NH2	2.46	0.48
13:CN:140:GLN:HG2	13:CN:173:LEU:HD21	1.96	0.48
1:C1:3067:G:OP2	1:C1:3078:C:N4	2.45	0.48
34:LN:56:LYS:NZ	34:LN:145:ASP:OD2	2.47	0.48
3:C3:35:C:O2'	5:CB:288:THR:O	2.30	0.48
24:LB:47:MET:HB3	24:LB:336:ILE:HD11	1.96	0.48
39:LS:66:GLU:HB3	39:LS:69:PRO:HG3	1.95	0.48
1:C1:278:A:H8	1:C1:297:G:H1'	1.78	0.48
1:C1:300:A:H2'	1:C1:301:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:410:A:H2'	1:C1:411:A:C8	2.49	0.48
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.49	0.48
1:C1:1939:U:O2'	1:C1:2045:G:N2	2.47	0.48
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.43	0.48
4:C4:75:A:O2'	19:Cf:94:LYS:NZ	2.44	0.48
45:LZ:56:MET:HG2	45:LZ:60:ARG:HD3	1.95	0.48
1:C1:1555:C:H5''	18:Ce:428:ALA:HB2	1.96	0.48
1:C1:2920:G:O2'	17:Cd:366:TYR:O	2.30	0.48
4:C4:44:C:OP2	30:LJ:138:ARG:NH2	2.47	0.48
7:CH:582:SER:N	7:CH:585:GLU:OE2	2.47	0.48
17:Cd:336:ASN:ND2	17:Cd:356:PRO:O	2.40	0.48
37:LQ:127:GLU:OE1	37:LQ:147:ARG:NH2	2.38	0.48
52:Lh:7:VAL:O	52:Lh:58:ARG:NH1	2.45	0.48
1:C1:129:G:OP2	52:Lh:79:LYS:NZ	2.46	0.48
3:C3:137:C:H5''	8:Cl:279:ARG:HD2	1.95	0.48
4:C4:6:C:O2'	26:LD:50:ARG:NH2	2.47	0.48
21:Ch:465:SER:OG	21:Ch:466:LYS:N	2.46	0.48
38:LR:105:LEU:HD23	38:LR:138:LEU:HD23	1.96	0.48
58:Lq:9:ILE:HG22	58:Lq:47:VAL:HG22	1.95	0.48
1:C1:515:G:H2'	1:C1:516:G:H8	1.79	0.48
1:C1:630:U:H2'	1:C1:631:U:C2	2.49	0.48
1:C1:3288:A:H2'	1:C1:3289:G:H8	1.78	0.48
1:C1:69:C:OP2	1:C1:294:G:N2	2.47	0.47
1:C1:1597:G:OP1	9:CJ:7:LYS:NZ	2.36	0.47
48:Ld:28:LEU:HD11	48:Ld:40:ALA:HB2	1.94	0.47
1:C1:1779:A:H2'	1:C1:1780:A:H8	1.79	0.47
24:LB:92:TYR:HB2	24:LB:158:VAL:HB	1.96	0.47
24:LB:146:THR:O	24:LB:150:GLU:HG2	2.14	0.47
45:LZ:21:LYS:NZ	45:LZ:128:TRP:O	2.42	0.47
1:C1:1864:A:OP2	48:Ld:39:ARG:NH2	2.46	0.47
3:C3:12:A:OP2	5:CB:188:ARG:NH2	2.47	0.47
9:CJ:161:PRO:HD2	9:CJ:164:MET:HE2	1.96	0.47
23:LA:129:THR:OG1	23:LA:132:ASN:ND2	2.42	0.47
47:Lc:44:LEU:HD23	47:Lc:95:ILE:HD12	1.96	0.47
1:C1:644:A:H2'	1:C1:645:A:C8	2.49	0.47
1:C1:1773:C:OP1	23:LA:177:LYS:NZ	2.45	0.47
1:C1:2648:A:OP1	26:LD:15:ARG:NH2	2.47	0.47
21:Ch:100:PRO:HG3	21:Ch:106:LEU:HD22	1.97	0.47
26:LD:214:LEU:HB3	26:LD:222:TYR:HB2	1.96	0.47
11:CL:70:GLU:HA	11:CL:73:ARG:HG2	1.96	0.47
39:LS:12:ARG:HB3	39:LS:24:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:21:A:H2'	1:C1:22:G:C8	2.50	0.47
1:C1:88:U:H2'	1:C1:89:A:H8	1.80	0.47
1:C1:1526:G:HO2'	1:C1:2131:A:HO2'	1.63	0.47
1:C1:3109:U:H3	1:C1:3338:C:H42	1.61	0.47
4:C4:26:C:H5'	26:LD:56:THR:HB	1.96	0.47
6:CF:94:ARG:NH2	6:CF:95:TYR:OH	2.47	0.47
12:LF:92:VAL:O	12:LF:120:GLY:HA2	2.14	0.47
30:LJ:38:LEU:HD13	30:LJ:70:VAL:HG23	1.97	0.47
1:C1:619:A:H2'	1:C1:620:G:C8	2.49	0.47
1:C1:652:A:H2'	1:C1:653:A:C8	2.50	0.47
5:CB:268:GLU:O	5:CB:274:LYS:NZ	2.48	0.47
7:CH:544:ILE:O	7:CH:549:ARG:NH1	2.45	0.47
31:LK:143:VAL:HB	31:LK:151:ILE:HD13	1.97	0.47
45:LZ:69:PRO:HG3	45:LZ:114:LYS:HB2	1.97	0.47
1:C1:523:G:H2'	1:C1:524:A:C8	2.50	0.47
1:C1:575:G:H2'	1:C1:576:A:H8	1.80	0.47
1:C1:1701:U:O2'	1:C1:1703:G:N7	2.47	0.47
5:CB:119:ASP:OD2	5:CB:119:ASP:N	2.48	0.47
8:CI:284:PRO:HB2	8:CI:287:LYS:HB2	1.97	0.47
8:CI:297:LEU:HD12	8:CI:301:GLN:HG3	1.96	0.47
12:CM:20:LYS:NZ	18:Ce:388:GLU:OE2	2.42	0.47
1:C1:231:A:H2'	1:C1:232:A:C8	2.50	0.47
1:C1:1726:C:O2'	55:Lk:4:GLU:OE1	2.31	0.47
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.50	0.47
12:CM:15:PRO:HG3	18:Ce:234:ILE:HD11	1.97	0.47
27:LE:86:PRO:HD2	27:LE:89:ILE:HD12	1.97	0.47
31:LK:62:LEU:HG	31:LK:71:VAL:HG22	1.96	0.47
53:Li:79:ARG:HH22	53:Li:93:LYS:HD3	1.80	0.47
1:C1:20:U:H2'	1:C1:21:A:C8	2.50	0.46
1:C1:663:C:O2'	1:C1:667:U:OP1	2.32	0.46
1:C1:706:G:OP2	1:C1:706:G:N2	2.34	0.46
1:C1:2218:A:N6	1:C1:2226:C:O2	2.48	0.46
1:C1:3132:A:H62	27:LE:191:LYS:HD3	1.79	0.46
46:La:133:GLU:OE1	46:La:136:ARG:NH2	2.46	0.46
1:C1:1041:U:OP2	12:LF:104:LYS:NZ	2.48	0.46
1:C1:1812:OMC:H2'	1:C1:1813:G:C8	2.49	0.46
1:C1:3079:U:H1'	1:C1:3080:A:H5''	1.97	0.46
26:LD:34:LYS:O	26:LD:38:THR:OG1	2.32	0.46
27:LE:61:LEU:HD11	27:LE:103:ILE:HG13	1.97	0.46
40:LT:42:ILE:HD11	40:LT:74:VAL:HG11	1.96	0.46
17:Cd:235:VAL:O	17:Cd:329:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LA:54:ARG:HG2	23:LA:56:ALA:H	1.80	0.46
1:C1:1559:G:OP2	1:C1:1559:G:N2	2.38	0.46
1:C1:2631:G:H5'	30:LJ:95:ARG:NH1	2.29	0.46
10:CK:87:PRO:HD2	10:CK:90:LEU:HD12	1.97	0.46
29:LH:154:ARG:HG2	29:LH:162:VAL:HG22	1.97	0.46
1:C1:1929:G:OP1	38:LR:104:ARG:NH1	2.46	0.46
1:C1:2513:C:OP1	51:Lg:103:LYS:NZ	2.43	0.46
19:Cf:36:THR:HA	19:Cf:63:LYS:HB3	1.98	0.46
58:Lq:11:GLU:HA	58:Lq:14:ARG:HD2	1.98	0.46
1:C1:1785:C:H2'	1:C1:1786:G:H8	1.81	0.46
16:Cb:52:CYS:SG	16:Cb:74:HIS:HE1	2.38	0.46
42:LV:106:ASN:HD21	42:LV:110:GLU:HB2	1.81	0.46
1:C1:1404:G:H2'	1:C1:1405:G:H8	1.80	0.46
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.50	0.46
8:CI:188:VAL:HG22	8:CI:234:GLU:HG2	1.97	0.46
18:Ce:258:ALA:HB2	45:LZ:123:SER:HB2	1.97	0.46
35:LO:62:MET:HA	35:LO:72:PRO:HD2	1.97	0.46
1:C1:230:G:H2'	1:C1:231:A:C8	2.51	0.46
1:C1:262:G:N2	1:C1:288:A:OP2	2.37	0.46
7:CH:647:HIS:O	7:CH:660:ARG:NH2	2.49	0.46
1:C1:2130:A:H2'	1:C1:2131:A:C8	2.51	0.46
7:CH:71:SER:O	17:Cd:178:ARG:NH1	2.49	0.46
7:CH:468:LEU:HD23	7:CH:473:PHE:CG	2.51	0.46
21:Ch:367:ILE:HD12	21:Ch:372:ALA:HB3	1.98	0.46
29:LH:68:ARG:NH1	29:LH:188:ASN:OD1	2.49	0.46
31:LK:143:VAL:HG23	31:LK:148:PRO:HG3	1.98	0.46
36:LP:40:LYS:HD3	36:LP:113:ILE:HG22	1.97	0.46
1:C1:2523:G:H2'	1:C1:2524:G:H8	1.81	0.46
7:CH:587:LEU:HD22	43:LX:146:LEU:HD13	1.98	0.46
1:C1:1778:A:H2'	1:C1:1779:A:C8	2.51	0.45
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.26	0.45
12:CM:102:PRO:HB2	12:CM:105:PRO:HD2	1.98	0.45
45:LZ:13:THR:HB	51:Lg:87:ARG:HG3	1.98	0.45
1:C1:293:G:H2'	1:C1:294:G:H8	1.81	0.45
1:C1:3111:C:C4	1:C1:3113:A:H1'	2.51	0.45
5:CB:19:ASP:N	5:CB:19:ASP:OD1	2.49	0.45
5:CB:263:ILE:HG12	5:CB:281:PHE:HE2	1.81	0.45
5:CB:263:ILE:HG12	5:CB:281:PHE:CE2	2.51	0.45
7:CH:168:THR:HA	7:CH:216:GLN:O	2.16	0.45
8:CI:191:ILE:HA	8:CI:259:THR:O	2.16	0.45
17:Cd:47:ILE:HB	17:Cd:56:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Cf:98:HIS:CD2	19:Cf:120:PRO:HG3	2.51	0.45
21:Ch:374:ARG:HH22	21:Ch:397:VAL:HG11	1.80	0.45
1:C1:111:G:OP2	32:LL:73:ARG:NH2	2.43	0.45
1:C1:1137:A:OP2	1:C1:2334:G:N1	2.42	0.45
1:C1:1433:OMG:H1'	1:C1:1433:OMG:HM23	1.76	0.45
1:C1:2225:A:H2'	1:C1:2226:C:C6	2.50	0.45
19:Cf:169:ARG:HG2	20:Cg:27:LEU:HD22	1.98	0.45
1:C1:213:A:HO2'	1:C1:214:G:H21	1.56	0.45
1:C1:1624:C:H5'	1:C1:1625:U:H5''	1.97	0.45
1:C1:2833:G:OP2	1:C1:2833:G:N2	2.36	0.45
1:C1:2991:A:H2	29:LH:159:GLU:HG2	1.81	0.45
4:C4:17:A:H2'	4:C4:18:G:C8	2.52	0.45
7:CH:628:ASN:O	36:LP:125:GLN:NE2	2.41	0.45
12:CM:149:SER:HG	12:CM:246:ARG:HH12	1.61	0.45
25:LC:136:LEU:HD23	25:LC:143:VAL:HG11	1.98	0.45
1:C1:575:G:H2'	1:C1:576:A:C8	2.52	0.45
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.52	0.45
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.82	0.45
58:Lq:31:ASP:HB3	58:Lq:34:ASN:HB2	1.98	0.45
1:C1:2318:G:OP1	36:LP:141:SER:OG	2.24	0.45
1:C1:2838:OMC:H5	1:C1:2906:G:H1	1.64	0.45
51:Lg:77:TYR:HB3	51:Lg:81:ARG:HB2	1.98	0.45
1:C1:1350:G:N2	1:C1:1351:U:O4	2.50	0.45
1:C1:1677:A:H5'	51:Lg:34:LEU:HD21	1.98	0.45
1:C1:2169:G:H2'	1:C1:2170:A:C8	2.51	0.45
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.81	0.45
3:C3:38:C:H2'	3:C3:39:G:H8	1.81	0.45
18:Ce:237:GLU:HA	18:Ce:240:ARG:HG2	1.99	0.45
29:LH:127:MET:HE2	29:LH:218:ILE:HG22	1.98	0.45
52:Lh:77:ASN:OD1	52:Lh:77:ASN:N	2.50	0.45
1:C1:159:U:H2'	1:C1:160:G:C8	2.52	0.45
1:C1:2074:G:C6	16:Cb:76:ARG:HD3	2.51	0.45
17:Cd:135:THR:HG22	17:Cd:138:ARG:HH12	1.82	0.45
32:LL:148:THR:HB	52:Lh:125:ALA:HB2	1.97	0.45
55:Lk:26:LYS:NZ	55:Lk:28:ASN:OD1	2.38	0.45
1:C1:64:A:N3	1:C1:79:U:O2'	2.39	0.45
1:C1:633:A:O5'	1:C1:1125:G:O2'	2.34	0.45
1:C1:980:A:H2'	1:C1:981:G:C8	2.51	0.45
1:C1:2642:U:HO2'	30:LJ:131:CYS:HG	1.64	0.45
13:CN:107:VAL:HG23	13:CN:108:ILE:HG13	1.99	0.45
17:Cd:315:ARG:NH1	17:Cd:370:MET:SD	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LL:189:ARG:HB2	53:Li:18:ARG:HD3	1.99	0.45
36:LP:41:LEU:HD21	36:LP:99:GLU:HB2	1.98	0.45
48:Ld:15:VAL:HA	48:Ld:85:ARG:O	2.17	0.45
1:C1:1142:A:OP1	37:LQ:31:GLY:N	2.50	0.45
1:C1:1187:A:N6	1:C1:2810:A:O4'	2.50	0.45
24:LB:76:VAL:HG12	24:LB:326:LYS:HA	1.99	0.45
46:La:112:LEU:HD22	46:La:125:VAL:HG11	1.99	0.45
1:C1:1615:G:N2	1:C1:1618:A:OP2	2.38	0.44
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.52	0.44
1:C1:2181:G:H2'	1:C1:2182:A:H8	1.82	0.44
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.52	0.44
19:Cf:135:PRO:HD2	19:Cf:138:MET:HE2	1.99	0.44
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.52	0.44
1:C1:2164:G:H21	1:C1:2205:A:H62	1.66	0.44
1:C1:2384:OMU:H1'	1:C1:2384:OMU:HM23	1.73	0.44
4:C4:16:C:N3	4:C4:64:A:N6	2.65	0.44
7:CH:426:ILE:O	15:CQ:80:ARG:NH1	2.49	0.44
27:LE:16:THR:HG23	12:LF:4:THR:HA	1.99	0.44
1:C1:151:G:H5''	1:C1:152:G:H2'	1.99	0.44
1:C1:351:G:N2	1:C1:354:A:OP2	2.41	0.44
4:C4:17:A:H2'	4:C4:18:G:H8	1.81	0.44
18:Ce:192:LYS:HD2	18:Ce:193:PRO:HD2	1.99	0.44
21:Ch:208:SER:OG	21:Ch:209:MET:N	2.50	0.44
23:LA:45:VAL:HG22	23:LA:61:VAL:HG22	1.98	0.44
34:LN:145:ASP:HB3	34:LN:148:ILE:HG22	1.98	0.44
3:C3:36:C:H2'	3:C3:37:G:C8	2.50	0.44
4:C4:78:A:H3'	4:C4:79:G:H8	1.82	0.44
7:CH:250:LEU:HD11	7:CH:334:VAL:HG11	1.98	0.44
13:CN:4:ARG:NH1	13:CN:210:THR:O	2.47	0.44
15:CQ:163:GLU:HA	15:CQ:166:LYS:HD2	1.98	0.44
17:Cd:121:PRO:HG2	21:Ch:404:GLN:HE21	1.83	0.44
19:Cf:227:LEU:HB3	19:Cf:253:MET:HB2	1.98	0.44
27:LE:77:ASP:OD2	27:LE:77:ASP:N	2.49	0.44
30:LJ:37:VAL:HA	30:LJ:40:GLN:OE1	2.18	0.44
50:Lf:55:TYR:CZ	50:Lf:67:ARG:HB2	2.51	0.44
1:C1:464:C:H2'	1:C1:465:G:C8	2.52	0.44
1:C1:1220:G:H22	1:C1:1234:A:H2	1.65	0.44
6:CF:97:THR:O	6:CF:243:ARG:NH2	2.50	0.44
7:CH:341:GLU:O	7:CH:345:GLN:HG3	2.17	0.44
7:CH:526:PRO:HB2	7:CH:529:GLN:HG3	1.97	0.44
26:LD:48:LYS:HE2	26:LD:148:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1783:C:H2'	1:C1:1784:G:C8	2.53	0.44
1:C1:2771:C:H2'	1:C1:2772:A:C8	2.52	0.44
1:C1:3314:G:OP2	48:Ld:110:LYS:NZ	2.35	0.44
7:CH:289:MET:HE3	7:CH:318:ARG:HG3	1.99	0.44
9:CJ:463:ASP:HB3	9:CJ:471:LYS:HE3	2.00	0.44
21:Ch:249:GLY:O	21:Ch:268:ASN:ND2	2.51	0.44
1:C1:2518:G:OP1	23:LA:69:TYR:OH	2.27	0.44
6:CF:41:PHE:HB2	6:CF:103:LEU:HB3	2.00	0.44
13:CN:21:ASN:HB2	13:CN:67:ARG:HB3	1.98	0.44
19:Cf:234:THR:OG1	26:LD:129:TYR:O	2.36	0.44
21:Ch:82:PRO:HB2	21:Ch:127:GLN:HB3	2.00	0.44
47:Lc:54:LEU:HD11	51:Lg:91:ILE:HG22	2.00	0.44
1:C1:382:A:H5''	36:LP:16:ARG:HG3	1.99	0.44
1:C1:768:A:H4'	1:C1:769:G:H5'	2.00	0.44
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.52	0.44
1:C1:3067:G:OP1	10:CK:23:ARG:HD2	2.18	0.44
9:CJ:141:LEU:HD23	9:CJ:141:LEU:HA	1.89	0.44
30:LJ:87:VAL:HG21	30:LJ:113:LEU:HD23	2.00	0.44
47:Lc:98:ALA:HB2	47:Lc:104:LEU:HD13	2.00	0.44
1:C1:582:G:H1'	27:LE:37:LYS:HG3	2.00	0.44
1:C1:604:G:H2'	1:C1:605:G:C8	2.53	0.44
1:C1:911:A:O2'	54:Lj:49:TRP:O	2.33	0.44
1:C1:2362:A:H5'	1:C1:2905:A:H61	1.83	0.44
5:CB:30:LEU:HD12	5:CB:30:LEU:HA	1.84	0.44
5:CB:237:PRO:HB2	8:CI:286:ASN:ND2	2.28	0.44
10:CK:133:PHE:HB3	10:CK:149:ARG:HB3	1.99	0.44
17:Cd:11:LEU:HD13	17:Cd:16:ARG:HE	1.81	0.44
24:LB:161:VAL:HG13	24:LB:184:ILE:HD11	1.99	0.44
43:LX:109:LYS:HE3	43:LX:109:LYS:HB2	1.83	0.44
1:C1:66:A:H1'	1:C1:78:A:H1'	1.99	0.43
6:CF:183:ASP:OD1	6:CF:184:GLU:N	2.51	0.43
1:C1:88:U:H2'	1:C1:89:A:C8	2.53	0.43
1:C1:448:C:H5	27:LE:15:ARG:HE	1.66	0.43
1:C1:1054:U:O2	1:C1:1070:G:N2	2.40	0.43
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.83	0.43
1:C1:3238:U:O4	24:LB:124:LYS:NZ	2.51	0.43
22:Cz:72:LYS:NZ	40:LT:160:ILE:O	2.49	0.43
27:LE:115:ASP:HB3	27:LE:118:LYS:HB2	2.00	0.43
30:LJ:22:ILE:HG12	30:LJ:126:MET:HG2	1.99	0.43
1:C1:966:G:N2	1:C1:1121:U:OP1	2.40	0.43
1:C1:1337:G:N2	1:C1:1339:U:O2'	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.83	0.43
2:C2:57:C:H4'	2:C2:63:G:N7	2.33	0.43
13:CN:15:VAL:HA	13:CN:61:ARG:HG2	1.99	0.43
27:LE:98:ASN:HB3	27:LE:101:TYR:HD1	1.83	0.43
33:LM:32:GLU:HB2	33:LM:40:LEU:HB3	1.99	0.43
46:La:101:VAL:HG22	46:La:124:VAL:HB	2.00	0.43
1:C1:2123:G:H2'	1:C1:2124:G:C8	2.53	0.43
1:C1:2157:G:O4'	17:Cd:307:ARG:NH1	2.51	0.43
1:C1:2335:A:OP1	11:CL:19:ARG:NH1	2.50	0.43
4:C4:38:U:N3	4:C4:41:G:OP2	2.40	0.43
5:CB:24:LEU:HD23	5:CB:28:LYS:NZ	2.32	0.43
5:CB:28:LYS:HE2	5:CB:28:LYS:HB2	1.81	0.43
5:CB:261:THR:HA	5:CB:264:ARG:HG2	2.00	0.43
14:CO:36:LYS:HB3	24:LB:208:THR:HG22	1.99	0.43
19:Cf:104:ARG:HB3	19:Cf:112:ASP:OD1	2.19	0.43
24:LB:242:LYS:HD2	24:LB:242:LYS:HA	1.86	0.43
27:LE:163:LYS:O	27:LE:167:LYS:HG2	2.17	0.43
39:LS:162:LYS:HG3	50:Lf:38:ASP:HB3	1.99	0.43
42:LV:19:LEU:HD11	42:LV:100:ASN:HB3	2.00	0.43
1:C1:222:U:OP1	44:LY:4:ARG:NH2	2.52	0.43
1:C1:2971:U:H2'	1:C1:2972:U:C6	2.53	0.43
5:CB:67:THR:HB	5:CB:280:ASN:HB2	2.01	0.43
9:CJ:415:ILE:HB	9:CJ:453:ARG:HH12	1.84	0.43
39:LS:77:ILE:HG12	39:LS:126:VAL:HG22	2.00	0.43
52:Lh:36:ILE:HA	52:Lh:39:ILE:HG12	2.00	0.43
54:Lj:32:LYS:HA	54:Lj:32:LYS:HD3	1.87	0.43
54:Lj:43:LYS:HE3	54:Lj:43:LYS:HB2	1.76	0.43
1:C1:1199:C:OP2	11:CL:57:ASN:ND2	2.50	0.43
1:C1:2315:A:H5''	36:LP:83:TRP:O	2.18	0.43
6:CF:91:ARG:O	6:CF:94:ARG:NH1	2.50	0.43
8:CI:255:GLY:O	28:LG:216:LYS:NZ	2.40	0.43
9:CJ:227:MET:HE3	18:Ce:407:TYR:HD1	1.83	0.43
13:CN:104:LEU:HA	13:CN:107:VAL:HG22	2.01	0.43
24:LB:304:LYS:NZ	24:LB:360:ILE:O	2.49	0.43
49:Le:68:MET:HE2	49:Le:68:MET:HB3	1.91	0.43
1:C1:2103:U:OP2	7:CH:657:LYS:NZ	2.39	0.43
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.82	0.43
8:CI:234:GLU:HB2	8:CI:273:PHE:CZ	2.53	0.43
21:Ch:470:LEU:HD11	21:Ch:505:SER:HB3	2.00	0.43
1:C1:414:G:O6	1:C1:2346:C:O2'	2.34	0.43
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2280:A:H5''	1:C1:2282:U:H5'	2.01	0.43
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.83	0.43
7:CH:275:PRO:HB2	17:Cd:161:VAL:HG12	2.01	0.43
27:LE:9:THR:HG22	27:LE:14:THR:HG22	2.01	0.43
28:LG:85:LEU:HD22	28:LG:89:LEU:HD23	1.99	0.43
1:C1:124:A:OP1	28:LG:108:LYS:NZ	2.51	0.43
1:C1:2706:A:H2'	1:C1:2707:A:C8	2.54	0.43
4:C4:4:U:H2'	4:C4:5:A:C8	2.53	0.43
5:CB:129:ASP:OD1	5:CB:129:ASP:N	2.47	0.43
6:CF:174:MET:HE3	6:CF:174:MET:HB3	1.91	0.43
