



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:04 AM UTC

PDB ID : 8PV7 / pdb_00008pv7
EMDB ID : EMD-17956
Title : Chaetomium thermophilum pre-60S State 1 - pre-5S rotation (Arx1/Nog2 state) - Composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.12 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:

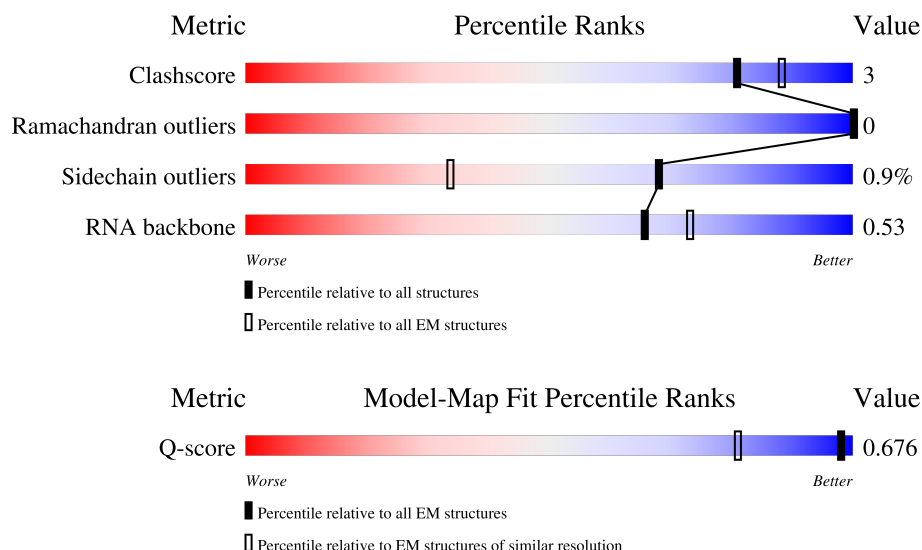
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

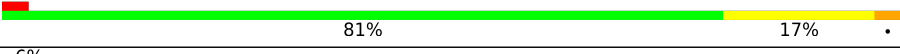
The reported resolution of this entry is 2.12 Å.

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	2398 (1.64 - 2.62)

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	

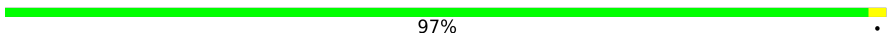
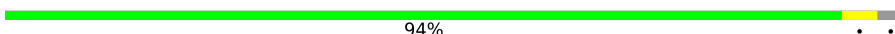
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Mol	Chain	Length	Quality of chain
4	C4	119	
5	CB	391	
6	CF	270	
7	CH	661	
8	CI	414	
9	CJ	679	
10	CK	261	
11	CL	558	
12	CM	249	
12	LF	249	
13	CN	246	
14	CO	120	
15	CQ	225	
16	Lq	147	
17	Cb	117	
18	Cd	627	
19	Ce	443	
20	Cf	350	
21	Cg	202	
22	Ch	517	
23	Cz	123	
24	LA	254	
25	LB	392	
26	LC	365	
27	LD	304	

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Mol	Chain	Length	Quality of chain
28	LE	200	
29	LG	262	
30	LH	229	
31	LJ	173	
32	LK	165	
33	LL	213	
34	LM	142	
35	LN	203	
36	LO	204	
37	LP	187	
38	LQ	213	
39	LR	2898	
40	LS	174	
41	LT	160	
42	LU	127	
43	LV	139	
44	LX	156	
45	LY	138	
46	LZ	135	
47	La	149	
48	Lc	108	
49	Ld	120	
50	Le	131	
51	Lf	109	
52	Lg	119	

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Mol	Chain	Length	Quality of chain
53	Lh	935	12%87%
54	Li	110	88%8%
55	Lj	95	82%11%7%
56	Lk	94	62%19%19%
57	Ll	51	94%
58	Lp	92	89%10%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 157262 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	267	Total	C	N	O	S	0	0
			2119	1359	373	384	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 Putative 60S ribosomal protein.

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

- Molecule 17 is a protein called Zinc finger domain-containing protein.

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

- Molecule 18 is a protein called Nucleolar GTP-binding protein 2.

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

- Molecule 19 is a protein called Ribosome biogenesis protein NOP53.

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

- Molecule 20 is a protein called Ribosome production factor 2 homolog.

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

- Molecule 21 is a protein called Ribosome biogenesis regulatory protein.

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

- Molecule 22 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	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 23 is a protein called rRNA-processing protein.

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

- Molecule 24 is a protein called 60S ribosomal protein L2-like protein.

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

- Molecule 25 is a protein called 60S ribosomal protein L3-like protein.

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

- Molecule 26 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 27 is a protein called 60S ribosomal protein l5-like protein.

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

- Molecule 28 is a protein called 60S ribosomal protein L6.

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

- Molecule 29 is a protein called 60S ribosomal protein L8.

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

- Molecule 30 is a protein called 60S ribosomal protein l9-like protein.

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

- Molecule 31 is a protein called Putative ribosomal protein.

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

- Molecule 32 is a protein called 60S ribosomal protein L12-like protein.

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

- Molecule 33 is a protein called 60S ribosomal protein L13.

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

- Molecule 34 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 35 is a protein called Ribosomal protein L15.

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

- Molecule 36 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 37 is a protein called 60S ribosomal protein l17-like protein.

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

- Molecule 38 is a protein called Ribosomal protein L18-like protein.

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

- Molecule 39 is a protein called Ribosomal protein L19.

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

- Molecule 40 is a protein called 60S ribosomal protein L20.

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

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 42 is a protein called 60S ribosomal protein L22-like protein.

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

- Molecule 43 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 44 is a protein called 60S ribosomal protein L25-like protein.

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

- Molecule 45 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 46 is a protein called 60S ribosomal protein L27.

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

- Molecule 47 is a protein called 60S ribosomal protein L28-like protein.

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

- Molecule 48 is a protein called 60S ribosomal protein l30-like protein.

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

- Molecule 49 is a protein called Putative 60S ribosomal protein.

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

- Molecule 50 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 51 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 52 is a protein called Ribosomal protein l34-like protein.

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

- Molecule 53 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 54 is a protein called 60S ribosomal protein L36.

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

- Molecule 55 is a protein called Ribosomal protein L37.

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

- Molecule 56 is a protein called 60S ribosomal protein L38-like protein.

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

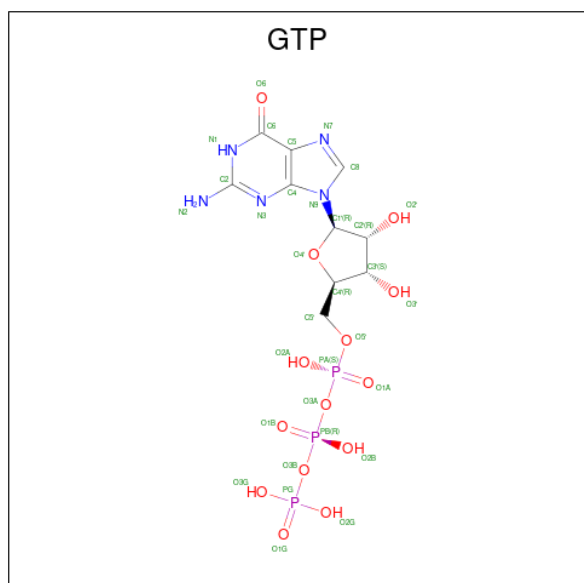
- Molecule 57 is a protein called Ribosomal protein eL39.

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

- Molecule 58 is a protein called 60S ribosomal protein L43-like protein.

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

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



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

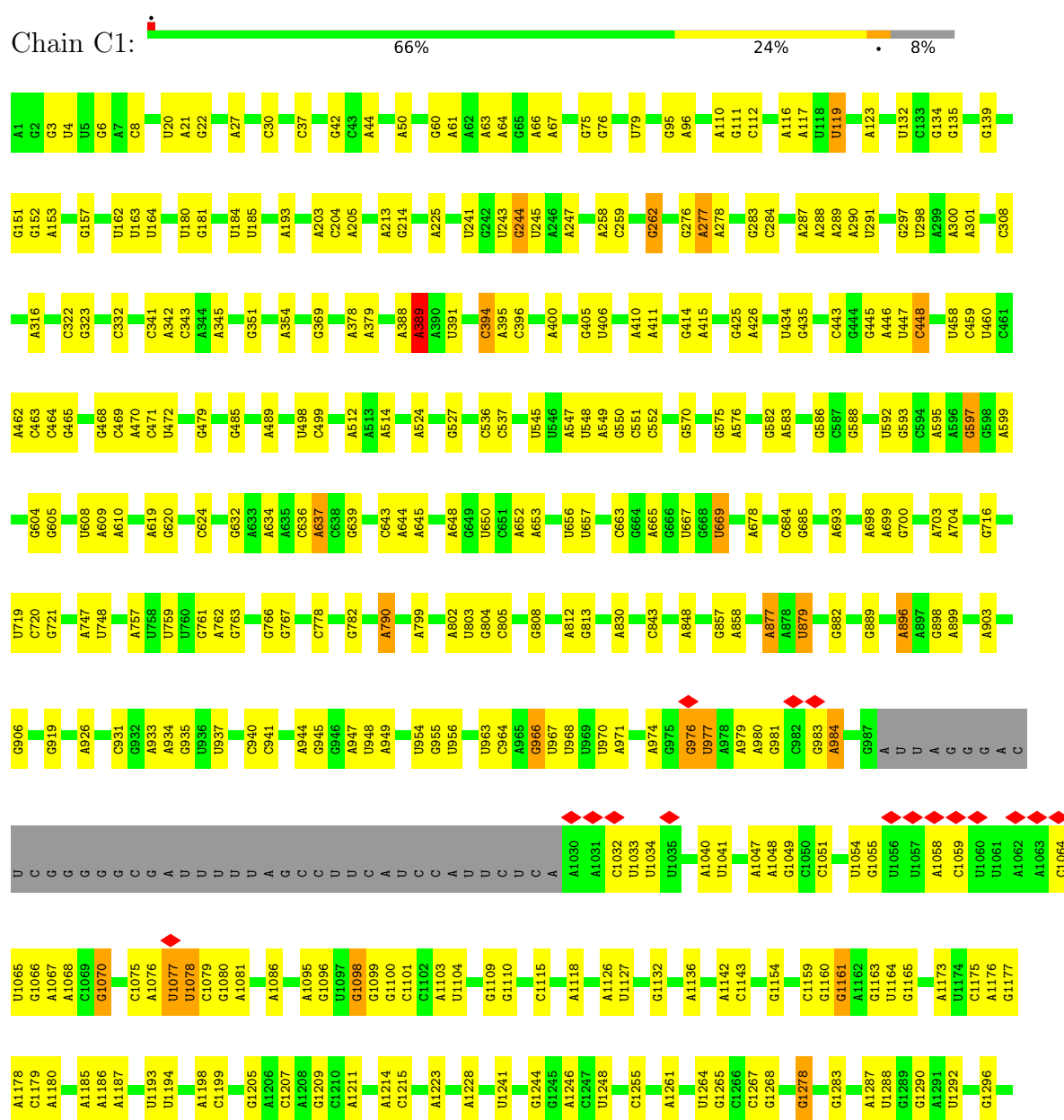
- Molecule 62 is water.

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

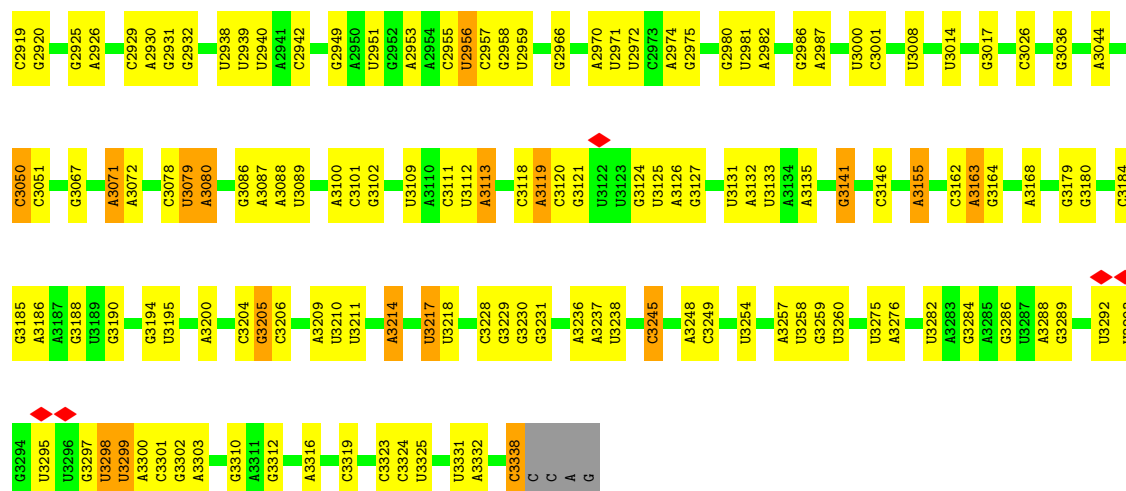
3 Residue-property plots

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

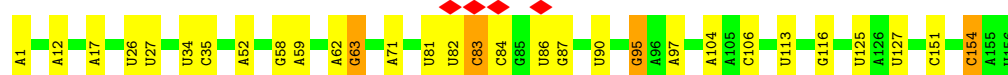
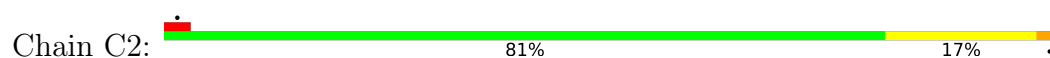
• Molecule 1: 26S rRNA



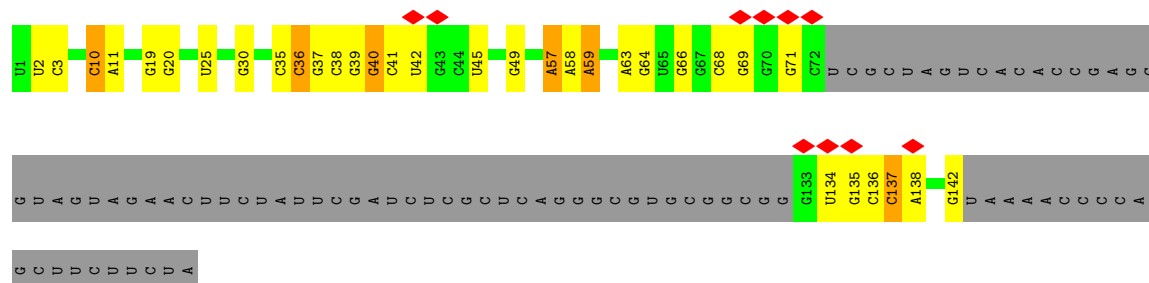
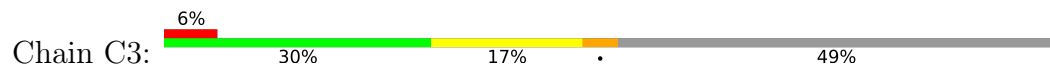
C2803	G2889	G2582	U2397	G	A2205	G2074	C	U	U1799	G1658	U1505	U1305
A2804	U2890	G2583	G2398	A	A2206	U2075	C	G	C1800	G1658	U1505	C1306
U2805	G2691	C2584	U2399	U2277	G2212	A2076	C	G	U1801	C1663	U1536	A1313
A2806	A2692	A2585	G2400	G2278	G2216	G2084	A	U	G1809	A1676	U1537	C1323
G2807	A2693	U2592	A2403	G2279	U2217	G2085	G	C	C1812	A1677	C1539	U1324
G2808	A2706	U	A2406	A2280	A2218	G2089	C	U	C1813	U1683	A1541	A1331
G2809	A2707	A	C	U2281	A2219	A2092	A	U	U1814	U1683	A1542	G1332
A2810	G2713	A	U	C2220	C2221	A2093	C	G	A1815	U1684	G1543	A1333
G2812	A2717	A	A	U2222	U2223	A2094	C	C	C1816	U1685	G1549	A1334
C2816	A2717	C	G	A2289	U2224	G2093	G	C	A1822	C1697	U1550	A1335
U2817	C2723	A	A	U2297	G2225	A2101	G	G	C1826	A1698	G1551	C1336
U	C2724	U	A	U2298	A2226	U2102	U	A	C1829	G1699	U1552	G1337
U2820	U2730	U	U	U2299	C2226	U2103	U	C	U1702	U1702	G1554	U1350
U2821	C2731	A	G	U2307	U2227	U2121	G	C	U1704	U1704	C1555	U1351
G2822	C2732	C	G	A2308	U2228	U2122	A	C	C1705	U1705	U1560	G1370
C2826	G2736	G2604	U	U2309	U2229	G2123	A	C	U1722	U1722	G1561	U1371
U2827	A2737	C2605	A	A2315	C2230	G2124	G	U	U1726	U1726	U1562	G1372
U2828	U2744	U2609	G	A2320	U2231	C2125	C	G	C1737	C1737	G1563	G1382
G2836	U2754	U2614	U	A2321	U	C2126	U	C	U1730	U1730	A1567	A1383
G2837	G2755	A2615	U	A2326	G2236	U2151	C	A	U1731	U1731	A1568	G1395
C2838	C2756	A2632	A	G2327	U2237	G2157	G	C	G1857	G1743	A1569	C1403
A2846	C2757	A2633	G	A2348	A2238	C2158	U	C	U1859	C1744	A1573	C1403
G2857	C2757	C2634	U	U2350	U2238	C2160	U	C	U1860	G1746	G1576	U1413
C2858	A2758	A2635	G	A2331	U	A2161	C	C	A1866	G1751	C1577	U1417
A2859	A2761	G2636	U	G2331	A2243	U2166	G	G	A1867	U1743	A1583	A1418
G2860	A2762	U2642	A	G2340	U	G2167	C	C	U1868	C1744	U1584	U1419
U2863	A2763	U2647	G	A2348	A	C2169	U	C	U1869	U1745	A1585	C1420
U2882	C2769	A2650	U	U2351	A	A2164	C	U	G1877	G1746	U1586	U1421
U2883	C2771	A2651	C	C2355	U	G2167	C	U	G1878	U1751	C1595	A1429
A2884	A2772	A2656	G	G2356	U	U2168	C	G	G1879	C1758	U1596	G1430
C2886	G2773	G2657	C	G2359	C	G2170	U	C	C1887	G1759	U1599	U1431
C2887	A2776	G2658	C	G2359	U	G2171	C	C	U1900	G1761	A1599	A1432
A2888	U	A2663	C	A2362	U	G2172	C	C	A1912	U1762	U1609	G1433
A2889	A	A2664	A	G2363	U	A2170	C	G	A1917	C1763	G1610	U1438
C2890	C	G2665	U	A2364	A	U2171	U	C	U1917	G1766	C1611	G1449
U2891	G2781	C2666	G	U2373	U	U2172	A	C	G1917	A1767	G1614	G1458
A2892	G2782	U2667	U	U2374	U	A2176	C	A	G1920	G1776	C1619	A1464
U2893	C2783	G2672	A	A2376	U	A2177	C	C	C1923	A1777	A1622	G1485
A2894	C2784	A2673	A	G2377	U	U2186	G	G	G1929	A1778	A1623	C1624
A2895	U2785	U2675	A	U2380	A	U2188	C	C	G1934	A1779	A1624	G1491
A2899	G2789	U2571	U	U2382	U	A2192	C	G	G1935	A1793	G1638	C1492
U2903	C2790	U2572	C	A2382	A	G2197	C	C	C1936	A1794	A1639	G1493
G2904	C2791	G2573	C	C2383	C	G2203	C	G	C1937	U1795	G1640	G1503
A2905	A2796	C2574	U	U2384	G	U2204	C	C	G1938	A1796	G1642	G1504
G2906	U2914	G2575	A	U2396	C	U2204	C	C	U1939			



• Molecule 2: 5.8S rRNA



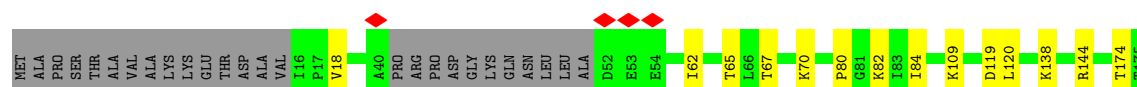
• Molecule 3: ITS2



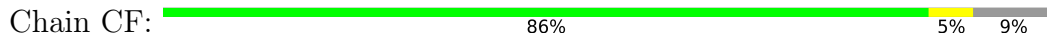
• Molecule 4: 5S rRNA



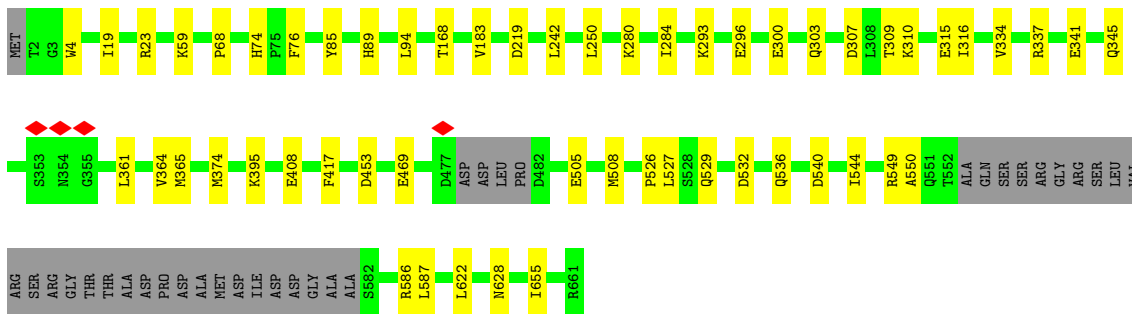
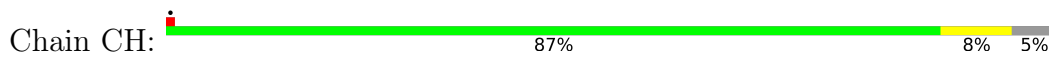
• Molecule 5: Utp30



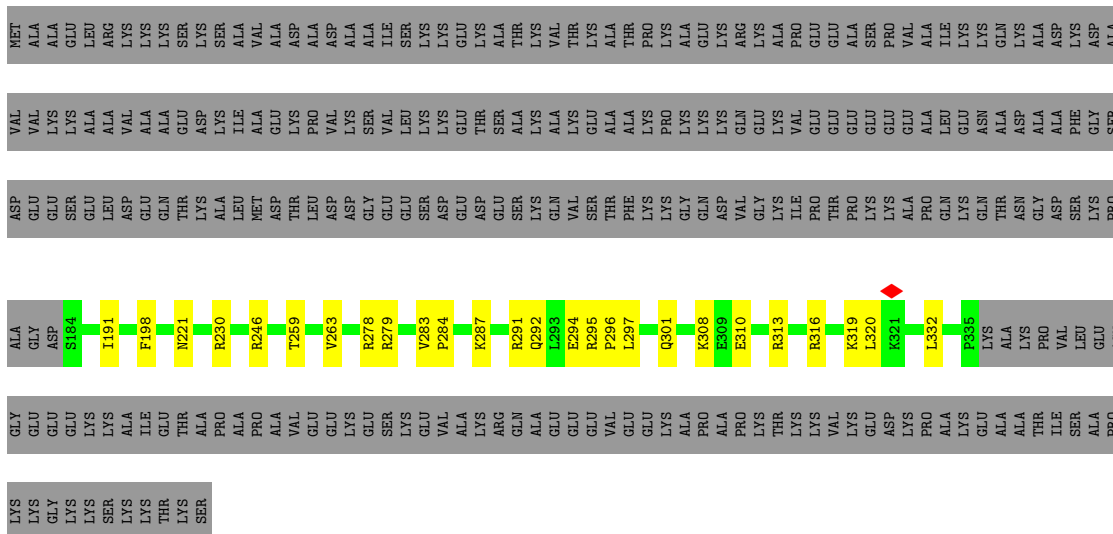
- Molecule 6: Large ribosomal subunit protein uL10



