



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:39 PM UTC

PDB ID : 9HUQ / pdb_00009huq
EMDB ID : EMD-52417
Title : Structure of WT E.coli ribosome with complexed filament nascent chain at length 47, with P-site tRNA
Authors : Mitropoulou, A.; Wlodarski, T.; Plessa, E.; Cabrita, L.D.; Christodoulou, J.
Deposited on : 2024-12-23
Resolution : 2.49 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:

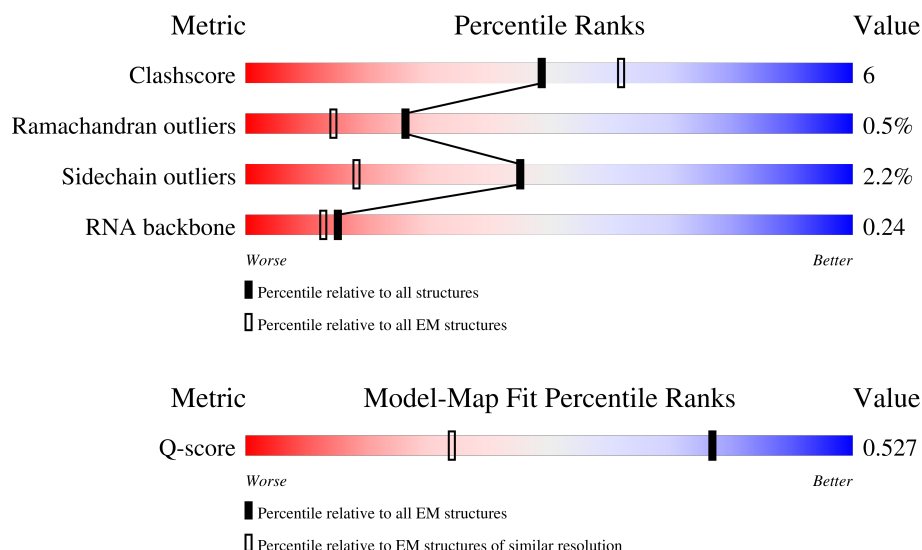
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.49 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	6237 (2.00 - 2.99)

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

Mol	Chain	Length	Quality of chain
1	0	78	
2	1	63	
3	2	59	

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Mol	Chain	Length	Quality of chain
4	3	57	
5	4	55	
6	6	46	
7	7	65	
8	8	38	
9	a	120	
10	c	273	
11	d	209	
12	e	201	
13	f	179	
14	g	177	
15	h	149	
16	j	142	
17	k	123	
18	l	144	
19	m	136	
20	n	127	
21	o	117	
22	p	115	
23	q	118	
24	r	103	
25	s	110	
26	t	100	
27	u	104	
28	w	94	

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Mol	Chain	Length	Quality of chain
29	y	85	7% 69% 24% 6%
30	z	161	7% 7% 89%
31	v	77	10% 39% 48% 13%
32	b	2904	11% 49% 43% 7%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 10 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 15 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 16 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 18 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 20 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	u	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 28 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	y	80	Total	C	N	O	S	0	0
			596	368	121	106	1		

- Molecule 30 is a protein called Gelation factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	z	18	Total	C	N	O	1	0
			178	127	29	22		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	7	MET	-	initiating methionine	UNP P13466
z	8	HIS	-	expression tag	UNP P13466
z	9	HIS	-	expression tag	UNP P13466
z	10	HIS	-	expression tag	UNP P13466
z	11	HIS	-	expression tag	UNP P13466
z	12	HIS	-	expression tag	UNP P13466
z	13	HIS	-	expression tag	UNP P13466
z	14	ALA	-	expression tag	UNP P13466
z	15	SER	-	expression tag	UNP P13466
z	149	GLU	-	expression tag	UNP P13466
z	150	LEU	-	expression tag	UNP P13466
z	151	PHE	-	expression tag	UNP P13466
z	152	SER	-	expression tag	UNP P13466
z	153	THR	-	expression tag	UNP P13466
z	154	PRO	-	expression tag	UNP P13466
z	155	VAL	-	expression tag	UNP P13466
z	156	TRP	-	expression tag	UNP P13466
z	157	ILE	-	expression tag	UNP P13466
z	158	TRP	-	expression tag	UNP P13466
z	159	TRP	-	expression tag	UNP P13466
z	160	TRP	-	expression tag	UNP P13466
z	161	PRO	-	expression tag	UNP P13466
z	162	ARG	-	expression tag	UNP P13466
z	163	ILE	-	expression tag	UNP P13466
z	164	ARG	-	expression tag	UNP P13466

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Chain	Residue	Modelled	Actual	Comment	Reference
z	165	GLY	-	expression tag	UNP P13466
z	166	PRO	-	expression tag	UNP P13466
z	167	PRO	-	expression tag	UNP P13466

- Molecule 31 is a RNA chain called Peptidyl Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

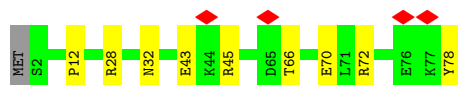
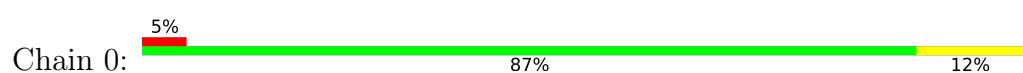
- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	2901	Total	C	N	O	P	0	0
			62281	27784	11464	20132	2901		

3 Residue-property plots [i](#)

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

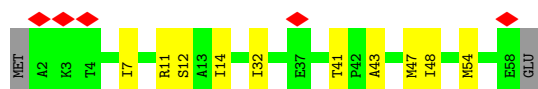
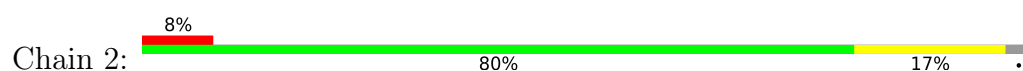
- Molecule 1: Large ribosomal subunit protein bL28



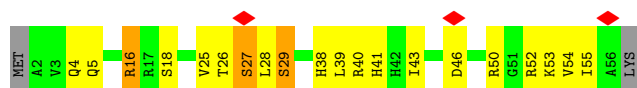
- Molecule 2: Large ribosomal subunit protein uL29



- Molecule 3: Large ribosomal subunit protein uL30



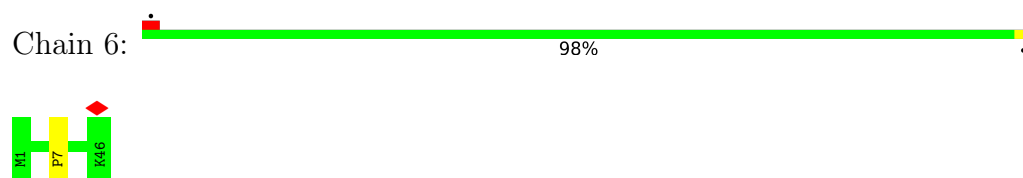
- Molecule 4: Large ribosomal subunit protein bL32



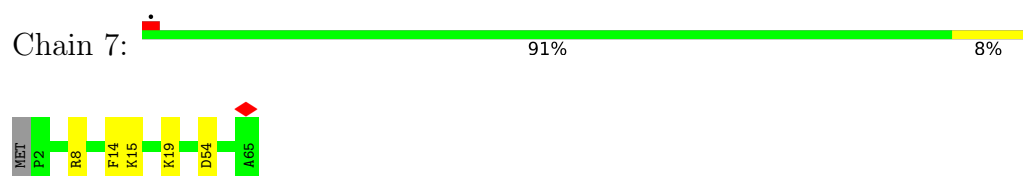
- Molecule 5: Large ribosomal subunit protein bL33



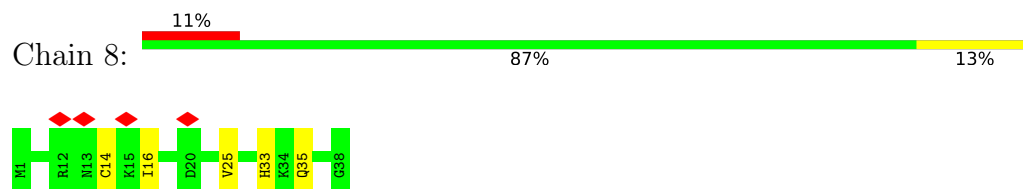
- Molecule 6: Large ribosomal subunit protein bL34



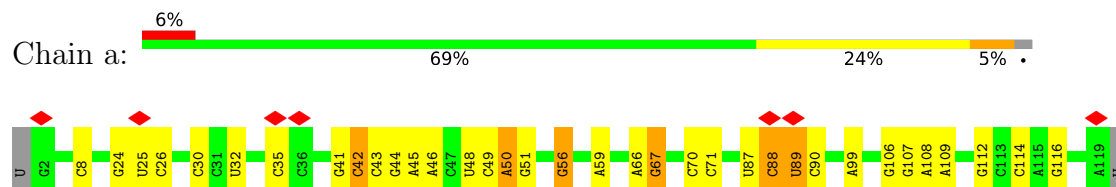
- Molecule 7: Large ribosomal subunit protein bL35



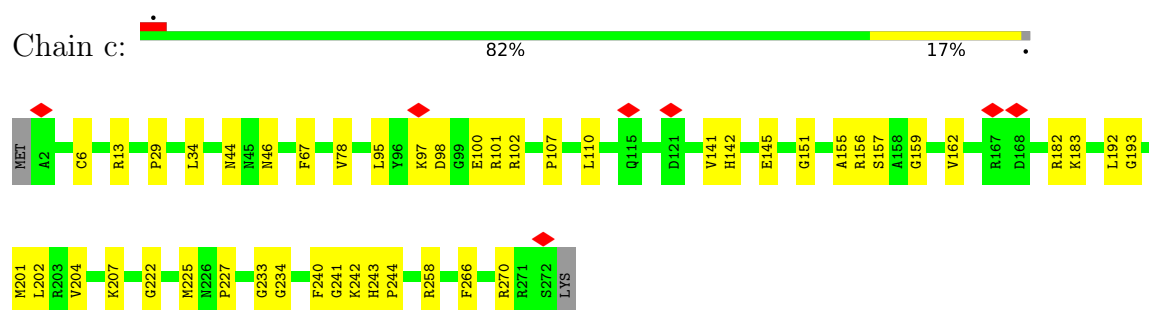
- Molecule 8: Large ribosomal subunit protein bL36A