9:CJ:223:ASP:HB3	9:CJ:226:ILE:HG22	2.01	0.43
15:CQ:23:ARG:NH2	15:CQ:25:ASP:OD2	2.47	0.43
24:LB:216:ILE:HD12	24:LB:339:LEU:HB3	2.01	0.43
34:LN:99:ARG:O	34:LN:103:GLU:HG3	2.18	0.43
1:C1:390:A:H4'	1:C1:391:U:H3'	2.00	0.43
7:CH:422:ARG:NH1	7:CH:435:ASP:O	2.44	0.43
10:CK:37:GLU:O	10:CK:41:ASN:HB2	2.19	0.43
19:Cf:123:TYR:HE1	19:Cf:253:MET:HE2	1.84	0.43
22:Cz:68:MET:HE2	40:LT:160:ILE:HG12	1.99	0.43
26:LD:98:ALA:HB1	26:LD:165:VAL:HG23	2.01	0.43
27:LE:194:LYS:HB3	27:LE:196:HIS:CE1	2.54	0.43
28:LG:78:ILE:HD11	34:LN:18:VAL:HG13	2.01	0.43
51:Lg:24:ILE:HD13	51:Lg:34:LEU:HD22	2.01	0.43
1:C1:1395:G:H5''	49:Le:125:ALA:HB2	2.00	0.42
1:C1:1449:G:N2	1:C1:1493:G:H5''	2.33	0.42
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.54	0.42
1:C1:2383:C:H2'	1:C1:2384:OMU:H6	2.01	0.42
1:C1:2711:U:H2'	1:C1:2712:G:C8	2.54	0.42
10:CK:2:PRO:HB2	10:CK:6:TYR:CG	2.54	0.42
13:CN:101:LEU:HB3	13:CN:107:VAL:HG11	2.00	0.42
19:Cf:291:LEU:HD23	19:Cf:291:LEU:HA	1.88	0.42
36:LP:91:LEU:HD23	36:LP:91:LEU:HA	1.91	0.42
44:LY:62:HIS:HB3	44:LY:65:LYS:HD2	2.01	0.42
52:Lh:107:GLU:HG3	52:Lh:111:LYS:HE3	2.00	0.42
1:C1:405:G:H2'	1:C1:406:U:C6	2.54	0.42
1:C1:882:G:H1'	1:C1:1569:A:N6	2.34	0.42
1:C1:1623:A:H5''	1:C1:1624:C:C5	2.54	0.42
1:C1:2495:U:H2'	1:C1:2496:G:C8	2.54	0.42
1:C1:2822:G:C2	7:CH:94:LEU:HD13	2.54	0.42
1:C1:2953:A:O2'	2:C2:1:A:N1	2.51	0.42
5:CB:67:THR:HA	5:CB:239:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CH:645:PRO:HG2	7:CH:648:LEU:HD12	2.02	0.42
11:CL:69:ILE:HD11	40:LT:156:TYR:HB3	2.01	0.42
24:LB:237:LYS:HB2	24:LB:237:LYS:HE2	1.77	0.42
44:LY:73:TYR:CE2	44:LY:76:LYS:HG3	2.54	0.42
1:C1:1577:C:H2'	1:C1:1578:G:C8	2.54	0.42
1:C1:3288:A:H2'	1:C1:3289:G:C8	2.54	0.42
5:CB:82:LYS:O	5:CB:269:ARG:NH2	2.52	0.42
9:CJ:141:LEU:HD11	9:CJ:241:VAL:HG11	2.02	0.42
15:CQ:89:THR:O	15:CQ:93:MET:HG3	2.18	0.42
18:Ce:156:THR:OG1	18:Ce:157:TYR:N	2.53	0.42
32:LL:115:ARG:NH2	32:LL:155:PHE:O	2.38	0.42
33:LM:21:LYS:HD2	33:LM:94:TRP:HH2	1.85	0.42
1:C1:364:G:O2'	1:C1:389:A2M:N6	2.50	0.42
1:C1:703:A:N1	1:C1:763:G:O2'	2.50	0.42
1:C1:3249:C:O2'	36:LP:69:ARG:O	2.33	0.42
4:C4:1:A:C8	26:LD:271:LYS:HG2	2.54	0.42
4:C4:62:U:H4'	26:LD:290:ARG:HH12	1.85	0.42
10:CK:149:ARG:HH22	17:Cd:44:GLY:HA2	1.85	0.42
12:LF:182:TYR:CZ	12:LF:203:GLN:HG2	2.54	0.42
29:LH:138:VAL:HG11	29:LH:183:LEU:HD21	2.00	0.42
32:LL:170:LYS:HA	32:LL:173:ILE:HG13	2.01	0.42
44:LY:39:ARG:HD2	44:LY:45:ARG:HA	2.01	0.42
1:C1:400:A:C2	2:C2:17:A:H1'	2.54	0.42
1:C1:524:A:H2'	1:C1:525:A:C8	2.55	0.42
1:C1:1917:OMU:H1'	1:C1:1917:OMU:HM23	1.72	0.42
1:C1:2570:U:H2'	1:C1:2571:U:C6	2.54	0.42
7:CH:167:ARG:NH1	13:CN:243:GLU:OE2	2.50	0.42
22:Cz:77:GLN:HA	22:Cz:80:ILE:HG22	2.01	0.42
40:LT:78:LYS:HE3	40:LT:87:LYS:HG3	2.01	0.42
45:LZ:114:LYS:O	45:LZ:118:GLU:HG3	2.19	0.42
53:Li:18:ARG:HA	53:Li:22:LYS:HD3	2.01	0.42
1:C1:30:C:H4'	1:C1:63:A:H4'	2.00	0.42
1:C1:219:C:OP1	44:LY:46:SER:OG	2.37	0.42
1:C1:551:C:H2'	1:C1:552:C:H6	1.84	0.42
1:C1:656:U:H2'	1:C1:657:U:C6	2.55	0.42
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.54	0.42
1:C1:2224:G:H3'	1:C1:2225:A:H8	1.85	0.42
1:C1:2958:G:H2'	1:C1:2959:U:C6	2.55	0.42
2:C2:103:G:OP2	2:C2:105:A:O2'	2.29	0.42
5:CB:109:LYS:HE3	5:CB:109:LYS:HB2	1.86	0.42
6:CF:62:ASP:OD2	6:CF:107:ARG:NH2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Cg:147:GLY:HA2	20:Cg:150:ASP:HB2	2.00	0.42
21:Ch:246:TRP:O	21:Ch:354:ARG:NH1	2.43	0.42
26:LD:95:TRP:CE3	26:LD:201:TYR:HB3	2.55	0.42
32:LL:141:ASP:N	32:LL:141:ASP:OD1	2.51	0.42
1:C1:404:U:H2'	1:C1:405:G:H8	1.84	0.42
1:C1:1476:G:OP2	1:C1:1476:G:N2	2.41	0.42
1:C1:2221:U:H2'	1:C1:2222:A:H8	1.85	0.42
1:C1:2728:A:H2'	1:C1:2729:G:C8	2.55	0.42
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.55	0.42
2:C2:47:C:H1'	2:C2:61:A:H2'	2.02	0.42
6:CF:224:LEU:HD11	6:CF:243:ARG:HH11	1.84	0.42
7:CH:459:GLN:NE2	7:CH:463:GLU:OE2	2.42	0.42
39:LS:110:MET:HE3	39:LS:110:MET:HB3	1.81	0.42
46:La:112:LEU:HB3	46:La:130:VAL:HG23	2.02	0.42
1:C1:498:U:H2'	1:C1:499:C:C6	2.55	0.42
1:C1:1577:C:H5'	1:C1:1676:A:H1'	2.01	0.42
1:C1:1809:G:O2'	9:CJ:2:GLY:N	2.48	0.42
16:Cb:35:TYR:O	16:Cb:38:THR:OG1	2.34	0.42
32:LL:124:ILE:HG23	32:LL:138:THR:HG21	2.01	0.42
49:Le:80:VAL:HA	49:Le:83:VAL:HG12	2.02	0.42
57:Lp:6:LYS:HB2	57:Lp:6:LYS:HE2	1.79	0.42
1:C1:425:G:H2'	1:C1:426:A:C8	2.55	0.42
1:C1:1583:A:OP1	38:LR:38:ARG:NH2	2.44	0.42
2:C2:83:C:O2	44:LY:109:HIS:NE2	2.43	0.42
5:CB:292:PRO:HD2	8:CI:320:LEU:HD11	2.02	0.42
22:Cz:82:ALA:HB1	22:Cz:86:ARG:HH12	1.85	0.42
1:C1:1901:A:H2'	1:C1:1902:A:C8	2.55	0.42
1:C1:2621:G:H2'	1:C1:2622:G:H8	1.85	0.42
3:C3:8:A:N6	3:C3:25:U:OP1	2.42	0.42
7:CH:309:THR:HG22	7:CH:314:VAL:HB	2.01	0.42
26:LD:214:LEU:HD12	26:LD:226:PHE:HE2	1.84	0.42
30:LJ:147:SER:OG	30:LJ:148:ARG:N	2.53	0.42
45:LZ:50:SER:HB2	45:LZ:64:ARG:HB3	2.02	0.42
1:C1:37:C:H4'	1:C1:790:A:C2	2.55	0.41
1:C1:2516:G:O2'	45:LZ:135:PHE:OXT	2.38	0.41
1:C1:2609:U:H4'	20:Cg:167:THR:HG22	2.02	0.41
1:C1:2729:G:H2'	1:C1:2732:C:H5	1.85	0.41
1:C1:3159:U:H5''	50:Lf:4:GLU:HB2	2.02	0.41
5:CB:133:LEU:HD21	5:CB:167:LEU:HD21	2.02	0.41
7:CH:357:ILE:HG23	7:CH:361:LEU:HD23	2.01	0.41
12:CM:241:ILE:HD12	12:CM:244:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Ce:429:LYS:HA	18:Ce:429:LYS:HD3	1.89	0.41
1:C1:698:A:H2'	1:C1:699:A:C8	2.55	0.41
1:C1:1480:C:H2'	1:C1:1481:A:H8	1.84	0.41
1:C1:1731:G:H5'	55:Lk:26:LYS:HE2	2.01	0.41
1:C1:1762:U:H2'	1:C1:1763:C:C6	2.54	0.41
1:C1:2801:U:OP1	11:CL:47:SER:N	2.50	0.41
1:C1:2843:C:H2'	1:C1:2844:C:H6	1.85	0.41
26:LD:226:PHE:HB3	26:LD:229:TYR:HB2	2.02	0.41
27:LE:139:GLU:HG3	27:LE:152:LYS:HE2	2.01	0.41
52:Lh:9:ALA:HB2	52:Lh:58:ARG:HD3	2.02	0.41
1:C1:269:A:H2'	1:C1:270:G:C8	2.55	0.41
1:C1:344:A:N6	56:Ll:37:TYR:O	2.47	0.41
1:C1:2562:G:HO2'	17:Cd:2:GLY:N	2.18	0.41
12:CM:114:LEU:HD21	12:CM:121:VAL:HG22	2.02	0.41
24:LB:386:LYS:HA	24:LB:389:GLN:HB2	2.03	0.41
29:LH:127:MET:HG2	29:LH:220:VAL:HA	2.01	0.41
37:LQ:174:ARG:HE	37:LQ:177:VAL:HG23	1.84	0.41
1:C1:243:U:O2'	1:C1:244:G:O5'	2.30	0.41
1:C1:405:G:OP1	36:LP:62:ARG:NH1	2.53	0.41
1:C1:705:C:OP1	1:C1:733:A:O2'	2.38	0.41
1:C1:2219:A:N6	1:C1:2221:U:OP1	2.53	0.41
1:C1:2642:U:H2'	1:C1:2643:C:C6	2.55	0.41
1:C1:2683:OMU:H1'	1:C1:2683:OMU:HM23	1.62	0.41
1:C1:2852:C:P	29:LH:207:ARG:HH22	2.43	0.41
2:C2:154:C:H5'	28:LG:184:LYS:HD3	2.01	0.41
6:CF:43:PHE:HB3	6:CF:223:LEU:HD23	2.02	0.41
9:CJ:371:THR:HB	9:CJ:415:ILE:HA	2.01	0.41
11:CL:53:PRO:HB2	39:LS:89:ASN:ND2	2.36	0.41
23:LA:83:TYR:HB3	57:Lp:64:MET:HG3	2.01	0.41
23:LA:177:LYS:HB2	57:Lp:29:GLN:HG2	2.03	0.41
24:LB:133:TYR:O	24:LB:136:LYS:HG2	2.20	0.41
55:Lk:63:PRO:HA	55:Lk:64:PRO:HD3	1.91	0.41
1:C1:1264:U:H2'	1:C1:1265:G:C8	2.50	0.41
1:C1:1595:C:H2'	1:C1:1596:U:C6	2.55	0.41
1:C1:2182:A:H2'	1:C1:2183:A:C8	2.56	0.41
7:CH:455:ASP:OD1	7:CH:456:ALA:N	2.53	0.41
12:LF:242:ASN:O	12:LF:246:ARG:HG2	2.21	0.41
1:C1:224:U:H2'	1:C1:225:A:C8	2.55	0.41
2:C2:26:U:H2'	2:C2:27:U:C6	2.55	0.41
7:CH:288:LYS:HG2	59:CH:701:GTP:C6	2.56	0.41
19:Cf:112:ASP:HB3	19:Cf:263:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LD:189:GLU:HG3	26:LD:190:THR:HG23	2.02	0.41
12:LF:102:PRO:HB2	12:LF:105:PRO:HD2	2.01	0.41
37:LQ:126:MET:O	37:LQ:146:GLY:HA3	2.20	0.41
1:C1:1211:A:H5'	6:CF:203:SER:HB3	2.02	0.41
22:Cz:96:TYR:HD2	22:Cz:99:LEU:HD12	1.85	0.41
22:Cz:108:LEU:HD12	22:Cz:108:LEU:HA	1.88	0.41
1:C1:1697:C:H2'	1:C1:1698:A:C8	2.56	0.41
1:C1:1799:U:O4	9:CJ:50:ARG:NH1	2.50	0.41
1:C1:2692:A:H2'	1:C1:2693:A:C8	2.56	0.41
1:C1:2984:G:H4'	10:CK:2:PRO:HD3	2.02	0.41
1:C1:3118:C:O2'	1:C1:3119:A:H8	2.04	0.41
3:C3:10:C:H2'	3:C3:11:A:H8	1.85	0.41
9:CJ:266:ALA:HB3	9:CJ:270:ALA:HB2	2.02	0.41
19:Cf:87:MET:HB2	19:Cf:103:VAL:HB	2.03	0.41
27:LE:30:ALA:HA	58:Lq:113:ALA:HB1	2.02	0.41
52:Lh:46:LEU:HA	52:Lh:49:ILE:HG12	2.02	0.41
1:C1:203:A:H4'	1:C1:205:A:N7	2.36	0.41
1:C1:813:G:O2'	1:C1:1844:A:N3	2.42	0.41
1:C1:1100:G:H2'	1:C1:1101:C:H6	1.86	0.41
1:C1:1159:C:OP2	1:C1:1160:G:O2'	2.35	0.41
1:C1:1361:U:H2'	1:C1:1362:G:H8	1.86	0.41
1:C1:1783:C:H2'	1:C1:1784:G:H8	1.85	0.41
1:C1:2320:A:H2'	1:C1:2321:A:C8	2.56	0.41
1:C1:2723:C:H2'	1:C1:2724:C:C6	2.56	0.41
1:C1:2771:C:H2'	1:C1:2772:A:H8	1.86	0.41
2:C2:83:C:N3	44:LY:50:ARG:NH2	2.60	0.41
6:CF:168:LEU:HD21	6:CF:207:ARG:HD3	2.02	0.41
7:CH:89:HIS:CE1	17:Cd:139:GLU:HG3	2.55	0.41
7:CH:360:ARG:HE	13:CN:246:TYR:C	2.29	0.41
12:CM:154:ILE:HD12	12:CM:191:ILE:HG12	2.02	0.41
19:Cf:23:ILE:HD13	20:Cg:97:PRO:HD2	2.02	0.41
25:LC:127:LEU:HD11	25:LC:240:LEU:HD13	2.02	0.41
12:LF:155:TYR:OH	12:LF:188:GLU:OE2	2.39	0.41
41:LU:56:LEU:HD22	41:LU:60:ILE:HB	2.02	0.41
45:LZ:14:ARG:HD2	45:LZ:78:HIS:CD2	2.56	0.41
1:C1:282:U:H2'	1:C1:283:G:C8	2.54	0.41
1:C1:596:A:OP1	25:LC:317:LYS:NZ	2.42	0.41
1:C1:651:C:H2'	1:C1:652:A:C8	2.56	0.41
1:C1:1866:A:O2'	24:LB:227:PHE:O	2.33	0.41
1:C1:2576:U:H1'	1:C1:2577:G:H5'	2.02	0.41
1:C1:2577:G:H21	1:C1:2578:OMG:HM23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2751:A:H2'	1:C1:2752:G:C8	2.55	0.41
1:C1:3245:C:O3'	24:LB:335:ARG:NH2	2.54	0.41
4:C4:17:A:OP1	30:LJ:154:ARG:NH2	2.54	0.41
8:CI:325:TYR:CE1	8:CI:327:PHE:HB2	2.55	0.41
19:Cf:232:ILE:HG23	19:Cf:244:VAL:HG13	2.02	0.41
20:Cg:79:VAL:HG23	26:LD:143:ARG:HH22	1.86	0.41
1:C1:2392:G:H2'	1:C1:2393:A:C8	2.57	0.40
6:CF:100:VAL:HG12	6:CF:243:ARG:HH12	1.85	0.40
12:CM:99:ASN:OD1	12:CM:100:LYS:N	2.54	0.40
30:LJ:132:MET:HE3	30:LJ:132:MET:HB3	1.80	0.40
35:LO:11:ASP:OD2	35:LO:38:ARG:HD3	2.22	0.40
1:C1:777:C:H2'	1:C1:778:OMC:H6	1.86	0.40
1:C1:804:G:H2'	1:C1:805:C:H6	1.86	0.40
1:C1:1316:C:OP1	37:LQ:31:GLY:N	2.54	0.40
1:C1:2101:A:C4	54:Lj:3:LYS:HB3	2.56	0.40
1:C1:2633:A:H5''	30:LJ:106:GLY:HA3	2.03	0.40
4:C4:108:G:OP1	26:LD:284:ARG:NH2	2.53	0.40
10:CK:174:PRO:HG2	10:CK:177:LEU:HD12	2.03	0.40
11:CL:56:PRO:HG3	39:LS:89:ASN:HB3	2.04	0.40
17:Cd:429:LEU:HD11	17:Cd:441:MET:HB3	2.03	0.40
24:LB:295:ALA:HB3	24:LB:304:LYS:HG3	2.04	0.40
25:LC:114:ILE:HB	25:LC:119:LYS:HE3	2.02	0.40
12:LF:11:ASP:HB3	58:Lq:92:LYS:HG3	2.03	0.40
33:LM:35:ASP:OD2	33:LM:38:ARG:N	2.48	0.40
42:LV:19:LEU:HD13	42:LV:25:MET:HE2	2.04	0.40
1:C1:1373:A:N6	1:C1:1401:A:O2'	2.54	0.40
5:CB:21:ASP:OD1	5:CB:22:GLN:N	2.54	0.40
9:CJ:453:ARG:HD2	9:CJ:455:TYR:CZ	2.57	0.40
20:Cg:152:ILE:HD13	40:LT:57:TYR:HB2	2.03	0.40
24:LB:89:LEU:HB2	24:LB:200:PHE:HZ	1.86	0.40
44:LY:127:GLN:HE21	44:LY:127:GLN:HB2	1.74	0.40
1:C1:1584:U:H2'	1:C1:1585:A:O4'	2.21	0.40
6:CF:175:ILE:HG22	6:CF:176:LYS:HE2	2.04	0.40
13:CN:100:ARG:HA	13:CN:100:ARG:HD3	1.88	0.40
15:CQ:4:GLU:HB2	15:CQ:13:ALA:HB3	2.03	0.40
21:Ch:107:LEU:HD22	21:Ch:112:VAL:HG21	2.04	0.40
21:Ch:362:GLU:O	21:Ch:366:LYS:HG3	2.20	0.40
1:C1:650:U:H2'	1:C1:651:C:C6	2.56	0.40
1:C1:651:C:H2'	1:C1:652:A:H8	1.85	0.40
1:C1:1158:C:H1'	35:LO:89:MET:HE3	2.02	0.40
1:C1:1159:C:H4'	35:LO:91:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2209:G:H2'	1:C1:2210:G:C8	2.57	0.40
1:C1:2307:U:H2'	1:C1:2308:A:C8	2.57	0.40
1:C1:2889:A:H2'	1:C1:2890:C:C6	2.56	0.40
2:C2:94:C:H5''	54:Lj:76:ASN:HD21	1.87	0.40
7:CH:584:LYS:HE3	7:CH:584:LYS:HB2	1.91	0.40
9:CJ:380:ARG:HD2	9:CJ:401:LEU:HB3	2.03	0.40
9:CJ:398:ASP:OD1	9:CJ:399:ALA:N	2.54	0.40
34:LN:28:TRP:O	34:LN:32:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CB	259/391 (66%)	254 (98%)	5 (2%)	0	100	100
6	CF	160/270 (59%)	157 (98%)	3 (2%)	0	100	100
7	CH	40/661 (6%)	39 (98%)	1 (2%)	0	100	100
8	CI	150/414 (36%)	149 (99%)	1 (1%)	0	100	100
9	CJ	376/679 (55%)	371 (99%)	5 (1%)	0	100	100
10	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
11	CL	77/558 (14%)	77 (100%)	0	0	100	100
12	CM	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
12	LF	246/249 (99%)	239 (97%)	7 (3%)	0	100	100
13	CN	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
14	CO	56/120 (47%)	56 (100%)	0	0	100	100
15	CQ	181/225 (80%)	180 (99%)	1 (1%)	0	100	100
16	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Cd	428/627 (68%)	422 (99%)	6 (1%)	0	100	100
19	Cf	4/350 (1%)	4 (100%)	0	0	100	100
21	Ch	242/517 (47%)	234 (97%)	8 (3%)	0	100	100
22	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
23	LA	189/254 (74%)	185 (98%)	4 (2%)	0	100	100
24	LB	387/392 (99%)	379 (98%)	7 (2%)	1 (0%)	36	44
25	LC	361/365 (99%)	354 (98%)	7 (2%)	0	100	100
26	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
27	LE	187/200 (94%)	184 (98%)	3 (2%)	0	100	100
28	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
29	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
30	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
31	LK	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
32	LL	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
33	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
34	LN	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
35	LO	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
36	LP	167/187 (89%)	165 (99%)	2 (1%)	0	100	100
37	LQ	148/213 (70%)	146 (99%)	2 (1%)	0	100	100
38	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
39	LS	172/174 (99%)	170 (99%)	2 (1%)	0	100	100
40	LT	127/160 (79%)	123 (97%)	4 (3%)	0	100	100
41	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
42	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
43	LX	143/156 (92%)	142 (99%)	1 (1%)	0	100	100
44	LY	131/138 (95%)	127 (97%)	4 (3%)	0	100	100
45	LZ	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
46	La	104/149 (70%)	103 (99%)	1 (1%)	0	100	100
47	Lc	93/108 (86%)	93 (100%)	0	0	100	100
48	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
49	Le	124/131 (95%)	124 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Lf	106/109 (97%)	105 (99%)	1 (1%)	0	100	100
51	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
52	Lh	120/935 (13%)	118 (98%)	2 (2%)	0	100	100
53	Li	99/110 (90%)	99 (100%)	0	0	100	100
54	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
55	Lk	74/94 (79%)	74 (100%)	0	0	100	100
56	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
57	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
58	Lq	137/147 (93%)	132 (96%)	5 (4%)	0	100	100
All	All	8708/15750 (55%)	8565 (98%)	142 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	LB	254	GLY