- Molecule 7: Nucleolar GTP-binding protein 1



- Molecule 8: Putative RNA-binding protein



- Molecule 9: Pescadillo homolog

53% . 44%



85% 5% 9%



Response	Percentage
Yes	13%
No	86%



MET	S2	I9	W10	E11	R14	L20	D31	N34	V47	R88	K92	K131	R140	ALA	ALA	ALA	ALA	GLY	LYS	GLN
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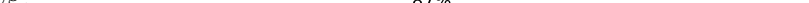
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | G2 | K11 | D25 | L26 | R27 | R30 | H31 | Q34 | H68 | R76 | M92 | Y97 | G102 | LYS | LYS | THR | THR | GLU | GLN | PRO | LYS | THR | GLN | ASP | VAL | GLU | MET | SER |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

- [illegible]

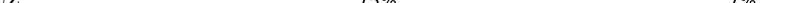
- 

VAL	ASN	MET
GLU	ASN	LEU
ALA	ASP	ARG
GLY	GLY	ILE
SER	GLU	GLN
GLY	ASN	LYS
GLU	PRO	P7
LYS	ALA	123
LYS	PRO	
LYS	LEU	
LYS	PRO	C30
LYS	GLY	L31
VAL	MET	F32
VAL	THR	
LYS	ASP	T36
GLY	PRO	
	ARG	M47
	SER	D48
	ILE	
	PRO	R59
	SER	
	SER	K62
	SER	K63
	Q221	
	L227	L86
	M253	R96
	D254	P97
	F255	H98
	R261	R104
	T277	D112
	P278	M113
	Q279	
	D290	F116
	D294	P120
		Y123
	R298	
	M301	A145
	R319	M159
GLY	GLY	D166
ARG	ARG	R169
ASP	GLU	
ASP	ASP	P172
GLU	GLU	
GLY	GLY	T188
GLY	GLY	
GLU	GLU	P192
ASP	ASP	THR
ARG	ARG	SER
THR	THR	THR
ASP	ASP	SER
VAL	VAL	THR

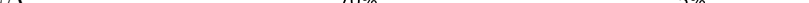
- Chain Cg:  87% 5% 7%

MET	THR	ASP	THR	SER	LYS	PRO	ALA	ARG	L11	V15	T19	D43	V46	Q49	D57	T71	T82	P97	D150	P151	I152	R170	K198	MET	GLY	LYS	LYS
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- Chain Ch:  84% 9% 6%

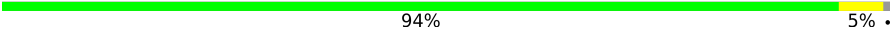
- Chain Cz:  75% 7% 18%

MET	ASN	MET	SER	GLU	THR	GLN	VAL	ASN	ILE	THR	ALA	ALA	PRO	ALA	PRO	ALA	THR	THR	LYS	K21	K64	K72	R86	K90	E94	E97	Q98	L99	R110	L121	ASN	SER
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- Chain LA:  70% 5% 25%

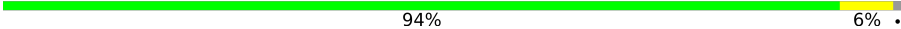
ARG	TYR	ALA	ALA	GLN	GLY	GLN	LYS	ALA	GLY	LEU	ILE	ALA	ARG	VAL	ARG	THR	THR	GLY	LEU	THR	GLN	LYS	THR	GLY	GLU																							
MET	GLY	ARG	VAL	ILE	ARG	ASN	GLN	ARG	LYS	GLY	ARG	GLY	VAL	PHE	THR	ALA	HIS	THR	ARG	LEU	R23	V45	V61	R64	R65	P66	Y67	S105	S114	N115	E118	R128	S160	M204	G213	GLY	ASN	HIS	GLN	HIS	ILE	GLY	LYS	ALA	SER	THR	ILE	SER

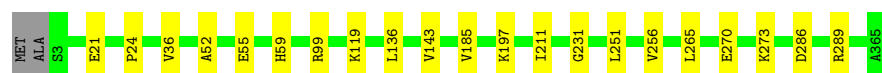
- 
- WORLDWIDE
PDB
PROTEIN DATA BANK

Chain LB:  94% 5% .



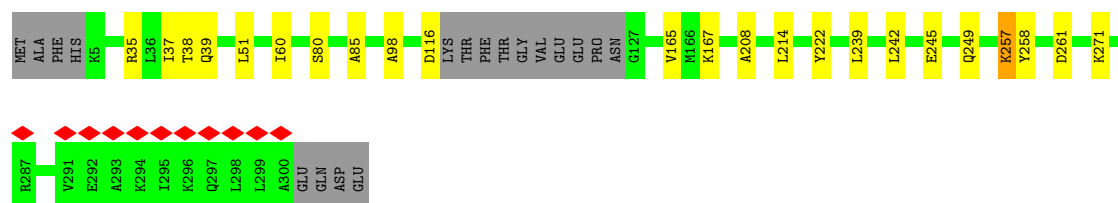
- Molecule 26: 60S ribosomal protein L4-like protein

Chain LC:  94% 6% .



- Molecule 27: 60S ribosomal protein l5-like protein

Chain LD:  87% 7% 6% .



- Molecule 28: 60S ribosomal protein L6

Chain LE:  86% 10% .



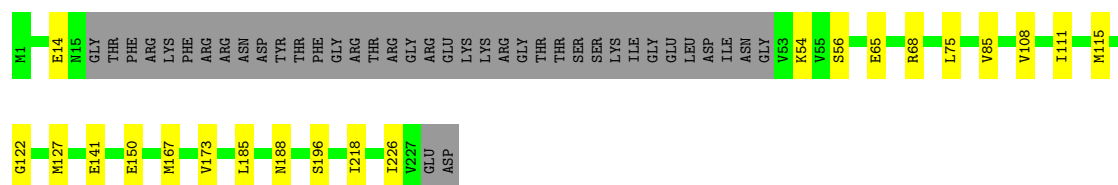
- Molecule 29: 60S ribosomal protein L8

Chain LG:  84% 5% 10% .



- Molecule 30: 60S ribosomal protein l9-like protein

Chain LH:  74% 9% 17% .



- Molecule 31: Putative ribosomal protein

Chain LJ:  84% 12% ..



- Molecule 32: 60S ribosomal protein L12-like protein

Chain LK:  88% 8% .



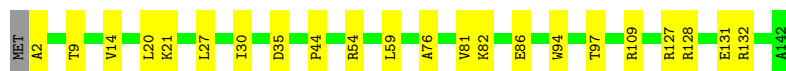
- Molecule 33: 60S ribosomal protein L13

Chain LL:  92% . 5%



- Molecule 34: 60S ribosomal protein L14-like protein

Chain LM:  84% 15% .

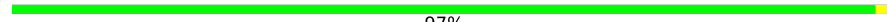


- Molecule 35: Ribosomal protein L15

Chain LN:  91% 8%



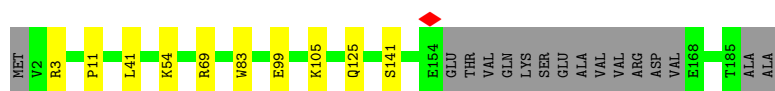
- Molecule 36: 60S ribosomal protein L16-like protein

Chain LO:  97% .



- Molecule 37: 60S ribosomal protein l17-like protein

Chain LP:  86% 5% 9%



- Molecule 38: Ribosomal protein L18-like protein

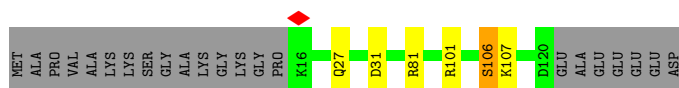
Response	Percentage
Used	65%
Not used	6%
Don't know	30%



Frequency	Percentage
Daily	5%
Not Daily	95%







- Molecule 43: 60S ribosomal protein l23-like protein

Chain LV: 94%



- Molecule 44: 60S ribosomal protein L25-like protein

Chain LX: 88% 5% 7%



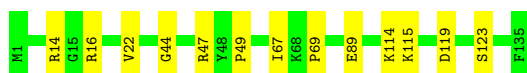
- Molecule 45: 60S ribosomal protein L26-like protein

Chain LY: 85% 12%



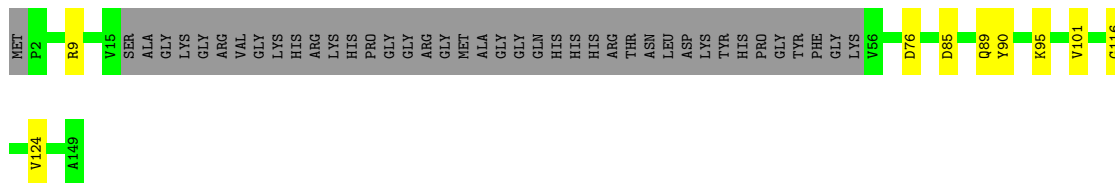
- Molecule 46: 60S ribosomal protein L27

Chain LZ: 90% 10%



- Molecule 47: 60S ribosomal protein L28-like protein

Chain La: 66% 6% 28%



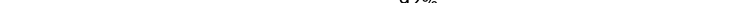
- Molecule 48: 60S ribosomal protein l30-like protein

Chain Lc: 80% 8% 12%

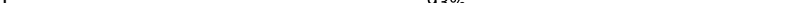


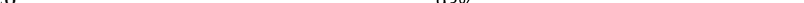
- Molecule 49: Putative 60S ribosomal protein

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 1.2. The x-axis shows amino acids: MET, SER, SER, THR, GLN, GLN, LYS, LYS, GLN, ARG, SER, and A11. MET, SER, SER, THR, GLN, GLN, LYS, LYS, GLN, ARG, and SER are all at 0 bits. A11 is at approximately 0.1 bits. L28 is at approximately 0.8 bits. T32 is at approximately 0.4 bits. A40 is at approximately 0.8 bits. K66 is at approximately 0.8 bits. R86 is at approximately 0.4 bits. E119 and E120 are both at approximately 1.1 bits, marked with red diamonds.

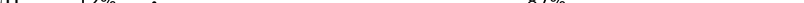
- Chain Le:  92% 5% .

MET	V2	I39	I56	I97	S102	R106	A125	K126	V127	THR	THR	GLU	VAL
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- Chain Lf:  93% 6%

- Chain Lg: 

Sequence logo for the 1000bp upstream region of the H19 gene. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions from -1000 to +1000. The sequence is: MET A2 R22 L34 R75 A76 Y77 R81 N84 K103 K114 K115 A116 S117 K118 K119. A red diamond marker is at position +1000.

- Chain Lh:  12% 87%

MET	SER	SER	N4	Q11	K15	L34	S41	S42	K45	L46	I49	K66	D84	E107	A125	ALA	THR	TYR	SER	SER	GLU	GLY	PRO	ALA	ALA	LEU	LEU	SER	SER	ILE	ILE	TYR	HIS	SER	HIS	GLN	GLN	ARG	ARG	GLU	GLY	ALA	ALA	ARG	CYS	CYS	LEU	VAL	PHE	THR	CYS	GLN	GLY	PRO	GLY	LEU
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GLU	SER	LEU	LEU	LEU	PRO	VAL	ALA	ALA	SER	LEU	LYS	GLY	PRO	GLU	ASN	PHE	THR	ARG	ARG	GLU	GLN	HIS	ARG	ASN	MET	SER	ALA	ALA	ALA	GLU	PRO	LEU	LYS	LEU	ALA	SER	ALA	ALA	GLY	LYS	GLY	LYS	SER	THR	ARG	SER	VAL	LEU	ARG	VAL	ALA	ILE	LEU	VAL
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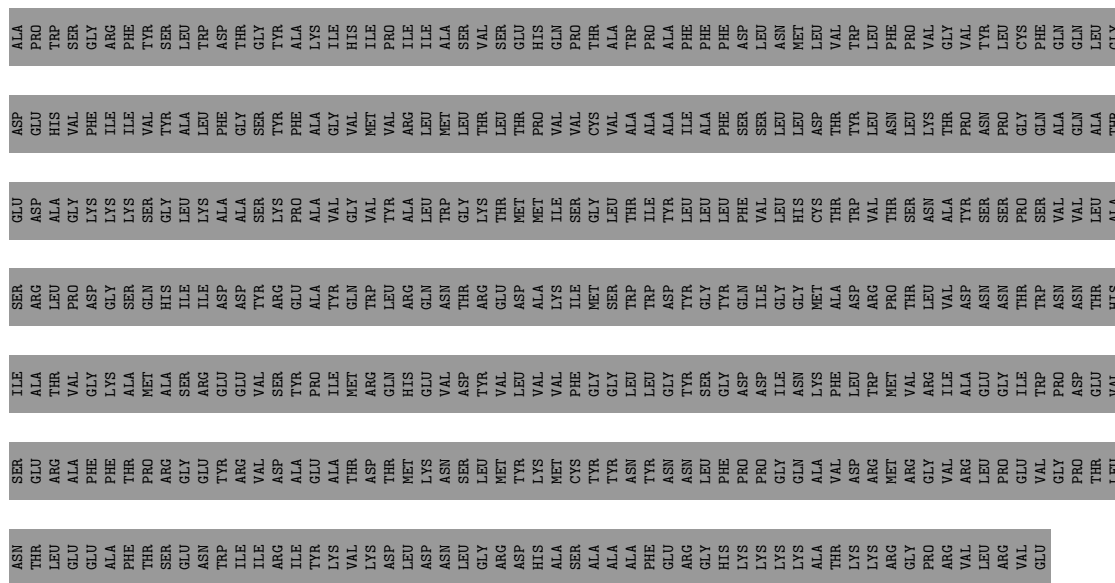
LEU	ILE	ALA	GLY	ALA	VAL	ALA	ALA	SER	ARG	LEU	PHE	SER	VAL	ILE	ILE	HIS	GLU	PHE	ASP	PRO	TRP	PHE	ASN	PHE	ARG	ALA	THR	LYS	TYR	TYR	LEU	VAL	ALA	ASN	GLY	PHE	PHE	TYR	LYS	PHE	TRP	TRP	PHE	ASP	ASP	ARG	THR	THR	HIS	PRO	PRO	LEU	GLY	ARG	VAL	THR
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GLY	THR	LEU	TYR	PRO	GLY	LEU	MET	VAL	THR	SER	GLY	VAL	ILE	TYR	HIS	LEU	LEU	ARG	PHE	LEU	THR	VAL	PRO	ASP	VAL	ILE	ARG	ASN	CYS	VAL	LEU	LEU	ALA	ALA	ALA	ALA	TYR	LEU	THR	ALA	PHE	GLY	SER	GLY	ASN	GLU	MET	THR	THR	SER	PRO	ALA
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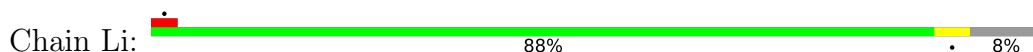
GLY	LEU	ALA	ALA	ALA	PHE	MET	GLY	ILE	ALA	PRO	GLY	TYR	ILE	ARG	SER	SER	VAL	ASP	ASN	GLU	ALA	ILE	ILE	ILE	PHE	LEU	LEU	VAL	PHE	PHE	PHE	TRP	TRP	ILE	LYS	LEU	LEU	LYS	GLN	GLY	SER	SER	MET	LEU	TRP	GLY	ALA	ALA	LEU	CYS	ALA	LEU	PHE	TYR	GLY
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TYR	MET	VAL	ALA	SER	TRP	GLY	GLY	TYR	ALA	ALA	ILE	THR	CYS	LEU	LEU	PRO	LEU	HIS	SER	PHE	VAL	VAL	LEU	ILE	CYS	MET	GLY	ARG	TYR	SER	THR	ARG	LEU	TYR	VAL	VAL	TYR	THR	THR	TRP	TRP	TYR	ALA	ALA	LEU	GLY	THR	LEU	LEU	ALA	SER	SER	MET	GLN	ILE	PRO	PHE	VAL	GLY	PHE	LEU	PRO	VAL	LYS
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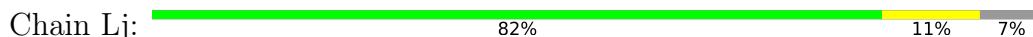
THR	SER	GLU	HIS	MET	PRO	ALA	LEU	GLY	ILE	PHE	GLY	PHE	LEU	GLN	ASP	TYR	VAL	ARG	SER	THR	ILE	SER	SER	ARG	GLN	PHE	GLN	THR	THR	PHE	LEU	TRP	LEU	PHE	ALA	ALA	GLY	GLY	ILE	ILE	PHE	GLY	LEU	GLY	LEU	VAL	ILE	ILE	THR	THR	ALA	GLY	ILE	ILE
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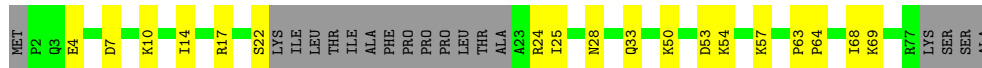
- Molecule 54: 60S ribosomal protein L36



- Molecule 55: Ribosomal protein L37



- Molecule 56: 60S ribosomal protein L38-like protein



- Molecule 57: Ribosomal protein eL39



- Molecule 58: 60S ribosomal protein L43-like protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	745895	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	10.768	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, A2M, ZN, GTP, OMG, OMC, MG

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	0.27	1/72882 (0.0%)	0.37	0/113631
2	C2	0.27	0/3710	0.35	0/5778
3	C3	0.22	0/1958	0.35	0/3050
4	C4	0.23	0/2833	0.34	0/4414
5	CB	0.21	0/2166	0.44	0/2945
6	CF	0.23	0/1972	0.42	1/2660 (0.0%)
7	CH	0.22	0/5147	0.43	0/6926
8	CI	0.26	0/1265	0.63	0/1702
9	CJ	0.23	0/3196	0.40	0/4319
10	CK	0.23	0/1939	0.43	0/2608
11	CL	0.20	0/631	0.42	0/843
12	CM	0.24	0/1805	0.48	0/2417
12	LF	0.26	0/2061	0.46	0/2765
13	CN	0.20	0/1878	0.48	0/2555
14	CO	0.22	0/470	0.42	0/619
15	CQ	0.23	0/1504	0.44	0/2000
16	Lq	0.20	0/1091	0.42	0/1468
17	Cb	0.19	0/845	0.41	0/1128
18	Cd	0.22	0/3770	0.42	1/5082 (0.0%)
19	Ce	0.21	0/2173	0.40	0/2890
20	Cf	0.20	0/2326	0.41	0/3113
21	Cg	0.23	0/1508	0.41	0/2051
22	Ch	0.24	0/3914	0.51	1/5319 (0.0%)
23	Cz	0.25	0/877	0.53	0/1148
24	LA	0.23	0/1488	0.47	0/2009
25	LB	0.23	0/3172	0.45	0/4260
26	LC	0.21	0/2808	0.40	0/3785
27	LD	0.21	0/2308	0.41	1/3105 (0.0%)
28	LE	0.20	0/1504	0.43	0/2027
29	LG	0.26	0/1918	0.46	0/2565
30	LH	0.25	0/1515	0.49	0/2037
31	LJ	0.20	0/1379	0.47	0/1844

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LK	0.22	0/1198	0.50	0/1611
33	LL	0.19	0/1614	0.38	0/2168
34	LM	0.23	0/1145	0.45	0/1539
35	LN	0.24	0/1741	0.41	0/2332
36	LO	0.24	0/1645	0.41	0/2205
37	LP	0.21	0/1364	0.42	0/1835
38	LQ	0.24	0/1218	0.43	0/1639
39	LR	0.21	0/1260	0.38	0/1683
40	LS	0.23	0/1461	0.45	0/1966
41	LT	0.24	0/1046	0.51	0/1409
42	LU	0.21	0/859	0.46	0/1151
43	LV	0.20	0/1009	0.40	0/1357
44	LX	0.25	0/1151	0.49	0/1547
45	LY	0.21	0/1070	0.47	0/1432
46	LZ	0.21	0/1135	0.41	0/1519
47	La	0.21	0/892	0.37	0/1200
48	Lc	0.19	0/714	0.39	0/960
49	Ld	0.21	0/889	0.38	0/1192
50	Le	0.22	0/1035	0.44	0/1379
51	Lf	0.22	0/883	0.35	0/1187
52	Lg	0.22	0/927	0.42	0/1244
53	Lh	0.22	0/1014	0.42	0/1349
54	Li	0.21	0/834	0.44	0/1099
55	Lj	0.23	0/712	0.50	2/944 (0.2%)
56	Lk	0.19	0/640	0.36	0/850
57	Ll	0.21	0/446	0.35	0/593
58	Lp	0.23	0/706	0.53	0/940
All	All	0.25	1/166621 (0.0%)	0.41	6/241393 (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	5.19	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Cd	95	MET	CB-CG-SD	5.77	130.02	112.70
55	Lj	69	THR	CA-C-N	5.52	123.72	120.24
55	Lj	69	THR	C-N-CA	5.52	123.72	120.24
27	LD	257	LYS	CB-CG-CD	5.41	123.74	111.30
6	CF	176	LYS	CB-CG-CD	5.32	123.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ch	338	ALA	CB-CA-C	-5.27	110.07	117.23