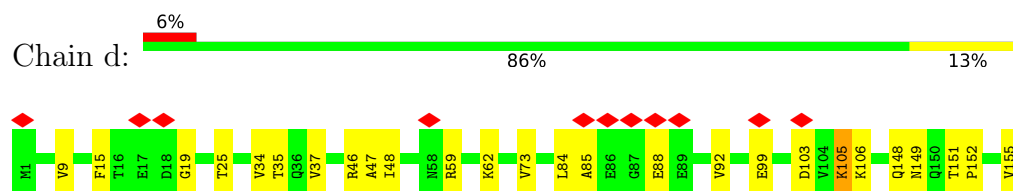
- Molecule 9: 5S rRNA



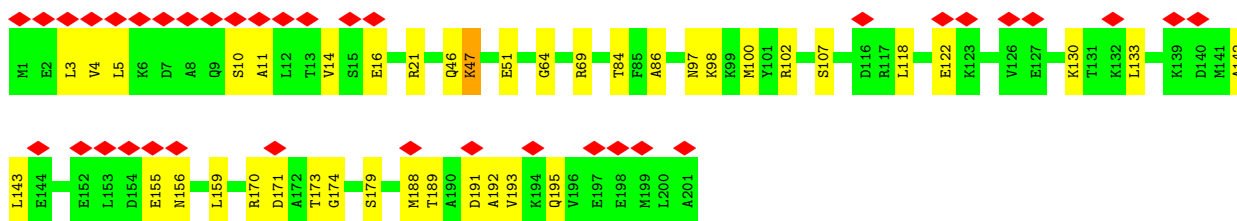
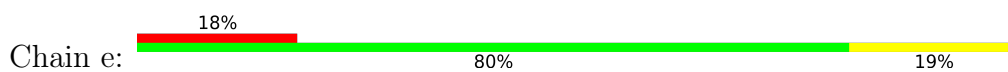
- Molecule 10: Large ribosomal subunit protein uL2



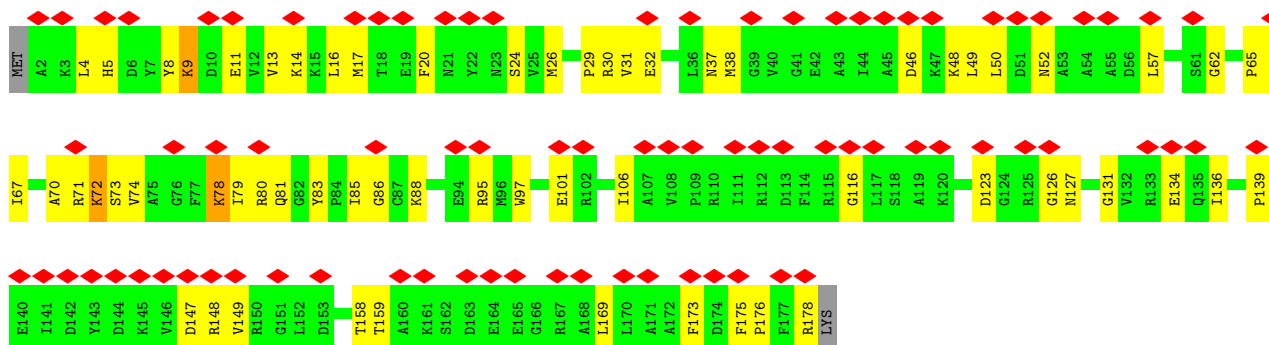
- Molecule 11: 50S ribosomal protein L3



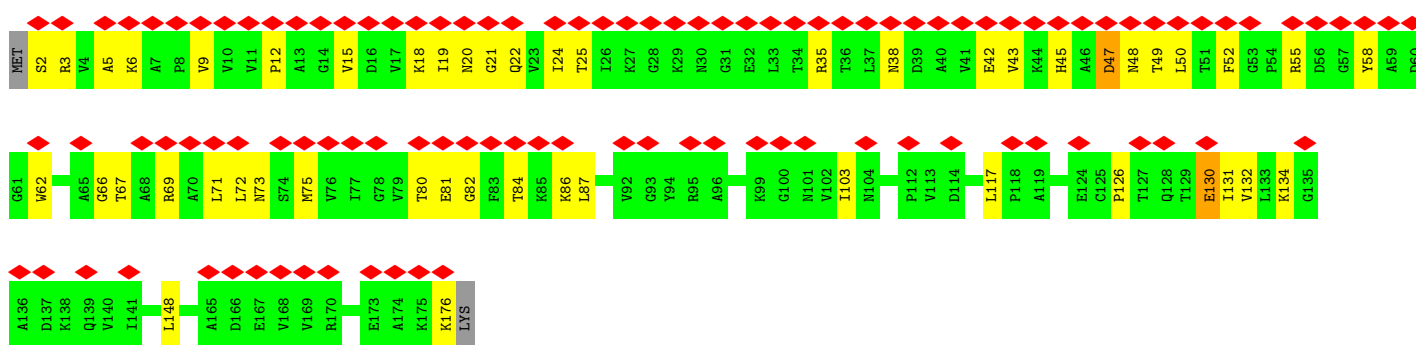
- Molecule 12: Large ribosomal subunit protein uL4



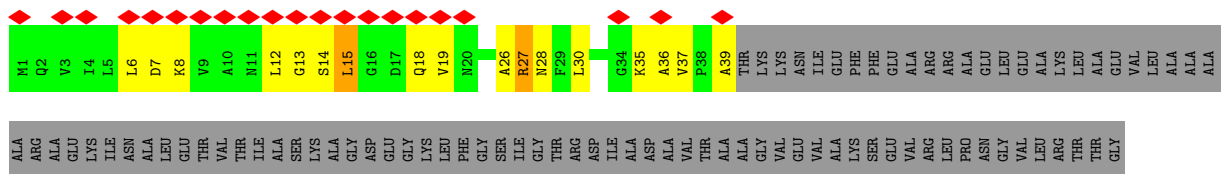
• Molecule 13: Large ribosomal subunit protein uL5



• Molecule 14: Large ribosomal subunit protein uL6



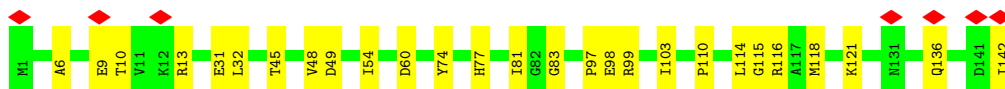
• Molecule 15: Large ribosomal subunit protein bL9



GLU HIS
GLU VAL
SER PHE
GLN VAL
HIS HIS
SER SER
GLU VAL
PHE PHE
ALA VAL
LYS VAL
ILE VAL
ASN VAL
VAL VAL
ALA VAL
GLU

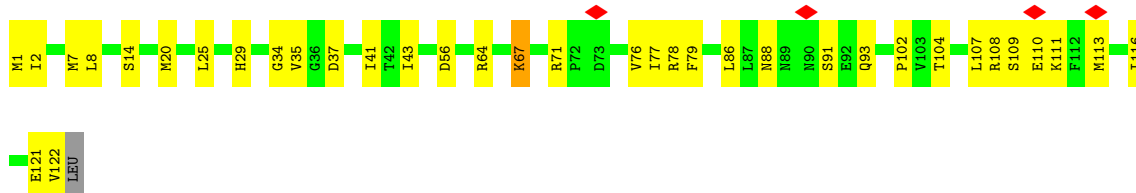
- Molecule 16: Large ribosomal subunit protein uL13

Chain j: 5% 81% 19%



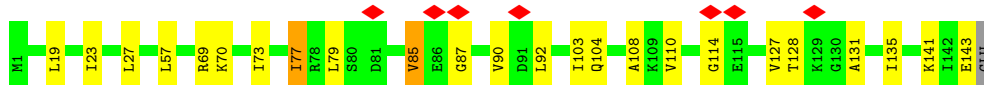
- Molecule 17: Large ribosomal subunit protein uL14

Chain k: 70% 28% ..



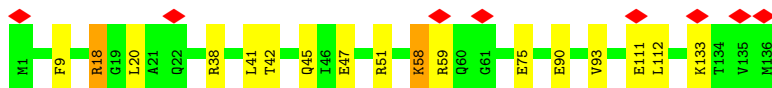
- Molecule 18: Large ribosomal subunit protein uL15

Chain l: 5% 83% 15% ..



- Molecule 19: 50S ribosomal protein L16

Chain m: 6% 88% 11% ..



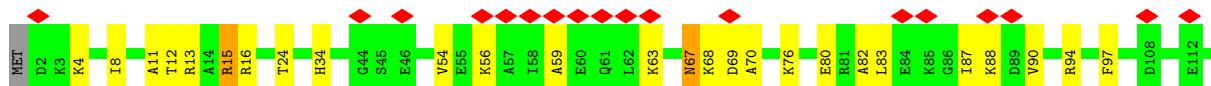
- Molecule 20: Large ribosomal subunit protein bL17

Chain n: 74% 19% .. 6%



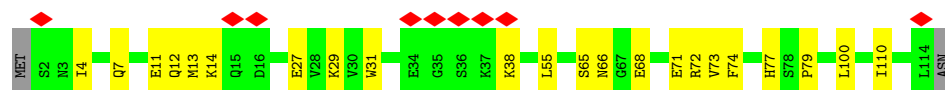
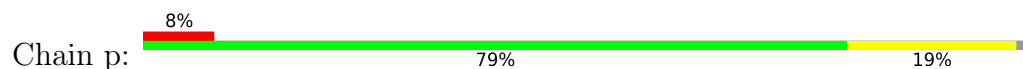
- Molecule 21: Large ribosomal subunit protein uL18

Chain o: 17% 76% 21% ..