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	
5	CB	227/329 (69%)	227 (100%)	0	100	100
6	CF	212/236 (90%)	212 (100%)	0	100	100
7	CH	549/575 (96%)	549 (100%)	0	100	100
8	CI	124/336 (37%)	124 (100%)	0	100	100
9	CJ	331/579 (57%)	331 (100%)	0	100	100
10	CK	206/225 (92%)	206 (100%)	0	100	100
11	CL	61/458 (13%)	61 (100%)	0	100	100
12	CM	185/215 (86%)	185 (100%)	0	100	100
12	LF	213/215 (99%)	213 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	CN	205/206 (100%)	205 (100%)	0	100	100
14	CO	48/99 (48%)	48 (100%)	0	100	100
15	CQ	144/192 (75%)	144 (100%)	0	100	100
16	Cb	85/101 (84%)	85 (100%)	0	100	100
17	Cd	403/541 (74%)	403 (100%)	0	100	100
18	Ce	223/383 (58%)	223 (100%)	0	100	100
19	Cf	250/310 (81%)	250 (100%)	0	100	100
20	Cg	158/176 (90%)	158 (100%)	0	100	100
21	Ch	408/436 (94%)	408 (100%)	0	100	100
22	Cz	89/107 (83%)	89 (100%)	0	100	100
23	LA	150/198 (76%)	150 (100%)	0	100	100
24	LB	329/331 (99%)	329 (100%)	0	100	100
25	LC	282/285 (99%)	282 (100%)	0	100	100
26	LD	221/253 (87%)	221 (100%)	0	100	100
27	LE	157/166 (95%)	157 (100%)	0	100	100
28	LG	200/222 (90%)	200 (100%)	0	100	100
29	LH	167/200 (84%)	167 (100%)	0	100	100
30	LJ	140/150 (93%)	140 (100%)	0	100	100
31	LK	127/136 (93%)	127 (100%)	0	100	100
32	LL	158/176 (90%)	158 (100%)	0	100	100
33	LM	116/117 (99%)	116 (100%)	0	100	100
34	LN	179/180 (99%)	179 (100%)	0	100	100
35	LO	162/163 (99%)	162 (100%)	0	100	100
36	LP	133/152 (88%)	133 (100%)	0	100	100
37	LQ	128/178 (72%)	128 (100%)	0	100	100
38	LR	125/2396 (5%)	125 (100%)	0	100	100
39	LS	152/154 (99%)	152 (100%)	0	100	100
40	LT	110/135 (82%)	110 (100%)	0	100	100
41	LU	92/108 (85%)	92 (100%)	0	100	100
42	LV	98/102 (96%)	98 (100%)	0	100	100
43	LX	122/129 (95%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	LY	116/119 (98%)	115 (99%)	1 (1%)	70	80
45	LZ	121/121 (100%)	121 (100%)	0	100	100
46	La	93/122 (76%)	93 (100%)	0	100	100
47	Lc	76/88 (86%)	76 (100%)	0	100	100
48	Ld	90/105 (86%)	90 (100%)	0	100	100
49	Le	109/114 (96%)	109 (100%)	0	100	100
50	Lf	89/90 (99%)	89 (100%)	0	100	100
51	Lg	95/102 (93%)	95 (100%)	0	100	100
52	Lh	109/781 (14%)	109 (100%)	0	100	100
53	Li	85/93 (91%)	85 (100%)	0	100	100
54	Lj	72/78 (92%)	72 (100%)	0	100	100
55	Lk	73/88 (83%)	73 (100%)	0	100	100
56	Ll	45/46 (98%)	45 (100%)	0	100	100
57	Lp	73/74 (99%)	73 (100%)	0	100	100
58	Lq	109/112 (97%)	109 (100%)	0	100	100
All	All	8824/13783 (64%)	8823 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
44	LY	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
5	CB	90	ASN
5	CB	150	HIS
7	CH	77	HIS
7	CH	82	ASN
7	CH	244	HIS
7	CH	306	ASN
7	CH	499	HIS
7	CH	641	HIS
8	CI	286	ASN
9	CJ	176	GLN
9	CJ	200	ASN