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	33239	280	0
2	C2	3319	0	1678	12	0
3	C3	1754	0	890	17	0
4	C4	2536	0	1286	17	0
5	CB	2119	0	2170	25	0
6	CF	1934	0	1945	8	0
7	CH	5063	0	5157	35	0
8	CI	1234	0	1245	19	0
9	CJ	3116	0	3122	14	0
10	CK	1903	0	1990	9	0
11	CL	622	0	641	8	0
12	CM	1773	0	1879	14	0
12	LF	2023	0	2132	9	0
13	CN	1853	0	1852	17	0
14	CO	468	0	503	5	0
15	CQ	1480	0	1523	11	0
16	Lq	1073	0	1130	7	0
17	Cb	830	0	838	5	0
18	Cd	3691	0	3817	21	0
19	Ce	2148	0	2250	19	0
20	Cf	2282	0	2347	21	0
21	Cg	1478	0	1517	7	0
22	Ch	3812	0	3715	25	0
23	Cz	869	0	956	5	0
24	LA	1454	0	1490	6	0
25	LB	3104	0	3221	16	0
26	LC	2751	0	2875	12	0
27	LD	2266	0	2219	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	LE	1477	0	1567	13	0
29	LG	1889	0	2043	9	0
30	LH	1495	0	1573	10	0
31	LJ	1357	0	1385	15	0
32	LK	1184	0	1249	8	0
33	LL	1587	0	1655	6	0
34	LM	1126	0	1198	14	0
35	LN	1704	0	1767	12	0
36	LO	1611	0	1702	5	0
37	LP	1343	0	1369	8	0
38	LQ	1200	0	1296	7	0
39	LR	1241	0	1298	11	0
40	LS	1426	0	1481	15	0
41	LT	1027	0	1076	11	0
42	LU	846	0	883	5	0
43	LV	991	0	1044	4	0
44	LX	1133	0	1234	5	0
45	LY	1056	0	1143	9	0
46	LZ	1112	0	1181	9	0
47	La	872	0	903	7	0
48	Lc	705	0	751	5	0
49	Ld	875	0	918	4	0
50	Le	1017	0	1092	5	0
51	Lf	862	0	891	3	0
52	Lg	914	0	960	6	0
53	Lh	1003	0	1116	7	0
54	Li	827	0	906	2	0
55	Lj	698	0	726	7	0
56	Lk	632	0	693	10	0
57	Ll	436	0	473	2	0
58	Lp	698	0	737	6	0
59	CH	32	0	12	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	157262	0	123961	728	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 (728) 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:C1:3289:G:H1	1:C1:3298:U:H3	1.19	0.90
3:C3:40:G:H1	3:C3:45:U:H3	1.22	0.88
1:C1:2400:G:H1	1:C1:2473:U:H3	1.13	0.87
41:LT:79:ARG:NH1	41:LT:81:LYS:O	2.18	0.77
45:LY:30:MET:HB3	45:LY:100:PRO:HG2	1.65	0.77
58:Lp:85:ARG:NH1	58:Lp:88:GLU:OE1	2.19	0.76
1:C1:1054:U:H3	1:C1:1070:G:H1	0.84	0.75
27:LD:85:ALA:HB2	27:LD:258:TYR:HB2	1.75	0.68
4:C4:99:C:H5'	20:Cf:96:ARG:HH12	1.58	0.68
1:C1:949:A:H62	1:C1:1098:G:H8	1.42	0.68
1:C1:1180:A:OP2	11:CL:16:LYS:NZ	2.27	0.67
58:Lp:84:ARG:HH11	58:Lp:85:ARG:HH21	1.42	0.67
1:C1:2796:A:O2'	1:C1:2810:A:N6	2.28	0.66
40:LS:117:ARG:HB3	40:LS:119:ARG:HH11	1.61	0.65
1:C1:2899:A:H2'	25:LB:256:TRP:HB3	1.79	0.65
29:LG:208:SER:HA	29:LG:211:LYS:HE3	1.78	0.65
8:CI:284:PRO:HB2	8:CI:287:LYS:HB2	1.78	0.65
37:LP:11:PRO:O	37:LP:105:LYS:NZ	2.30	0.65
3:C3:57:A:OP2	5:CB:144:ARG:NH2	2.30	0.64
13:CN:118:HIS:HB3	13:CN:121:LEU:HD13	1.78	0.64
1:C1:2932:G:N7	10:CK:140:LYS:NZ	2.44	0.64
7:CH:395:LYS:H	7:CH:395:LYS:HE2	1.63	0.64
18:Cd:285:ILE:HD11	18:Cd:296:ALA:HB2	1.80	0.64
8:CI:246:ARG:NH2	19:Ce:443:ILE:OXT	2.31	0.63
22:Ch:489:ASP:HB3	22:Ch:508:LYS:HB3	1.79	0.63
3:C3:71:G:H1	3:C3:134:U:H3	1.45	0.63
20:Cf:227:LEU:HB3	20:Cf:253:MET:HB2	1.81	0.63
1:C1:984:A:N1	1:C1:1033:U:O2'	2.33	0.62
1:C1:2544:G:H5'	19:Ce:436:TRP:HE1	1.64	0.62
2:C2:12:A:OP1	37:LP:3:ARG:NH1	2.33	0.62
1:C1:1619:C:OP2	52:Lg:75:ARG:NH1	2.32	0.61
11:CL:73:ARG:NH2	41:LT:157:GLU:OE1	2.33	0.61
7:CH:303:GLN:NE2	7:CH:307:ASP:OD1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1809:G:HO2'	9:CJ:2:GLY:N	1.98	0.61
16:Lq:88:ARG:NH1	28:LE:24:ALA:O	2.34	0.61
2:C2:154:C:H5'	29:LG:184:LYS:HD3	1.81	0.60
30:LH:14:GLU:OE2	34:LM:2:ALA:N	2.34	0.60
1:C1:948:U:H2'	1:C1:949:A:H8	1.66	0.60
18:Cd:133:LYS:HE2	18:Cd:133:LYS:H	1.64	0.60
37:LP:41:LEU:HD21	37:LP:99:GLU:HG3	1.83	0.60
53:Lh:15:LYS:O	53:Lh:66:LYS:NZ	2.31	0.60
15:CQ:145:LEU:HD22	15:CQ:159:LEU:HB3	1.84	0.60
1:C1:2101:A:HO2'	55:Lj:2:THR:N	1.98	0.60
20:Cf:112:ASP:HB2	20:Cf:159:MET:HE2	1.82	0.60
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.37	0.60
1:C1:3109:U:H3	1:C1:3338:C:H42	1.50	0.59
45:LY:86:ARG:HB3	45:LY:96:ILE:HD11	1.84	0.59
1:C1:448:C:H41	28:LE:15:ARG:HH21	1.49	0.59
47:La:85:ASP:OD1	47:La:85:ASP:N	2.35	0.59
1:C1:2197:G:HO2'	18:Cd:2:GLY:N	2.01	0.59
1:C1:2591:G:H21	1:C1:2605:C:H41	1.49	0.59
1:C1:1611:C:OP2	46:LZ:47:ARG:NH2	2.33	0.59
7:CH:527:LEU:HD13	7:CH:550:ALA:HB2	1.84	0.59
3:C3:137:C:H3'	8:CI:279:ARG:HH21	1.67	0.59
4:C4:44:C:OP2	31:LJ:138:ARG:NH2	2.35	0.59
28:LE:131:GLU:OE1	28:LE:134:LYS:NZ	2.36	0.58
46:LZ:115:LYS:NZ	46:LZ:119:ASP:OD1	2.36	0.58
4:C4:88:G:N2	4:C4:91:A:OP2	2.35	0.58
34:LM:44:PRO:HG3	34:LM:81:VAL:HG12	1.85	0.58
24:LA:105:SER:HB3	24:LA:160:SER:HB3	1.84	0.58
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.32	0.58
7:CH:242:LEU:O	7:CH:280:LYS:NZ	2.36	0.58
3:C3:40:G:O6	3:C3:45:U:O4	2.22	0.58
22:Ch:35:GLY:O	22:Ch:56:ASN:ND2	2.37	0.58
46:LZ:49:PRO:HD3	46:LZ:67:ILE:HG12	1.85	0.58
2:C2:86:U:O2	55:Lj:87:ARG:NH1	2.37	0.58
37:LP:125:GLN:HB3	37:LP:141:SER:HB2	1.86	0.58
3:C3:64:G:O6	8:CI:278:ARG:NH2	2.38	0.57
9:CJ:112:LEU:H	9:CJ:115:LYS:HE3	1.68	0.57
5:CB:67:THR:HB	5:CB:280:ASN:HB2	1.87	0.57
53:Lh:34:LEU:HB3	53:Lh:49:ILE:HG22	1.86	0.57
3:C3:37:G:OP1	8:CI:316:ARG:NH1	2.38	0.57
1:C1:277:A:N1	1:C1:2744:A:O2'	2.37	0.57
21:Cg:152:ILE:HD13	41:LT:57:TYR:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C4:39:C:H4'	31:LJ:45:THR:HG23	1.85	0.57
7:CH:74:HIS:HD1	7:CH:76:PHE:H	1.52	0.57
33:LL:115:ARG:NH2	33:LL:155:PHE:O	2.35	0.57
11:CL:5:ILE:HD13	36:LO:49:PHE:HB2	1.87	0.56
12:CM:110:GLN:HG3	12:CM:115:ARG:HD3	1.85	0.56
12:CM:178:ASN:N	12:CM:178:ASN:HD22	2.03	0.56
18:Cd:427:TYR:O	18:Cd:445:LYS:NZ	2.39	0.56
7:CH:540:ASP:OD2	15:CQ:143:ARG:NH1	2.34	0.56
13:CN:109:VAL:HB	13:CN:149:GLY:HA2	1.86	0.56
19:Ce:258:ALA:HB2	46:LZ:123:SER:HB2	1.85	0.56
1:C1:278:A:H8	1:C1:297:G:H1'	1.70	0.56
1:C1:716:G:H5''	38:LQ:71:PRO:HB2	1.87	0.56
10:CK:163:ARG:HH12	18:Cd:228:LYS:HG2	1.71	0.56
38:LQ:110:VAL:HG12	38:LQ:112:ALA:H	1.70	0.56
1:C1:1842:U:OP1	39:LR:70:ARG:NH2	2.37	0.56
22:Ch:53:VAL:HG21	22:Ch:68:LEU:HD21	1.88	0.56
22:Ch:264:ILE:HD12	22:Ch:274:HIS:HB2	1.88	0.56
45:LY:1:MET:HE3	45:LY:2:LYS:HG3	1.87	0.56
34:LM:59:LEU:O	40:LS:155:ARG:NH2	2.38	0.56
34:LM:94:TRP:O	34:LM:97:THR:OG1	2.24	0.56
42:LU:106:SER:OG	42:LU:107:LYS:N	2.39	0.56
1:C1:3284:G:H21	1:C1:3303:A:H2	1.54	0.55
22:Ch:41:PHE:HD2	22:Ch:69:LEU:HD13	1.72	0.55
22:Ch:195:VAL:HG12	22:Ch:206:THR:HG22	1.89	0.55
1:C1:974:A:H5''	41:LT:43:LYS:HD2	1.89	0.55
1:C1:1095:A:H2'	1:C1:1096:G:C8	2.41	0.55
7:CH:505:GLU:OE2	15:CQ:174:LYS:NZ	2.38	0.55
9:CJ:143:ASP:OD2	19:Ce:413:ARG:NH2	2.36	0.55
20:Cf:47:ASN:OD1	20:Cf:59:ARG:NH1	2.40	0.55
1:C1:1939:U:O2'	1:C1:2045:G:N2	2.39	0.55
4:C4:86:C:N4	4:C4:87:G:O6	2.40	0.55
15:CQ:18:GLY:HA3	15:CQ:31:PHE:O	2.07	0.55
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.25	0.55
1:C1:1077:U:O2'	1:C1:1078:U:O2	2.24	0.55
1:C1:1420:OMC:HM22	1:C1:1421:U:H5'	1.89	0.55
1:C1:1685:U:O2	1:C1:1766:G:O2'	2.25	0.55
20:Cf:145:ALA:HB3	20:Cf:188:THR:HG22	1.89	0.55
1:C1:3:G:H1'	44:LX:36:LYS:HE3	1.88	0.55
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.23	0.55
29:LG:165:LEU:HA	35:LN:7:LEU:HD11	1.89	0.55
1:C1:1041:U:OP2	12:LF:104:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1920:G:H21	1:C1:3303:A:H8	1.52	0.54
9:CJ:42:ILE:HG13	9:CJ:72:LEU:HD11	1.89	0.54
22:Ch:470:LEU:HB2	22:Ch:484:LEU:HB2	1.88	0.54
18:Cd:411:ILE:HG13	18:Cd:439:LEU:HD11	1.90	0.54
22:Ch:178:SER:O	27:LD:167:LYS:NZ	2.41	0.54
1:C1:3204:C:H2'	1:C1:3205:G:H8	1.72	0.54
34:LM:20:LEU:HD21	34:LM:30:ILE:HD11	1.89	0.54
45:LY:26:ARG:O	45:LY:30:MET:HG3	2.08	0.54
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.73	0.54
1:C1:2632:A:OP1	31:LJ:96:ASN:ND2	2.40	0.54
1:C1:877:A:O2'	1:C1:879:U:OP2	2.26	0.53
34:LM:54:ARG:NH2	34:LM:76:ALA:O	2.37	0.53
1:C1:643:C:H2'	1:C1:644:A:H8	1.73	0.53
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.44	0.53
22:Ch:40:ASN:OD1	22:Ch:48:GLN:NE2	2.40	0.53
26:LC:211:ILE:HG13	26:LC:256:VAL:HB	1.90	0.53
26:LC:36:VAL:HG21	26:LC:251:LEU:HD21	1.89	0.53
24:LA:115:ASN:OD1	24:LA:128:ARG:NH1	2.40	0.53
18:Cd:406:HIS:ND1	18:Cd:408:GLU:OE2	2.39	0.53
5:CB:281:PHE:HB2	5:CB:294:TYR:HB3	1.91	0.53
7:CH:549:ARG:NH2	42:LU:27:GLN:OE1	2.41	0.53
19:Ce:417:GLU:OE2	19:Ce:419:ARG:NH1	2.41	0.53
17:Cb:92:MET:HG2	17:Cb:97:TYR:HB3	1.91	0.53
39:LR:136:ARG:O	39:LR:140:GLU:HG3	2.09	0.53
15:CQ:138:ARG:HB2	15:CQ:141:GLU:HG2	1.90	0.53
1:C1:244:G:N2	1:C1:245:U:O4	2.33	0.52
1:C1:669:U:O4	26:LC:119:LYS:NZ	2.40	0.52
30:LH:173:VAL:HG22	30:LH:185:LEU:HG	1.90	0.52
53:Lh:34:LEU:HD11	53:Lh:45:LYS:HD2	1.90	0.52
1:C1:8:C:OP1	9:CJ:93:ARG:NH1	2.42	0.52
14:CO:40:ILE:HD12	25:LB:208:THR:HG21	1.92	0.52
45:LY:54:GLU:HB2	45:LY:107:LYS:HB3	1.91	0.52
1:C1:1599:A:OP2	9:CJ:52:LYS:NZ	2.42	0.52
18:Cd:307:ARG:NH1	18:Cd:346:LEU:O	2.43	0.52
1:C1:259:C:OP1	35:LN:5:LYS:NZ	2.36	0.52
1:C1:1154:G:OP2	12:LF:223:ARG:NH1	2.42	0.52
13:CN:32:GLU:OE1	13:CN:50:ARG:NH1	2.43	0.52
51:Lf:16:LEU:HD11	51:Lf:33:LYS:HB2	1.91	0.52
22:Ch:338:ALA:O	22:Ch:360:ARG:NH1	2.40	0.52
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.38	0.52
7:CH:453:ASP:OD1	7:CH:453:ASP:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Cf:277:THR:HG22	20:Cf:279:GLN:H	1.75	0.52
28:LE:139:GLU:HG3	28:LE:152:LYS:HG2	1.92	0.52
40:LS:117:ARG:HB3	40:LS:119:ARG:NH1	2.24	0.52
1:C1:2892:A:OP2	43:LV:6:ARG:NH1	2.41	0.52
46:LZ:14:ARG:NH2	52:Lg:84:ASN:OD1	2.35	0.52
1:C1:3000:U:OP2	1:C1:3050:C:N4	2.42	0.52
1:C1:3079:U:H1'	1:C1:3080:A:H5''	1.91	0.52
12:CM:129:THR:HA	12:CM:132:MET:HE2	1.91	0.52
22:Ch:88:HIS:HB2	22:Ch:121:THR:HB	1.91	0.52
1:C1:2157:G:O6	18:Cd:315:ARG:NH2	2.37	0.52
9:CJ:75:GLU:HG3	9:CJ:77:LEU:H	1.74	0.51
12:CM:173:ALA:O	12:CM:177:GLU:HG3	2.10	0.51
1:C1:643:C:H2'	1:C1:644:A:C8	2.45	0.51
8:CI:292:GLN:HE22	8:CI:295:ARG:HH12	1.58	0.51
1:C1:966:G:O4'	41:LT:79:ARG:NH2	2.43	0.51
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.46	0.51
13:CN:186:VAL:HG12	13:CN:218:ILE:HD11	1.92	0.51
1:C1:2074:G:C6	17:Cb:76:ARG:HD3	2.45	0.51
1:C1:2231:U:O4	20:Cf:298:ARG:NH1	2.43	0.51
30:LH:54:LYS:HB3	30:LH:65:GLU:HB2	1.92	0.51
30:LH:127:MET:HE2	30:LH:218:ILE:HG22	1.92	0.51
41:LT:145:ASP:OD1	41:LT:145:ASP:N	2.43	0.51
1:C1:1142:A:OP1	38:LQ:31:GLY:N	2.44	0.51
1:C1:1552:G:O2'	19:Ce:425:ARG:NH1	2.43	0.51
9:CJ:25:LYS:HE3	9:CJ:73:LEU:HD11	1.92	0.51
34:LM:127:ARG:O	34:LM:131:GLU:HG3	2.11	0.51
17:Cb:25:ASP:OD1	17:Cb:31:HIS:ND1	2.40	0.51
34:LM:54:ARG:HG2	40:LS:70:LEU:HD22	1.92	0.51
3:C3:49:G:H4'	5:CB:238:SER:HB2	1.93	0.51
16:Lq:92:LYS:HG3	12:LF:11:ASP:HB3	1.93	0.51
19:Ce:363:ASP:OD1	19:Ce:363:ASP:N	2.38	0.51
25:LB:84:MET:O	25:LB:203:PRO:HA	2.11	0.51
1:C1:1698:A:H4'	39:LR:117:LYS:HD2	1.93	0.51
1:C1:3289:G:O6	1:C1:3298:U:O4	2.28	0.51
10:CK:11:ARG:CZ	10:CK:16:ARG:HD2	2.41	0.51
1:C1:967:U:H2'	1:C1:968:U:C6	2.46	0.51
9:CJ:400:VAL:HG21	12:CM:192:HIS:HA	1.92	0.51
1:C1:1929:G:OP2	39:LR:135:LYS:NZ	2.34	0.50
22:Ch:84:ARG:NH1	22:Ch:97:ASP:OD1	2.44	0.50
1:C1:2231:U:H1'	20:Cf:301:MET:HB2	1.93	0.50
25:LB:92:TYR:HB2	25:LB:158:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Cz:94:GLU:HA	23:Cz:97:GLU:HG3	1.92	0.50
1:C1:979:A:N6	1:C1:1033:U:O4	2.44	0.50
1:C1:1737:G:OP1	42:LU:101:ARG:NH2	2.35	0.50
2:C2:71:A:O2'	2:C2:83:C:N4	2.44	0.50
5:CB:295:GLN:HB3	8:CI:313:ARG:NH2	2.26	0.50
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.44	0.50
6:CF:44:SER:HG	6:CF:222:SER:HG	1.58	0.50
1:C1:1186:A:H62	1:C1:1283:G:H21	1.58	0.50
1:C1:1866:A:O2'	25:LB:227:PHE:O	2.27	0.50
31:LJ:118:ASP:OD1	31:LJ:120:SER:OG	2.29	0.50
41:LT:107:ARG:NH1	41:LT:111:GLU:OE2	2.44	0.50
1:C1:1816:C:O2'	1:C1:1822:A:N1	2.44	0.50
1:C1:2400:G:O6	1:C1:2473:U:O4	2.30	0.50
1:C1:3001:C:OP1	43:LV:47:ARG:NE	2.41	0.50
1:C1:300:A:H2'	1:C1:301:A:C8	2.46	0.50
18:Cd:364:TRP:HA	18:Cd:377:ASP:O	2.12	0.50
1:C1:3275:U:H4'	1:C1:3276:A:H5'	1.94	0.49
1:C1:1677:A:OP1	52:Lg:22:ARG:NH2	2.45	0.49
1:C1:2615:A:N6	1:C1:2672:U:O2'	2.43	0.49
21:Cg:71:THR:HG23	21:Cg:82:THR:HB	1.93	0.49
56:Lk:28:ASN:HB2	56:Lk:33:GLN:HG2	1.94	0.49
1:C1:1244:G:O2'	1:C1:1261:A:N1	2.37	0.49
5:CB:65:THR:HG23	5:CB:240:ASN:HD21	1.76	0.49
15:CQ:89:THR:O	15:CQ:93:MET:HG3	2.13	0.49
7:CH:183:VAL:HG21	7:CH:219:ASP:HB2	1.94	0.49
33:LL:167:GLU:OE1	47:La:95:LYS:NZ	2.45	0.49
1:C1:394:C:H2'	7:CH:622:LEU:HD23	1.95	0.49
1:C1:2176:A:H2'	1:C1:2177:A:C8	2.48	0.49
28:LE:61:LEU:HD11	28:LE:103:ILE:HG13	1.94	0.49
1:C1:1704:U:H1'	1:C1:1705:C:C6	2.48	0.49
1:C1:2396:U:H1'	35:LN:125:SER:HB3	1.94	0.49
5:CB:18:VAL:HG22	5:CB:294:TYR:HB2	1.93	0.49
7:CH:307:ASP:HA	7:CH:310:LYS:HG3	1.95	0.49
1:C1:644:A:H2'	1:C1:645:A:C8	2.47	0.49
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.48	0.49
5:CB:62:ILE:HG13	5:CB:255:LEU:HD11	1.94	0.49
13:CN:210:THR:HG23	13:CN:214:GLU:HG3	1.94	0.49
27:LD:214:LEU:HB3	27:LD:222:TYR:HB2	1.95	0.49
29:LG:175:LYS:HD2	54:Li:52:LEU:HD13	1.94	0.49
3:C3:30:G:OP1	8:CI:221:ASN:ND2	2.36	0.49
20:Cf:36:THR:HA	20:Cf:63:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LC:185:VAL:HG11	26:LC:231:GLY:HA3	1.94	0.48
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.48	0.48
1:C1:489:A:O2'	1:C1:3214:A:N1	2.41	0.48
1:C1:1193:U:H5	6:CF:3:LYS:HB2	1.78	0.48
8:CI:191:ILE:HA	8:CI:259:THR:O	2.13	0.48
12:CM:238:GLU:HB3	12:CM:239:GLU:H	1.47	0.48
28:LE:117:ALA:O	28:LE:121:GLU:HG3	2.13	0.48
1:C1:586:G:H1	1:C1:597:G:H5''	1.78	0.48
7:CH:19:ILE:HG21	7:CH:59:LYS:HE2	1.96	0.48
1:C1:1658:G:O6	42:LU:81:ARG:NH2	2.46	0.48
1:C1:2218:A:N6	1:C1:2226:C:O2	2.46	0.48
5:CB:82:LYS:O	5:CB:269:ARG:NH2	2.46	0.48
15:CQ:137:LEU:HD21	15:CQ:163:GLU:HB3	1.95	0.48
1:C1:388:A:H2'	1:C1:389:A2M:H8	1.95	0.48
1:C1:967:U:H2'	1:C1:968:U:H6	1.78	0.48
1:C1:2130:A:H2'	1:C1:2131:A:C8	2.48	0.48
1:C1:3008:U:O2'	15:CQ:16:SER:O	2.30	0.48
1:C1:3163:A:N6	1:C1:3217:U:O2	2.42	0.48
9:CJ:397:TRP:HB2	9:CJ:401:LEU:HD12	1.96	0.48
29:LG:27:ASN:HB3	29:LG:30:LEU:HG	1.95	0.48
1:C1:64:A:H5''	35:LN:174:LEU:HD13	1.95	0.48
19:Ce:434:GLU:HB3	19:Ce:439:LYS:HE3	1.96	0.48
25:LB:59:ASP:HB2	25:LB:358:LYS:HD3	1.95	0.48
38:LQ:98:ASN:HB3	38:LQ:165:LEU:HD21	1.96	0.48
1:C1:1054:U:O2	1:C1:1070:G:N2	2.37	0.48
1:C1:2476:U:H4'	29:LG:241:MET:HE2	1.96	0.48
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.79	0.48
8:CI:319:LYS:HE2	8:CI:319:LYS:HB3	1.60	0.48
13:CN:91:ASP:OD1	13:CN:91:ASP:N	2.47	0.48
25:LB:90:VAL:HG13	25:LB:104:THR:HG22	1.96	0.48
1:C1:2919:C:H2'	1:C1:2920:G:H8	1.78	0.48
4:C4:11:A:N1	4:C4:67:G:O2'	2.45	0.48
12:CM:22:ARG:NH2	19:Ce:378:GLU:OE1	2.46	0.48
27:LD:35:ARG:HA	27:LD:39:GLN:HG3	1.96	0.48
27:LD:37:ILE:HG13	27:LD:38:THR:HG23	1.96	0.48
32:LK:10:ILE:HG12	32:LK:65:GLN:HG3	1.96	0.48
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.49	0.47
3:C3:35:C:O2'	5:CB:288:THR:O	2.32	0.47
7:CH:250:LEU:HD11	7:CH:334:VAL:HG11	1.95	0.47
32:LK:8:ASN:OD1	32:LK:65:GLN:NE2	2.47	0.47
21:Cg:15:VAL:HG11	21:Cg:57:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LF:182:TYR:CZ	12:LF:203:GLN:HG2	2.49	0.47
32:LK:46:ILE:HA	32:LK:71:VAL:HG11	1.95	0.47
48:Lc:44:LEU:HD23	48:Lc:95:ILE:HD12	1.96	0.47
1:C1:652:A:H2'	1:C1:653:A:C8	2.48	0.47
5:CB:80:PRO:HD2	5:CB:181:PRO:HD3	1.96	0.47
36:LO:194:LYS:HE2	36:LO:194:LYS:H	1.78	0.47
1:C1:1812:OMC:H2'	1:C1:1813:G:H8	1.79	0.47
13:CN:152:MET:HE2	13:CN:154:LEU:HB2	1.94	0.47
19:Ce:260:GLU:OE2	46:LZ:89:GLU:N	2.47	0.47
1:C1:448:C:H42	1:C1:468:G:H1'	1.80	0.47
1:C1:2308:A:H5''	49:Ld:32:THR:HG23	1.97	0.47
2:C2:58:G:N7	55:Lj:63:ARG:NH2	2.44	0.47
3:C3:38:C:H5'	5:CB:67:THR:HG21	1.96	0.47
16:Lq:9:ILE:HG22	16:Lq:47:VAL:HG22	1.94	0.47
45:LY:112:LYS:HB3	45:LY:112:LYS:HE3	1.63	0.47
1:C1:410:A:H2'	1:C1:411:A:C8	2.49	0.47
7:CH:586:ARG:HH21	44:LX:156:VAL:HG12	1.79	0.47
20:Cf:113:MET:HB2	20:Cf:261:ARG:HB3	1.96	0.47
40:LS:12:ARG:HB3	40:LS:24:LEU:HD23	1.97	0.47
1:C1:948:U:H2'	1:C1:949:A:C8	2.47	0.47
1:C1:1726:C:O2'	56:Lk:4:GLU:OE1	2.30	0.47
1:C1:3141:G:C8	34:LM:9:THR:HG22	2.50	0.47
5:CB:174:THR:HG22	5:CB:176:THR:H	1.78	0.47
7:CH:526:PRO:HB2	7:CH:529:GLN:HG3	1.96	0.47
27:LD:261:ASP:OD1	27:LD:261:ASP:N	2.37	0.47
1:C1:341:C:O2	1:C1:345:A:O2'	2.32	0.47
1:C1:1054:U:O4	1:C1:1070:G:O6	2.33	0.47
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.50	0.47
15:CQ:181:ARG:NH1	15:CQ:182:ARG:O	2.47	0.47
35:LN:159:ARG:HB3	35:LN:164:LEU:HB2	1.96	0.47
7:CH:587:LEU:HD22	44:LX:146:LEU:HD13	1.96	0.47
11:CL:52:ASP:OD1	40:LS:80:ARG:NH2	2.43	0.47
36:LO:62:MET:HA	36:LO:72:PRO:HD2	1.97	0.47
51:Lf:55:TYR:CZ	51:Lf:67:ARG:HB2	2.49	0.47
1:C1:2801:U:OP1	11:CL:47:SER:N	2.48	0.47
1:C1:604:G:H2'	1:C1:605:G:C8	2.49	0.46
1:C1:1067:A:H2'	1:C1:1068:A:C8	2.50	0.46
22:Ch:60:ALA:HA	22:Ch:65:ILE:HD11	1.95	0.46
30:LH:141:GLU:HG2	30:LH:150:GLU:HB2	1.97	0.46
32:LK:40:LYS:HB2	32:LK:40:LYS:HE2	1.73	0.46
1:C1:1595:C:H2'	1:C1:1596:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ch:159[B]:SER:OG	22:Ch:499:ASP:OD1	2.33	0.46
30:LH:111:ILE:O	30:LH:115:MET:HG3	2.15	0.46
31:LJ:111:ILE:HD13	31:LJ:123:ILE:HG13	1.96	0.46
1:C1:1278:G:OP2	40:LS:84:ARG:NH1	2.48	0.46
11:CL:69:ILE:HG21	41:LT:160:ILE:HG21	1.97	0.46
47:La:76:ASP:HB3	47:La:116:GLY:HA3	1.96	0.46
2:C2:26:U:H2'	2:C2:27:U:C6	2.51	0.46
10:CK:132:MET:HE1	10:CK:214:VAL:HG11	1.97	0.46
1:C1:1264:U:H2'	1:C1:1265:G:C8	2.50	0.46
1:C1:1350:G:N2	1:C1:1351:U:O4	2.47	0.46
1:C1:1778:A:H2'	1:C1:1779:A:C8	2.51	0.46
27:LD:257:LYS:HE3	27:LD:257:LYS:HA	1.97	0.46
4:C4:37:G:N7	23:Cz:110:ARG:NH2	2.56	0.46
19:Ce:87:LYS:HE3	19:Ce:91:ILE:HD11	1.97	0.46
1:C1:464:C:H2'	1:C1:465:G:H8	1.80	0.46
1:C1:1395:G:H5''	50:Le:125:ALA:HB2	1.97	0.46
13:CN:107:VAL:HG23	13:CN:108:ILE:HG13	1.98	0.46
19:Ce:397:LYS:HE3	19:Ce:397:LYS:HB2	1.76	0.46
31:LJ:94:ARG:O	31:LJ:157:ARG:NH2	2.49	0.46
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.50	0.46
1:C1:2642:U:HO2'	31:LJ:131:CYS:HG	1.61	0.46
4:C4:93:G:H2'	4:C4:94:A:C8	2.50	0.46
34:LM:128:ARG:HD3	34:LM:132:ARG:CZ	2.46	0.46
3:C3:142:G:H1	8:CI:283:VAL:HG22	1.81	0.46
4:C4:53:U:O2'	4:C4:55:A:N7	2.48	0.46
7:CH:315:GLU:OE2	7:CH:337:ARG:NH1	2.48	0.46
22:Ch:320:HIS:CE1	22:Ch:385:TYR:HD2	2.34	0.46
30:LH:75:LEU:HD13	30:LH:108:VAL:HG13	1.98	0.46
35:LN:177:GLY:O	35:LN:184:ARG:NH1	2.49	0.46
1:C1:262:G:H5''	35:LN:14:LYS:HE2	1.97	0.46
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.97	0.46
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.51	0.46
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.51	0.46
1:C1:2221:U:H2'	1:C1:2222:A:H8	1.81	0.46
12:LF:114:LEU:HD21	12:LF:121:VAL:HG22	1.97	0.46
1:C1:1702:U:O4'	39:LR:96:MET:HG3	2.17	0.45
12:CM:23:LYS:O	12:CM:27:LYS:HG2	2.15	0.45
17:Cb:30:ARG:O	17:Cb:34:GLN:HG3	2.17	0.45
20:Cf:98:HIS:CD2	20:Cf:120:PRO:HG3	2.50	0.45
31:LJ:33:ARG:O	31:LJ:37:VAL:HG23	2.16	0.45
1:C1:20:U:H2'	1:C1:21:A:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:976:G:H4'	1:C1:977:U:H5'	1.98	0.45
27:LD:245:GLU:HG3	27:LD:249:GLN:HE21	1.81	0.45
46:LZ:22:VAL:HG12	46:LZ:44:GLY:HA3	1.98	0.45
46:LZ:69:PRO:HG3	46:LZ:114:LYS:HB2	1.98	0.45
1:C1:1677:A:H5'	52:Lg:34:LEU:HD21	1.97	0.45
9:CJ:131:TYR:OH	9:CJ:140:ASP:OD2	2.33	0.45
12:CM:126:THR:H	12:CM:129:THR:HG1	1.63	0.45
30:LH:68:ARG:NH1	30:LH:188:ASN:OD1	2.49	0.45
55:Lj:32:LYS:HA	55:Lj:32:LYS:HD3	1.80	0.45
1:C1:1100:G:H2'	1:C1:1101:C:H6	1.82	0.45
1:C1:2882:U:H2'	18:Cd:221:ARG:HD3	1.99	0.45
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.52	0.45
1:C1:2966:G:H5''	36:LO:62:MET:HE1	1.99	0.45
7:CH:361:LEU:O	7:CH:365:MET:HG2	2.16	0.45
21:Cg:150:ASP:O	21:Cg:170:ARG:NH1	2.30	0.45
25:LB:161:VAL:HG13	25:LB:184:ILE:HD11	1.97	0.45
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.81	0.45
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.82	0.45
53:Lh:46:LEU:O	53:Lh:49:ILE:HG13	2.16	0.45
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.52	0.45
13:CN:101:LEU:HA	43:LV:137:VAL:HG22	1.98	0.45
15:CQ:179:GLU:OE1	49:Ld:86:ARG:NH1	2.47	0.45
25:LB:288:LYS:HA	25:LB:288:LYS:HD2	1.75	0.45
1:C1:1698:A:H2'	1:C1:1699:G:H8	1.82	0.45
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.28	0.45
1:C1:2838:OMC:H5	1:C1:2906:G:H1	1.64	0.45
31:LJ:47:VAL:O	31:LJ:68:VAL:HA	2.16	0.45
33:LL:124:ILE:HG23	33:LL:138:THR:HG21	1.98	0.45
56:Lk:24:ARG:HA	56:Lk:69:LYS:O	2.16	0.45
1:C1:2169:G:H2'	1:C1:2170:A:C8	2.51	0.44
1:C1:2315:A:H5''	37:LP:83:TRP:O	2.17	0.44
1:C1:2971:U:H2'	1:C1:2972:U:C6	2.53	0.44
5:CB:70:LYS:HD2	5:CB:301:LEU:HD21	1.98	0.44
14:CO:13:ASN:OD1	14:CO:16:ARG:NH2	2.50	0.44
1:C1:1306:C:H4'	40:LS:2:GLY:N	2.33	0.44
19:Ce:237:GLU:OE2	19:Ce:240:ARG:NH2	2.51	0.44
40:LS:106:MET:HE3	40:LS:106:MET:HB3	1.78	0.44
2:C2:63:G:H22	2:C2:97:A:H2	1.64	0.44
5:CB:67:THR:HA	5:CB:239:THR:O	2.17	0.44
7:CH:532:ASP:O	7:CH:536:GLN:HG3	2.17	0.44