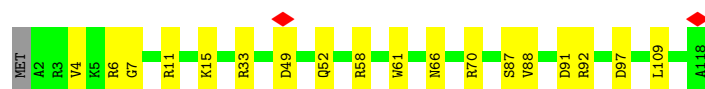
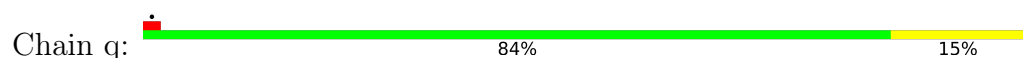




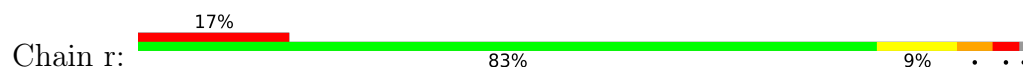
- Molecule 22: Large ribosomal subunit protein bL19



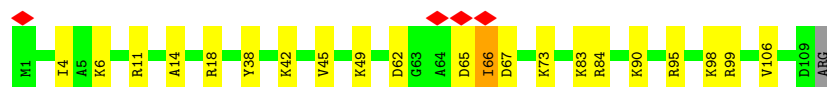
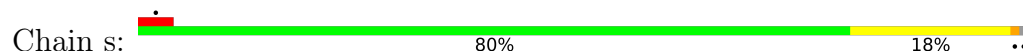
- Molecule 23: Large ribosomal subunit protein bL20



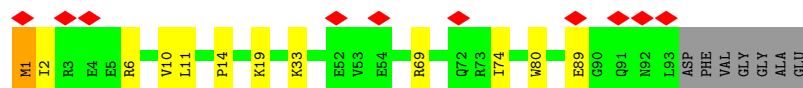
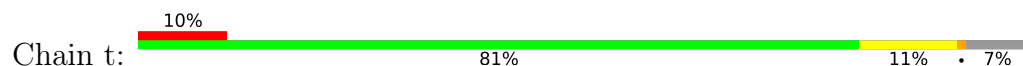
- Molecule 24: Large ribosomal subunit protein bL21



- Molecule 25: Large ribosomal subunit protein uL22

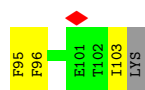


- Molecule 26: Large ribosomal subunit protein uL23

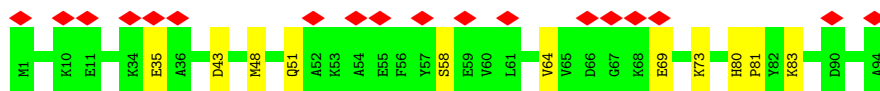
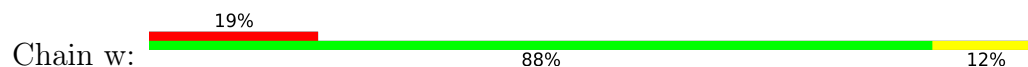


- Molecule 27: Large ribosomal subunit protein uL24

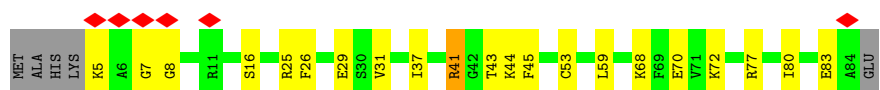




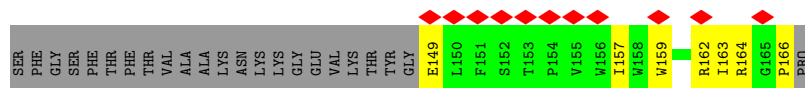
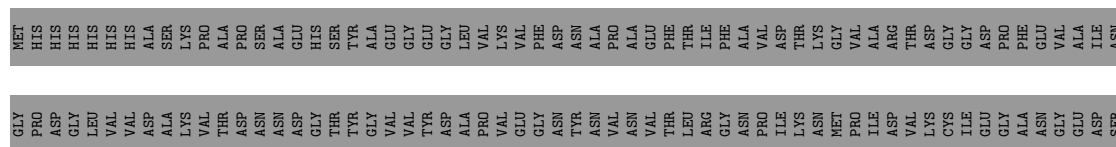
- Molecule 28: Large ribosomal subunit protein bL25



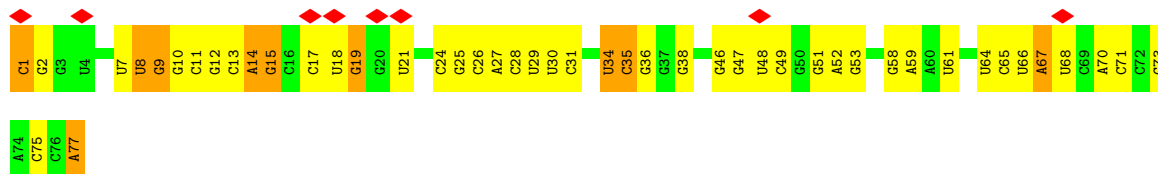
- Molecule 29: Large ribosomal subunit protein bL27



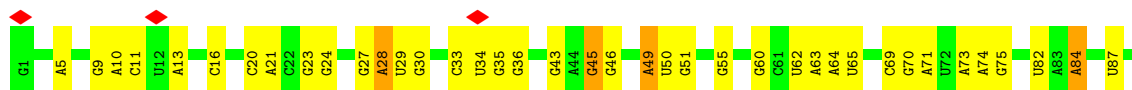
- Molecule 30: Gelation factor

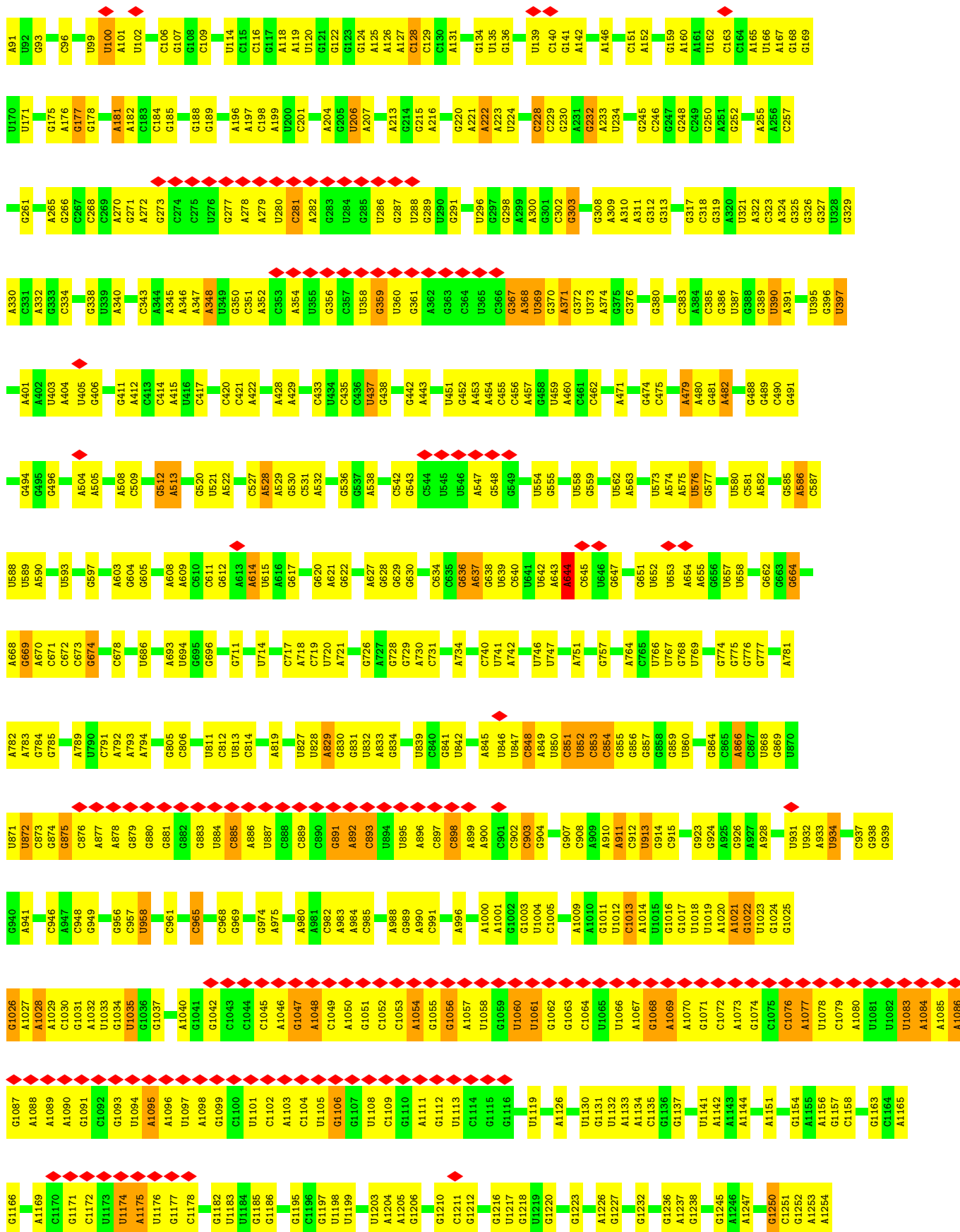


- Molecule 31: Peptidyl Pro-tRNA



- Molecule 32: 23S rRNA







A2820	A2821	A2822	A2823	A2824	A2825	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2871	A2879	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2893	A2894	A2895	A2898	A2899	A2900	A2901	C	U	U			
A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	C2771	C2772	C2773	C2777	C2778	C2779	C2780	A2781	C2782	C2783	C2784	C2785	C2786	C2787	C2788	C2789	C2790	C2794	C2795	C2796	C2797	C2798	A2799	A2800	C2801	C2802	C2803	U2804	U2807	C2808	A2809	A2810	A2814	U2818	U2819
A2662	A2663	A2664	A2668	A2669	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2688	A2689	A2690	A2691	A2692	A2696	A2697	A2700	A2701	A2702	A2705	U2713	A2716	C2717	C2718	U2724	A2725	A2726	A2727	U2728	C2731	C2732	A2733	A2736	A2737	A2738	U2739	C2744	C2745	U2746	C2747								
C2573	C2574	C2575	C2579	C2580	C2581	C2582	C2583	C2584	C2585	A2590	C2597	C2602	C2603	U2604	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2623	C2624	C2625	C2626	U2629	C2630	A2634	A2635	C2636	A2639	C2643	C2645	C2646	C2655	C2656	A2657	C2658	C2659	A2660	C2661										
G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	A2497	C2498	C2499	G2502	A2503	U2504	U2505	U2506	A2513	U2514	A2516	C2517	U2519	C2520	G2526	C2527	U2528	C2529	U2533	A2534	C2535	C2536	U2537	G2543	U2546	C2547	G2550	U2554	C2555	A2560	U2561	U2562	C2563	A2564	C2565	A2567	C2568	G2567	A2572									
U2408	U2409	U2410	U2416	U2419	U2420	U2421	U2422	U2423	U2424	U2425	A2426	C2427	U2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	U2441	G2445	G2446	A2448	C2452	A2453	G2454	U2457	G2458	A2459	U2464	A2468	A2469	C2470	A2471	G2472	U2473	U2474	C2475	U2476	A2477	A2478	U2479	C2480	G2481	A2482	C2483	G2484	G2485	C2486					
U2323	U2324	U2325	A2326	A2327	A2328	U2331	A2332	A2333	U2334	A2335	A2336	C2337	C2338	C2339	A2340	U2345	A2346	C2347	C2350	C2351	C2352	C2353	C2354	C2355	U2361	C2364	U2367	C2368	A2369	A2377	A2378	C2379	U2383	U2384	C2385	U2389	G2389	U2390	C2391	C2396	C2397	U2398	C2399	U2402	C2403	U2404	G2405	A2406	A2407						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	14.45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.39	0/635	0.52	0/848
2	1	0.36	0/496	0.51	0/660
3	2	0.37	0/443	0.44	0/593
4	3	0.57	0/440	0.98	4/588 (0.7%)
5	4	0.55	0/416	0.74	1/554 (0.2%)
6	6	0.43	0/380	0.53	0/498
7	7	0.47	0/513	0.57	0/676
8	8	0.39	0/302	0.48	0/397
9	a	0.38	0/2828	0.36	0/4410
10	c	0.39	0/2121	0.49	0/2852
11	d	0.45	0/1586	0.53	0/2134
12	e	0.33	0/1571	0.43	1/2113 (0.0%)
13	f	0.43	0/1434	0.64	0/1926
14	g	0.40	0/1333	0.57	0/1805
15	h	0.51	0/290	0.80	0/392
16	j	0.44	0/1152	0.50	1/1551 (0.1%)
17	k	0.46	0/947	0.60	1/1268 (0.1%)
18	l	0.65	0/1052	0.83	0/1401
19	m	0.40	0/1093	0.55	0/1460
20	n	0.42	0/973	0.59	1/1301 (0.1%)
21	o	0.42	0/902	0.59	0/1209
22	p	0.39	0/920	0.44	0/1231
23	q	0.42	0/960	0.47	0/1278
24	r	0.52	0/823	0.65	0/1100
25	s	0.42	0/852	0.44	0/1142
26	t	0.42	0/744	0.57	0/994
27	u	0.46	0/787	0.61	0/1051
28	w	0.34	0/766	0.43	0/1025
29	y	0.48	0/603	0.63	0/799
30	z	0.41	0/194	0.69	0/270
31	v	1.42	3/1838 (0.2%)	0.79	5/2862 (0.2%)
32	b	0.53	2/69755 (0.0%)	0.73	30/108819 (0.0%)
All	All	0.53	5/99149 (0.0%)	0.69	44/149207 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	k	0	1
19	m	0	2
20	n	0	1
21	o	0	1
24	r	0	1
29	y	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	v	1	C	O3'-P	-57.37	0.75	1.61
32	b	2059	A	O3'-P	25.70	1.99	1.61
32	b	2058	A	O3'-P	20.93	1.92	1.61
31	v	1	C	C1'-N1	6.54	1.58	1.48
31	v	35	C	C1'-N1	6.52	1.58	1.48