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Mol	Chain	Res	Type
10	CK	41	ASN
10	CK	60	GLN
10	CK	95	ASN
10	CK	143	HIS
10	CK	190	ASN
12	CM	116	GLN
12	CM	119	ASN
12	CM	172	ASN
15	CQ	5	ASN
16	Cb	68	HIS
17	Cd	89	GLN
18	Ce	329	GLN
20	Cg	98	GLN
21	Ch	64	ASN
21	Ch	274	HIS
21	Ch	411	GLN
21	Ch	426	ASN
23	LA	205	ASN
24	LB	262	GLN
24	LB	389	GLN
25	LC	111	HIS
25	LC	330	ASN
26	LD	89	ASN
26	LD	247	HIS
27	LE	196	HIS
12	LF	9	GLN
12	LF	119	ASN
12	LF	200	ASN
28	LG	106	GLN
28	LG	194	HIS
29	LH	5	HIS
29	LH	133	HIS
29	LH	202	GLN
31	LK	14	HIS
33	LM	24	ASN
34	LN	32	GLN
36	LP	34	GLN
36	LP	75	GLN
37	LQ	86	ASN
38	LR	143	HIS
43	LX	92	GLN
43	LX	107	GLN

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Mol	Chain	Res	Type
45	LZ	77	ASN
46	La	62	HIS
46	La	94	GLN
50	Lf	7	HIS
52	Lh	64	ASN
53	Li	42	GLN
53	Li	100	GLN
54	Lj	13	ASN
58	Lq	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3069/3342 (91%)	556 (18%)	23 (0%)
2	C2	155/156 (99%)	21 (13%)	0
3	C3	80/162 (49%)	20 (25%)	0
4	C4	118/119 (99%)	22 (18%)	0
All	All	3422/3779 (90%)	619 (18%)	23 (0%)

All (619) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	4	U
1	C1	6	G
1	C1	27	A
1	C1	44	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	72	A
1	C1	95	G
1	C1	96	A
1	C1	110	A
1	C1	111	G
1	C1	112	C
1	C1	116	A
1	C1	117	A
1	C1	123	A
1	C1	132	U

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Mol	Chain	Res	Type
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	144	G
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	178	U
1	C1	181	G
1	C1	184	U
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	226	G
1	C1	241	U
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	262	G
1	C1	276	G
1	C1	277	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	331	A
1	C1	332	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	389	A2M
1	C1	391	U
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	434	U
1	C1	435	G

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Mol	Chain	Res	Type
1	C1	443	C
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	535	U
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	549	A
1	C1	570	G
1	C1	583	A
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	632	G
1	C1	634	A
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G

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Mol	Chain	Res	Type
1	C1	703	A
1	C1	704	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	743	A
1	C1	747	A
1	C1	748	U
1	C1	756	G
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	766	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	830	A
1	C1	839	G
1	C1	843	C
1	C1	857	G
1	C1	877	A
1	C1	878	A
1	C1	879	U
1	C1	889	G
1	C1	890	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	905	C
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C

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Mol	Chain	Res	Type
1	C1	941	C
1	C1	943	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	976	G
1	C1	977	U
1	C1	983	G
1	C1	984	A
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1051	C
1	C1	1055	G
1	C1	1058	A
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1075	C
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1098	G
1	C1	1099	G
1	C1	1109	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G

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Mol	Chain	Res	Type
1	C1	1136	A
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1182	C
1	C1	1185	A
1	C1	1188	A
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1229	G
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G
1	C1	1270	A
1	C1	1278	G
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1369	A
1	C1	1370	G
1	C1	1375	G
1	C1	1382	A
1	C1	1383	G

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Mol	Chain	Res	Type
1	C1	1401	A
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1451	A
1	C1	1458	G
1	C1	1464	A
1	C1	1466	G
1	C1	1477	U
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	U
1	C1	1506	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1560	U
1	C1	1561	G
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	A
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1623	A
1	C1	1624	C
1	C1	1637	C
1	C1	1683	U
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U

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Mol	Chain	Res	Type
1	C1	1721	A
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G
1	C1	1751	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1828	G
1	C1	1829	C
1	C1	1830	A
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1873	A
1	C1	1886	G
1	C1	1887	C
1	C1	1917	OMU
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2048	U
1	C1	2050	C
1	C1	2052	G
1	C1	2056	A
1	C1	2076	A
1	C1	2084	G

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Mol	Chain	Res	Type
1	C1	2085	G
1	C1	2094	A
1	C1	2103	U
1	C1	2121	A
1	C1	2126	C
1	C1	2132	G
1	C1	2151	A
1	C1	2156	U
1	C1	2157	G
1	C1	2158	C
1	C1	2161	A
1	C1	2167	C
1	C1	2168	U
1	C1	2169	G
1	C1	2171	A
1	C1	2172	U
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2203	G
1	C1	2205	A
1	C1	2206	A
1	C1	2212	G
1	C1	2216	G
1	C1	2217	U
1	C1	2218	A
1	C1	2219	A
1	C1	2220	C
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2225	A
1	C1	2226	C
1	C1	2229	U
1	C1	2230	C
1	C1	2231	U
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2284	A

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Mol	Chain	Res	Type
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2326	A
1	C1	2340	G
1	C1	2348	A
1	C1	2351	U
1	C1	2355	C
1	C1	2356	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2403	A
1	C1	2405	G
1	C1	2472	U
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2489	C
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2515	G
1	C1	2516	G
1	C1	2521	A
1	C1	2527	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C

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Mol	Chain	Res	Type
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2582	G
1	C1	2584	C
1	C1	2585	A
1	C1	2592	U
1	C1	2613	C
1	C1	2615	A
1	C1	2631	G
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2647	U
1	C1	2651	A
1	C1	2656	A
1	C1	2657	G
1	C1	2663	A
1	C1	2664	A
1	C1	2667	C
1	C1	2671	U
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2689	G
1	C1	2690	OMU
1	C1	2691	G
1	C1	2713	G
1	C1	2717	A
1	C1	2731	C
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2754	U
1	C1	2755	G
1	C1	2756	C
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A

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Mol	Chain	Res	Type
1	C1	2763	A
1	C1	2769	C
1	C1	2773	G
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2804	A
1	C1	2805	U
1	C1	2806	A
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2834	U
1	C1	2836	G
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2894	U
1	C1	2895	A
1	C1	2900	A
1	C1	2903	U
1	C1	2905	A
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2949	G
1	C1	2951	U
1	C1	2953	A
1	C1	2955	C
1	C1	2956	U

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Mol	Chain	Res	Type
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3032	G
1	C1	3036	G
1	C1	3044	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3118	C
1	C1	3119	A
1	C1	3125	U
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3168	A
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U

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Mol	Chain	Res	Type
1	C1	3214	A
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G
1	C1	3231	G
1	C1	3244	G
1	C1	3245	C
1	C1	3248	A
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3276	A
1	C1	3282	U
1	C1	3292	U
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3316	A
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3328	G
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C

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Mol	Chain	Res	Type
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	104	A
2	C2	106	C
2	C2	113	U
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
2	C2	154	C
3	C3	2	U
3	C3	4	A
3	C3	10	C
3	C3	19	G
3	C3	20	G
3	C3	25	U
3	C3	33	A
3	C3	36	C
3	C3	40	G
3	C3	50	G
3	C3	57	A
3	C3	58	A
3	C3	59	A
3	C3	63	A
3	C3	68	C
3	C3	69	G
3	C3	135	G
3	C3	136	C
3	C3	138	A
3	C3	139	G
4	C4	6	C
4	C4	7	G
4	C4	22	A
4	C4	29	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	66	G
4	C4	75	A
4	C4	76	G

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Mol	Chain	Res	Type
4	C4	77	U
4	C4	82	G
4	C4	83	G
4	C4	84	G
4	C4	85	U
4	C4	86	C
4	C4	89	U
4	C4	91	A
4	C4	97	A
4	C4	100	G
4	C4	101	A
4	C4	111	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	898	G
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U
1	C1	1267	C
1	C1	1537	U
1	C1	2157	G
1	C1	2160	C
1	C1	2225	A
1	C1	2280	A
1	C1	2575	C
1	C1	2883	U
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	C