7:CH:549:ARG:NH2	42:LU:31:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LK:143:VAL:HG23	32:LK:148:PRO:HG3	1.99	0.44
39:LR:71:ARG:HE	39:LR:71:ARG:HB2	1.58	0.44
50:Le:97:ILE:HG21	50:Le:106:ARG:HG2	1.99	0.44
1:C1:30:C:H4'	1:C1:63:A:H4'	1.99	0.44
1:C1:656:U:H2'	1:C1:657:U:C6	2.52	0.44
1:C1:804:G:H2'	1:C1:805:C:H6	1.82	0.44
1:C1:1812:OMC:HM23	57:L1:7:PHE:HB2	1.98	0.44
1:C1:2164:G:H1	1:C1:2204:U:H3	1.64	0.44
1:C1:2512:U:OP1	52:Lg:103:LYS:NZ	2.44	0.44
1:C1:3111:C:C4	1:C1:3113:A:H1'	2.52	0.44
8:CI:292:GLN:NE2	8:CI:295:ARG:HH12	2.13	0.44
20:Cf:23:ILE:HD13	21:Cg:97:PRO:HD2	1.98	0.44
12:LF:174:ILE:O	12:LF:178:ASN:ND2	2.43	0.44
1:C1:980:A:H2'	1:C1:981:G:C8	2.52	0.44
1:C1:1449:G:N2	1:C1:1493:G:H5''	2.32	0.44
1:C1:1877:G:OP2	17:Cb:11:LYS:NZ	2.38	0.44
1:C1:2658:G:OP1	20:Cf:62:LYS:NZ	2.45	0.44
4:C4:78:A:H3'	4:C4:79:G:H8	1.82	0.44
13:CN:74:THR:OG1	15:CQ:74:ARG:NH2	2.50	0.44
31:LJ:92:LEU:O	31:LJ:172:VAL:HA	2.17	0.44
1:C1:2307:U:H2'	1:C1:2308:A:C8	2.53	0.44
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.82	0.44
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.53	0.44
6:CF:148:GLU:HG3	6:CF:214:ILE:HG12	2.00	0.44
7:CH:284:ILE:HB	7:CH:316:ILE:HD13	1.99	0.44
16:Lq:131:LYS:HA	16:Lq:131:LYS:HD3	1.70	0.44
39:LR:105:LEU:HD23	39:LR:138:LEU:HD23	2.00	0.44
41:LT:85:ILE:HD11	41:LT:87:LYS:HE2	2.00	0.44
1:C1:37:C:H4'	1:C1:790:A:C2	2.53	0.44
1:C1:351:G:N2	1:C1:354:A:OP2	2.46	0.44
1:C1:1159:C:H2'	1:C1:1160:G:N2	2.33	0.44
1:C1:2822:G:C2	7:CH:94:LEU:HD13	2.53	0.44
1:C1:3249:C:O2'	37:LP:69:ARG:O	2.35	0.44
5:CB:120:LEU:HD12	5:CB:221:VAL:HG13	1.99	0.44
7:CH:628:ASN:O	37:LP:125:GLN:NE2	2.51	0.44
26:LC:136:LEU:HD23	26:LC:143:VAL:HG11	2.00	0.44
44:LX:109:LYS:HE3	44:LX:109:LYS:HB2	1.79	0.44
4:C4:17:A:H2'	4:C4:18:G:H8	1.82	0.44
6:CF:94:ARG:HD2	6:CF:245:LYS:HD3	1.98	0.44
8:CI:297:LEU:HD23	8:CI:301:GLN:HB3	1.98	0.44
18:Cd:86:ASP:OD1	18:Cd:86:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Ce:318:LYS:HE3	19:Ce:318:LYS:HB3	1.77	0.44
25:LB:154:LYS:HE3	25:LB:154:LYS:HB2	1.84	0.44
28:LE:5:PRO:HB2	28:LE:16:THR:HG22	2.00	0.44
37:LP:54:LYS:HA	37:LP:83:TRP:CD1	2.53	0.44
1:C1:619:A:H2'	1:C1:620:G:C8	2.53	0.44
1:C1:698:A:H2'	1:C1:699:A:C8	2.52	0.44
1:C1:1555:C:H5''	19:Ce:428:ALA:HB2	2.00	0.44
1:C1:1623:A:H5''	1:C1:1624:C:C5	2.53	0.44
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.83	0.44
1:C1:2576:U:H1'	1:C1:2577:G:H5'	1.98	0.44
1:C1:3155:A:OP1	34:LM:109:ARG:NH1	2.51	0.44
12:CM:178:ASN:N	12:CM:178:ASN:ND2	2.65	0.44
53:Lh:107:GLU:H	53:Lh:107:GLU:CD	2.26	0.44
56:Lk:14:ILE:HA	56:Lk:17:ARG:HD3	1.99	0.44
1:C1:498:U:H2'	1:C1:499:C:C6	2.53	0.43
1:C1:663:C:O2'	1:C1:667:U:OP1	2.31	0.43
1:C1:1207:C:O2'	6:CF:8:ARG:NH2	2.51	0.43
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.82	0.43
13:CN:61:ARG:NH2	13:CN:105:GLY:O	2.49	0.43
25:LB:123:TYR:CZ	25:LB:124:LYS:HG3	2.53	0.43
32:LK:92:ARG:HH12	32:LK:98:ILE:HG12	1.83	0.43
7:CH:89:HIS:NE2	18:Cd:139:GLU:O	2.51	0.43
28:LE:86:PRO:HB3	28:LE:166:ASP:HB2	1.98	0.43
12:LF:56:LYS:HB3	12:LF:56:LYS:HE3	1.73	0.43
12:LF:92:VAL:O	12:LF:120:GLY:HA2	2.17	0.43
58:Lp:84:ARG:HG2	58:Lp:85:ARG:NH2	2.33	0.43
1:C1:652:A:H2'	1:C1:653:A:H8	1.82	0.43
1:C1:804:G:H2'	1:C1:805:C:C6	2.53	0.43
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.53	0.43
1:C1:2225:A:H2'	1:C1:2226:C:C6	2.52	0.43
1:C1:2666:U:H2'	1:C1:2667:C:C6	2.54	0.43
1:C1:3071:A:H2'	1:C1:3072:A:O4'	2.18	0.43
5:CB:109:LYS:HE3	5:CB:109:LYS:HB2	1.89	0.43
10:CK:61:MET:HE3	10:CK:61:MET:HB3	1.88	0.43
13:CN:21:ASN:HB2	13:CN:67:ARG:HB3	2.01	0.43
32:LK:88:PRO:HA	32:LK:89:PRO:HD3	1.92	0.43
1:C1:180:U:H1'	45:LY:128:VAL:HG11	2.00	0.43
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.52	0.43
1:C1:2953:A:O2'	2:C2:1:A:N1	2.47	0.43
18:Cd:273:ILE:HD13	18:Cd:296:ALA:HB1	2.00	0.43
19:Ce:331:GLU:HG3	56:Lk:54:LYS:HG3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Cf:104:ARG:HB3	20:Cf:112:ASP:OD1	2.17	0.43
22:Ch:465:SER:OG	22:Ch:466:LYS:N	2.52	0.43
58:Lp:78:ALA:O	58:Lp:82:THR:HG23	2.18	0.43
1:C1:2159:C:H2'	1:C1:2160:C:C6	2.54	0.43
1:C1:2771:C:H2'	1:C1:2772:A:C8	2.53	0.43
7:CH:300:GLU:OE2	7:CH:300:GLU:N	2.51	0.43
13:CN:14:GLY:O	13:CN:61:ARG:NH1	2.51	0.43
16:Lq:11:GLU:HA	16:Lq:14:ARG:HD2	2.00	0.43
20:Cf:169:ARG:HH12	20:Cf:172:PRO:HB3	1.84	0.43
24:LA:45:VAL:HG22	24:LA:61:VAL:HG22	1.99	0.43
48:Lc:47:ILE:HG21	48:Lc:56:LYS:HG3	1.99	0.43
1:C1:37:C:H4'	1:C1:790:A:H2	1.83	0.43
1:C1:1762:U:H2'	1:C1:1763:C:C6	2.53	0.43
1:C1:3078:C:OP2	10:CK:26:LYS:NZ	2.51	0.43
5:CB:305:LYS:HA	8:CI:296:PRO:HB3	2.01	0.43
7:CH:408:GLU:HG3	7:CH:417:PHE:HB3	2.00	0.43
10:CK:185:THR:HG23	10:CK:258:VAL:HG22	2.00	0.43
22:Ch:437:LYS:HD2	22:Ch:438:PHE:N	2.34	0.43
35:LN:73:ARG:HA	35:LN:74:PRO:HD3	1.90	0.43
47:La:101:VAL:HG22	47:La:124:VAL:HB	2.00	0.43
1:C1:448:C:H5	28:LE:15:ARG:HE	1.66	0.43
1:C1:882:G:H1'	1:C1:1569:A:N6	2.33	0.43
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.36	0.43
3:C3:10:C:H2'	3:C3:11:A:H8	1.82	0.43
4:C4:17:A:H2'	4:C4:18:G:C8	2.54	0.43
27:LD:98:ALA:HB1	27:LD:165:VAL:HG23	2.00	0.43
45:LY:79:ILE:HG23	45:LY:100:PRO:HG3	2.01	0.43
52:Lg:77:TYR:HB3	52:Lg:81:ARG:HB2	2.00	0.43
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.53	0.43
47:La:85:ASP:O	47:La:89:GLN:HG3	2.19	0.43
53:Lh:84:ASP:OD1	53:Lh:84:ASP:N	2.48	0.43
1:C1:42:G:H21	1:C1:2571:U:H4'	1.84	0.43
1:C1:425:G:H2'	1:C1:426:A:C8	2.54	0.43
1:C1:684:C:H2'	1:C1:685:G:C8	2.54	0.43
1:C1:2320:A:H2'	1:C1:2321:A:C8	2.54	0.43
1:C1:2888:C:H4'	18:Cd:209:ALA:HB2	2.00	0.43
10:CK:2:PRO:HB2	10:CK:6:TYR:CG	2.54	0.43
22:Ch:97:ASP:HB3	22:Ch:476:ARG:HG2	2.01	0.43
29:LG:117:THR:O	29:LG:121:GLU:HG3	2.19	0.43
1:C1:3238:U:O4	25:LB:124:LYS:NZ	2.52	0.43
27:LD:208:ALA:HB2	27:LD:239:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LE:118:LYS:HA	28:LE:118:LYS:HD3	1.82	0.43
38:LQ:150:THR:OG1	38:LQ:152:ASP:OD2	2.33	0.43
49:Ld:28:LEU:HD11	49:Ld:40:ALA:HB2	2.01	0.43
1:C1:21:A:H2'	1:C1:22:G:C8	2.54	0.42
1:C1:551:C:H2'	1:C1:552:C:H6	1.83	0.42
1:C1:1403:C:OP2	26:LC:197:LYS:NZ	2.51	0.42
1:C1:2692:A:H2'	1:C1:2693:A:C8	2.54	0.42
1:C1:2889:A:H2'	1:C1:2890:C:C6	2.54	0.42
5:CB:282:TYR:HB3	5:CB:290:ALA:HB1	2.01	0.42
23:Cz:99:LEU:HD23	23:Cz:99:LEU:HA	1.88	0.42
56:Lk:7:ASP:OD2	56:Lk:10:LYS:N	2.41	0.42
1:C1:2518:G:C6	24:LA:64:ARG:HD2	2.54	0.42
3:C3:59:A:HO2'	8:CI:230:ARG:HE	1.61	0.42
5:CB:70:LYS:HG2	5:CB:277:ASN:HD21	1.84	0.42
7:CH:4:TRP:CH2	7:CH:68:PRO:HB3	2.54	0.42
14:CO:106:ILE:HG23	14:CO:107:VAL:HG13	2.00	0.42
18:Cd:358:PRO:HD2	18:Cd:400:ARG:HG2	2.00	0.42
20:Cf:32:PHE:HB2	20:Cf:59:ARG:HG2	2.00	0.42
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.83	0.42
1:C1:3288:A:H2'	1:C1:3289:G:H8	1.84	0.42
3:C3:41:C:H41	8:CI:308:LYS:HE3	1.84	0.42
7:CH:293:LYS:HB2	7:CH:296:GLU:HG3	2.01	0.42
12:CM:94:ARG:NH1	12:CM:95:ILE:O	2.52	0.42
26:LC:286:ASP:OD2	26:LC:289:ARG:NH2	2.52	0.42
30:LH:167:MET:SD	30:LH:196:SER:HB3	2.59	0.42
31:LJ:127:ASP:OD1	31:LJ:127:ASP:N	2.52	0.42
53:Lh:11:GLN:H	53:Lh:11:GLN:HG2	1.68	0.42
6:CF:62:ASP:OD1	6:CF:62:ASP:N	2.45	0.42
20:Cf:116:PHE:HB3	20:Cf:255:PHE:CD1	2.55	0.42
23:Cz:90:LYS:HE3	23:Cz:90:LYS:HB3	1.86	0.42
28:LE:194:LYS:HB3	28:LE:196:HIS:CE1	2.54	0.42
38:LQ:69:GLU:H	38:LQ:69:GLU:CD	2.26	0.42
1:C1:1161:G:O6	51:Lf:22:ARG:HG2	2.19	0.42
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.54	0.42
21:Cg:170:ARG:NH2	41:LT:90:ASN:O	2.53	0.42
1:C1:582:G:H1'	28:LE:37:LYS:HG3	2.02	0.42
1:C1:2473:U:O2'	1:C1:2474:A:O5'	2.34	0.42
1:C1:3245:C:O3'	25:LB:335:ARG:NH2	2.53	0.42
1:C1:3299:U:H2'	1:C1:3300:A:H8	1.84	0.42
7:CH:544:ILE:HB	7:CH:549:ARG:HH12	1.84	0.42
18:Cd:135:THR:HG22	18:Cd:138:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LK:45:ASP:OD1	32:LK:45:ASP:N	2.49	0.42
1:C1:162:U:H5'	33:LL:135:LYS:HE2	2.01	0.42
1:C1:289:A:H2'	1:C1:290:A:C8	2.55	0.42
1:C1:2219:A:N6	1:C1:2221:U:OP1	2.53	0.42
1:C1:2723:C:H2'	1:C1:2724:C:C6	2.55	0.42
8:CI:313:ARG:NH1	8:CI:332:LEU:HD21	2.34	0.42
20:Cf:30:CYS:HA	20:Cf:86:LEU:O	2.18	0.42
22:Ch:148:PRO:HB3	22:Ch:508:LYS:HA	2.01	0.42
50:Le:56:ILE:HD12	50:Le:56:ILE:HA	1.91	0.42
1:C1:76:G:H5'	33:LL:58:VAL:HB	2.02	0.42
1:C1:970:U:H2'	1:C1:971:A:C8	2.54	0.42
7:CH:341:GLU:OE1	7:CH:345:GLN:NE2	2.53	0.42
1:C1:1126:A:H5''	50:Le:39:ILE:HD11	2.02	0.42
4:C4:55:A:H5''	31:LJ:5:LYS:HD3	2.01	0.42
13:CN:152:MET:HG3	13:CN:161:VAL:HG12	2.02	0.42
24:LA:66:PRO:HG2	24:LA:67:TYR:CE2	2.55	0.42
39:LR:8:LYS:HG2	39:LR:19:GLU:HG2	2.02	0.42
40:LS:40:ARG:HA	40:LS:40:ARG:HD2	1.92	0.42
1:C1:575:G:H2'	1:C1:576:A:H8	1.85	0.42
22:Ch:173:ILE:HD11	22:Ch:204:LEU:HD22	2.02	0.42
48:Lc:19:LEU:O	48:Lc:23:SER:OG	2.38	0.42
48:Lc:77:ASN:OD1	48:Lc:77:ASN:N	2.53	0.42
56:Lk:50:LYS:HD2	56:Lk:50:LYS:HA	1.85	0.42
1:C1:119:U:H5''	19:Ce:106:ARG:HH22	1.85	0.41
1:C1:1614:G:N7	46:LZ:16:ARG:NH2	2.67	0.41
1:C1:2226:C:H2'	1:C1:2227:U:H6	1.85	0.41
5:CB:292:PRO:HD2	8:CI:320:LEU:HD11	2.01	0.41
6:CF:196:LYS:HE2	6:CF:196:LYS:HB2	1.82	0.41
8:CI:291:ARG:HA	8:CI:294:GLU:HB2	2.01	0.41
11:CL:14:LYS:HE2	11:CL:14:LYS:HB3	1.82	0.41
16:Lq:20:LEU:HD12	16:Lq:20:LEU:HA	1.89	0.41
22:Ch:339:TYR:CZ	22:Ch:353:ARG:HD2	2.55	0.41
34:LM:27:LEU:HD11	34:LM:94:TRP:CG	2.55	0.41
38:LQ:126:MET:O	38:LQ:146:GLY:HA3	2.20	0.41
1:C1:405:G:H2'	1:C1:406:U:C6	2.55	0.41
1:C1:1929:G:OP1	39:LR:104:ARG:NH1	2.48	0.41
1:C1:2884:C:H2'	1:C1:2885:A:C4	2.55	0.41
2:C2:83:C:N3	45:LY:50:ARG:NH2	2.57	0.41
5:CB:84:ILE:HD12	5:CB:226:LYS:HG2	2.02	0.41
7:CH:309:THR:HG21	7:CH:316:ILE:HG12	2.01	0.41
58:Lp:73:THR:HG22	58:Lp:76:ALA:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:203:A:H4'	1:C1:205:A:N7	2.35	0.41
1:C1:283:G:H2'	1:C1:284:C:C6	2.55	0.41
1:C1:1584:U:H2'	1:C1:1585:A:O4'	2.19	0.41
1:C1:1814:U:OP2	57:Ll:10:LYS:NZ	2.50	0.41
1:C1:2101:A:C4	55:Lj:3:LYS:HB3	2.55	0.41
1:C1:3184:C:O2	14:CO:93:ARG:NH2	2.44	0.41
4:C4:88:G:O2'	4:C4:91:A:N6	2.53	0.41
7:CH:374:MET:HE2	13:CN:175:SER:HB3	2.02	0.41
30:LH:122:GLY:HA3	30:LH:226:ILE:HD12	2.03	0.41
33:LL:167:GLU:OE2	47:La:90:TYR:OH	2.24	0.41
1:C1:1372:G:H5''	50:Le:102:SER:HB3	2.00	0.41
1:C1:1503:G:O2'	1:C1:1583:A:N1	2.48	0.41
1:C1:3120:C:H2'	1:C1:3121:G:C8	2.56	0.41
5:CB:119:ASP:OD1	5:CB:119:ASP:N	2.53	0.41
20:Cf:290:ASP:OD1	20:Cf:294:ASP:N	2.53	0.41
22:Ch:470:LEU:HD11	22:Ch:505:SER:HB3	2.01	0.41
12:LF:61:TYR:O	12:LF:65:GLU:HG3	2.19	0.41
34:LM:82:LYS:O	34:LM:86:GLU:HG2	2.21	0.41
43:LV:61:MET:HE3	43:LV:75:VAL:HG12	2.02	0.41
1:C1:2801:U:O2'	1:C1:2805:U:N3	2.54	0.41
1:C1:2981:U:H2'	1:C1:2982:A:H8	1.86	0.41
2:C2:26:U:O2'	26:LC:52:ALA:O	2.38	0.41
5:CB:138:LYS:H	5:CB:138:LYS:HG2	1.71	0.41
20:Cf:48:ASP:OD2	20:Cf:123:TYR:OH	2.38	0.41
1:C1:464:C:H2'	1:C1:465:G:C8	2.56	0.41
1:C1:1584:U:H4'	1:C1:1815:A:H4'	2.02	0.41
1:C1:2123:G:H2'	1:C1:2124:G:C8	2.55	0.41
1:C1:2277:OMU:H6	1:C1:2277:OMU:O5'	2.20	0.41
1:C1:2633:A:H5''	31:LJ:106:GLY:HA3	2.01	0.41
7:CH:508:MET:HE1	49:Ld:66:LYS:HB2	2.01	0.41
11:CL:67:GLN:HG3	23:Cz:64:LYS:NZ	2.36	0.41
12:CM:90:VAL:HG23	12:CM:123:VAL:HB	2.02	0.41
34:LM:21:LYS:HD2	34:LM:94:TRP:HH2	1.86	0.41
1:C1:802:A:H2'	1:C1:803:U:C6	2.56	0.41
1:C1:1198:A:H2'	1:C1:1199:C:C6	2.56	0.41
1:C1:1305:U:O2'	40:LS:1:MET:SD	2.74	0.41
1:C1:3118:C:O2'	1:C1:3119:A:H8	2.04	0.41
1:C1:3209:A:C5	28:LE:154:VAL:HG21	2.55	0.41
3:C3:10:C:H2'	3:C3:11:A:C8	2.55	0.41
9:CJ:189:PHE:HB3	9:CJ:196:TYR:HB2	2.02	0.41
9:CJ:401:LEU:HD23	9:CJ:401:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ch:100:PRO:HG3	22:Ch:106:LEU:HD22	2.03	0.41
26:LC:273:LYS:HE2	26:LC:273:LYS:HB2	1.87	0.41
39:LR:98:ARG:NH1	39:LR:130:ASN:OD1	2.43	0.41
44:LX:69:ARG:HH12	44:LX:102:LYS:NZ	2.19	0.41
1:C1:284:C:OP1	35:LN:68:ARG:HB2	2.21	0.41
1:C1:287:A:OP2	35:LN:15:GLN:NE2	2.49	0.41
1:C1:896:A:N3	24:LA:204:MET:HG2	2.36	0.41
1:C1:2236:G:N3	1:C1:2238:A:H1'	2.36	0.41
7:CH:19:ILE:O	7:CH:23:ARG:HG2	2.21	0.41
10:CK:149:ARG:HH22	18:Cd:44:GLY:HA2	1.85	0.41
13:CN:168:GLN:H	13:CN:168:GLN:CD	2.28	0.41
26:LC:59:HIS:NE2	26:LC:99:ARG:HD3	2.36	0.41
40:LS:96:GLU:HG3	40:LS:102:ALA:HA	2.03	0.41
1:C1:64:A:N3	1:C1:79:U:O2'	2.47	0.41
1:C1:636:C:H2'	1:C1:637:A2M:O4'	2.20	0.41
1:C1:1211:A:H5''	6:CF:203:SER:HB3	2.03	0.41
1:C1:2224:G:H3'	1:C1:2225:A:H8	1.86	0.41
1:C1:2504:G:H2'	1:C1:2505:U:H6	1.85	0.41
1:C1:2706:A:H2'	1:C1:2707:A:C8	2.56	0.41
1:C1:2958:G:H2'	1:C1:2959:U:C6	2.56	0.41
1:C1:3236:A:H2'	1:C1:3237:A:C8	2.56	0.41
2:C2:95:G:O2'	55:Lj:81:GLY:O	2.31	0.41
3:C3:36:C:H2'	3:C3:37:G:H8	1.86	0.41
5:CB:251:GLU:H	5:CB:254:LYS:HZ3	1.68	0.41
9:CJ:376:ARG:NH1	9:CJ:398:ASP:OD2	2.53	0.41
12:CM:182:TYR:CZ	12:CM:203:GLN:HG2	2.55	0.41
18:Cd:235:VAL:O	18:Cd:329:VAL:HA	2.21	0.41
18:Cd:481:GLU:HA	18:Cd:482:PRO:HD3	1.94	0.41
19:Ce:391:ASP:OD2	19:Ce:391:ASP:N	2.54	0.41
21:Cg:43:ASP:HB3	21:Cg:46:VAL:HG22	2.03	0.41
26:LC:24:PRO:HG2	26:LC:265:LEU:HD23	2.02	0.41
31:LJ:76:LYS:HB2	31:LJ:76:LYS:HE2	1.89	0.41
40:LS:100:VAL:O	40:LS:104:GLU:HG3	2.21	0.41
41:LT:111:GLU:HA	41:LT:114:GLU:HG3	2.03	0.41
55:Lj:43:LYS:HB2	55:Lj:43:LYS:HE3	1.79	0.41
58:Lp:84:ARG:NH1	58:Lp:85:ARG:HE	2.19	0.41
1:C1:378:A:H2'	1:C1:379:A:C8	2.56	0.41
1:C1:2508:A:H2'	1:C1:2509:A:C8	2.56	0.41
1:C1:2986:G:H2'	1:C1:2987:A:C8	2.56	0.41
4:C4:93:G:H2'	4:C4:94:A:H8	1.85	0.41
14:CO:89:LYS:HA	14:CO:89:LYS:HD2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Lq:31:ASP:HB3	16:Lq:34:ASN:HB2	2.03	0.41
25:LB:262:GLN:HG2	36:LO:65:TYR:HA	2.03	0.41
27:LD:60:ILE:HB	27:LD:80:SER:HB3	2.03	0.41
1:C1:575:G:H2'	1:C1:576:A:C8	2.57	0.40
1:C1:2687:G:C6	18:Cd:325:LYS:HG2	2.56	0.40
1:C1:3026:C:OP2	39:LR:62:ARG:NH2	2.49	0.40
4:C4:99:C:OP1	20:Cf:96:ARG:NH2	2.53	0.40
22:Ch:61:THR:O	22:Ch:65:ILE:HG12	2.20	0.40
22:Ch:145:HIS:CE1	22:Ch:172:ARG:HD2	2.56	0.40
29:LG:85:LEU:HD22	29:LG:89:LEU:HD23	2.02	0.40
31:LJ:38:LEU:HD13	31:LJ:70:VAL:HG23	2.02	0.40
56:Lk:63:PRO:HA	56:Lk:64:PRO:HD3	1.88	0.40
1:C1:1323:C:H2'	1:C1:1324:U:C6	2.56	0.40
19:Ce:316:LYS:O	19:Ce:320:GLU:HG3	2.20	0.40
35:LN:28:TRP:O	35:LN:32:GLN:HG2	2.20	0.40
48:Lc:93:MET:HE3	48:Lc:93:MET:HB2	1.97	0.40
1:C1:163:U:H2'	1:C1:164:U:C6	2.57	0.40
1:C1:1103:A:H2'	1:C1:1104:U:H6	1.86	0.40
1:C1:1214:A:H5''	1:C1:1215:C:H5'	2.02	0.40
27:LD:116:ASP:OD1	27:LD:116:ASP:N	2.38	0.40
29:LG:73:LYS:HB3	29:LG:73:LYS:HE2	1.92	0.40
40:LS:45:LEU:HD23	40:LS:45:LEU:HA	1.83	0.40
1:C1:400:A:C2	2:C2:17:A:H1'	2.56	0.40
1:C1:813:G:O2'	1:C1:1844:A:N3	2.43	0.40
1:C1:1900:U:O2'	1:C1:1912:A:N7	2.45	0.40
1:C1:2925:G:H2'	1:C1:2926:A:C8	2.56	0.40
12:CM:114:LEU:HD21	12:CM:121:VAL:HG22	2.02	0.40
35:LN:9:GLU:HB2	54:Li:53:ILE:HG13	2.04	0.40
56:Lk:25:ILE:HG13	56:Lk:68:ILE:HD11	2.03	0.40
1:C1:462:A:H2'	1:C1:463:C:C6	2.57	0.40
1:C1:1413:U:H2'	47:La:9:ARG:HH22	1.87	0.40
1:C1:3194:G:H2'	1:C1:3195:U:C6	2.56	0.40
4:C4:1:A:C8	27:LD:271:LYS:HG2	2.57	0.40
13:CN:21:ASN:ND2	13:CN:112:ASP:OD2	2.46	0.40
25:LB:313:VAL:HG23	25:LB:365:GLU:HG3	2.03	0.40
25:LB:358:LYS:HE3	25:LB:358:LYS:HB3	1.95	0.40
26:LC:55:GLU:H	26:LC:55:GLU:HG3	1.64	0.40
40:LS:135:VAL:HG12	40:LS:141:LYS:HG2	2.02	0.40
56:Lk:53:ASP:O	56:Lk:57:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CB	261/391 (67%)	256 (98%)	5 (2%)	0	100	100
6	CF	243/270 (90%)	238 (98%)	5 (2%)	0	100	100
7	CH	621/661 (94%)	614 (99%)	7 (1%)	0	100	100
8	CI	150/414 (36%)	149 (99%)	1 (1%)	0	100	100
9	CJ	376/679 (55%)	374 (100%)	2 (0%)	0	100	100
10	CK	231/261 (88%)	226 (98%)	5 (2%)	0	100	100
11	CL	77/558 (14%)	77 (100%)	0	0	100	100
12	CM	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
12	LF	246/249 (99%)	240 (98%)	6 (2%)	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%)	179 (99%)	2 (1%)	0	100	100
16	Lq	137/147 (93%)	132 (96%)	5 (4%)	0	100	100
17	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
18	Cd	458/627 (73%)	454 (99%)	4 (1%)	0	100	100
19	Ce	252/443 (57%)	251 (100%)	1 (0%)	0	100	100
20	Cf	281/350 (80%)	279 (99%)	2 (1%)	0	100	100
21	Cg	186/202 (92%)	186 (100%)	0	0	100	100
22	Ch	484/517 (94%)	471 (97%)	13 (3%)	0	100	100
23	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
24	LA	189/254 (74%)	187 (99%)	2 (1%)	0	100	100
25	LB	387/392 (99%)	381 (98%)	6 (2%)	0	100	100
26	LC	361/365 (99%)	355 (98%)	6 (2%)	0	100	100
27	LD	282/304 (93%)	278 (99%)	4 (1%)	0	100	100
28	LE	187/200 (94%)	184 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LG	233/262 (89%)	228 (98%)	5 (2%)	0	100	100
30	LH	188/229 (82%)	186 (99%)	2 (1%)	0	100	100
31	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
32	LK	156/165 (94%)	155 (99%)	1 (1%)	0	100	100
33	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
34	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
35	LN	200/203 (98%)	196 (98%)	4 (2%)	0	100	100
36	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
37	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
38	LQ	148/213 (70%)	147 (99%)	1 (1%)	0	100	100
39	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
40	LS	172/174 (99%)	170 (99%)	2 (1%)	0	100	100
41	LT	127/160 (79%)	126 (99%)	1 (1%)	0	100	100
42	LU	103/127 (81%)	101 (98%)	2 (2%)	0	100	100
43	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
44	LX	143/156 (92%)	142 (99%)	1 (1%)	0	100	100
45	LY	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
46	LZ	133/135 (98%)	132 (99%)	1 (1%)	0	100	100
47	La	104/149 (70%)	104 (100%)	0	0	100	100
48	Lc	93/108 (86%)	93 (100%)	0	0	100	100
49	Ld	108/120 (90%)	108 (100%)	0	0	100	100
50	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
51	Lf	106/109 (97%)	106 (100%)	0	0	100	100
52	Lg	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
53	Lh	120/935 (13%)	117 (98%)	3 (2%)	0	100	100
54	Li	99/110 (90%)	99 (100%)	0	0	100	100
55	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
56	Lk	74/94 (79%)	74 (100%)	0	0	100	100
57	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
58	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
All	All	10361/16395 (63%)	10225 (99%)	136 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	228/329 (69%)	227 (100%)	1 (0%)	84	89
6	CF	212/236 (90%)	211 (100%)	1 (0%)	81	87
7	CH	549/575 (96%)	544 (99%)	5 (1%)	70	78
8	CI	124/336 (37%)	121 (98%)	3 (2%)	43	48
9	CJ	331/579 (57%)	330 (100%)	1 (0%)	86	91
10	CK	206/225 (92%)	203 (98%)	3 (2%)	57	65
11	CL	61/458 (13%)	60 (98%)	1 (2%)	55	63
12	CM	185/215 (86%)	181 (98%)	4 (2%)	45	52
12	LF	213/215 (99%)	212 (100%)	1 (0%)	81	87
13	CN	205/206 (100%)	203 (99%)	2 (1%)	68	76
14	CO	48/99 (48%)	48 (100%)	0	100	100
15	CQ	144/192 (75%)	143 (99%)	1 (1%)	76	83
16	Lq	109/112 (97%)	109 (100%)	0	100	100
17	Cb	85/101 (84%)	83 (98%)	2 (2%)	43	48
18	Cd	403/541 (74%)	403 (100%)	0	100	100
19	Ce	223/383 (58%)	221 (99%)	2 (1%)	70	78
20	Cf	250/310 (81%)	249 (100%)	1 (0%)	84	89
21	Cg	158/176 (90%)	155 (98%)	3 (2%)	50	57
22	Ch	408/436 (94%)	404 (99%)	4 (1%)	68	76
23	Cz	89/107 (83%)	86 (97%)	3 (3%)	32	35
24	LA	150/198 (76%)	148 (99%)	2 (1%)	61	69
25	LB	329/331 (99%)	329 (100%)	0	100	100
26	LC	282/285 (99%)	280 (99%)	2 (1%)	76	83
27	LD	221/253 (87%)	219 (99%)	2 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LE	157/166 (95%)	156 (99%)	1 (1%)	78	85
29	LG	200/222 (90%)	199 (100%)	1 (0%)	81	87
30	LH	167/200 (84%)	165 (99%)	2 (1%)	63	71
31	LJ	140/150 (93%)	137 (98%)	3 (2%)	47	54
32	LK	127/136 (93%)	127 (100%)	0	100	100
33	LL	158/176 (90%)	157 (99%)	1 (1%)	78	85
34	LM	116/117 (99%)	114 (98%)	2 (2%)	53	61
35	LN	179/180 (99%)	178 (99%)	1 (1%)	78	85
36	LO	162/163 (99%)	162 (100%)	0	100	100
37	LP	133/152 (88%)	133 (100%)	0	100	100
38	LQ	128/178 (72%)	127 (99%)	1 (1%)	73	80
39	LR	125/2396 (5%)	123 (98%)	2 (2%)	55	63
40	LS	152/154 (99%)	152 (100%)	0	100	100
41	LT	110/135 (82%)	107 (97%)	3 (3%)	39	44
42	LU	92/108 (85%)	91 (99%)	1 (1%)	65	74
43	LV	98/102 (96%)	98 (100%)	0	100	100
44	LX	122/129 (95%)	120 (98%)	2 (2%)	55	63
45	LY	116/119 (98%)	113 (97%)	3 (3%)	40	45
46	LZ	121/121 (100%)	121 (100%)	0	100	100
47	La	93/122 (76%)	93 (100%)	0	100	100
48	Lc	76/88 (86%)	75 (99%)	1 (1%)	61	69
49	Ld	90/105 (86%)	90 (100%)	0	100	100
50	Le	109/114 (96%)	109 (100%)	0	100	100
51	Lf	89/90 (99%)	87 (98%)	2 (2%)	45	52
52	Lg	95/102 (93%)	95 (100%)	0	100	100
53	Lh	109/781 (14%)	109 (100%)	0	100	100
54	Li	85/93 (91%)	83 (98%)	2 (2%)	43	48
55	Lj	72/78 (92%)	70 (97%)	2 (3%)	38	42
56	Lk	73/88 (83%)	72 (99%)	1 (1%)	59	67
57	Ll	45/46 (98%)	45 (100%)	0	100	100
58	Lp	73/74 (99%)	71 (97%)	2 (3%)	39	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	8825/13783 (64%)	8748 (99%)	77 (1%)	68	78