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	v	1	C	OP2-P-O3'	-23.81	36.56	108.00
32	b	2059	A	P-O3'-C3'	-23.46	85.01	120.20
31	v	1	C	O3'-P-O5'	22.34	137.50	104.00
32	b	2058	A	O3'-P-O5'	21.48	136.22	104.00
32	b	2059	A	OP2-P-O3'	10.47	139.42	108.00
31	v	1	C	P-O3'-C3'	-8.87	106.89	120.20
32	b	2864	G	C2'-C3'-O3'	8.65	126.67	113.70
32	b	390	U	C2'-C3'-O3'	8.38	122.07	109.50
32	b	2604	U	P-O3'-C3'	-7.95	108.28	120.20
32	b	1595	C	C2'-C3'-O3'	7.91	125.57	113.70
32	b	2832	U	C4'-C3'-O3'	7.80	121.10	109.40
32	b	2602	A	P-O3'-C3'	7.63	131.64	120.20
20	n	41	ALA	N-CA-C	-7.58	101.08	110.41
17	k	67	LYS	N-CA-C	-7.50	102.02	112.45
32	b	2059	A	OP1-P-O3'	-7.47	85.60	108.00
31	v	1	C	OP1-P-O3'	-7.26	86.22	108.00
32	b	1626	A	C2'-C3'-O3'	7.08	124.31	113.70
32	b	228	C	C4'-C3'-O3'	6.94	119.81	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	29	SER	CA-C-N	-6.87	114.67	123.19
4	3	29	SER	C-N-CA	-6.87	114.67	123.19
32	b	2584	U	P-O3'-C3'	-6.80	109.99	120.20
32	b	9	G	C2'-C3'-O3'	6.62	123.63	113.70
32	b	479	A	C2'-C3'-O3'	-6.41	99.89	109.50
32	b	1538	G	C2'-C3'-O3'	6.22	123.04	113.70
32	b	2655	G	C4'-C3'-O3'	6.16	118.64	109.40
4	3	27	SER	CA-C-N	-6.10	110.57	120.87
4	3	27	SER	C-N-CA	-6.10	110.57	120.87
31	v	34	U	O3'-P-O5'	-6.08	94.89	104.00
32	b	1930	G	C4'-C3'-O3'	5.92	118.28	109.40
32	b	2334	U	C2'-C3'-O3'	5.79	122.38	113.70
32	b	45	G	C2'-C3'-O3'	-5.68	105.18	113.70
32	b	1762	A	C4'-C3'-O3'	-5.58	104.63	113.00
32	b	2058	A	P-O3'-C3'	5.57	128.56	120.20
32	b	2585	U	P-O3'-C3'	-5.52	111.92	120.20
32	b	644	A	O4'-C1'-C2'	-5.41	102.19	107.60
16	j	136	GLN	CA-C-O	-5.39	116.33	120.48
32	b	2655	G	C2'-C3'-O3'	5.34	117.51	109.50
32	b	2055	C	C4'-C3'-O3'	5.29	120.93	113.00
32	b	2333	A	P-O3'-C3'	-5.18	112.42	120.20
32	b	1299	G	C2'-C3'-O3'	5.15	121.42	113.70
5	4	50	LYS	O-C-N	5.10	129.19	123.27
32	b	2055	C	C3'-C2'-O2'	5.09	118.33	110.70
12	e	47	LYS	CB-CG-CD	5.04	122.90	111.30
32	b	204	A	C2'-C3'-O3'	-5.00	101.99	109.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	k	108	ARG	Sidechain
19	m	18	ARG	Sidechain
19	m	38	ARG	Sidechain
20	n	118	ARG	Sidechain
21	o	16	ARG	Sidechain
24	r	47	VAL	Mainchain
29	y	41	ARG	Sidechain

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	0	625	0	652	5	0
2	1	495	0	526	13	0
3	2	439	0	482	6	0
4	3	434	0	445	25	0
5	4	409	0	440	8	0
6	6	377	0	418	1	0
7	7	504	0	572	3	0
8	8	301	0	341	3	0
9	a	2529	0	1281	15	0
10	c	2082	0	2154	28	0
11	d	1565	0	1616	22	0
12	e	1552	0	1619	26	0
13	f	1410	0	1444	48	0
14	g	1313	0	1358	28	0
15	h	287	0	307	13	0
16	j	1129	0	1162	19	0
17	k	938	0	1012	24	0
18	l	1043	0	1123	10	0
19	m	1074	0	1157	13	0
20	n	960	0	1000	17	0
21	o	892	0	923	25	0
22	p	908	0	956	19	0
23	q	947	0	1019	18	0
24	r	810	0	834	17	0
25	s	845	0	909	27	0
26	t	738	0	807	7	0
27	u	779	0	831	27	0
28	w	753	0	780	7	0
29	y	596	0	611	23	0
30	z	178	0	168	19	0
31	v	1646	0	830	70	0
32	b	62281	0	31324	409	0
All	All	90839	0	59101	860	0