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

34 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	OMU	C1	2277	1	19,22,23	3.11	6 (31%)	25,31,34	1.77	5 (20%)
1	OMG	C1	646	1	23,26,27	0.48	0	32,38,41	0.53	0
1	OMG	C1	2774	1	23,26,27	0.49	0	32,38,41	0.50	0
1	OMG	C1	2876	1	23,26,27	0.47	0	32,38,41	0.47	0
1	OMU	C1	2683	1	19,22,23	3.08	6 (31%)	25,31,34	1.74	5 (20%)
1	OMU	C1	2688	1	19,22,23	3.10	6 (31%)	25,31,34	1.78	5 (20%)
1	OMG	C1	2881	1	23,26,27	0.46	0	32,38,41	0.47	0
1	A2M	C1	1432	1	22,25,26	3.97	11 (50%)	30,36,39	3.38	13 (43%)
1	A2M	C1	389	1	22,25,26	3.98	11 (50%)	30,36,39	3.38	13 (43%)
1	OMU	C1	1868	1	19,22,23	3.12	6 (31%)	25,31,34	1.83	4 (16%)
1	OMC	C1	1491	1	19,22,23	0.52	0	25,31,34	0.70	0
1	OMG	C1	385	1	23,26,27	0.50	0	32,38,41	0.52	0
1	OMG	C1	2578	1	23,26,27	0.47	0	32,38,41	0.59	0
1	OMC	C1	778	1	19,22,23	0.56	0	25,31,34	0.94	1 (4%)
1	OMG	C1	1433	1	23,26,27	0.50	0	32,38,41	0.51	0
1	OMC	C1	1836	1	19,22,23	0.56	0	25,31,34	0.85	1 (4%)
1	OMC	C1	2838	1	19,22,23	0.69	0	25,31,34	1.60	4 (16%)
1	OMU	C1	2384	1	19,22,23	3.13	6 (31%)	25,31,34	1.75	5 (20%)
1	OMC	C1	1812	1	19,22,23	0.58	0	25,31,34	1.27	2 (8%)
1	A2M	C1	637	1	22,25,26	3.98	11 (50%)	30,36,39	3.37	13 (43%)
1	OMG	C1	2358	1	23,26,27	0.50	0	32,38,41	0.53	0
1	A2M	C1	1223	1	22,25,26	3.98	12 (54%)	30,36,39	3.33	13 (43%)
1	OMC	C1	2300	1	19,22,23	0.53	0	25,31,34	0.71	0
1	A2M	C1	858	1	22,25,26	4.01	12 (54%)	30,36,39	3.37	12 (40%)
1	OMU	C1	2380	1	19,22,23	3.06	6 (31%)	25,31,34	1.75	5 (20%)
1	A2M	C1	1847	1	22,25,26	4.00	12 (54%)	30,36,39	3.43	14 (46%)
1	OMU	C1	1917	1	19,22,23	3.15	6 (31%)	25,31,34	1.88	5 (20%)
1	OMU	C1	2690	1	19,22,23	3.11	6 (31%)	25,31,34	1.79	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	C1	627	1	23,26,27	0.48	0	32,38,41	0.54	0
1	A2M	C1	848	1	22,25,26	3.97	12 (54%)	30,36,39	3.42	14 (46%)
1	A2M	C1	2289	1	22,25,26	3.98	10 (45%)	30,36,39	3.33	13 (43%)
1	OMG	C1	787	1	23,26,27	0.49	0	32,38,41	0.59	0
1	OMC	C1	1420	1	19,22,23	0.64	0	25,31,34	1.39	4 (16%)
1	OMC	C1	2918	1	19,22,23	0.58	0	25,31,34	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	2277	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2876	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2881	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	389	1	-	3/9/27/28	0/3/3/3
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1491	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	2/9/27/28	0/3/3/3
1	OMG	C1	2578	1	-	3/9/27/28	0/3/3/3
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	1433	1	-	3/9/27/28	0/3/3/3
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	637	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1223	1	-	1/9/27/28	0/3/3/3
1	OMC	C1	2300	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	1/9/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMU	C1	1917	1	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	627	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	1420	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	858	A2M	C3'-C2'	-13.04	1.24	1.53
1	C1	637	A2M	C3'-C2'	-13.01	1.24	1.53
1	C1	2289	A2M	C3'-C2'	-13.00	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-12.97	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.94	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.93	1.24	1.53
1	C1	848	A2M	C3'-C2'	-12.91	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.83	1.24	1.53
1	C1	1917	OMU	C2-N1	7.85	1.50	1.38
1	C1	1868	OMU	C2-N1	7.62	1.50	1.38
1	C1	2384	OMU	C2-N1	7.56	1.50	1.38
1	C1	2690	OMU	C2-N1	7.51	1.50	1.38
1	C1	2277	OMU	C2-N1	7.41	1.50	1.38
1	C1	2683	OMU	C2-N1	7.38	1.50	1.38
1	C1	2688	OMU	C2-N1	7.36	1.50	1.38
1	C1	2384	OMU	C2-N3	7.32	1.50	1.38
1	C1	2688	OMU	C2-N3	7.29	1.50	1.38
1	C1	2277	OMU	C2-N3	7.28	1.50	1.38
1	C1	2683	OMU	C2-N3	7.26	1.50	1.38
1	C1	1868	OMU	C2-N3	7.26	1.50	1.38
1	C1	2690	OMU	C2-N3	7.24	1.50	1.38
1	C1	2380	OMU	C2-N1	7.24	1.49	1.38
1	C1	1917	OMU	C2-N3	7.21	1.50	1.38
1	C1	2380	OMU	C2-N3	7.19	1.50	1.38
1	C1	1847	A2M	O4'-C4'	-6.63	1.30	1.45
1	C1	389	A2M	O4'-C4'	-6.60	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.58	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.54	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.46	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.36	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O4'-C4'	-6.29	1.31	1.45
1	C1	2277	OMU	C6-C5	6.21	1.49	1.35
1	C1	1917	OMU	C6-C5	6.20	1.49	1.35
1	C1	2688	OMU	C6-C5	6.17	1.49	1.35
1	C1	2683	OMU	C6-C5	6.15	1.49	1.35
1	C1	2690	OMU	C6-C5	6.14	1.49	1.35
1	C1	2384	OMU	C6-C5	6.13	1.49	1.35
1	C1	2380	OMU	C6-C5	6.12	1.49	1.35
1	C1	1868	OMU	C6-C5	6.12	1.49	1.35
1	C1	858	A2M	C3'-C4'	5.38	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.37	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.36	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.30	1.66	1.53
1	C1	1847	A2M	C3'-C4'	5.23	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.22	1.66	1.53
1	C1	389	A2M	C3'-C4'	5.14	1.66	1.53
1	C1	637	A2M	C3'-C4'	5.07	1.65	1.53
1	C1	2289	A2M	O4'-C1'	4.54	1.52	1.42
1	C1	848	A2M	O4'-C1'	4.49	1.52	1.42
1	C1	1847	A2M	C1'-N9	-4.48	1.33	1.46
1	C1	858	A2M	O4'-C1'	4.48	1.52	1.42
1	C1	1847	A2M	O4'-C1'	4.47	1.52	1.42
1	C1	1432	A2M	O4'-C1'	4.41	1.52	1.42
1	C1	2384	OMU	C4-N3	4.40	1.46	1.38
1	C1	637	A2M	C6-N6	4.40	1.45	1.34
1	C1	1223	A2M	C6-N6	4.40	1.45	1.34
1	C1	858	A2M	C1'-N9	-4.38	1.34	1.46
1	C1	2289	A2M	C6-N6	4.38	1.45	1.34
1	C1	2277	OMU	C4-N3	4.38	1.46	1.38
1	C1	1432	A2M	C6-N6	4.38	1.45	1.34
1	C1	848	A2M	C6-N6	4.37	1.45	1.34
1	C1	2688	OMU	C4-N3	4.36	1.46	1.38
1	C1	389	A2M	O4'-C1'	4.35	1.52	1.42
1	C1	858	A2M	C6-N6	4.35	1.45	1.34
1	C1	1223	A2M	C1'-N9	-4.33	1.34	1.46
1	C1	389	A2M	C1'-N9	-4.32	1.34	1.46
1	C1	637	A2M	O4'-C1'	4.31	1.52	1.42
1	C1	848	A2M	C1'-N9	-4.31	1.34	1.46
1	C1	2690	OMU	C4-N3	4.30	1.46	1.38
1	C1	389	A2M	C6-N6	4.29	1.45	1.34
1	C1	637	A2M	C1'-N9	-4.29	1.34	1.46
1	C1	1847	A2M	C6-N6	4.29	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2683	OMU	C4-N3	4.28	1.45	1.38
1	C1	1223	A2M	O4'-C1'	4.25	1.51	1.42
1	C1	1868	OMU	C4-N3	4.22	1.45	1.38
1	C1	2289	A2M	C1'-N9	-4.22	1.34	1.46
1	C1	1917	OMU	C4-N3	4.22	1.45	1.38
1	C1	2380	OMU	C4-N3	4.18	1.45	1.38
1	C1	1432	A2M	C1'-N9	-4.14	1.34	1.46
1	C1	389	A2M	O2'-C2'	3.83	1.52	1.42
1	C1	858	A2M	O2'-C2'	3.62	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.58	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.57	1.51	1.42
1	C1	637	A2M	O2'-C2'	3.57	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.55	1.51	1.42
1	C1	389	A2M	C2'-C1'	3.29	1.61	1.53
1	C1	848	A2M	C2'-C1'	3.08	1.60	1.53
1	C1	1847	A2M	C2'-C1'	3.05	1.60	1.53
1	C1	389	A2M	C5-C4	-3.05	1.33	1.39
1	C1	858	A2M	C5-C4	-3.03	1.33	1.39
1	C1	1847	A2M	C5-C4	-3.01	1.33	1.39
1	C1	637	A2M	C5-C4	-2.98	1.33	1.39
1	C1	848	A2M	C5-C4	-2.97	1.33	1.39
1	C1	1223	A2M	C5-C4	-2.97	1.33	1.39
1	C1	2289	A2M	C5-C4	-2.96	1.33	1.39
1	C1	1223	A2M	C2'-C1'	2.96	1.60	1.53
1	C1	1432	A2M	C2'-C1'	2.95	1.60	1.53
1	C1	1432	A2M	C5-C4	-2.94	1.33	1.39
1	C1	2289	A2M	C2'-C1'	2.94	1.60	1.53
1	C1	637	A2M	C2'-C1'	2.91	1.60	1.53
1	C1	858	A2M	C2'-C1'	2.75	1.59	1.53
1	C1	1432	A2M	C5-N7	-2.75	1.34	1.39
1	C1	1868	OMU	C6-N1	2.71	1.44	1.38
1	C1	2277	OMU	C6-N1	2.71	1.44	1.38
1	C1	858	A2M	C5-N7	-2.70	1.34	1.39
1	C1	2688	OMU	C6-N1	2.70	1.44	1.38
1	C1	1917	OMU	C6-N1	2.69	1.44	1.38
1	C1	389	A2M	C5-N7	-2.69	1.34	1.39
1	C1	2384	OMU	C6-N1	2.68	1.44	1.38
1	C1	2690	OMU	C6-N1	2.67	1.44	1.38
1	C1	1223	A2M	C5-N7	-2.67	1.34	1.39
1	C1	2380	OMU	C6-N1	2.67	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C5-N7	-2.63	1.34	1.39
1	C1	2683	OMU	C6-N1	2.61	1.44	1.38
1	C1	637	A2M	C5-N7	-2.60	1.34	1.39
1	C1	848	A2M	C5-N7	-2.56	1.34	1.39
1	C1	1847	A2M	C5-N7	-2.51	1.34	1.39
1	C1	2688	OMU	C5-C4	2.29	1.48	1.43
1	C1	2277	OMU	C5-C4	2.26	1.48	1.43
1	C1	2380	OMU	C5-C4	2.23	1.48	1.43
1	C1	1868	OMU	C5-C4	2.22	1.48	1.43
1	C1	1917	OMU	C5-C4	2.21	1.48	1.43
1	C1	2690	OMU	C5-C4	2.20	1.48	1.43
1	C1	1847	A2M	C8-N9	-2.17	1.33	1.37
1	C1	2683	OMU	C5-C4	2.15	1.48	1.43
1	C1	2384	OMU	C5-C4	2.14	1.48	1.43
1	C1	389	A2M	C8-N9	-2.11	1.34	1.37
1	C1	1847	A2M	O3'-C3'	2.10	1.48	1.43
1	C1	1223	A2M	C8-N9	-2.10	1.34	1.37
1	C1	858	A2M	C8-N9	-2.09	1.34	1.37
1	C1	637	A2M	C8-N9	-2.08	1.34	1.37
1	C1	1432	A2M	C8-N9	-2.07	1.34	1.37
1	C1	848	A2M	O3'-C3'	2.07	1.48	1.43
1	C1	1223	A2M	O3'-C3'	2.04	1.48	1.43
1	C1	848	A2M	C8-N9	-2.03	1.34	1.37
1	C1	858	A2M	O3'-C3'	2.01	1.47	1.43