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	CB	255	LEU
6	CF	149	VAL
7	CH	85	TYR
7	CH	168	THR
7	CH	364	VAL
7	CH	469	GLU
7	CH	655	ILE
8	CI	198	PHE
8	CI	263	VAL
8	CI	310	GLU
9	CJ	381	GLN
10	CK	57	GLN
10	CK	98	THR
10	CK	185	THR
11	CL	67	GLN
12	CM	132	MET
12	CM	162	VAL
12	CM	178	ASN
12	CM	238	GLU
13	CN	121	LEU
13	CN	168	GLN
15	CQ	173	SER
17	Cb	27	ARG
17	Cb	68	HIS
19	Ce	102	SER
19	Ce	396	LEU
20	Cf	166	ASP
21	Cg	19	THR
21	Cg	49	GLN
21	Cg	71	THR
22	Ch	142	ILE
22	Ch	222	LYS
22	Ch	426	ASN
22	Ch	488	GLU
23	Cz	72	LYS
23	Cz	86	ARG
23	Cz	98	GLN

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Mol	Chain	Res	Type
24	LA	114	SER
24	LA	118	GLU
26	LC	21	GLU
26	LC	270	GLU
27	LD	51	LEU
27	LD	242	LEU
28	LE	6	THR
12	LF	90	VAL
29	LG	169	LEU
30	LH	56	SER
30	LH	85	VAL
31	LJ	45	THR
31	LJ	127	ASP
31	LJ	171	ILE
33	LL	177	ILE
34	LM	14	VAL
34	LM	35	ASP
35	LN	64	VAL
38	LQ	41	SER
39	LR	51	ILE
39	LR	68	LEU
41	LT	72	VAL
41	LT	115	LEU
41	LT	124	VAL
42	LU	106	SER
44	LX	37	THR
44	LX	83	GLU
45	LY	46	SER
45	LY	78	VAL
45	LY	93	THR
48	Lc	101	SER
51	Lf	3	SER
51	Lf	51	VAL
54	Li	67	ILE
54	Li	105	GLU
55	Lj	6	SER
55	Lj	7	SER
56	Lk	22	SER
58	Lp	11	SER
58	Lp	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
6	CF	11	HIS
6	CF	14	GLN
7	CH	14	GLN
7	CH	77	HIS
7	CH	345	GLN
7	CH	459	GLN
8	CI	303	GLN
8	CI	311	GLN
9	CJ	200	ASN
9	CJ	369	ASN
9	CJ	381	GLN
10	CK	14	HIS
10	CK	53	GLN
12	CM	165	GLN
12	CM	172	ASN
13	CN	140	GLN
14	CO	14	HIS
15	CQ	82	ASN
16	Lq	43	HIS
18	Cd	99	GLN
18	Cd	131	GLN
18	Cd	170	GLN
18	Cd	176	HIS
18	Cd	409	GLN
19	Ce	223	GLN
19	Ce	224	GLN
21	Cg	31	ASN
21	Cg	185	GLN
22	Ch	325	ASN
23	Cz	22	ASN
24	LA	205	ASN
25	LB	319	ASN
26	LC	118	GLN
26	LC	203	HIS
26	LC	217	HIS
26	LC	330	ASN
27	LD	42	ASN
27	LD	247	HIS
28	LE	116	GLN
12	LF	9	GLN
12	LF	41	GLN
12	LF	200	ASN
12	LF	249	ASN