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

All (860) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:v:35:C:C1'	31:v:36:G:C8	2.01	1.40
31:v:14:A:N7	32:b:1924:C:C2	1.98	1.31
31:v:35:C:H1'	31:v:36:G:C8	1.64	1.27
32:b:2059:A:O3'	32:b:2060:A:P	1.99	1.19
32:b:851:C:O2'	32:b:852:U:H5'	1.41	1.17
32:b:2059:A:H3'	32:b:2060:A:P	1.84	1.15
32:b:2059:A:C3'	32:b:2060:A:P	2.34	1.15
31:v:35:C:O4'	31:v:36:G:C8	1.99	1.12
29:y:5:LYS:N	31:v:1:C:H1'	1.66	1.10
32:b:1997:C:H4'	32:b:1997:C:OP1	1.54	1.07
31:v:35:C:C1'	31:v:36:G:H8	1.50	1.07
32:b:644:A:H8	32:b:644:A:C5'	1.69	1.04
32:b:368:A:H2'	32:b:369:U:O5'	1.57	1.04
32:b:643:A:H2'	32:b:644:A:H5''	1.43	0.99
32:b:644:A:H8	32:b:644:A:H5'	1.28	0.96
32:b:368:A:C2'	32:b:369:U:O5'	2.11	0.96
31:v:35:C:H1'	31:v:36:G:N9	1.79	0.95
32:b:644:A:H5'	32:b:644:A:C8	2.03	0.94
32:b:851:C:C2'	32:b:852:U:H5'	1.97	0.93
32:b:852:U:H2'	32:b:853:C:H6	1.35	0.91
32:b:851:C:H2'	32:b:852:U:C6	2.06	0.91
32:b:644:A:C5'	32:b:644:A:C8	2.54	0.91
32:b:851:C:H2'	32:b:852:U:H6	1.34	0.90
32:b:643:A:C2'	32:b:644:A:H5''	2.02	0.89
32:b:874:G:H2'	32:b:875:G:H5'	1.56	0.87
32:b:2041:U:H2'	32:b:2042:A:C8	2.10	0.86
32:b:1997:C:OP1	32:b:1997:C:C4'	2.24	0.85
32:b:2783:U:H2'	32:b:2784:U:C6	2.12	0.84
17:k:110:GLU:H	17:k:113:MET:HE3	1.42	0.84
21:o:13:ARG:NH2	32:b:2334:U:H3'	1.92	0.84
31:v:14:A:C8	32:b:1924:C:C2	2.65	0.84
31:v:19:G:O2'	31:v:58:G:N2	2.10	0.84
31:v:35:C:H1'	31:v:36:G:O4'	1.76	0.83
31:v:35:C:H1'	31:v:36:G:C1'	2.08	0.83
31:v:14:A:N7	32:b:1924:C:N1	2.22	0.83
31:v:35:C:N1	31:v:36:G:H8	1.77	0.82
32:b:270:A:C2	32:b:369:U:H4'	2.15	0.82
21:o:12:THR:CG2	32:b:2334:U:H4'	2.10	0.81
4:3:28:LEU:HD11	25:s:38:TYR:CD2	2.15	0.81
31:v:34:U:H2'	31:v:35:C:H6	1.45	0.81
32:b:673:C:O2'	32:b:674:G:H5'	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1875:G:H8	32:b:1875:G:H5''	1.46	0.80
30:z:166:PRO:O	31:v:77:A:H5'	1.82	0.80
14:g:18:LYS:HB3	14:g:25:THR:HB	1.64	0.80
30:z:157:ILE:HG21	32:b:2611:C:C2	2.17	0.80
32:b:852:U:H2'	32:b:853:C:C6	2.16	0.79
32:b:874:G:C2'	32:b:875:G:H5'	2.12	0.79
31:v:14:A:N7	32:b:1924:C:O2	2.15	0.79
4:3:28:LEU:HD21	25:s:38:TYR:CD2	2.17	0.79
32:b:2690:U:H4'	32:b:2691:C:OP1	1.83	0.78
30:z:166:PRO:HA	31:v:77:A:O3'	1.83	0.78
32:b:948:C:O4'	32:b:984:A:C2	2.36	0.78
32:b:643:A:C3'	32:b:644:A:H5''	2.14	0.78
11:d:15:PHE:H	22:p:12:GLN:HE22	1.32	0.77
25:s:6:LYS:HB2	32:b:494:G:H4'	1.67	0.77
4:3:28:LEU:HD21	25:s:38:TYR:CG	2.20	0.77
13:f:80:ARG:HD2	13:f:83:TYR:OH	1.82	0.77
32:b:2657:A:C2'	32:b:2658:C:H5'	2.16	0.76
32:b:2682:A:H61	32:b:2728:U:H1'	1.51	0.76
21:o:13:ARG:HH21	32:b:2334:U:H3'	1.49	0.75
31:v:9:G:H21	31:v:24:C:H41	1.32	0.74
29:y:5:LYS:CB	31:v:1:C:O2	2.35	0.74
29:y:5:LYS:N	31:v:1:C:C1'	2.48	0.74
32:b:1875:G:H5''	32:b:1875:G:C8	2.21	0.74
32:b:1954:G:H5'	32:b:2550:G:H21	1.53	0.74
12:e:130:LYS:HB2	12:e:133:LEU:HD13	1.70	0.73
29:y:5:LYS:N	31:v:1:C:HO2'	1.85	0.73
32:b:2059:A:C2	32:b:2503:A:C6	2.75	0.73
12:e:84:THR:HG21	32:b:586:A:H5'	1.68	0.73
12:e:64:GLY:O	32:b:2059:A:H5''	1.86	0.73
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.70	0.73
31:v:34:U:H2'	31:v:35:C:C6	2.23	0.73
32:b:281:C:H2'	32:b:282:A:C8	2.23	0.73
31:v:35:C:C1'	31:v:36:G:O4'	2.36	0.72
32:b:851:C:O2'	32:b:852:U:C5'	2.32	0.72
32:b:1992:G:N2	32:b:1996:C:O2'	2.22	0.72
11:d:9:VAL:HG11	22:p:4:ILE:HD11	1.72	0.72
32:b:1964:G:H4'	32:b:1965:C:OP2	1.89	0.71
29:y:43:THR:O	29:y:45:PHE:N	2.24	0.71
32:b:637:A:H4'	32:b:638:G:O5'	1.91	0.71
31:v:9:G:N2	31:v:24:C:H41	1.88	0.71
32:b:1997:C:H2'	32:b:1998:A:H5'	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:2111:U:H2'	32:b:2143:C:H5''	1.74	0.70
19:m:41:LEU:HA	19:m:45:GLN:HE21	1.54	0.70
32:b:612:G:C6	32:b:614:A:C8	2.79	0.70
32:b:2758:A:H2'	32:b:2759:G:H5'	1.73	0.70
21:o:94:ARG:HH22	32:b:2293:G:H5''	1.56	0.70
21:o:67:ASN:H	21:o:70:ALA:HB3	1.57	0.69
32:b:1889:A:H8	32:b:1889:A:OP2	1.73	0.69
23:q:6:ARG:HD3	32:b:1250:G:H5''	1.74	0.69
32:b:852:U:C2	32:b:853:C:C5	2.80	0.69
32:b:612:G:N2	32:b:617:G:C6	2.61	0.69
13:f:48:LYS:O	13:f:52:ASN:ND2	2.26	0.69
32:b:1283:G:N2	32:b:1285:A:H3'	2.08	0.69
32:b:2690:U:C4'	32:b:2691:C:OP1	2.41	0.68
20:n:86:ARG:HH21	20:n:117:ASP:HB2	1.58	0.68
32:b:612:G:C2	32:b:617:G:O6	2.47	0.68
32:b:2506:U:H3	32:b:2583:G:H1	1.41	0.68
4:3:40:ARG:HG3	4:3:41:HIS:ND1	2.08	0.68
14:g:35:ARG:HG2	14:g:75:MET:HE1	1.74	0.68
31:v:7:U:H3'	31:v:8:U:H5'	1.74	0.68
32:b:2059:A:C2	32:b:2503:A:C5	2.81	0.68
32:b:644:A:H8	32:b:644:A:H5''	1.59	0.67
22:p:7:GLN:NE2	22:p:11:GLU:OE1	2.25	0.67
13:f:116:GLY:O	13:f:178:ARG:NH2	2.27	0.67
14:g:42:GLU:OE1	14:g:55:ARG:NE	2.28	0.66
32:b:272:A:H2'	32:b:273:G:C8	2.29	0.66
32:b:612:G:C5	32:b:614:A:C8	2.84	0.66
20:n:12:ARG:HD3	20:n:16:HIS:CD2	2.31	0.66
9:a:51:G:OP1	21:o:63:LYS:NZ	2.28	0.66
20:n:37:THR:HG22	20:n:110:MET:HE1	1.76	0.66
16:j:118:MET:HA	16:j:121:LYS:HZ3	1.61	0.66
32:b:1889:A:OP2	32:b:1889:A:C8	2.49	0.65
13:f:80:ARG:CD	13:f:83:TYR:OH	2.43	0.65
23:q:91:ASP:HB2	24:r:11:GLN:NE2	2.11	0.65
13:f:46:ASP:HB3	13:f:49:LEU:HD23	1.77	0.65
11:d:59:ARG:HG3	32:b:2830:C:OP1	1.95	0.65
31:v:12:G:H5''	32:b:1908:C:O2'	1.96	0.65
32:b:1997:C:C2'	32:b:1998:A:H5'	2.26	0.65
32:b:2758:A:C2'	32:b:2759:G:H5'	2.26	0.65
32:b:2041:U:H2'	32:b:2042:A:H8	1.59	0.65
32:b:902:C:C4	32:b:903:C:C5	2.85	0.65
15:h:12:LEU:HD13	15:h:19:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:r:46:GLU:HB3	24:r:48:LYS:HG3	1.79	0.65
16:j:49:ASP:OD2	16:j:121:LYS:NZ	2.29	0.64
2:1:11:VAL:O	2:1:15:ASN:ND2	2.30	0.64
10:c:67:PHE:CE1	10:c:156:ARG:HD2	2.32	0.64
28:w:64:VAL:HG22	28:w:69:GLU:HG2	1.79	0.64
32:b:2543:G:H21	32:b:2646:C:H5'	1.61	0.64
4:3:28:LEU:CD1	25:s:38:TYR:CE2	2.79	0.64
10:c:182:ARG:NH2	10:c:183:LYS:O	2.30	0.64
2:1:2:LYS:HE3	2:1:6:LEU:HD11	1.79	0.64
32:b:2617:U:C2'	32:b:2618:G:H5'	2.28	0.64
7:7:54:ASP:HB3	18:l:57:LEU:HD22	1.80	0.64
30:z:166:PRO:CA	31:v:77:A:O3'	2.46	0.64
32:b:948:C:O4'	32:b:984:A:H2	1.80	0.64
32:b:612:G:C2	32:b:617:G:C6	2.85	0.64
32:b:2110:G:H22	32:b:2179:C:H2'	1.61	0.64
32:b:852:U:C2	32:b:853:C:C6	2.86	0.64
14:g:103:ILE:HG13	14:g:117:LEU:HD11	1.80	0.63
27:u:34:VAL:HG13	27:u:67:VAL:HG12	1.79	0.63