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.32	106.41	127.09
1	C1	389	A2M	C1'-N9-C8	-9.25	106.57	127.09
1	C1	1432	A2M	C1'-N9-C8	-9.14	106.81	127.09
1	C1	637	A2M	C1'-N9-C8	-9.10	106.89	127.09
1	C1	858	A2M	C1'-N9-C8	-9.10	106.89	127.09
1	C1	848	A2M	C1'-N9-C8	-9.06	107.00	127.09
1	C1	1223	A2M	C1'-N9-C8	-8.89	107.36	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.78	107.62	127.09
1	C1	1432	A2M	C4-N9-C1'	7.99	145.33	126.63
1	C1	389	A2M	C4-N9-C1'	7.92	145.16	126.63
1	C1	1847	A2M	C4-N9-C1'	7.89	145.08	126.63
1	C1	637	A2M	C4-N9-C1'	7.87	145.04	126.63
1	C1	858	A2M	C4-N9-C1'	7.76	144.79	126.63
1	C1	848	A2M	C4-N9-C1'	7.72	144.69	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1223	A2M	C4-N9-C1'	7.63	144.48	126.63
1	C1	2289	A2M	C4-N9-C1'	7.55	144.29	126.63
1	C1	858	A2M	N3-C2-N1	-5.90	119.66	128.58
1	C1	2289	A2M	N3-C2-N1	-5.80	119.80	128.58
1	C1	1847	A2M	N3-C2-N1	-5.79	119.82	128.58
1	C1	389	A2M	N3-C2-N1	-5.79	119.82	128.58
1	C1	1223	A2M	N3-C2-N1	-5.78	119.83	128.58
1	C1	848	A2M	N3-C2-N1	-5.78	119.83	128.58
1	C1	1432	A2M	N3-C2-N1	-5.76	119.86	128.58
1	C1	637	A2M	N3-C2-N1	-5.75	119.88	128.58
1	C1	1847	A2M	N6-C6-N1	-5.73	105.62	118.38
1	C1	858	A2M	N6-C6-N1	-5.68	105.72	118.38
1	C1	1223	A2M	N6-C6-N1	-5.62	105.86	118.38
1	C1	848	A2M	N6-C6-N1	-5.59	105.92	118.38
1	C1	637	A2M	N6-C6-N1	-5.57	105.97	118.38
1	C1	2688	OMU	C4-N3-C2	-5.54	119.73	126.61
1	C1	1868	OMU	C4-N3-C2	-5.54	119.74	126.61
1	C1	1432	A2M	N6-C6-N1	-5.53	106.07	118.38
1	C1	2690	OMU	C4-N3-C2	-5.49	119.80	126.61
1	C1	1917	OMU	C4-N3-C2	-5.45	119.84	126.61
1	C1	2289	A2M	N6-C6-N1	-5.41	106.32	118.38
1	C1	389	A2M	N6-C6-N1	-5.40	106.36	118.38
1	C1	2380	OMU	C4-N3-C2	-5.40	119.91	126.61
1	C1	2277	OMU	C4-N3-C2	-5.32	120.00	126.61
1	C1	2683	OMU	C4-N3-C2	-5.26	120.08	126.61
1	C1	2384	OMU	C4-N3-C2	-5.15	120.22	126.61
1	C1	1432	A2M	C5-C4-N3	-5.04	119.77	126.72
1	C1	2838	OMC	C1'-N1-C2	4.95	129.37	118.44
1	C1	637	A2M	C5-C4-N3	-4.87	120.01	126.72
1	C1	848	A2M	C5-C4-N3	-4.85	120.04	126.72
1	C1	2289	A2M	C5-C4-N3	-4.79	120.13	126.72
1	C1	389	A2M	C5-C4-N3	-4.78	120.13	126.72
1	C1	1847	A2M	C5-C4-N3	-4.71	120.23	126.72
1	C1	1223	A2M	C5-C4-N3	-4.63	120.34	126.72
1	C1	858	A2M	C5-C4-N3	-4.57	120.43	126.72
1	C1	858	A2M	C5-C6-N6	4.46	134.34	123.29
1	C1	1223	A2M	C5-C6-N6	4.44	134.28	123.29
1	C1	1847	A2M	C5-C6-N6	4.43	134.25	123.29
1	C1	1812	OMC	CM2-O2'-C2'	4.43	125.85	114.47
1	C1	637	A2M	C5-C6-N6	4.41	134.20	123.29
1	C1	1847	A2M	N9-C8-N7	-4.39	107.70	113.94
1	C1	848	A2M	N9-C8-N7	-4.36	107.75	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	858	A2M	N9-C8-N7	-4.33	107.80	113.94
1	C1	848	A2M	C5-C6-N6	4.31	133.96	123.29
1	C1	1432	A2M	C5-C6-N6	4.29	133.90	123.29
1	C1	2289	A2M	O4'-C1'-N9	4.28	116.31	108.09
1	C1	389	A2M	N9-C8-N7	-4.24	107.93	113.94
1	C1	2289	A2M	C5-C6-N6	4.22	133.75	123.29
1	C1	1917	OMU	N3-C2-N1	4.21	120.37	114.89
1	C1	1223	A2M	N9-C8-N7	-4.17	108.02	113.94
1	C1	389	A2M	C5-C6-N6	4.16	133.59	123.29
1	C1	2289	A2M	N9-C8-N7	-4.16	108.03	113.94
1	C1	848	A2M	O4'-C1'-N9	4.15	116.06	108.09
1	C1	637	A2M	N9-C8-N7	-4.14	108.07	113.94
1	C1	1420	OMC	C1'-N1-C2	4.12	127.54	118.44
1	C1	1432	A2M	N9-C8-N7	-4.03	108.22	113.94
1	C1	1223	A2M	O4'-C1'-N9	3.99	115.76	108.09
1	C1	858	A2M	O4'-C1'-N9	3.85	115.48	108.09
1	C1	2384	OMU	N3-C2-N1	3.80	119.83	114.89
1	C1	2277	OMU	N3-C2-N1	3.79	119.82	114.89
1	C1	2690	OMU	N3-C2-N1	3.78	119.82	114.89
1	C1	2688	OMU	N3-C2-N1	3.78	119.81	114.89
1	C1	637	A2M	O4'-C1'-N9	3.77	115.34	108.09
1	C1	1868	OMU	N3-C2-N1	3.73	119.75	114.89
1	C1	389	A2M	O4'-C1'-N9	3.73	115.25	108.09
1	C1	1432	A2M	O4'-C1'-N9	3.72	115.24	108.09
1	C1	2838	OMC	C1'-N1-C6	-3.72	112.83	120.78
1	C1	2380	OMU	C5-C4-N3	3.70	119.98	114.80
1	C1	1868	OMU	C5-C4-N3	3.67	119.95	114.80
1	C1	2380	OMU	N3-C2-N1	3.64	119.64	114.89
1	C1	2688	OMU	C5-C4-N3	3.61	119.86	114.80
1	C1	2683	OMU	N3-C2-N1	3.61	119.59	114.89
1	C1	2683	OMU	C5-C4-N3	3.59	119.83	114.80
1	C1	2690	OMU	C5-C4-N3	3.56	119.78	114.80
1	C1	1432	A2M	C2-N3-C4	3.51	120.40	111.83
1	C1	2277	OMU	C5-C4-N3	3.49	119.68	114.80
1	C1	848	A2M	C2-N3-C4	3.42	120.19	111.83
1	C1	1847	A2M	C2-N3-C4	3.40	120.15	111.83
1	C1	389	A2M	C2-N3-C4	3.38	120.10	111.83
1	C1	1917	OMU	C5-C4-N3	3.38	119.54	114.80
1	C1	2384	OMU	C5-C4-N3	3.38	119.53	114.80
1	C1	637	A2M	C2-N3-C4	3.38	120.08	111.83
1	C1	2289	A2M	C2-N3-C4	3.37	120.07	111.83
1	C1	1847	A2M	O4'-C1'-N9	3.35	114.52	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	858	A2M	C2-N3-C4	3.32	119.94	111.83
1	C1	1223	A2M	C2-N3-C4	3.30	119.89	111.83
1	C1	1432	A2M	N3-C4-N9	3.09	132.41	127.17
1	C1	848	A2M	N3-C4-N9	3.06	132.37	127.17
1	C1	389	A2M	N3-C4-N9	3.05	132.36	127.17
1	C1	848	A2M	C5-N7-C8	3.01	108.18	103.45
1	C1	2289	A2M	N3-C4-N9	2.99	132.25	127.17
1	C1	1868	OMU	O4-C4-C5	-2.96	120.06	125.16
1	C1	2688	OMU	O4-C4-C5	-2.94	120.08	125.16
1	C1	1847	A2M	N3-C4-N9	2.93	132.15	127.17
1	C1	2838	OMC	O2-C2-N3	-2.92	117.73	122.33
1	C1	2683	OMU	O4-C4-C5	-2.92	120.13	125.16
1	C1	637	A2M	N3-C4-N9	2.92	132.13	127.17
1	C1	2380	OMU	O4-C4-C5	-2.92	120.13	125.16
1	C1	1847	A2M	C5-N7-C8	2.91	108.02	103.45
1	C1	2384	OMU	O4-C4-C5	-2.90	120.16	125.16
1	C1	1420	OMC	C1'-N1-C6	-2.88	114.61	120.78
1	C1	2277	OMU	O4-C4-C5	-2.88	120.19	125.16
1	C1	389	A2M	C5-N7-C8	2.87	107.95	103.45
1	C1	2690	OMU	O4-C4-C5	-2.87	120.22	125.16
1	C1	858	A2M	C5-N7-C8	2.83	107.90	103.45
1	C1	1917	OMU	C1'-N1-C2	2.83	122.67	117.59
1	C1	1432	A2M	C5-N7-C8	2.82	107.89	103.45
1	C1	858	A2M	N3-C4-N9	2.81	131.95	127.17
1	C1	1917	OMU	O4-C4-C5	-2.81	120.32	125.16
1	C1	848	A2M	C2'-C1'-N9	-2.80	109.14	113.75
1	C1	1223	A2M	N3-C4-N9	2.80	131.94	127.17
1	C1	2289	A2M	C5-N7-C8	2.80	107.86	103.45
1	C1	1847	A2M	C2'-C1'-N9	-2.80	109.15	113.75
1	C1	637	A2M	C5-N7-C8	2.79	107.83	103.45
1	C1	1223	A2M	C5-N7-C8	2.77	107.81	103.45
1	C1	1847	A2M	C4-N9-C8	2.64	108.51	105.74
1	C1	1812	OMC	C2'-C1'-N1	-2.59	109.33	114.24
1	C1	778	OMC	C1'-N1-C2	2.55	124.08	118.44
1	C1	1836	OMC	C1'-N1-C2	2.46	123.88	118.44
1	C1	858	A2M	C4-N9-C8	2.46	108.32	105.74
1	C1	2838	OMC	O2-C2-N1	2.45	123.70	118.90
1	C1	848	A2M	C4-N9-C8	2.44	108.31	105.74
1	C1	389	A2M	C4-N9-C8	2.41	108.27	105.74
1	C1	1420	OMC	O2-C2-N1	2.36	123.53	118.90
1	C1	1420	OMC	O2-C2-N3	-2.31	118.68	122.33
1	C1	1223	A2M	C4-N9-C8	2.30	108.16	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2289	A2M	C2'-C1'-N9	-2.26	110.03	113.75
1	C1	2289	A2M	C4-N9-C8	2.24	108.09	105.74
1	C1	2380	OMU	O2-C2-N1	-2.22	119.90	122.80
1	C1	637	A2M	C4-N9-C8	2.21	108.06	105.74
1	C1	2384	OMU	C1'-N1-C2	2.17	121.49	117.59
1	C1	2277	OMU	O2-C2-N1	-2.15	119.99	122.80
1	C1	2688	OMU	O2-C2-N1	-2.13	120.02	122.80
1	C1	1847	A2M	C4-C5-N7	-2.12	108.16	110.58
1	C1	848	A2M	C4-C5-N7	-2.10	108.18	110.58
1	C1	389	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
1	C1	637	A2M	C4-C5-N7	-2.09	108.19	110.58
1	C1	1432	A2M	C4-C5-N7	-2.06	108.22	110.58
1	C1	2683	OMU	O2-C2-N1	-2.02	120.17	122.80
1	C1	1432	A2M	C4-N9-C8	2.01	107.85	105.74
1	C1	1223	A2M	C4-C5-N7	-2.01	108.29	110.58

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1433	OMG	C1'-C2'-O2'-CM2
1	C1	1812	OMC	C1'-C2'-O2'-CM2
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1917	OMU	C1'-C2'-O2'-CM2
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2384	OMU	C1'-C2'-O2'-CM2
1	C1	2578	OMG	O4'-C4'-C5'-O5'
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2690	OMU	O4'-C4'-C5'-O5'
1	C1	2838	OMC	O4'-C1'-N1-C2
1	C1	2838	OMC	O4'-C1'-N1-C6
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	2690	OMU	C3'-C4'-C5'-O5'
1	C1	2578	OMG	C3'-C4'-C5'-O5'
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	1917	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	2300	OMC	C1'-C2'-O2'-CM2
1	C1	1420	OMC	C2'-C1'-N1-C6
1	C1	858	A2M	O4'-C4'-C5'-O5'
1	C1	1420	OMC	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	2683	OMU	1	0
1	C1	1432	A2M	1	0
1	C1	389	A2M	2	0
1	C1	2578	OMG	1	0
1	C1	778	OMC	1	0
1	C1	1433	OMG	1	0
1	C1	2838	OMC	1	0
1	C1	2384	OMU	2	0
1	C1	1812	OMC	3	0
1	C1	1917	OMU	1	0
1	C1	1420	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GTP	CH	701	60	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
59	GTP	Cd	1000	60	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)

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
59	GTP	CH	701	60	-	5/22/38/38	0/3/3/3
59	GTP	Cd	1000	60	-	3/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CH	701	GTP	C2-N3	2.13	1.38	1.33
59	Cd	1000	GTP	C2-N3	2.04	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CH	701	GTP	C5-C4-N3	-5.03	120.38	128.39
59	Cd	1000	GTP	C5-C4-N3	-4.94	120.53	128.39
59	CH	701	GTP	C2-N3-C4	4.61	120.25	112.30
59	Cd	1000	GTP	C2-N3-C4	4.58	120.19	112.30
59	CH	701	GTP	N9-C4-N3	3.22	132.40	125.95
59	Cd	1000	GTP	N9-C4-N3	3.07	132.10	125.95
59	Cd	1000	GTP	C2-N1-C6	-2.93	119.81	125.11
59	CH	701	GTP	C2-N1-C6	-2.90	119.85	125.11
59	Cd	1000	GTP	N9-C8-N7	-2.66	108.47	113.40
59	CH	701	GTP	N9-C8-N7	-2.63	108.52	113.40
59	Cd	1000	GTP	C8-N7-C5	2.56	108.82	104.26
59	CH	701	GTP	C5-C6-N1	2.51	119.63	113.25
59	CH	701	GTP	C8-N7-C5	2.46	108.65	104.26
59	Cd	1000	GTP	C5-C6-N1	2.46	119.50	113.25
59	CH	701	GTP	O6-C6-C5	-2.38	120.25	126.53
59	Cd	1000	GTP	O6-C6-C5	-2.25	120.59	126.53
59	CH	701	GTP	C3'-C2'-C1'	2.23	105.68	101.46
59	Cd	1000	GTP	C3'-C2'-C1'	2.07	105.37	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	Cd	1000	GTP	O4'-C4'-C5'-O5'
59	Cd	1000	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3B-PG-O2G
59	Cd	1000	GTP	C5'-O5'-PA-O1A
59	CH	701	GTP	PB-O3A-PA-O2A
59	CH	701	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3B-PG-O3G
59	CH	701	GTP	PB-O3A-PA-O1A

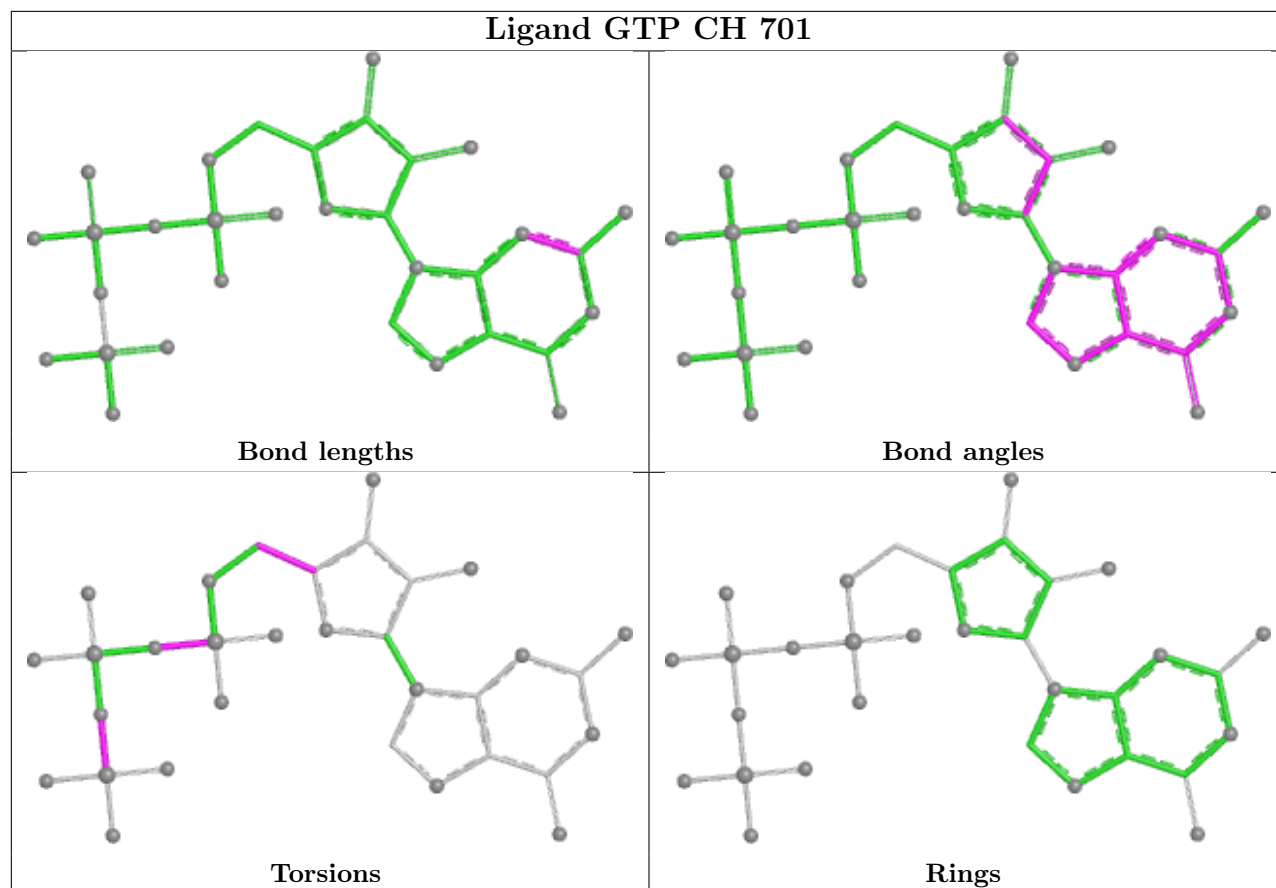
There are no ring outliers.

1 monomer is involved in 1 short contact:

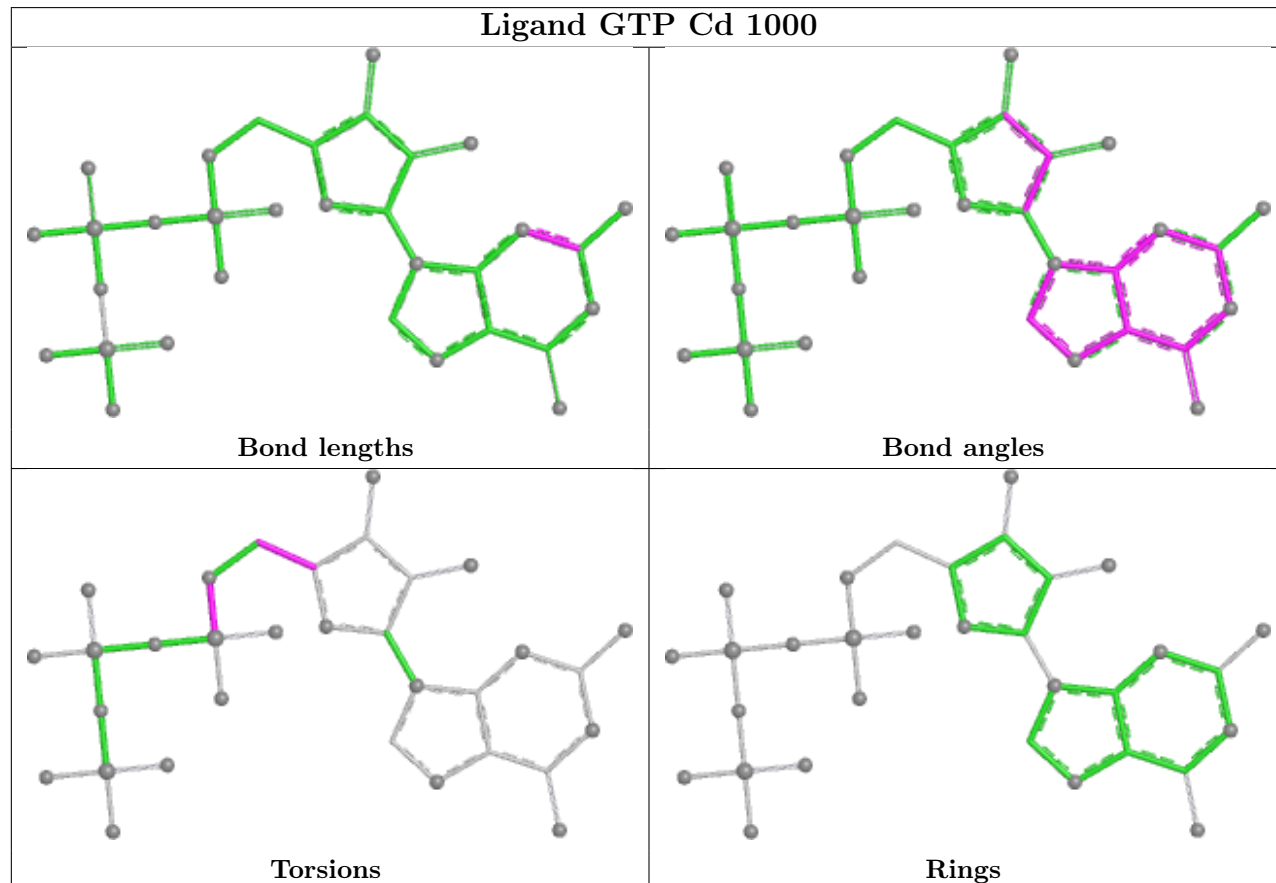
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	CH	701	GTP	1	0

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

Ligand GTP CH 701



Ligand GTP Cd 1000



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

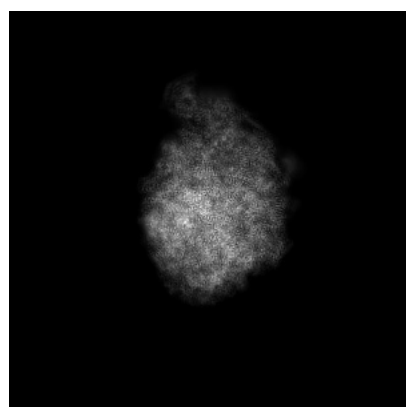
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17950. These allow visual inspection of the internal detail of the map and identification of artifacts.