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Mol	Chain	Res	Type
29	LG	194	HIS
29	LG	246	GLN
30	LH	5	HIS
30	LH	95	HIS
32	LK	14	HIS
32	LK	65	GLN
33	LL	142	GLN
34	LM	103	GLN
35	LN	95	GLN
35	LN	138	ASN
37	LP	42	GLN
38	LQ	86	ASN
39	LR	125	HIS
39	LR	143	HIS
41	LT	127	GLN
44	LX	124	ASN
47	La	62	HIS
49	Ld	29	HIS
49	Ld	62	GLN
49	Ld	64	ASN
49	Ld	88	ASN
50	Le	21	HIS
51	Lf	7	HIS
51	Lf	58	GLN
53	Lh	64	ASN
54	Li	42	GLN
58	Lp	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3069/3342 (91%)	550 (17%)	23 (0%)
2	C2	155/156 (99%)	21 (13%)	0
3	C3	80/162 (49%)	21 (26%)	0
4	C4	118/119 (99%)	23 (19%)	0
All	All	3422/3779 (90%)	615 (17%)	23 (0%)

All (615) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	4	U

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Mol	Chain	Res	Type
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	75	G
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	119	U
1	C1	123	A
1	C1	132	U
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	151	G
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	185	U
1	C1	193	A
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	225	A
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

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Mol	Chain	Res	Type
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	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
1	C1	443	C
1	C1	445	G
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	485	G
1	C1	512	A
1	C1	514	A
1	C1	524	A
1	C1	527	G
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	548	U

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Mol	Chain	Res	Type
1	C1	549	A
1	C1	550	G
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
1	C1	703	A
1	C1	704	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	747	A
1	C1	748	U
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	808	G
1	C1	812	A

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Mol	Chain	Res	Type
1	C1	830	A
1	C1	843	C
1	C1	857	G
1	C1	877	A
1	C1	879	U
1	C1	889	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	906	G
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
1	C1	941	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	954	U
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	966	G
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

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Mol	Chain	Res	Type
1	C1	1059	C
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
1	C1	1136	A
1	C1	1143	C
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1173	A
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1185	A
1	C1	1187	A
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1241	U
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G

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Mol	Chain	Res	Type
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	1370	G
1	C1	1382	A
1	C1	1383	G
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1458	G
1	C1	1464	A
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	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

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Mol	Chain	Res	Type
1	C1	1573	A
1	C1	1576	C
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1663	C
1	C1	1683	U
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U
1	C1	1705	C
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1743	U
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	1799	U
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A

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Mol	Chain	Res	Type
1	C1	1886	G
1	C1	1887	C
1	C1	1917	OMU
1	C1	1923	C
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	2054	U
1	C1	2056	A
1	C1	2076	A
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
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

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Mol	Chain	Res	Type
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
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	2398	G
1	C1	2403	A
1	C1	2406	A
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2489	C
1	C1	2499	C
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C

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Mol	Chain	Res	Type
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
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	2609	U
1	C1	2615	A
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2647	U
1	C1	2650	A
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	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

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Mol	Chain	Res	Type
1	C1	2713	G
1	C1	2717	A
1	C1	2730	U
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
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	2803	C
1	C1	2805	U
1	C1	2806	A
1	C1	2808	C
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	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	2887	C
1	C1	2894	U
1	C1	2895	A

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Mol	Chain	Res	Type
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	2955	C
1	C1	2956	U
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3036	G
1	C1	3044	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3071	A
1	C1	3080	A
1	C1	3086	G
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	3119	A
1	C1	3124	G
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

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Mol	Chain	Res	Type
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
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	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	3282	U
1	C1	3286	G
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

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Mol	Chain	Res	Type
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	52	A
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
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	3	C
3	C3	10	C
3	C3	19	G
3	C3	20	G
3	C3	25	U
3	C3	36	C
3	C3	39	G
3	C3	40	G
3	C3	42	U
3	C3	57	A
3	C3	58	A
3	C3	59	A
3	C3	63	A
3	C3	66	G
3	C3	68	C
3	C3	69	G
3	C3	135	G

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Mol	Chain	Res	Type
3	C3	136	C
3	C3	137	C
3	C3	138	A
4	C4	6	C
4	C4	7	G
4	C4	42	C
4	C4	52	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
4	C4	78	A
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	90	G
4	C4	93	G
4	C4	97	A
4	C4	98	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

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Mol	Chain	Res	Type
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 [i](#)

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	A2M	C1	2289	1	22,25,26	4.01	11 (50%)	30,36,39	3.31	13 (43%)
1	A2M	C1	637	1	22,25,26	3.97	11 (50%)	30,36,39	3.35	13 (43%)
1	OMG	C1	646	1	23,26,27	0.55	0	32,38,41	0.59	0
1	A2M	C1	858	1	22,25,26	4.03	12 (54%)	30,36,39	3.36	14 (46%)
1	OMG	C1	385	1	23,26,27	0.53	0	32,38,41	0.51	0
1	A2M	C1	1223	1	22,25,26	3.98	11 (50%)	30,36,39	3.28	15 (50%)
1	OMU	C1	1868	1	19,22,23	3.02	7 (36%)	25,31,34	2.00	5 (20%)
1	OMU	C1	2690	1	19,22,23	3.02	7 (36%)	25,31,34	1.84	4 (16%)
1	OMC	C1	1420	1	19,22,23	0.70	0	25,31,34	1.27	4 (16%)
1	A2M	C1	1847	1	22,25,26	3.97	12 (54%)	30,36,39	3.48	14 (46%)
1	OMG	C1	787	1	23,26,27	0.53	0	32,38,41	0.61	0
1	OMU	C1	2380	1	19,22,23	3.01	7 (36%)	25,31,34	1.79	5 (20%)
1	A2M	C1	389	1	22,25,26	3.99	11 (50%)	30,36,39	3.35	12 (40%)
1	OMG	C1	2881	1	23,26,27	0.50	0	32,38,41	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	C1	2683	1	19,22,23	3.01	7 (36%)	25,31,34	1.84	5 (20%)
1	OMU	C1	2384	1	19,22,23	3.07	7 (36%)	25,31,34	1.81	5 (20%)
1	OMC	C1	2918	1	19,22,23	0.62	0	25,31,34	0.79	0
1	OMU	C1	1917	1	19,22,23	3.06	6 (31%)	25,31,34	1.85	6 (24%)
1	OMG	C1	2578	1	23,26,27	0.53	0	32,38,41	0.65	0
1	OMG	C1	2876	1	23,26,27	0.50	0	32,38,41	0.51	0
1	OMU	C1	2277	1	19,22,23	3.04	6 (31%)	25,31,34	1.79	5 (20%)
1	OMC	C1	778	1	19,22,23	0.58	0	25,31,34	0.86	1 (4%)
1	OMC	C1	2300	1	19,22,23	0.60	0	25,31,34	0.67	0
1	OMG	C1	2774	1	23,26,27	0.56	0	32,38,41	0.55	0
1	OMG	C1	627	1	23,26,27	0.55	0	32,38,41	0.63	0
1	OMG	C1	1433	1	23,26,27	0.58	0	32,38,41	0.51	0
1	OMG	C1	2358	1	23,26,27	0.54	0	32,38,41	0.56	0
1	OMC	C1	2838	1	19,22,23	0.76	1 (5%)	25,31,34	1.59	4 (16%)
1	OMC	C1	1836	1	19,22,23	0.61	0	25,31,34	0.72	0
1	OMC	C1	1491	1	19,22,23	0.60	0	25,31,34	0.69	0
1	A2M	C1	848	1	22,25,26	3.98	11 (50%)	30,36,39	3.44	15 (50%)
1	A2M	C1	1432	1	22,25,26	3.97	11 (50%)	30,36,39	3.38	13 (43%)
1	OMU	C1	2688	1	19,22,23	3.04	6 (31%)	25,31,34	1.77	5 (20%)
1	OMC	C1	1812	1	19,22,23	0.63	0	25,31,34	1.44	2 (8%)

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	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	858	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	385	1	-	2/9/27/28	0/3/3/3
1	A2M	C1	1223	1	-	1/9/27/28	0/3/3/3
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	1420	1	-	2/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	C1	389	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2881	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	2384	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	2578	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2876	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2277	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	627	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	1433	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1491	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	2/9/27/28	0/2/2/2

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-13.20	1.24	1.53
1	C1	858	A2M	C3'-C2'	-13.11	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.99	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.98	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-12.93	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.93	1.24	1.53
1	C1	848	A2M	C3'-C2'	-12.93	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.82	1.24	1.53
1	C1	1917	OMU	C2-N1	7.63	1.50	1.38
1	C1	1868	OMU	C2-N1	7.44	1.50	1.38
1	C1	2384	OMU	C2-N1	7.42	1.50	1.38
1	C1	2277	OMU	C2-N1	7.23	1.49	1.38
1	C1	2690	OMU	C2-N1	7.23	1.49	1.38
1	C1	2688	OMU	C2-N1	7.22	1.49	1.38
1	C1	2277	OMU	C2-N3	7.16	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2683	OMU	C2-N1	7.14	1.49	1.38
1	C1	2384	OMU	C2-N3	7.13	1.50	1.38
1	C1	2688	OMU	C2-N3	7.12	1.50	1.38
1	C1	2380	OMU	C2-N1	7.08	1.49	1.38
1	C1	2683	OMU	C2-N3	7.04	1.50	1.38
1	C1	2690	OMU	C2-N3	7.02	1.50	1.38
1	C1	2380	OMU	C2-N3	6.99	1.50	1.38
1	C1	1868	OMU	C2-N3	6.94	1.50	1.38
1	C1	1917	OMU	C2-N3	6.92	1.50	1.38
1	C1	389	A2M	O4'-C4'	-6.77	1.29	1.45
1	C1	637	A2M	O4'-C4'	-6.63	1.30	1.45
1	C1	1847	A2M	O4'-C4'	-6.62	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.57	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.53	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.33	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.32	1.30	1.45
1	C1	2380	OMU	C6-C5	6.12	1.49	1.35
1	C1	1917	OMU	C6-C5	6.10	1.49	1.35
1	C1	2688	OMU	C6-C5	6.07	1.49	1.35
1	C1	2277	OMU	C6-C5	6.04	1.49	1.35
1	C1	1868	OMU	C6-C5	6.01	1.49	1.35
1	C1	2384	OMU	C6-C5	6.00	1.49	1.35
1	C1	2690	OMU	C6-C5	5.99	1.49	1.35
1	C1	2683	OMU	C6-C5	5.92	1.48	1.35
1	C1	848	A2M	C3'-C4'	5.40	1.66	1.53
1	C1	858	A2M	C3'-C4'	5.38	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.33	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.30	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.26	1.66	1.53
1	C1	389	A2M	C3'-C4'	5.02	1.65	1.53
1	C1	637	A2M	C3'-C4'	5.01	1.65	1.53
1	C1	1847	A2M	C3'-C4'	4.90	1.65	1.53
1	C1	1847	A2M	O4'-C1'	4.45	1.52	1.42
1	C1	848	A2M	O4'-C1'	4.43	1.52	1.42
1	C1	2289	A2M	O4'-C1'	4.42	1.52	1.42
1	C1	858	A2M	O4'-C1'	4.39	1.52	1.42
1	C1	1432	A2M	O4'-C1'	4.39	1.52	1.42
1	C1	848	A2M	C1'-N9	-4.34	1.34	1.46
1	C1	858	A2M	C6-N6	4.34	1.45	1.34
1	C1	637	A2M	C1'-N9	-4.33	1.34	1.46
1	C1	1847	A2M	C1'-N9	-4.32	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2384	OMU	C4-N3	4.32	1.46	1.38
1	C1	1223	A2M	C1'-N9	-4.30	1.34	1.46
1	C1	2289	A2M	C1'-N9	-4.28	1.34	1.46
1	C1	858	A2M	C1'-N9	-4.28	1.34	1.46
1	C1	637	A2M	C6-N6	4.28	1.45	1.34
1	C1	848	A2M	C6-N6	4.27	1.45	1.34
1	C1	389	A2M	O4'-C1'	4.27	1.51	1.42
1	C1	2289	A2M	C6-N6	4.26	1.45	1.34
1	C1	2683	OMU	C4-N3	4.25	1.45	1.38
1	C1	1432	A2M	C6-N6	4.24	1.45	1.34
1	C1	1847	A2M	C6-N6	4.23	1.45	1.34
1	C1	389	A2M	C1'-N9	-4.23	1.34	1.46
1	C1	389	A2M	C6-N6	4.23	1.45	1.34
1	C1	2277	OMU	C4-N3	4.22	1.45	1.38
1	C1	1223	A2M	C6-N6	4.22	1.45	1.34
1	C1	2688	OMU	C4-N3	4.19	1.45	1.38
1	C1	637	A2M	O4'-C1'	4.18	1.51	1.42
1	C1	1432	A2M	C1'-N9	-4.08	1.35	1.46
1	C1	1223	A2M	O4'-C1'	4.03	1.51	1.42
1	C1	2690	OMU	C4-N3	4.01	1.45	1.38
1	C1	2380	OMU	C4-N3	3.99	1.45	1.38
1	C1	389	A2M	O2'-C2'	3.90	1.52	1.42
1	C1	1917	OMU	C4-N3	3.88	1.45	1.38
1	C1	1868	OMU	C4-N3	3.84	1.45	1.38
1	C1	848	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.54	1.51	1.42
1	C1	637	A2M	O2'-C2'	3.54	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.54	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.53	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.52	1.51	1.42
1	C1	858	A2M	C5-C4	-3.22	1.33	1.39
1	C1	2289	A2M	C5-C4	-3.18	1.33	1.39
1	C1	389	A2M	C5-C4	-3.17	1.33	1.39
1	C1	848	A2M	C2'-C1'	3.16	1.60	1.53
1	C1	389	A2M	C2'-C1'	3.14	1.60	1.53
1	C1	1223	A2M	C5-C4	-3.11	1.33	1.39
1	C1	848	A2M	C5-C4	-3.10	1.33	1.39
1	C1	637	A2M	C5-C4	-3.09	1.33	1.39
1	C1	1432	A2M	C5-C4	-3.08	1.33	1.39
1	C1	1847	A2M	C2'-C1'	3.05	1.60	1.53
1	C1	1847	A2M	C5-C4	-3.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	C2'-C1'	3.02	1.60	1.53
1	C1	1223	A2M	C5-N7	-2.98	1.33	1.39
1	C1	389	A2M	C5-N7	-2.94	1.33	1.39
1	C1	1432	A2M	C2'-C1'	2.90	1.60	1.53
1	C1	2289	A2M	C2'-C1'	2.89	1.60	1.53
1	C1	1432	A2M	C5-N7	-2.82	1.33	1.39
1	C1	637	A2M	C2'-C1'	2.82	1.60	1.53
1	C1	858	A2M	C2'-C1'	2.82	1.60	1.53
1	C1	637	A2M	C5-N7	-2.81	1.33	1.39
1	C1	2289	A2M	C5-N7	-2.80	1.34	1.39
1	C1	858	A2M	C5-N7	-2.76	1.34	1.39
1	C1	1847	A2M	C5-N7	-2.75	1.34	1.39
1	C1	848	A2M	C5-N7	-2.66	1.34	1.39
1	C1	2380	OMU	C6-N1	2.66	1.44	1.38
1	C1	2688	OMU	C6-N1	2.60	1.44	1.38
1	C1	1917	OMU	C6-N1	2.58	1.44	1.38
1	C1	1868	OMU	C6-N1	2.58	1.44	1.38
1	C1	2277	OMU	C6-N1	2.57	1.44	1.38
1	C1	2384	OMU	C6-N1	2.54	1.44	1.38
1	C1	2690	OMU	C6-N1	2.52	1.44	1.38
1	C1	2683	OMU	C6-N1	2.43	1.43	1.38
1	C1	1847	A2M	C8-N9	-2.22	1.33	1.37
1	C1	637	A2M	C8-N9	-2.22	1.33	1.37
1	C1	858	A2M	C8-N9	-2.19	1.33	1.37
1	C1	389	A2M	C8-N9	-2.17	1.33	1.37
1	C1	1868	OMU	C5-C4	2.16	1.48	1.43
1	C1	1917	OMU	C5-C4	2.15	1.48	1.43
1	C1	2683	OMU	C5-C4	2.13	1.48	1.43
1	C1	2380	OMU	C5-C4	2.13	1.48	1.43
1	C1	2688	OMU	C5-C4	2.12	1.48	1.43
1	C1	2690	OMU	C5-C4	2.11	1.48	1.43
1	C1	848	A2M	O3'-C3'	2.11	1.48	1.43
1	C1	1223	A2M	C8-N9	-2.10	1.34	1.37
1	C1	1432	A2M	C8-N9	-2.10	1.34	1.37
1	C1	2277	OMU	C5-C4	2.09	1.48	1.43
1	C1	2683	OMU	O4-C4	-2.08	1.20	1.24
1	C1	2384	OMU	C5-C4	2.08	1.48	1.43
1	C1	2838	OMC	C4-N3	-2.06	1.30	1.34
1	C1	1847	A2M	O3'-C3'	2.06	1.48	1.43
1	C1	2289	A2M	C8-N9	-2.04	1.34	1.37
1	C1	1868	OMU	O4-C4	-2.03	1.20	1.24
1	C1	2690	OMU	O4-C4	-2.03	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2384	OMU	O4-C4	-2.03	1.20	1.24
1	C1	2380	OMU	O4-C4	-2.01	1.20	1.24
1	C1	858	A2M	O3'-C3'	2.01	1.47	1.43