25:s:11:ARG:NH2	25:s:98:LYS:HD3	2.14	0.63
32:b:1935:G:H1'	32:b:1964:G:N2	2.13	0.63
16:j:114:LEU:HG	16:j:118:MET:HE3	1.81	0.63
31:v:35:C:O4'	31:v:36:G:N7	2.29	0.63
23:q:4:VAL:HG22	32:b:1199:U:H1'	1.80	0.62
17:k:78:ARG:NH2	22:p:71:GLU:OE2	2.26	0.62
32:b:272:A:H2'	32:b:273:G:H8	1.63	0.62
11:d:148:GLN:HB2	11:d:152:PRO:HG2	1.82	0.62
31:v:14:A:O3'	32:b:1925:C:P	2.57	0.62
32:b:628:G:O2'	32:b:629:G:H5'	1.99	0.62
12:e:21:ARG:NH2	12:e:107:SER:OG	2.33	0.62
12:e:98:LYS:HB3	12:e:102:ARG:HH22	1.64	0.62
14:g:43:VAL:HG23	14:g:52:PHE:HE1	1.64	0.62
18:l:128:THR:HG22	32:b:636:G:OP2	2.00	0.62
30:z:164:ARG:HD2	32:b:2452:C:C2	2.34	0.62
32:b:851:C:C2	32:b:852:U:C5	2.88	0.62
10:c:227:PRO:HG3	10:c:234:GLY:H	1.65	0.62
32:b:2657:A:H2'	32:b:2658:C:H5'	1.82	0.61
32:b:2834:G:H2'	32:b:2879:A:H61	1.65	0.61
2:1:10:SER:N	2:1:13:GLU:OE2	2.25	0.61
12:e:69:ARG:HD3	32:b:674:G:H1'	1.83	0.61
32:b:933:A:C5'	32:b:934:U:OP2	2.49	0.61
31:v:14:A:C1'	32:b:1924:C:HO2'	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1269:A:H61	32:b:2011:U:H3	1.48	0.61
23:q:91:ASP:HB2	24:r:11:GLN:HE21	1.64	0.61
5:4:32:GLU:OE2	5:4:32:GLU:N	2.28	0.60
10:c:155:ALA:HB2	10:c:162:VAL:HG23	1.82	0.60
13:f:66:LEU:O	13:f:67:ILE:HD13	1.99	0.60
9:a:89:U:O2	32:b:958:U:H2'	2.01	0.60
24:r:51:VAL:HG22	24:r:52:PRO:HD2	1.82	0.60
27:u:94:ARG:HB3	27:u:103:ILE:HD12	1.83	0.60
29:y:7:GLY:HA3	31:v:2:G:H4'	1.83	0.60
31:v:25:G:O2'	32:b:1923:U:OP1	2.18	0.60
8:8:16:ILE:HD13	8:8:25:VAL:HG22	1.84	0.60
31:v:11:C:O3'	32:b:1909:C:H4'	2.01	0.60
29:y:43:THR:C	29:y:45:PHE:H	2.10	0.60
32:b:373:U:H2'	32:b:374:A:H8	1.67	0.59
21:o:12:THR:HB	32:b:2334:U:H4'	1.84	0.59
32:b:2074:U:H2'	32:b:2075:U:C6	2.36	0.59
32:b:874:G:O2'	32:b:875:G:H5'	2.02	0.59
13:f:134:GLU:OE1	13:f:136:ILE:HG22	2.02	0.59
32:b:2128:G:H1'	32:b:2174:C:H1'	1.83	0.59
32:b:671:C:H2'	32:b:672:C:C6	2.36	0.59
27:u:7:ARG:NH1	27:u:28:VAL:HG23	2.18	0.59
14:g:35:ARG:HG2	14:g:75:MET:CE	2.33	0.59
17:k:107:LEU:HB2	17:k:116:ILE:HD11	1.84	0.59
31:v:35:C:C6	31:v:36:G:H8	2.21	0.59
20:n:96:ARG:HG3	20:n:116:VAL:HG12	1.83	0.58
21:o:13:ARG:N	32:b:2334:U:O3'	2.35	0.58
24:r:51:VAL:O	24:r:52:PRO:C	2.45	0.58
32:b:669:G:H2'	32:b:669:G:N3	2.16	0.58
15:h:8:LYS:HE2	15:h:15:LEU:HD23	1.84	0.58
32:b:28:A:N6	32:b:512:G:H1'	2.19	0.58
17:k:76:VAL:HG12	22:p:73:VAL:HB	1.86	0.58
23:q:66:ASN:O	23:q:70:ARG:HG3	2.04	0.58
5:4:34:LEU:HB3	5:4:51:GLU:OE1	2.04	0.58
10:c:159:GLY:HA3	32:b:1820:U:C4	2.37	0.58
22:p:14:LYS:HD2	22:p:77:HIS:HA	1.84	0.58
20:n:29:VAL:O	20:n:78:LYS:NZ	2.30	0.58
21:o:12:THR:CB	32:b:2334:U:H4'	2.33	0.58
21:o:13:ARG:HH21	32:b:2334:U:C3'	2.17	0.58
13:f:147:ASP:OD1	13:f:148:ARG:N	2.37	0.57
32:b:581:C:H2'	32:b:582:A:C8	2.39	0.57
13:f:31:VAL:HG12	13:f:158:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:956:G:H2'	32:b:957:C:H2'	1.86	0.57
2:1:30:MET:HE1	26:t:14:PRO:HD3	1.85	0.57
32:b:2059:A:N3	32:b:2503:A:C6	2.72	0.57
18:l:79:LEU:HB2	18:l:114:GLY:H	1.69	0.57
32:b:673:C:C2'	32:b:674:G:H5'	2.34	0.57
16:j:118:MET:HA	16:j:121:LYS:NZ	2.19	0.57
32:b:2617:U:H2'	32:b:2618:G:H5'	1.86	0.57
32:b:2140:G:H3'	32:b:2141:G:H8	1.69	0.57
10:c:78:VAL:HG21	10:c:110:LEU:HD11	1.87	0.57
30:z:157:ILE:CG2	32:b:2611:C:C2	2.88	0.57
32:b:898:C:C2'	32:b:899:A:O5'	2.53	0.57
2:1:29:ARG:NH2	26:t:11:LEU:O	2.38	0.57
14:g:43:VAL:HG23	14:g:52:PHE:CE1	2.40	0.57
30:z:159[B]:TRP:HE3	30:z:163:ILE:HD11	1.70	0.57
32:b:368:A:O2'	32:b:369:U:O5'	2.23	0.56
32:b:833:A:H2'	32:b:834:G:C8	2.40	0.56
17:k:29:HIS:CE1	32:b:2547:G:H4'	2.40	0.56
21:o:12:THR:HG22	32:b:2334:U:H4'	1.86	0.56
5:4:10:LYS:O	5:4:52:ALA:N	2.39	0.56
13:f:57:LEU:HD23	13:f:65:PRO:HB3	1.87	0.56
32:b:2659:G:H2'	32:b:2660:A:H2'	1.88	0.56
11:d:46:ARG:NH1	11:d:85:ALA:O	2.39	0.56
21:o:56:LYS:O	21:o:59:ALA:N	2.39	0.56
9:a:42:C:C4	13:f:66:LEU:HD21	2.41	0.56
32:b:933:A:H5'	32:b:934:U:OP2	2.06	0.56
32:b:1384:A:H1'	32:b:1405:U:H1'	1.88	0.56
31:v:14:A:C1'	32:b:1924:C:O2'	2.35	0.56
31:v:64:U:H2'	31:v:65:C:H6	1.70	0.56
32:b:866:A:H61	32:b:913:U:H1'	1.71	0.55
32:b:2751:G:H3'	32:b:2752:C:H6	1.70	0.55
14:g:22:GLN:NE2	14:g:38:ASN:O	2.40	0.55
14:g:9:VAL:HG12	14:g:50:LEU:HB2	1.87	0.55
2:1:44:LYS:O	2:1:48:ARG:HG2	2.06	0.55
13:f:126:GLY:O	13:f:158:THR:OG1	2.20	0.55
32:b:1469:A:H2'	32:b:1470:A:C8	2.42	0.55
32:b:2324:U:H1'	32:b:2337:G:H5''	1.86	0.55
32:b:2845:U:H2'	32:b:2846:G:C8	2.41	0.55
29:y:77:ARG:HG3	29:y:77:ARG:HH11	1.70	0.55
32:b:898:C:H2'	32:b:899:A:O5'	2.06	0.55
4:3:28:LEU:CD1	25:s:38:TYR:CD2	2.90	0.55
12:e:98:LYS:HB3	12:e:102:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1095:A:H5'	32:b:1096:A:H5''	1.89	0.55
32:b:2273:A:H2'	32:b:2274:A:C8	2.42	0.55
32:b:2829:A:C6	32:b:2830:C:C4	2.95	0.55
25:s:4:ILE:HG13	25:s:106:VAL:HG22	1.88	0.55
27:u:81:ASP:OD1	27:u:82:ARG:N	2.40	0.55
2:1:12:GLU:O	2:1:16:THR:HG23	2.07	0.55
1:0:72:ARG:NH1	1:0:78:TYR:OH	2.38	0.54
4:3:28:LEU:HD11	25:s:38:TYR:CE2	2.40	0.54
15:h:6:LEU:HD13	15:h:36:ALA:HA	1.89	0.54
15:h:26:ALA:C	15:h:28:ASN:H	2.15	0.54
21:o:88:LYS:NZ	21:o:116:GLN:HE22	2.05	0.54
9:a:87:U:O2'	9:a:88:C:O5'	2.24	0.54
32:b:643:A:H2'	32:b:644:A:C5'	2.28	0.54
32:b:948:C:C4'	32:b:984:A:C2	2.89	0.54
13:f:38:MET:HE2	13:f:57:LEU:HD13	1.89	0.54
23:q:92:ARG:HG3	23:q:92:ARG:HH11	1.71	0.54
20:n:37:THR:OG1	20:n:40:LYS:HG3	2.08	0.54
32:b:874:G:C2'	32:b:875:G:C5'	2.85	0.54
32:b:2074:U:H2'	32:b:2075:U:O4'	2.08	0.54
32:b:644:A:C8	32:b:644:A:C4'	2.91	0.54
31:v:67:A:H2'	31:v:68:U:H6	1.73	0.54
4:3:29:SER:N	4:3:38:HIS:O	2.28	0.54
32:b:2086:U:H2'	32:b:2087:G:C8	2.43	0.54
5:4:5:ILE:HG21	5:4:28:ARG:NH2	2.23	0.54
8:8:14:CYS:SG	8:8:33:HIS:ND1	2.81	0.54
30:z:166:PRO:O	31:v:77:A:C5'	2.55	0.53
32:b:852:U:N3	32:b:853:C:C5	2.76	0.53
32:b:2233:U:H2'	32:b:2234:G:C8	2.43	0.53
13:f:80:ARG:HB2	13:f:83:TYR:CZ	2.42	0.53
16:j:99:ARG:HE	16:j:103:ILE:HG23	1.74	0.53
25:s:65:ASP:C	25:s:67:ASP:N	2.66	0.53
10:c:240:PHE:O	10:c:242:LYS:HE3	2.09	0.53
11:d:149:ASN:HD22	32:b:2575:C:H5'	1.73	0.53
12:e:97:ASN:HB2	12:e:100:MET:HG3	1.88	0.53
24:r:39:LEU:O	24:r:49:ILE:HB	2.08	0.53
27:u:66:GLN:HB2	27:u:69:ASN:OD1	2.08	0.53
32:b:720:U:H2'	32:b:721:A:C8	2.43	0.53
4:3:4:GLN:HA	32:b:2615:U:C2	2.43	0.53
32:b:891:G:H4'	32:b:892:A:C8	2.42	0.53