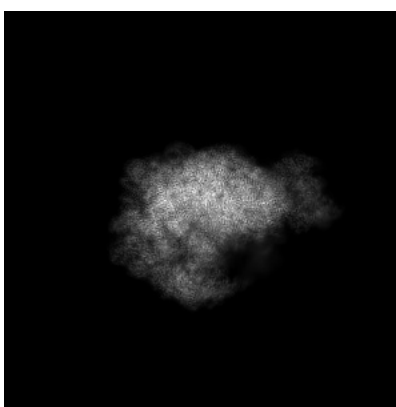
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

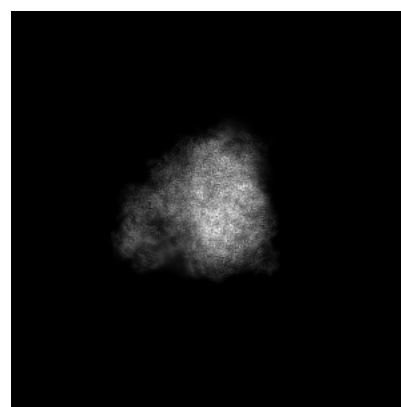
6.1.1 Primary map



X



Y

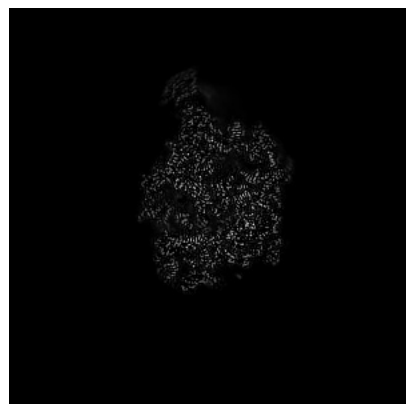


Z

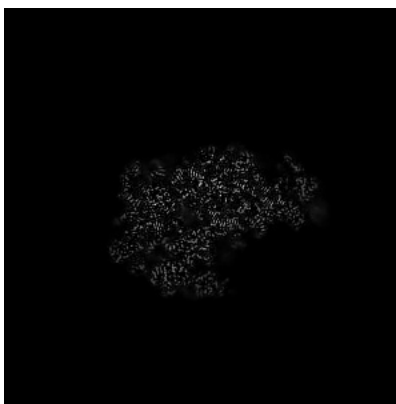
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

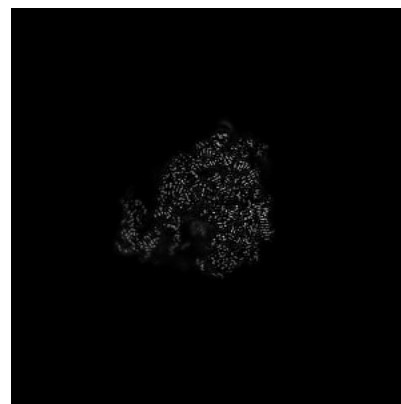
6.2.1 Primary map



X Index: 250



Y Index: 250

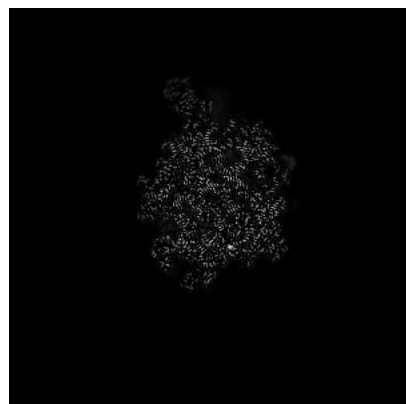


Z Index: 250

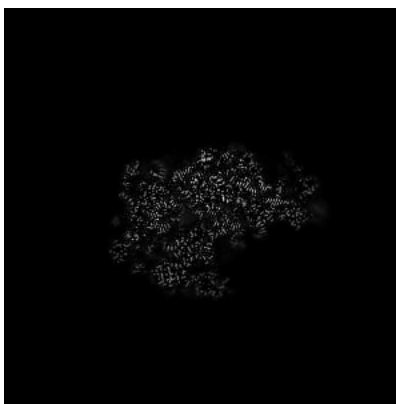
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

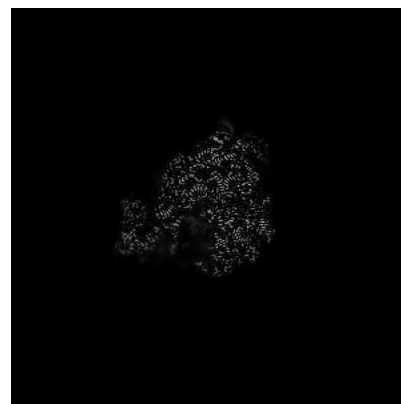
6.3.1 Primary map



X Index: 259



Y Index: 248

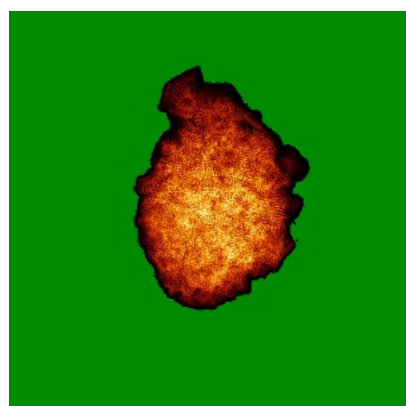


Z Index: 252

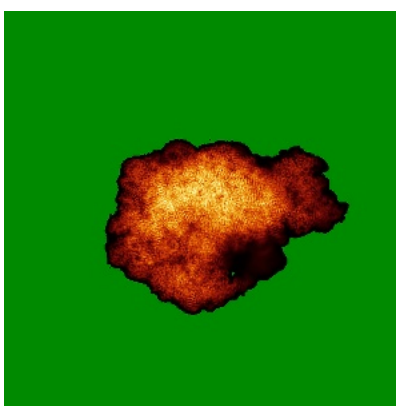
The images above show the largest variance slices of the map in three orthogonal directions.

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

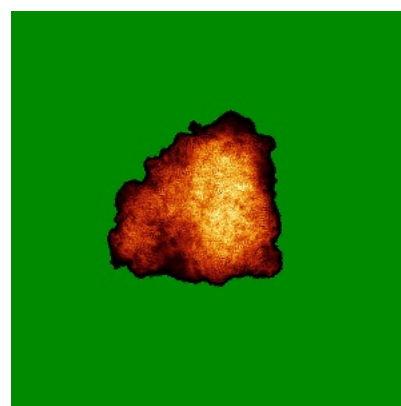
6.4.1 Primary map



X



Y

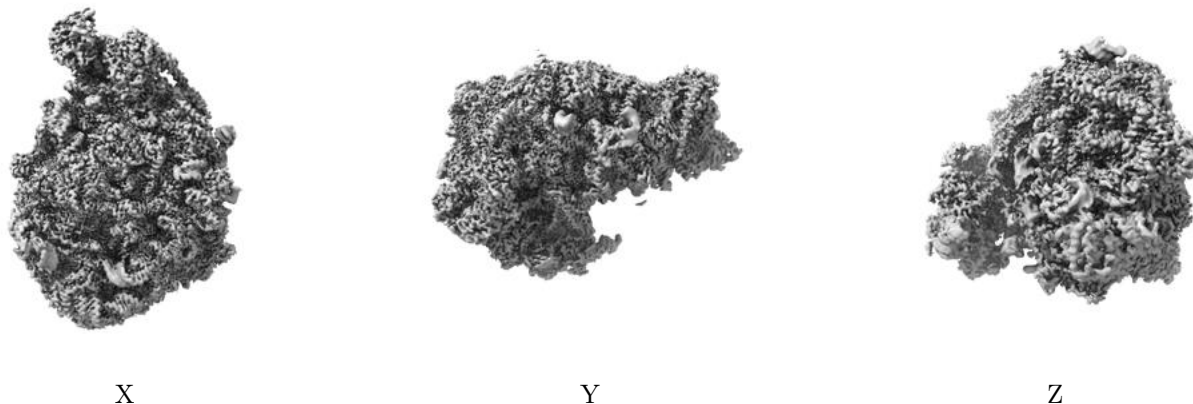


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

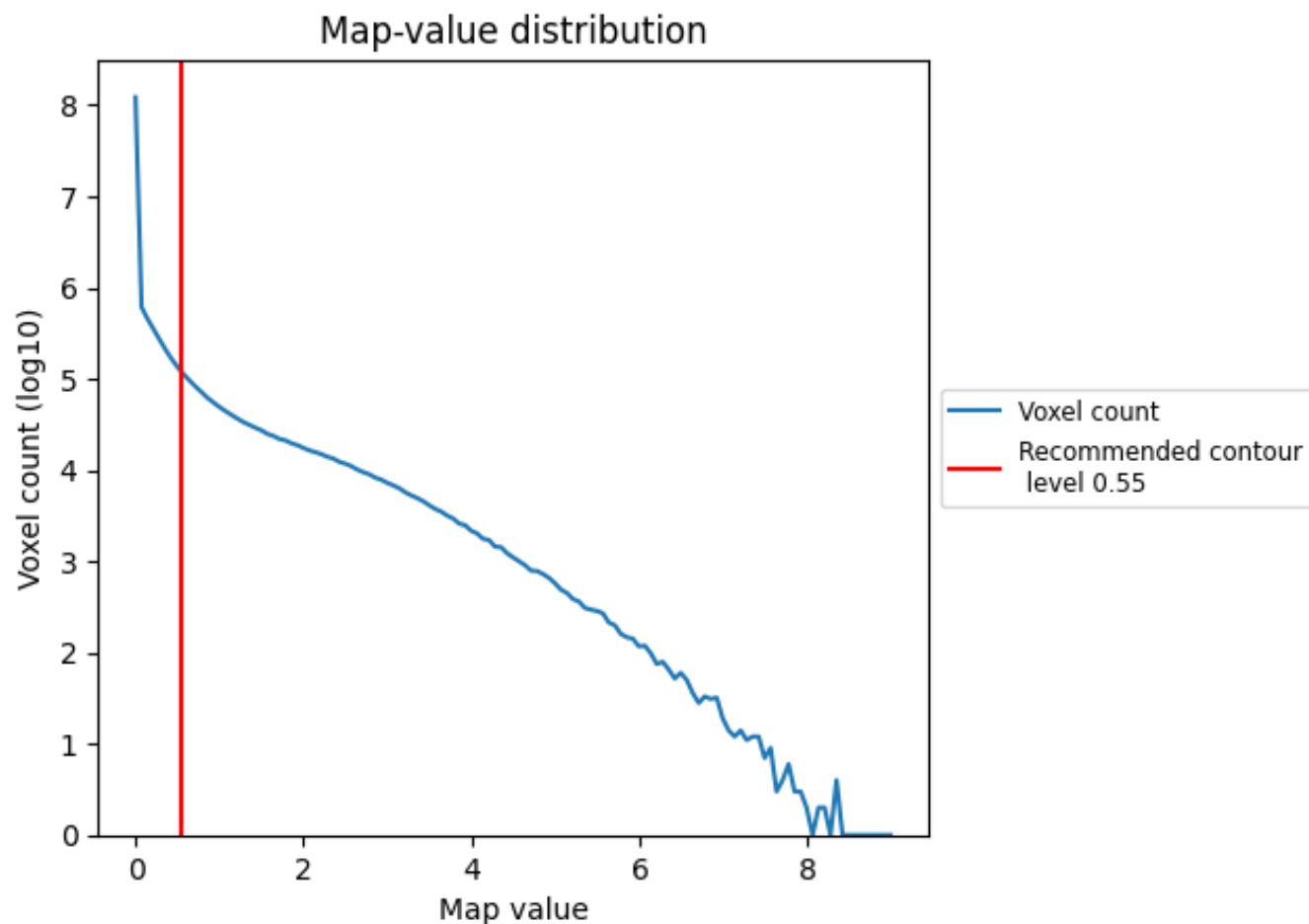
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

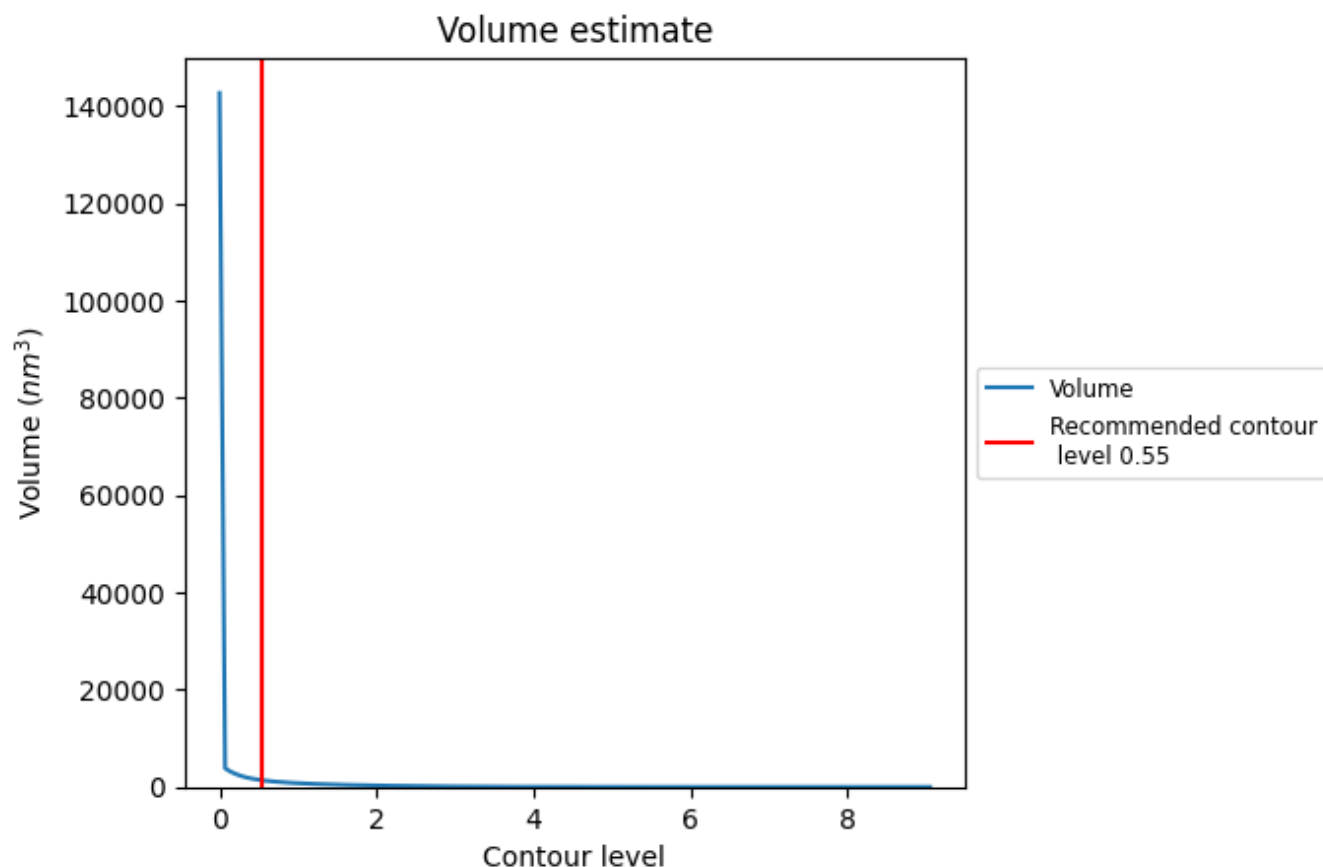
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