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.40	106.23	127.09
1	C1	389	A2M	C1'-N9-C8	-9.03	107.05	127.09
1	C1	637	A2M	C1'-N9-C8	-8.95	107.23	127.09
1	C1	848	A2M	C1'-N9-C8	-8.87	107.42	127.09
1	C1	1432	A2M	C1'-N9-C8	-8.82	107.52	127.09
1	C1	858	A2M	C1'-N9-C8	-8.75	107.67	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.43	108.39	127.09
1	C1	1223	A2M	C1'-N9-C8	-8.33	108.60	127.09
1	C1	1847	A2M	C4-N9-C1'	8.13	145.66	126.63
1	C1	389	A2M	C4-N9-C1'	7.91	145.13	126.63
1	C1	1432	A2M	C4-N9-C1'	7.79	144.85	126.63
1	C1	637	A2M	C4-N9-C1'	7.73	144.70	126.63
1	C1	858	A2M	C4-N9-C1'	7.58	144.35	126.63
1	C1	848	A2M	C4-N9-C1'	7.54	144.28	126.63
1	C1	1223	A2M	C4-N9-C1'	7.29	143.68	126.63
1	C1	2289	A2M	C4-N9-C1'	7.27	143.62	126.63
1	C1	1868	OMU	C4-N3-C2	-6.17	118.95	126.61
1	C1	858	A2M	N6-C6-N1	-6.12	104.75	118.38
1	C1	848	A2M	N3-C2-N1	-5.99	119.51	128.58
1	C1	389	A2M	N3-C2-N1	-5.99	119.52	128.58
1	C1	1847	A2M	N6-C6-N1	-5.97	105.08	118.38
1	C1	1432	A2M	N3-C2-N1	-5.96	119.56	128.58
1	C1	858	A2M	N3-C2-N1	-5.94	119.58	128.58
1	C1	2289	A2M	N3-C2-N1	-5.94	119.59	128.58
1	C1	1432	A2M	N6-C6-N1	-5.88	105.27	118.38
1	C1	1223	A2M	N3-C2-N1	-5.87	119.70	128.58
1	C1	1223	A2M	N6-C6-N1	-5.84	105.36	118.38
1	C1	637	A2M	N3-C2-N1	-5.76	119.86	128.58
1	C1	637	A2M	N6-C6-N1	-5.75	105.56	118.38
1	C1	1847	A2M	N3-C2-N1	-5.67	120.00	128.58
1	C1	848	A2M	N6-C6-N1	-5.66	105.77	118.38
1	C1	2690	OMU	C4-N3-C2	-5.64	119.61	126.61
1	C1	2683	OMU	C4-N3-C2	-5.58	119.69	126.61
1	C1	2289	A2M	N6-C6-N1	-5.52	106.08	118.38
1	C1	2380	OMU	C4-N3-C2	-5.48	119.81	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2688	OMU	C4-N3-C2	-5.46	119.83	126.61
1	C1	2277	OMU	C4-N3-C2	-5.45	119.85	126.61
1	C1	2384	OMU	C4-N3-C2	-5.43	119.87	126.61
1	C1	1812	OMC	CM2-O2'-C2'	5.38	128.30	114.47
1	C1	389	A2M	N6-C6-N1	-5.38	106.40	118.38
1	C1	1917	OMU	C4-N3-C2	-5.37	119.95	126.61
1	C1	1432	A2M	C5-C4-N3	-5.02	119.80	126.72
1	C1	2838	OMC	C1'-N1-C2	4.97	129.41	118.44
1	C1	1847	A2M	C5-C4-N3	-4.90	119.97	126.72
1	C1	848	A2M	C5-C4-N3	-4.88	120.00	126.72
1	C1	858	A2M	C5-C6-N6	4.82	135.22	123.29
1	C1	389	A2M	C5-C4-N3	-4.72	120.22	126.72
1	C1	1223	A2M	C5-C6-N6	4.70	134.92	123.29
1	C1	2289	A2M	C5-C4-N3	-4.66	120.30	126.72
1	C1	637	A2M	C5-C6-N6	4.63	134.76	123.29
1	C1	858	A2M	C5-C4-N3	-4.59	120.40	126.72
1	C1	637	A2M	C5-C4-N3	-4.59	120.40	126.72
1	C1	1432	A2M	C5-C6-N6	4.55	134.55	123.29
1	C1	1847	A2M	C5-C6-N6	4.55	134.54	123.29
1	C1	1223	A2M	C5-C4-N3	-4.51	120.51	126.72
1	C1	848	A2M	N9-C8-N7	-4.45	107.63	113.94
1	C1	2289	A2M	O4'-C1'-N9	4.41	116.56	108.09
1	C1	848	A2M	O4'-C1'-N9	4.38	116.51	108.09
1	C1	2289	A2M	C5-C6-N6	4.36	134.09	123.29
1	C1	1868	OMU	N3-C2-N1	4.36	120.57	114.89
1	C1	848	A2M	C5-C6-N6	4.32	133.99	123.29
1	C1	1847	A2M	N9-C8-N7	-4.27	107.87	113.94
1	C1	858	A2M	N9-C8-N7	-4.22	107.94	113.94
1	C1	389	A2M	C5-C6-N6	4.21	133.71	123.29
1	C1	1917	OMU	N3-C2-N1	4.18	120.34	114.89
1	C1	637	A2M	N9-C8-N7	-4.16	108.03	113.94
1	C1	2289	A2M	N9-C8-N7	-4.15	108.05	113.94
1	C1	1223	A2M	O4'-C1'-N9	4.09	115.94	108.09
1	C1	1432	A2M	N9-C8-N7	-4.03	108.22	113.94
1	C1	2683	OMU	C5-C4-N3	4.00	120.41	114.80
1	C1	1223	A2M	N9-C8-N7	-4.00	108.27	113.94
1	C1	2690	OMU	N3-C2-N1	3.98	120.07	114.89
1	C1	389	A2M	N9-C8-N7	-3.93	108.35	113.94
1	C1	858	A2M	O4'-C1'-N9	3.93	115.64	108.09
1	C1	637	A2M	O4'-C1'-N9	3.88	115.53	108.09
1	C1	2380	OMU	N3-C2-N1	3.86	119.92	114.89
1	C1	2277	OMU	N3-C2-N1	3.85	119.90	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1868	OMU	C5-C4-N3	3.84	120.18	114.80
1	C1	1432	A2M	O4'-C1'-N9	3.81	115.40	108.09
1	C1	2384	OMU	N3-C2-N1	3.74	119.77	114.89
1	C1	2688	OMU	N3-C2-N1	3.74	119.77	114.89
1	C1	2380	OMU	C5-C4-N3	3.72	120.01	114.80
1	C1	2838	OMC	C1'-N1-C6	-3.71	112.84	120.78
1	C1	2683	OMU	N3-C2-N1	3.68	119.68	114.89
1	C1	1420	OMC	C1'-N1-C2	3.66	126.53	118.44
1	C1	1432	A2M	C2-N3-C4	3.63	120.71	111.83
1	C1	2384	OMU	C5-C4-N3	3.61	119.86	114.80
1	C1	2688	OMU	C5-C4-N3	3.61	119.86	114.80
1	C1	1847	A2M	O4'-C1'-N9	3.60	115.01	108.09
1	C1	2690	OMU	C5-C4-N3	3.60	119.84	114.80
1	C1	2277	OMU	C5-C4-N3	3.58	119.81	114.80
1	C1	389	A2M	O4'-C1'-N9	3.53	114.86	108.09
1	C1	848	A2M	C2-N3-C4	3.51	120.41	111.83
1	C1	1847	A2M	C2-N3-C4	3.43	120.20	111.83
1	C1	848	A2M	C2'-C1'-N9	-3.42	108.12	113.75
1	C1	1917	OMU	C5-C4-N3	3.42	119.59	114.80
1	C1	389	A2M	C2-N3-C4	3.41	120.17	111.83
1	C1	858	A2M	C2-N3-C4	3.40	120.13	111.83
1	C1	1223	A2M	C2-N3-C4	3.32	119.94	111.83
1	C1	2289	A2M	C2-N3-C4	3.32	119.94	111.83
1	C1	637	A2M	C2-N3-C4	3.26	119.79	111.83
1	C1	2683	OMU	O4-C4-C5	-3.11	119.80	125.16
1	C1	2384	OMU	O4-C4-C5	-3.06	119.89	125.16
1	C1	848	A2M	C5-N7-C8	3.05	108.24	103.45
1	C1	1847	A2M	C5-N7-C8	3.04	108.23	103.45
1	C1	2838	OMC	O2-C2-N3	-3.04	117.54	122.33
1	C1	848	A2M	N3-C4-N9	3.04	132.33	127.17
1	C1	1847	A2M	N3-C4-N9	3.00	132.27	127.17
1	C1	1868	OMU	O4-C4-C5	-2.96	120.05	125.16
1	C1	2380	OMU	O4-C4-C5	-2.94	120.10	125.16
1	C1	2690	OMU	O4-C4-C5	-2.93	120.11	125.16
1	C1	1812	OMC	C2'-C1'-N1	-2.93	108.68	114.24
1	C1	2277	OMU	O4-C4-C5	-2.93	120.11	125.16
1	C1	1432	A2M	C5-N7-C8	2.92	108.03	103.45
1	C1	2688	OMU	O4-C4-C5	-2.91	120.15	125.16
1	C1	389	A2M	N3-C4-N9	2.90	132.10	127.17
1	C1	858	A2M	C5-N7-C8	2.85	107.93	103.45
1	C1	1432	A2M	N3-C4-N9	2.82	131.97	127.17
1	C1	637	A2M	C5-N7-C8	2.81	107.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2289	A2M	N3-C4-N9	2.79	131.91	127.17
1	C1	2289	A2M	C5-N7-C8	2.77	107.81	103.45
1	C1	1223	A2M	C5-N7-C8	2.76	107.79	103.45
1	C1	1917	OMU	C1'-N1-C2	2.76	122.54	117.59
1	C1	637	A2M	N3-C4-N9	2.70	131.76	127.17
1	C1	389	A2M	C5-N7-C8	2.70	107.70	103.45
1	C1	2289	A2M	C2'-C1'-N9	-2.69	109.33	113.75
1	C1	858	A2M	N3-C4-N9	2.55	131.50	127.17
1	C1	1223	A2M	N3-C4-N9	2.52	131.46	127.17
1	C1	848	A2M	C4-N9-C8	2.43	108.29	105.74
1	C1	1917	OMU	O4-C4-C5	-2.43	120.97	125.16
1	C1	2384	OMU	C1'-N1-C2	2.39	121.88	117.59
1	C1	1420	OMC	C1'-N1-C6	-2.38	115.69	120.78
1	C1	2380	OMU	O2-C2-N1	-2.34	119.75	122.80
1	C1	2683	OMU	O2-C2-N1	-2.32	119.78	122.80
1	C1	778	OMC	C1'-N1-C2	2.32	123.56	118.44
1	C1	1432	A2M	C4-C5-N7	-2.31	107.94	110.58
1	C1	2838	OMC	O2-C2-N1	2.28	123.38	118.90
1	C1	1847	A2M	C4-N9-C8	2.26	108.11	105.74
1	C1	1847	A2M	C4-C5-N7	-2.24	108.02	110.58
1	C1	1432	A2M	C5-C4-N9	2.22	108.23	105.81
1	C1	858	A2M	C4-C5-N7	-2.22	108.05	110.58
1	C1	637	A2M	C4-N9-C8	2.21	108.06	105.74
1	C1	1847	A2M	C5'-C4'-C3'	-2.21	107.27	115.21
1	C1	1223	A2M	C2'-C1'-N9	-2.17	110.18	113.75
1	C1	858	A2M	C4-N9-C8	2.14	107.98	105.74
1	C1	2289	A2M	C4-N9-C8	2.14	107.98	105.74
1	C1	1420	OMC	O2-C2-N1	2.14	123.08	118.90
1	C1	1868	OMU	O2-C2-N1	-2.11	120.05	122.80
1	C1	1223	A2M	O4'-C1'-C2'	-2.11	102.96	106.59
1	C1	848	A2M	C4-C5-N7	-2.11	108.17	110.58
1	C1	1223	A2M	C4-C5-N7	-2.10	108.18	110.58
1	C1	858	A2M	C5-C4-N9	2.09	108.09	105.81
1	C1	848	A2M	O4'-C1'-C2'	-2.08	103.01	106.59
1	C1	637	A2M	C4-C5-N7	-2.08	108.21	110.58
1	C1	389	A2M	C4'-O4'-C1'	-2.06	104.92	109.47
1	C1	1223	A2M	C5-C4-N9	2.04	108.04	105.81
1	C1	2277	OMU	O2-C2-N1	-2.03	120.15	122.80
1	C1	1420	OMC	O2-C2-N3	-2.03	119.13	122.33
1	C1	1917	OMU	O2-C2-N3	-2.02	117.77	121.49
1	C1	2688	OMU	O2-C2-N1	-2.01	120.18	122.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	1812	OMC	C1'-C2'-O2'-CM2
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2578	OMG	O4'-C4'-C5'-O5'
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2690	OMU	C3'-C4'-C5'-O5'
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	389	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1812	OMC	C3'-C2'-O2'-CM2
1	C1	1917	OMU	C3'-C4'-C5'-O5'
1	C1	2578	OMG	C3'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	2300	OMC	C1'-C2'-O2'-CM2
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	1420	OMC	C3'-C2'-O2'-CM2
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	1433	OMG	C1'-C2'-O2'-CM2
1	C1	1420	OMC	C2'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	637	A2M	1	0
1	C1	1420	OMC	1	0
1	C1	389	A2M	1	0
1	C1	2277	OMU	1	0
1	C1	2838	OMC	1	0
1	C1	1432	A2M	1	0
1	C1	1812	OMC	2	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	Cd	1000	60	33,34,34	0.86	0	50,54,54	1.56	9 (18%)
59	GTP	CH	701	60	33,34,34	0.91	0	50,54,54	1.58	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	Cd	1000	60	-	3/22/38/38	0/3/3/3
59	GTP	CH	701	60	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CH	701	GTP	C5-C4-N3	-4.84	120.69	128.39
59	Cd	1000	GTP	C5-C4-N3	-4.65	121.00	128.39
59	Cd	1000	GTP	C2-N3-C4	4.50	120.06	112.30
59	CH	701	GTP	C2-N3-C4	4.36	119.81	112.30
59	CH	701	GTP	N9-C4-N3	3.15	132.25	125.95
59	CH	701	GTP	O2G-PG-O3B	3.10	115.02	104.64
59	CH	701	GTP	C2-N1-C6	-2.91	119.84	125.11
59	Cd	1000	GTP	N9-C4-N3	2.84	131.62	125.95
59	CH	701	GTP	N9-C8-N7	-2.74	108.33	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Cd	1000	GTP	N9-C8-N7	-2.72	108.36	113.40
59	Cd	1000	GTP	C2-N1-C6	-2.71	120.19	125.11
59	CH	701	GTP	C8-N7-C5	2.53	108.77	104.26
59	Cd	1000	GTP	C8-N7-C5	2.51	108.74	104.26
59	CH	701	GTP	C5-C6-N1	2.46	119.52	113.25
59	Cd	1000	GTP	C5-C6-N1	2.43	119.45	113.25
59	CH	701	GTP	O6-C6-C5	-2.41	120.16	126.53
59	Cd	1000	GTP	O6-C6-C5	-2.32	120.42	126.53
59	Cd	1000	GTP	O3G-PG-O3B	2.12	111.73	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

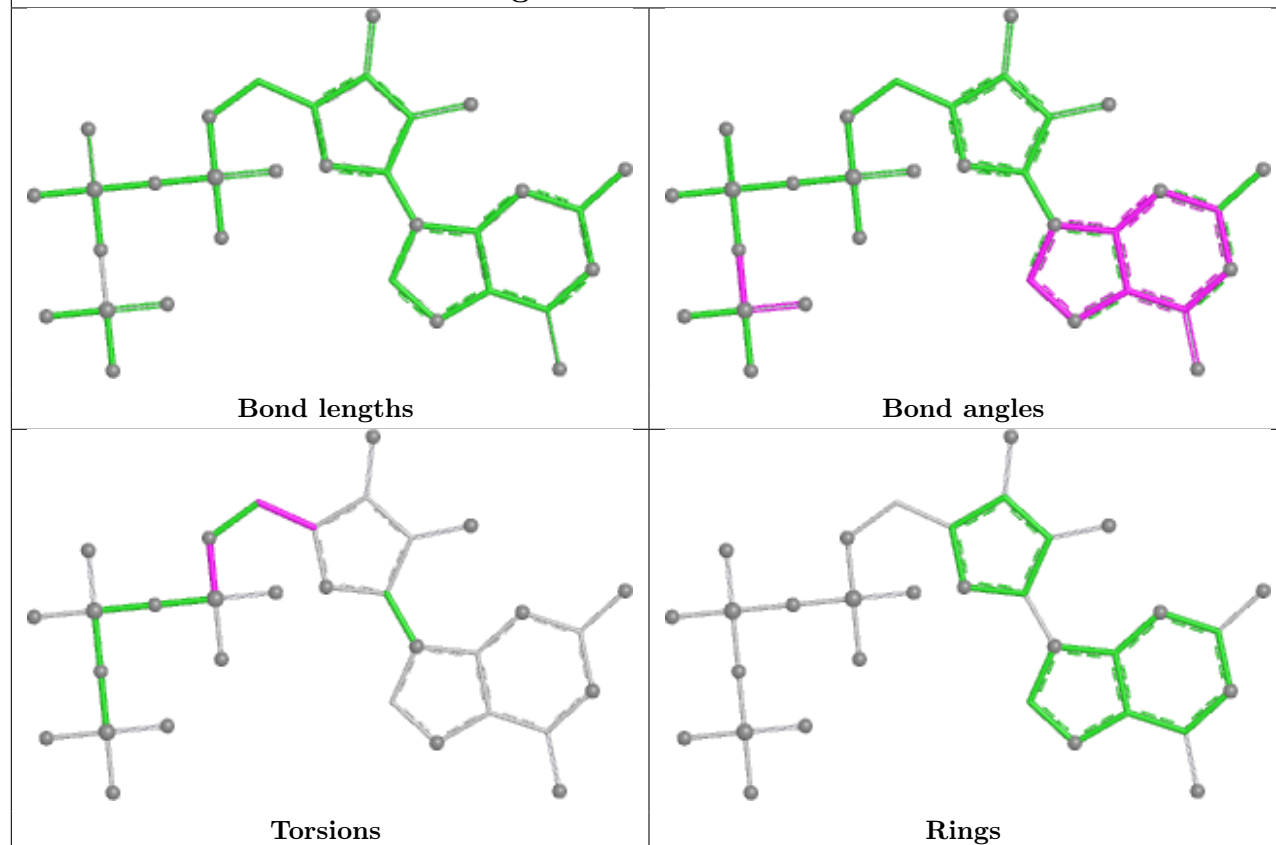
Mol	Chain	Res	Type	Atoms
59	CH	701	GTP	O4'-C4'-C5'-O5'
59	CH	701	GTP	C3'-C4'-C5'-O5'
59	Cd	1000	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	C5'-O5'-PA-O3A
59	CH	701	GTP	C5'-O5'-PA-O1A
59	CH	701	GTP	C5'-O5'-PA-O2A
59	Cd	1000	GTP	C5'-O5'-PA-O1A
59	Cd	1000	GTP	O4'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3A-PA-O2A
59	CH	701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

There are no ring outliers.

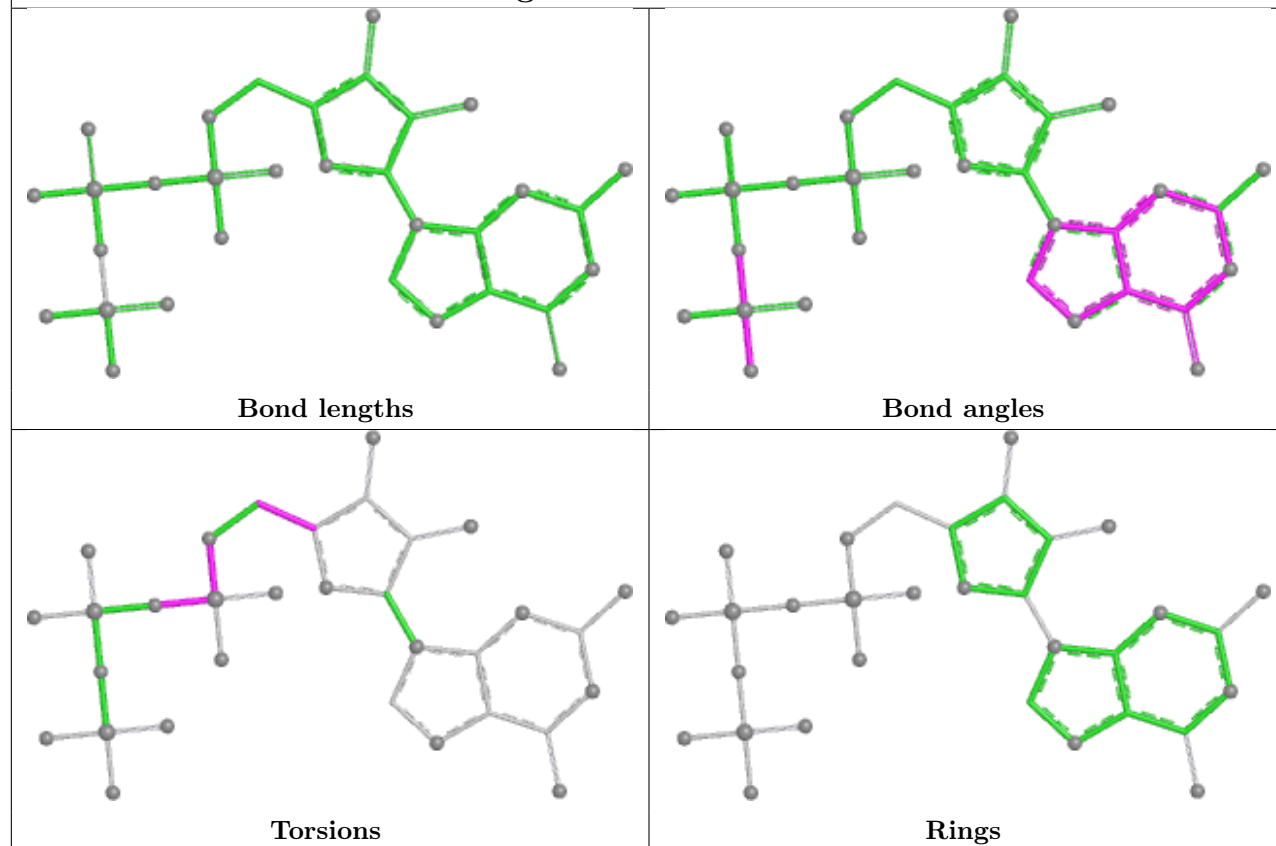
No monomer is involved in short contacts.

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

Ligand GTP Cd 1000



Ligand GTP CH 701



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.

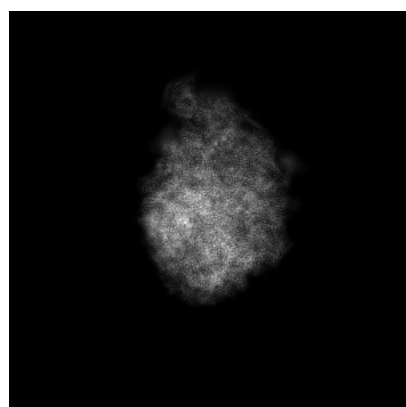
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17956. These allow visual inspection of the internal detail of the map and identification of artifacts.

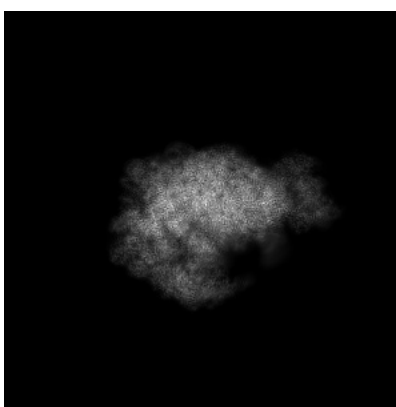
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

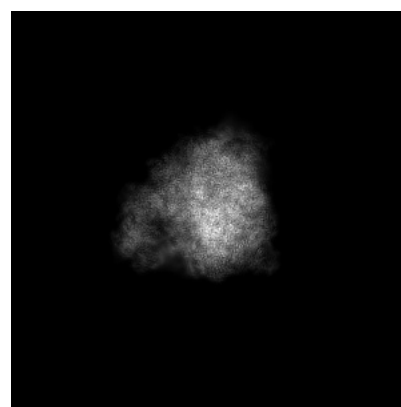
6.1.1 Primary map



X



Y

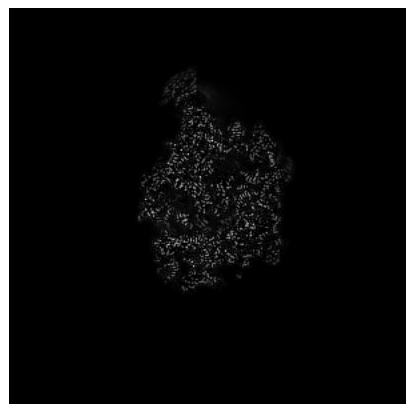


Z

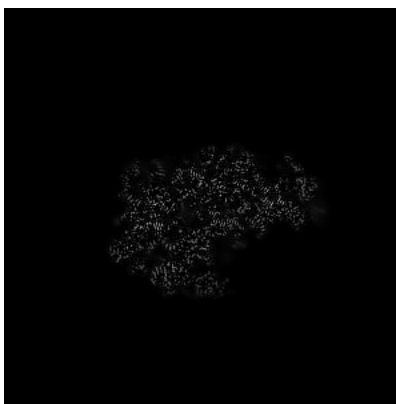
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

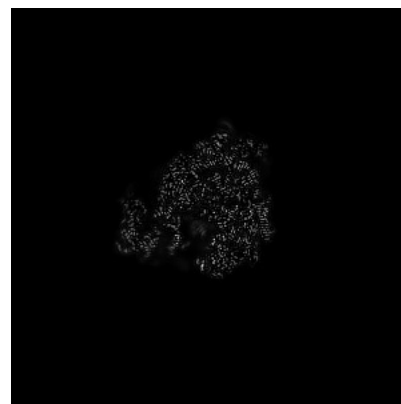
6.2.1 Primary map



X Index: 250



Y Index: 250

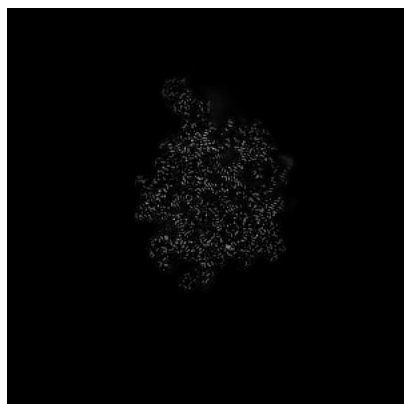


Z Index: 250

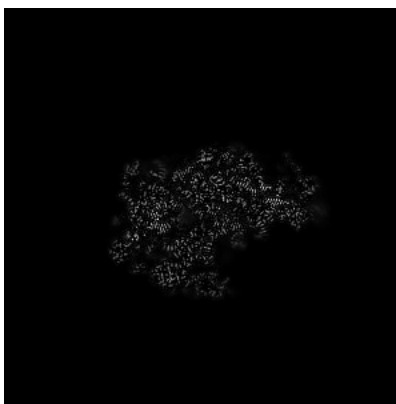
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

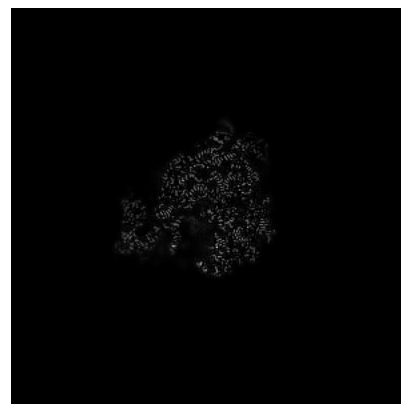
6.3.1 Primary map



X Index: 259



Y Index: 248

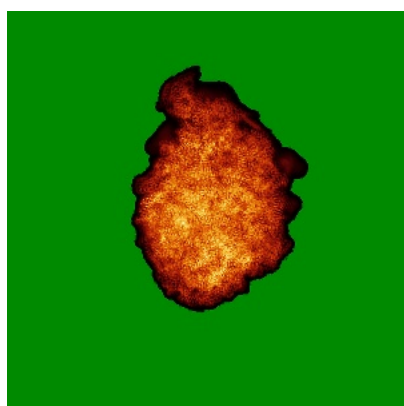


Z Index: 252

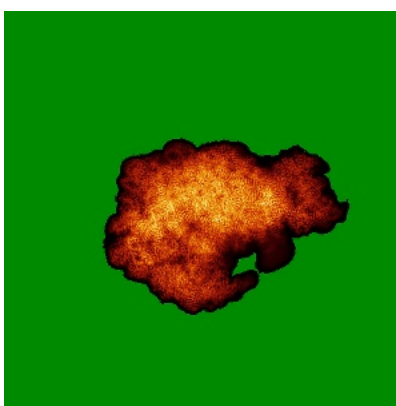
The images above show the largest variance slices of the map in three orthogonal directions.