12:e:191:ASP:OD1	12:e:192:ALA:N	2.42	0.53
13:f:37:ASN:OD1	13:f:38:MET:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:k:121:GLU:OE1	22:p:65:SER:OG	2.26	0.53
18:l:141:LYS:NZ	18:l:143:GLU:OE2	2.42	0.53
32:b:2547:G:H1	32:b:2561:U:H3	1.57	0.53
4:3:28:LEU:CD2	25:s:38:TYR:CD2	2.91	0.53
14:g:55:ARG:HB2	14:g:58:TYR:HD2	1.73	0.53
18:l:110:VAL:HB	18:l:127:VAL:HG22	1.90	0.53
25:s:83:LYS:HB3	25:s:95:ARG:HD2	1.91	0.53
10:c:141:VAL:HG12	10:c:192:LEU:HD23	1.91	0.53
10:c:201:MET:HG3	10:c:202:LEU:HD23	1.89	0.53
14:g:69:ARG:NH1	14:g:73:ASN:HB2	2.24	0.53
32:b:850:U:H2'	32:b:851:C:C6	2.43	0.53
11:d:156:PHE:CE1	16:j:81:ILE:HD13	2.44	0.53
10:c:182:ARG:NH2	10:c:266:PHE:HB3	2.24	0.52
20:n:57:THR:HG23	20:n:62:ASN:ND2	2.23	0.52
24:r:55:ASP:C	24:r:57:GLY:H	2.17	0.52
32:b:605:G:H1'	32:b:657:U:O2'	2.09	0.52
10:c:95:LEU:HD13	10:c:101:ARG:HG3	1.89	0.52
16:j:31:GLU:HG2	16:j:142:ILE:HD12	1.92	0.52
17:k:121:GLU:HG2	17:k:122:VAL:HG23	1.89	0.52
31:v:67:A:H2'	31:v:68:U:C6	2.44	0.52
14:g:67:THR:O	14:g:71:LEU:HG	2.10	0.52
4:3:46:ASP:O	4:3:53:LYS:NZ	2.41	0.52
10:c:258:ARG:HD3	10:c:270:ARG:NH1	2.24	0.52
32:b:1964:G:C4'	32:b:1965:C:OP2	2.58	0.52
32:b:1752:C:H2'	32:b:1753:G:C8	2.44	0.52
32:b:2334:U:C5	32:b:2335:A:H4'	2.45	0.52
13:f:50:LEU:HD21	13:f:67:ILE:HG23	1.92	0.52
4:3:28:LEU:HD13	25:s:38:TYR:CE2	2.44	0.52
11:d:155:VAL:HG21	32:b:2618:G:H21	1.75	0.52
30:z:166:PRO:O	31:v:77:A:C3'	2.58	0.52
32:b:1000:A:H2'	32:b:1001:A:C8	2.45	0.52
32:b:2125:G:H2'	32:b:2126:A:H4'	1.91	0.52
25:s:42:LYS:HB2	32:b:2010:G:H5''	1.92	0.52
27:u:5:ILE:C	27:u:6:ARG:HD2	2.35	0.52
32:b:2663:G:C6	32:b:2664:G:C5	2.98	0.52
14:g:84:THR:HG22	14:g:134:LYS:HG2	1.93	0.51
32:b:1047:G:O2'	32:b:1048:A:C8	2.61	0.51
32:b:2783:U:H2'	32:b:2784:U:H6	1.70	0.51
5:4:38:LYS:HB2	5:4:49:TYR:CD2	2.45	0.51
11:d:37:VAL:HG22	11:d:48:ILE:HG22	1.92	0.51
12:e:47:LYS:HG3	12:e:51:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:49:LEU:HA	13:f:52:ASN:HD22	1.75	0.51
21:o:94:ARG:HD2	21:o:97:PHE:O	2.10	0.51
22:p:72:ARG:HD2	22:p:74:PHE:CZ	2.45	0.51
1:0:12:PRO:HG2	1:0:28:ARG:HH21	1.76	0.51
4:3:40:ARG:HG3	4:3:41:HIS:CE1	2.46	0.51
10:c:97:LYS:HG2	32:b:1490:A:H62	1.76	0.51
4:3:28:LEU:CD2	25:s:38:TYR:CE2	2.93	0.51
32:b:29:U:H2'	32:b:30:G:C8	2.45	0.51
32:b:1047:G:HO2'	32:b:1048:A:H8	1.57	0.51
20:n:103:ARG:HB2	20:n:110:MET:HE3	1.93	0.51
24:r:49:ILE:HD12	24:r:50:GLY:H	1.76	0.51
27:u:54:GLN:C	27:u:56:GLY:H	2.19	0.51
32:b:28:A:H61	32:b:512:G:H1'	1.76	0.51
32:b:1311:G:H21	32:b:1603:A:H62	1.57	0.51
32:b:1408:G:H1	32:b:1594:U:H3	1.58	0.51
32:b:2291:U:H2'	32:b:2292:U:C6	2.46	0.51
32:b:367:G:C2'	32:b:368:A:H5'	2.41	0.51
32:b:612:G:N2	32:b:617:G:O6	2.43	0.51
32:b:2663:G:C4	32:b:2664:G:C8	2.99	0.51
13:f:70:ALA:C	13:f:72:LYS:H	2.19	0.51
23:q:11:ARG:O	23:q:15:LYS:HG2	2.11	0.50
23:q:87:SER:HB3	24:r:52:PRO:HD3	1.93	0.50
31:v:35:C:N1	31:v:36:G:C8	2.63	0.50
13:f:32:GLU:OE2	13:f:159:THR:OG1	2.20	0.50
10:c:6:CYS:SG	10:c:13:ARG:NH2	2.84	0.50
27:u:82:ARG:HH21	27:u:82:ARG:HG3	1.76	0.50
32:b:853:C:H2'	32:b:853:C:O2	2.11	0.50
32:b:1884:G:H5''	32:b:1884:G:H8	1.77	0.50
32:b:2886:A:H3'	32:b:2887:A:H8	1.75	0.50
13:f:85:ILE:HG13	13:f:86:GLY:N	2.26	0.50
15:h:6:LEU:HD11	15:h:37:VAL:HG22	1.92	0.50
32:b:854:C:H2'	32:b:854:C:O2	2.12	0.50
32:b:1028:A:H2'	32:b:1029:A:C8	2.46	0.50
32:b:1802:A:H2'	32:b:1803:A:C8	2.46	0.50
32:b:2151:U:H5''	32:b:2152:G:H8	1.75	0.50
32:b:2756:U:H1'	32:b:2757:A:H5''	1.94	0.50
19:m:20:LEU:HD13	28:w:81:PRO:HG2	1.94	0.50
27:u:96:PHE:CE1	27:u:103:ILE:HG12	2.46	0.50
31:v:64:U:H2'	31:v:65:C:C6	2.46	0.50
32:b:2334:U:H5''	32:b:2335:A:P	2.51	0.50
11:d:34:VAL:HG12	11:d:92:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:62:GLY:HA3	13:f:95:ARG:NH2	2.26	0.50
25:s:73:LYS:HB2	25:s:106:VAL:HB	1.94	0.50
29:y:26:PHE:N	29:y:29:GLU:HG3	2.26	0.50
27:u:16:GLY:O	27:u:17:LYS:HG3	2.11	0.50
32:b:2764:A:N6	32:b:2766:A:C6	2.79	0.50
13:f:85:ILE:HD11	32:b:2312:U:H5'	1.94	0.50
32:b:1721:G:H2'	32:b:1738:G:H22	1.77	0.50
32:b:2339:C:H2'	32:b:2340:A:C8	2.47	0.50
9:a:45:A:C4	9:a:46:A:C8	3.00	0.49
22:p:13:MET:HE2	22:p:55:LEU:N	2.28	0.49
25:s:65:ASP:O	25:s:67:ASP:N	2.45	0.49
32:b:373:U:H2'	32:b:374:A:C8	2.46	0.49
3:2:12:SER:OG	3:2:14:ILE:HG12	2.13	0.49
27:u:4:LYS:O	27:u:5:ILE:HD13	2.13	0.49
10:c:29:PRO:HG2	10:c:34:LEU:HD11	1.92	0.49
12:e:3:LEU:HD12	12:e:14:VAL:HG11	1.94	0.49
19:m:42:THR:OG1	19:m:45:GLN:HG2	2.12	0.49
29:y:5:LYS:CB	31:v:73:G:H22	2.25	0.49
32:b:612:G:N2	32:b:617:G:C5	2.80	0.49
32:b:965:C:H4'	32:b:2273:A:H1'	1.94	0.49
13:f:70:ALA:O	13:f:72:LYS:N	2.45	0.49
20:n:41:ALA:C	20:n:43:GLU:H	2.20	0.49
32:b:639:U:H2'	32:b:640:C:C6	2.47	0.49
2:1:54:LYS:HA	2:1:57:LEU:HB2	1.94	0.49
5:4:40:ASP:HB3	5:4:43:VAL:HG12	1.95	0.49
26:t:19:LYS:HD3	32:b:1339:G:H5''	1.95	0.49
32:b:2241:A:H2'	32:b:2242:G:C8	2.48	0.49
32:b:2408:U:H2'	32:b:2409:G:C8	2.48	0.49
13:f:13:VAL:O	13:f:17:MET:HG2	2.13	0.49
32:b:558:U:H2'	32:b:559:G:H8	1.77	0.49
32:b:1061:U:H1'	32:b:1068:G:H1'	1.94	0.49
11:d:105:LYS:HG2	11:d:106:LYS:HG2	1.94	0.49
30:z:166:PRO:O	31:v:77:A:H3'	2.12	0.49
32:b:853:C:C2	32:b:854:C:C5	3.01	0.49
15:h:7:ASP:OD1	15:h:8:LYS:N	2.46	0.49
19:m:42:THR:HG22	19:m:93:VAL:HG12	1.95	0.49
31:v:25:G:O2'	32:b:1923:U:H5'	2.12	0.49
32:b:2840:C:H2'	32:b:2841:C:C6	2.48	0.49
32:b:1174:U:H5''	32:b:1175:A:H8	1.77	0.49
32:b:1265:A:H61	32:b:2013:A:H3'	1.76	0.49
4:3:43:ILE:HD11	20:n:98:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1483:G:H1	32:b:1506:U:H3	1.60	0.49
5:4:38:LYS:HB2	5:4:49:TYR:CE2	2.47	0.48
18:l:85:VAL:HG21	18:l:90:VAL:HA	1.94	0.48
19:m:75:GLU:HB2	19:m:90:GLU:HG3	1.94	0.48
32:b:184:C:H2'	32:b:185:G:C8	2.48	0.48
32:b:184:C:H2'	32:b:185:G:H8	1.78	0.48
32:b:589:U:H2'	32:b:590:A:C8	2.47	0.48
13:f:5:HIS:HB2	13:f:97:TRP:CD1	2.48	0.48
31:v:24:C:H2'	31:v:25:G:C8	2.48	0.48
31:v:59:A:O2'	31:v:61:U:OP2	2.26	0.48
32:b:27:G:H22	32:b:512:G:H2'	1.79	0.48
32:b:1927:A:H2'	32:b:1928:A:C8	2.48	0.48
32:b:2458:G:H8	32:b:2459:A:H62	1.61	0.48
32:b:2543:G:N2	32:b:2646:C:H5''	2.28	0.48
10:c:157:SER:HB2	32:b:1818:U:H5''	1.94	0.48
14:g:2:SER:HB2	14:g:62:TRP:HB3	1.95	0.48
16:j:6:ALA:HB3	16:j:48:VAL:HG11	1.94	0.48