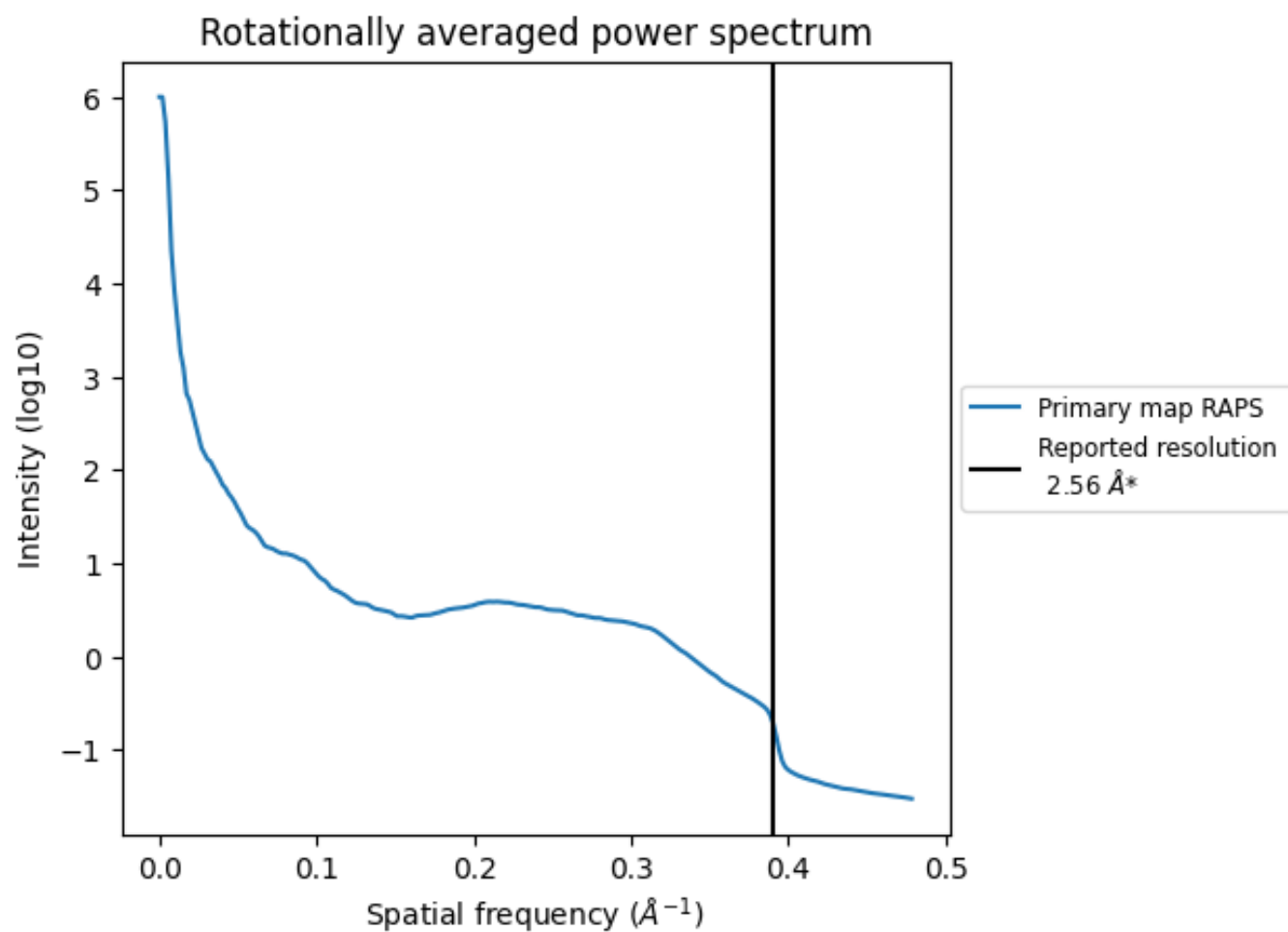
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1366 nm^3 ; this corresponds to an approximate mass of 1234 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 0.391 Å⁻¹

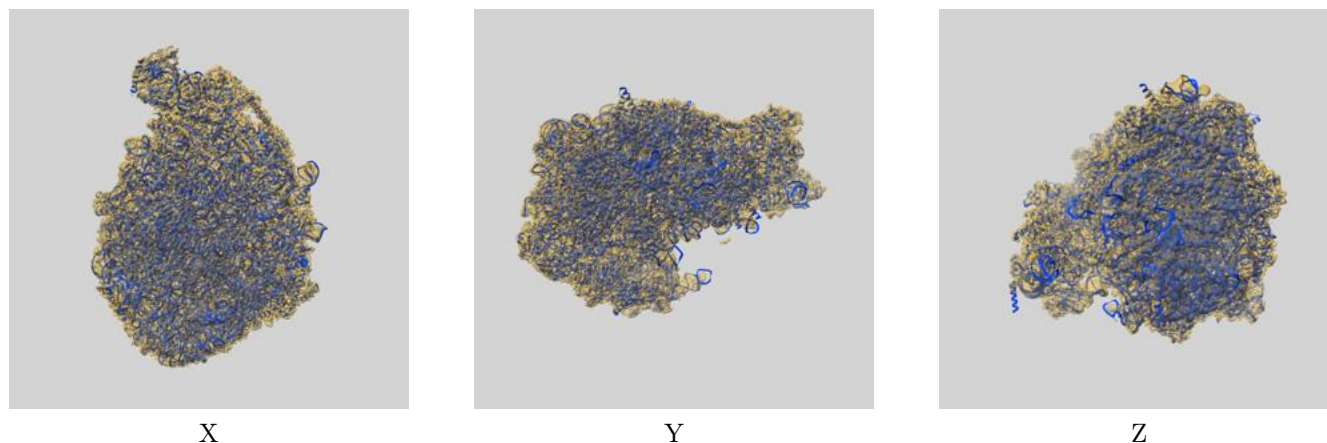
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

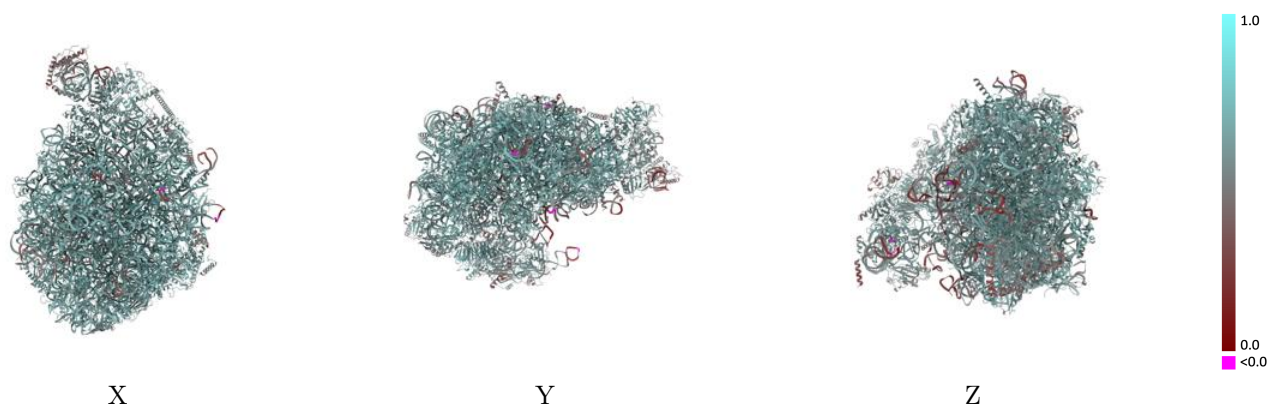
This section contains information regarding the fit between EMDB map EMD-17950 and PDB model 8PV1. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



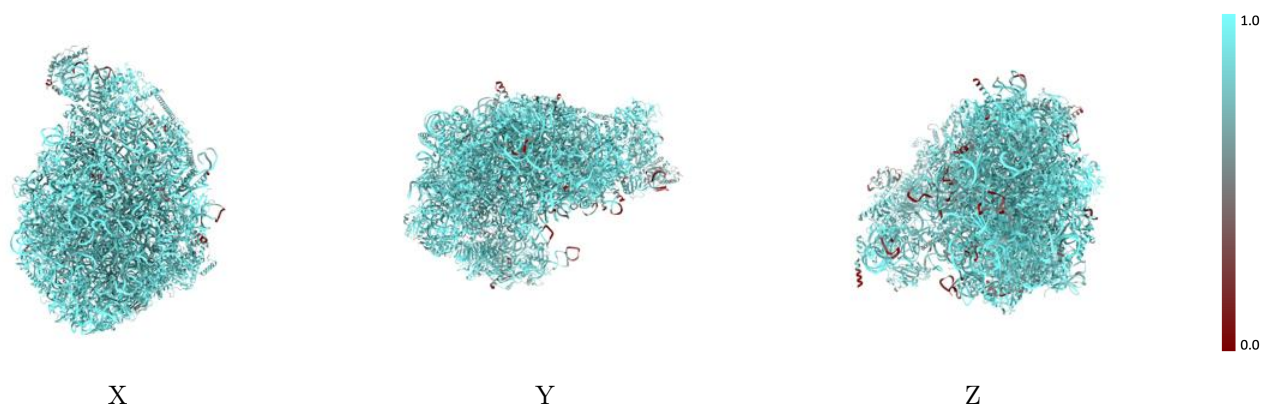
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



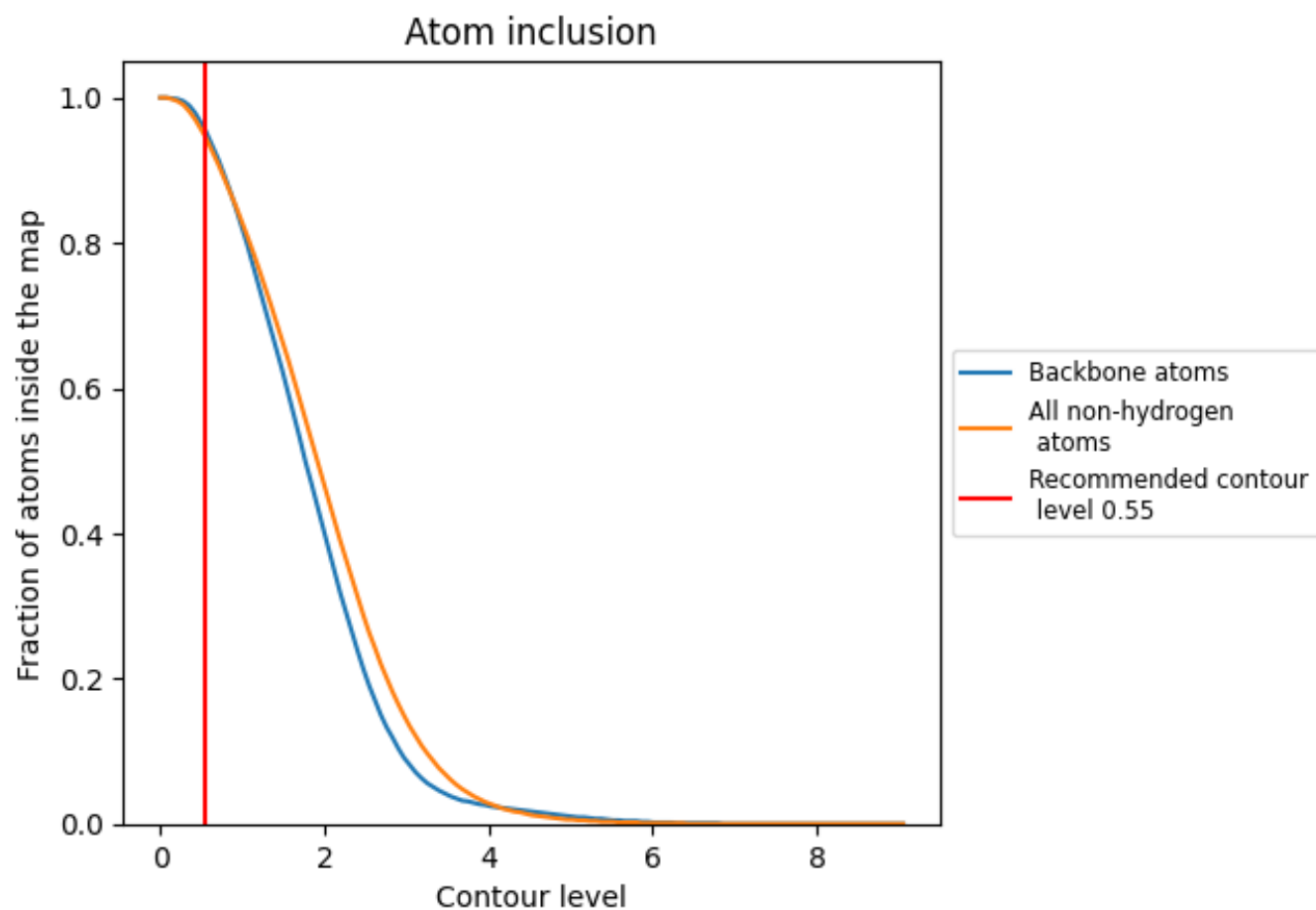
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.6180
C1	 0.9700	 0.6200
C2	 0.9720	 0.6490
C3	 0.7660	 0.4470
C4	 0.9080	 0.5310
CB	 0.7780	 0.4950
CF	 0.9210	 0.5950
CH	 0.9190	 0.6190
CI	 0.8300	 0.5240
CJ	 0.9600	 0.6200
CK	 0.9710	 0.6530
CL	 0.8890	 0.5630
CM	 0.9060	 0.5750
CN	 0.9630	 0.6520
CO	 0.9100	 0.6370
CQ	 0.8810	 0.6140
Cb	 0.9560	 0.6450
Cd	 0.9580	 0.6340
Ce	 0.8510	 0.5650
Cf	 0.9350	 0.5990
Cg	 0.9280	 0.5810
Ch	 0.8870	 0.5910
Cz	 0.8380	 0.5240
LA	 0.9690	 0.6540
LB	 0.9810	 0.6850
LC	 0.9770	 0.6680
LD	 0.9090	 0.5860
LE	 0.9260	 0.6220
LF	 0.9590	 0.6480
LG	 0.9480	 0.6270
LH	 0.9520	 0.6460
LJ	 0.8900	 0.5120
LK	 0.8580	 0.5450
LL	 0.9390	 0.6360
LM	 0.9580	 0.6450



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Chain	Atom inclusion	Q-score
LN	 0.9900	 0.6750
LO	 0.9830	 0.6790
LP	 0.9810	 0.6790
LQ	 0.9600	 0.6390
LR	 0.9510	 0.6580
LS	 0.9670	 0.6470
LT	 0.8620	 0.5280
LU	 0.9250	 0.6050
LV	 0.9890	 0.6820
LX	 0.9530	 0.6370
LY	 0.9590	 0.6440
LZ	 0.9550	 0.6370
La	 0.9550	 0.6410
Lc	 0.9320	 0.6220
Ld	 0.9730	 0.6770
Le	 0.9810	 0.6750
Lf	 0.9920	 0.6930
Lg	 0.9150	 0.6400
Lh	 0.9270	 0.6000
Li	 0.9240	 0.6060
Lj	 0.9880	 0.6900
Lk	 0.8950	 0.6060
Ll	 0.9950	 0.6980
Lp	 0.9200	 0.6340
Lq	 0.9580	 0.6410