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

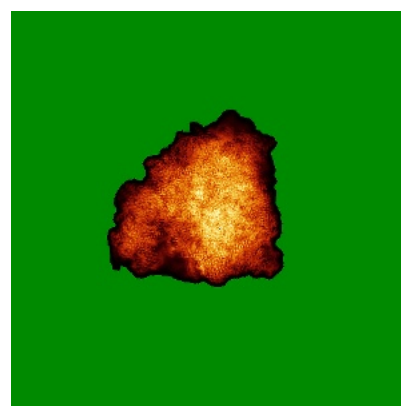
6.4.1 Primary map



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

This section was not generated.

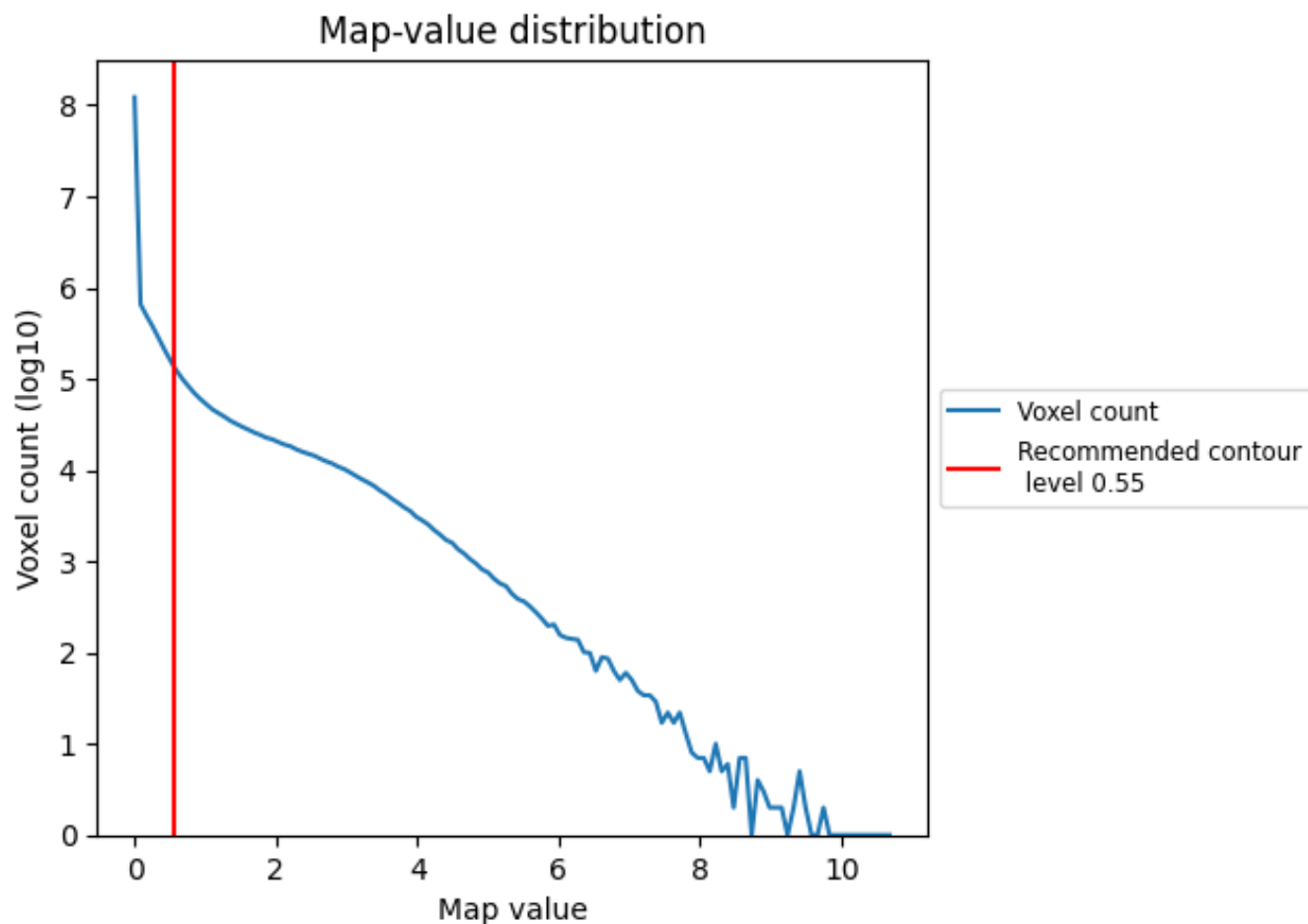
6.6 Mask visualisation

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

7 Map analysis [i](#)

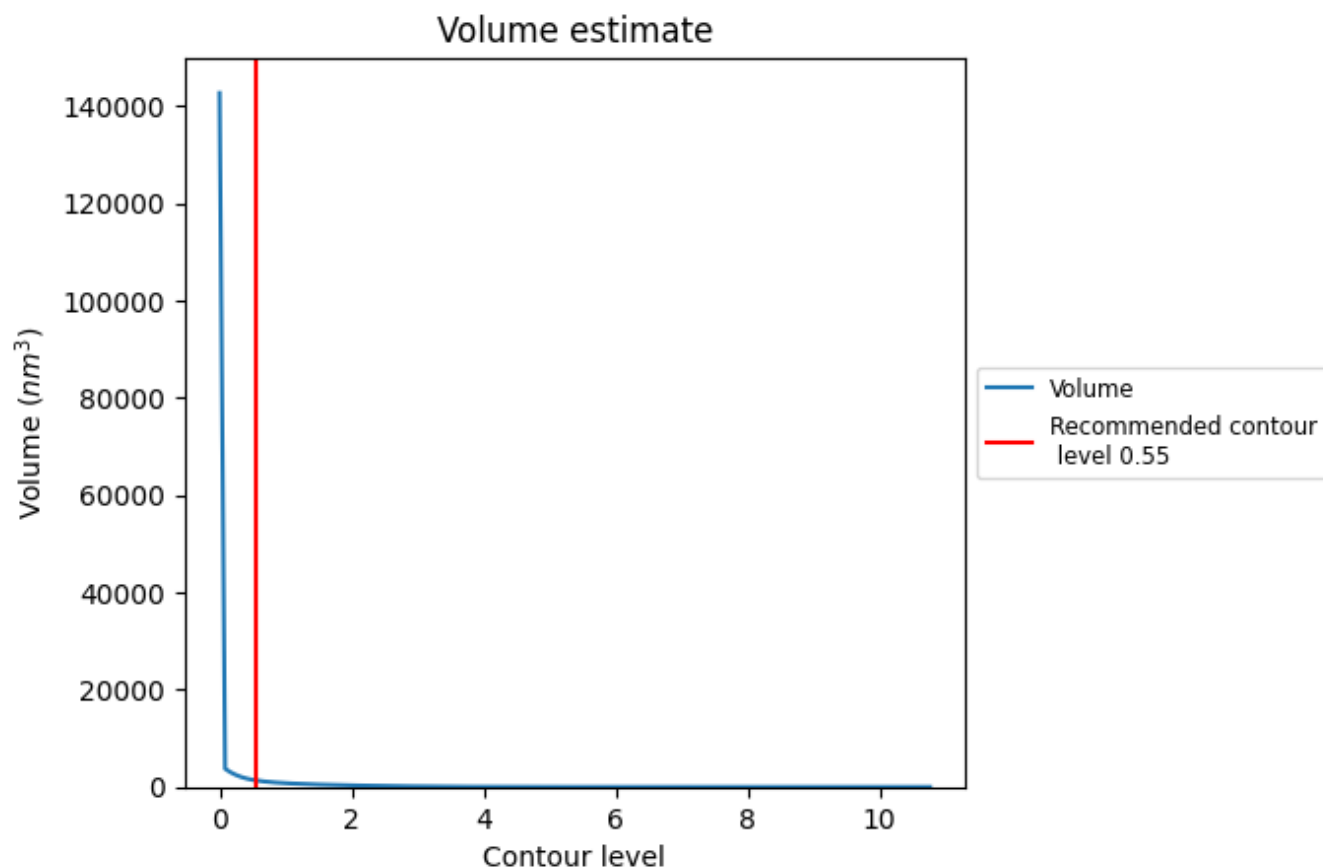
This section contains the results of statistical analysis of the map.

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.

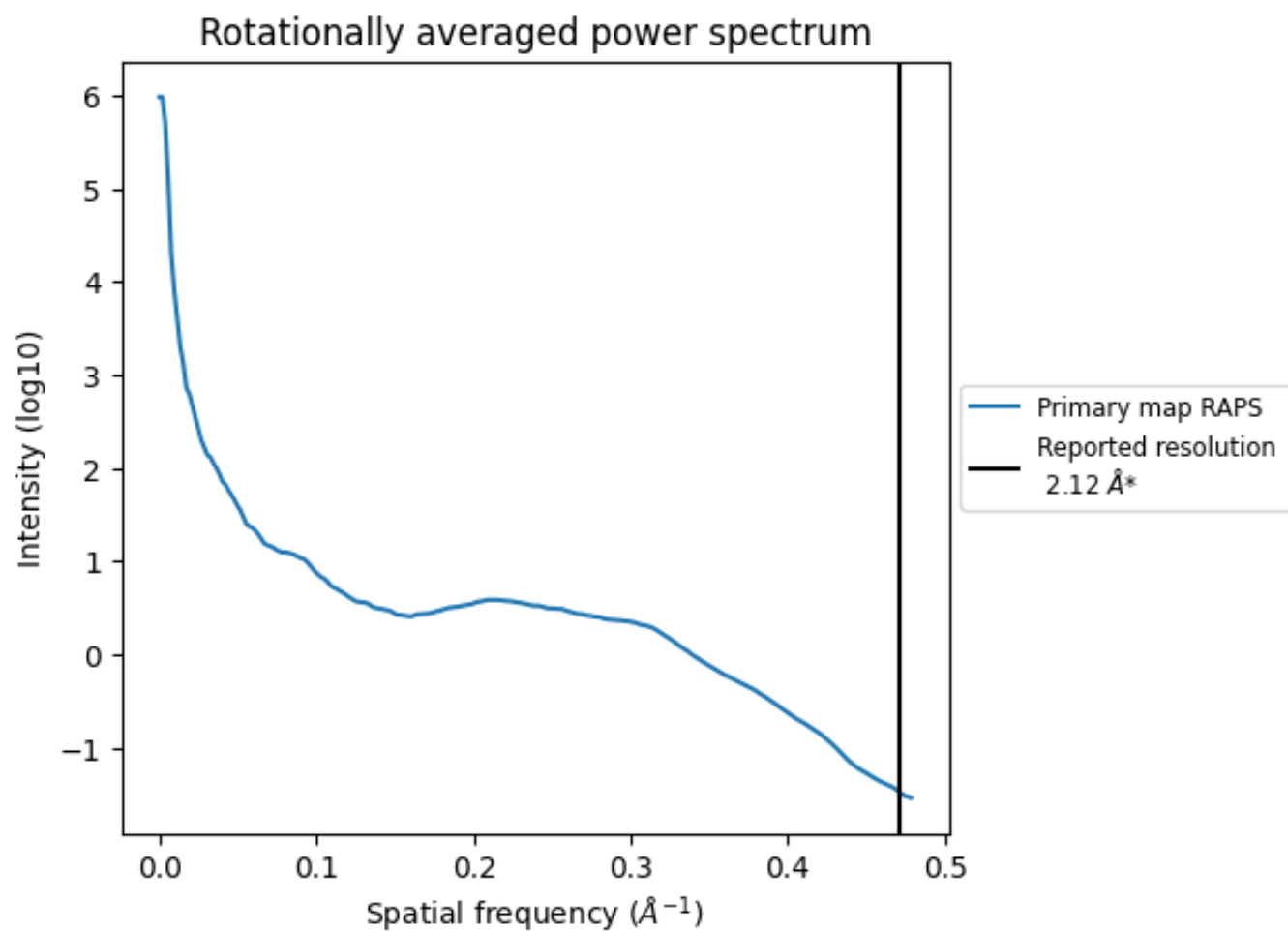
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1355 nm^3 ; this corresponds to an approximate mass of 1224 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 0.472 Å⁻¹

8 Fourier-Shell correlation

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

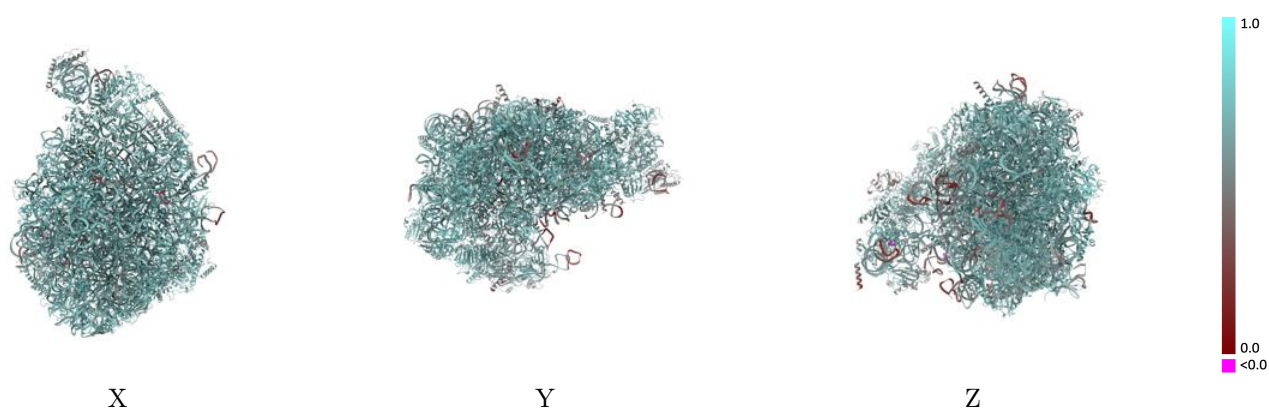
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17956 and PDB model 8PV7. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

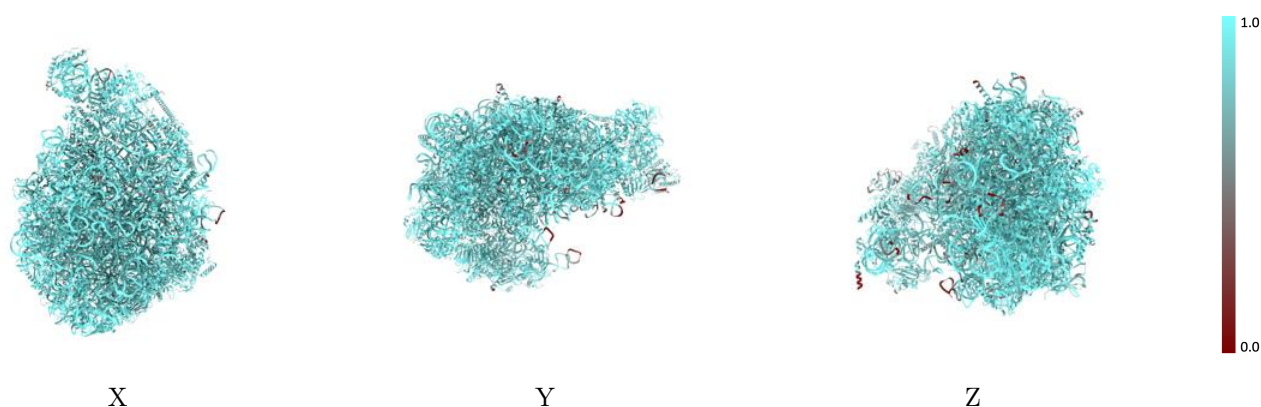
This section was not generated.

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



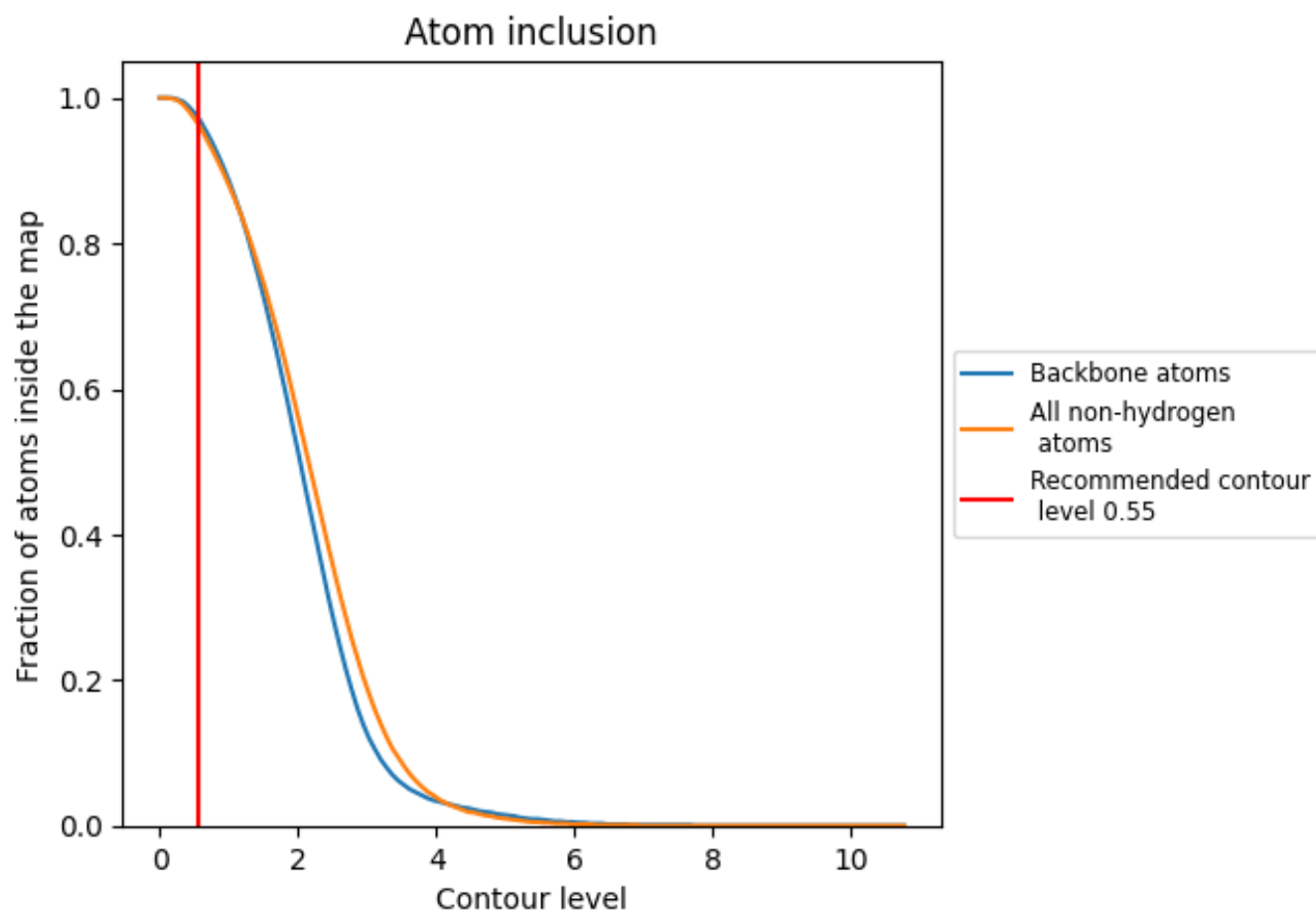
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.6760
C1	 0.9770	 0.6650
C2	 0.9770	 0.6890
C3	 0.8300	 0.5370
C4	 0.9280	 0.5990
CB	 0.9290	 0.6250
CF	 0.9670	 0.6860
CH	 0.9490	 0.6920
CI	 0.9200	 0.6380
CJ	 0.9840	 0.6940
CK	 0.9860	 0.7230
CL	 0.9440	 0.6420
CM	 0.9520	 0.6590
CN	 0.9730	 0.7110
CO	 0.9520	 0.7060
CQ	 0.9210	 0.6770
Cb	 0.9750	 0.7070
Cd	 0.9690	 0.7000
Ce	 0.8940	 0.6380
Cf	 0.9640	 0.6740
Cg	 0.9650	 0.6590
Ch	 0.9210	 0.6570
Cz	 0.8810	 0.5970
LA	 0.9870	 0.7100
LB	 0.9850	 0.7300
LC	 0.9810	 0.7230
LD	 0.9300	 0.6620
LE	 0.9440	 0.6810
LF	 0.9770	 0.7050
LG	 0.9720	 0.6990
LH	 0.9730	 0.7150
LJ	 0.9290	 0.5920
LK	 0.9410	 0.6470
LL	 0.9610	 0.7030
LM	 0.9730	 0.7060



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Chain	Atom inclusion	Q-score
LN	 0.9960	 0.7310
LO	 0.9890	 0.7290
LP	 0.9870	 0.7210
LQ	 0.9860	 0.7000
LR	 0.9620	 0.7080
LS	 0.9880	 0.7080
LT	 0.9490	 0.6280
LU	 0.9410	 0.6620
LV	 0.9910	 0.7310
LX	 0.9730	 0.6940
LY	 0.9770	 0.7080
LZ	 0.9670	 0.7020
La	 0.9730	 0.7060
Lc	 0.9600	 0.6890
Ld	 0.9660	 0.7160
Le	 0.9880	 0.7310
Lf	 0.9960	 0.7380
Lg	 0.9340	 0.6940
Lh	 0.9460	 0.6620
Li	 0.9500	 0.6780
Lj	 0.9930	 0.7390
Lk	 0.9170	 0.6740
Ll	 0.9980	 0.7390
Lp	 0.9480	 0.6910
Lq	 0.9690	 0.6970