17:k:1:MET:HE1	32:b:1664:A:H2	1.78	0.48
20:n:72:ASP:OD2	20:n:75:ILE:HG12	2.13	0.48
32:b:2432:A:H2'	32:b:2433:A:C8	2.48	0.48
13:f:9:LYS:HB2	13:f:9:LYS:HE2	1.59	0.48
19:m:47:GLU:OE2	19:m:51:ARG:NH1	2.46	0.48
32:b:1429:G:H2'	32:b:1430:G:C8	2.48	0.48
32:b:2515:C:H2'	32:b:2516:A:H8	1.78	0.48
32:b:2543:G:H21	32:b:2646:C:C5'	2.25	0.48
13:f:131:GLY:HA3	32:b:2305:U:H5''	1.96	0.48
15:h:8:LYS:NZ	15:h:14:SER:HA	2.28	0.48
24:r:48:LYS:HB2	24:r:48:LYS:HE2	1.65	0.48
25:s:14:ALA:O	25:s:18:ARG:HG3	2.14	0.48
32:b:871:U:H2'	32:b:872:U:C6	2.49	0.48
15:h:8:LYS:HB2	15:h:15:LEU:HD23	1.95	0.48
16:j:74:TYR:CE1	16:j:103:ILE:HD11	2.48	0.48
21:o:34:HIS:CE1	21:o:54:VAL:HA	2.49	0.48
32:b:1021:A:H2'	32:b:1022:G:H4'	1.95	0.48
32:b:1056:G:H1'	32:b:1086:A:H62	1.78	0.48
32:b:1326:U:H2'	32:b:1327:A:H8	1.78	0.48
32:b:1991:U:H2'	32:b:1992:G:C5'	2.43	0.48
23:q:88:VAL:HG22	24:r:49:ILE:HG22	1.94	0.48
32:b:2061:G:H5'	32:b:2502:G:H5'	1.96	0.48
25:s:65:ASP:C	25:s:67:ASP:H	2.22	0.48
29:y:37:ILE:HG21	29:y:80:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:875:G:H3'	32:b:875:G:C8	2.49	0.48
32:b:2497:A:H1'	32:b:2498:C:H5	1.79	0.48
32:b:2829:A:C5	32:b:2830:C:C5	3.01	0.48
19:m:58:LYS:HB3	19:m:59:ARG:HH11	1.79	0.47
21:o:13:ARG:HH12	32:b:2335:A:H5'	1.78	0.47
23:q:6:ARG:NH1	32:b:585:G:N7	2.62	0.47
32:b:358:U:H2'	32:b:359:G:C8	2.49	0.47
32:b:368:A:O2'	32:b:369:U:C5'	2.63	0.47
32:b:437:U:H2'	32:b:438:G:C8	2.49	0.47
32:b:852:U:N3	32:b:853:C:C4	2.81	0.47
32:b:2008:C:H2'	32:b:2009:A:C8	2.49	0.47
2:1:56:LEU:HA	2:1:59:GLU:HG2	1.95	0.47
13:f:30:ARG:H	13:f:159:THR:HB	1.80	0.47
17:k:88:ASN:HB3	17:k:91:SER:O	2.14	0.47
32:b:856:G:H2'	32:b:857:G:C8	2.49	0.47
13:f:38:MET:HE2	13:f:57:LEU:HB2	1.95	0.47
16:j:9:GLU:HG2	16:j:10:THR:HG23	1.96	0.47
17:k:102:PRO:HD2	22:p:68:GLU:OE2	2.14	0.47
31:v:24:C:H2'	31:v:25:G:H8	1.79	0.47
32:b:151:C:H2'	32:b:152:A:C8	2.49	0.47
10:c:222:GLY:O	10:c:225:MET:HG3	2.15	0.47
23:q:58:ARG:HA	23:q:61:TRP:CE3	2.50	0.47
32:b:2308:G:H2'	32:b:2310:C:H5	1.80	0.47
12:e:118:LEU:HD11	12:e:188:MET:HE3	1.97	0.47
29:y:68:LYS:HD2	29:y:83:GLU:OE2	2.13	0.47
4:3:52:ARG:CZ	4:3:54:VAL:HG12	2.45	0.47
9:a:90:C:H5'	19:m:18:ARG:HG3	1.95	0.47
14:g:24:ILE:HD13	14:g:72:LEU:HD11	1.96	0.47
17:k:102:PRO:HD3	22:p:66:ASN:HB2	1.97	0.47
18:l:77:ILE:HD12	18:l:108:ALA:HB1	1.96	0.47
29:y:43:THR:H	32:b:2331:G:H4'	1.78	0.47
30:z:166:PRO:C	31:v:77:A:H3'	2.40	0.47
32:b:206:U:H2'	32:b:207:A:H8	1.79	0.47
32:b:272:A:C2	32:b:273:G:C5	3.03	0.47
32:b:903:C:H4'	32:b:903:C:OP1	2.14	0.47
32:b:2173:A:H5''	32:b:2174:C:H5	1.80	0.47
32:b:2751:G:H3'	32:b:2752:C:C6	2.50	0.47
16:j:77:HIS:CE1	16:j:83:GLY:HA3	2.50	0.47
27:u:54:GLN:O	27:u:56:GLY:N	2.48	0.47
30:z:157:ILE:CD1	32:b:2058:A:H2	2.27	0.47
32:b:1469:A:H2'	32:b:1470:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:t:1:MET:HB3	26:t:1:MET:HE3	1.70	0.47
15:h:26:ALA:O	15:h:28:ASN:N	2.48	0.47
29:y:25:ARG:HH11	29:y:31:VAL:HG12	1.78	0.47
29:y:26:PHE:H	29:y:29:GLU:HG3	1.79	0.47
29:y:43:THR:C	29:y:45:PHE:N	2.69	0.47
32:b:513:A:H2	32:b:582:A:H4'	1.79	0.47
32:b:459:U:H2'	32:b:460:A:H8	1.80	0.46
32:b:669:G:N3	32:b:669:G:C2'	2.77	0.46
32:b:850:U:H3'	32:b:851:C:C5	2.50	0.46
3:2:41:THR:HG22	3:2:43:ALA:H	1.79	0.46
9:a:42:C:C5	13:f:66:LEU:HD21	2.50	0.46
13:f:8:TYR:HB2	13:f:173:PHE:HZ	1.79	0.46
31:v:8:U:H5	31:v:15:G:N7	2.13	0.46
32:b:839:U:H3	32:b:939:G:H1	1.64	0.46
32:b:1340:U:H4'	32:b:1394:U:H4'	1.97	0.46
17:k:71:ARG:HA	17:k:71:ARG:HD3	1.67	0.46
20:n:8:ARG:HG3	20:n:43:GLU:OE2	2.16	0.46
21:o:88:LYS:HZ2	21:o:116:GLN:HE22	1.63	0.46
25:s:84:ARG:O	25:s:95:ARG:HD3	2.16	0.46
31:v:26:C:C2	31:v:27:A:C8	3.04	0.46
32:b:2346:A:H3'	32:b:2347:C:H5''	1.97	0.46
12:e:5:LEU:HD13	12:e:10:SER:O	2.15	0.46
23:q:109:LEU:HD23	24:r:48:LYS:HE3	1.97	0.46
25:s:65:ASP:O	25:s:66:ILE:C	2.56	0.46
32:b:643:A:H3'	32:b:644:A:H5''	1.94	0.46
23:q:97:ASP:OD2	24:r:13:ARG:NE	2.49	0.46
32:b:848:C:H2'	32:b:849:A:C8	2.51	0.46
32:b:903:C:H2'	32:b:903:C:O2	2.15	0.46
27:u:45:HIS:HB2	32:b:482:A:H5''	1.96	0.46
32:b:1689:A:H2'	32:b:1690:A:C8	2.51	0.46
11:d:105:LYS:HB3	11:d:105:LYS:HE3	1.63	0.46
27:u:48:PRO:HB3	27:u:55:PRO:O	2.15	0.46
32:b:414:C:H2'	32:b:415:A:C8	2.50	0.46
32:b:1076:C:H2'	32:b:1077:A:C8	2.51	0.46
32:b:1716:U:H2'	32:b:1717:A:H8	1.80	0.46
32:b:580:U:H2'	32:b:581:C:C6	2.50	0.45
32:b:2657:A:O2'	32:b:2658:C:H5'	2.16	0.45
1:0:43:GLU:HB3	1:0:45:ARG:HG2	1.98	0.45
17:k:34:GLY:N	17:k:37:ASP:OD2	2.44	0.45
17:k:77:ILE:HG12	22:p:72:ARG:HE	1.80	0.45
32:b:368:A:O2'	32:b:369:U:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:741:U:H2'	32:b:742:A:C8	2.52	0.45
32:b:891:G:O2'	32:b:893:C:N4	2.49	0.45
32:b:2208:C:H2'	32:b:2209:G:C8	2.51	0.45
17:k:43:ILE:HD12	17:k:56:ASP:HB2	1.99	0.45
17:k:91:SER:O	17:k:93:GLN:N	2.48	0.45
22:p:31:TRP:CE3	22:p:38:LYS:HG2	2.51	0.45
30:z:163:ILE:HG23	32:b:2062:A:N1	2.32	0.45
31:v:29:U:H2'	31:v:30:U:H6	1.81	0.45
32:b:657:U:H2'	32:b:658:U:C6	2.51	0.45
32:b:1026:G:H2'	32:b:1027:A:C8	2.51	0.45
32:b:1996:C:O2	32:b:1997:C:H1'	2.16	0.45
2:1:12:GLU:HG2	2:1:13:GLU:N	2.30	0.45
9:a:48:U:H2'	9:a:49:C:C6	2.52	0.45
32:b:82:U:H5''	32:b:296:U:H5'	1.98	0.45
32:b:948:C:H2'	32:b:949:G:C8	2.51	0.45
32:b:1035:U:O2	32:b:1035:U:H2'	2.17	0.45
11:d:59:ARG:HH11	32:b:2830:C:H3'	1.82	0.45
17:k:35:VAL:HG11	17:k:104:THR:CG2	2.46	0.45
25:s:45:VAL:O	25:s:49:LYS:HG2	2.16	0.45
30:z:166:PRO:O	31:v:77:A:C4'	2.65	0.45
32:b:222:A:H3'	32:b:421:C:H5'	1.97	0.45
4:3:38:HIS:ND1	4:3:39:LEU:O	2.41	0.45
12:e:155:GLU:O	12:e:159:LEU:HG	2.17	0.45
28:w:35:GLU:OE1	28:w:35:GLU:N	2.44	0.45
31:v:75:C:OP2	32:b:2602:A:H5''	2.16	0.45
32:b:1493:C:H3'	32:b:1494:A:H8	1.81	0.45
9:a:8:C:H5''	21:o:15:ARG:HH12	1.82	0.45
14:g:80:THR:C	14:g:82:GLY:H	2.24	0.45
32:b:581:C:H2'	32:b:582:A:H8	1.80	0.45
32:b:2765:A:N3	32:b:2765:A:H2'	2.31	0.45
6:6:7:PRO:HB2	32:b:1309:G:H4'	1.99	0.45
16:j:60:ASP:HB3	16:j:97:PRO:HB3	1.98	0.45
16:j:110:PRO:O	16:j:115:GLY:HA3	2.17	0.45
23:q:33:ARG:HG3	32:b:581:C:OP1	2.16	0.45
29:y:8:GLY:N	31:v:2:G:H4'	2.31	0.45
31:v:28:C:H2'	31:v:29:U:H6	1.82	0.45
32:b:2134:A:H1'	32:b:2161:C:H5'	1.98	0.45
11:d:47:ALA:HA	11:d:84:LEU:HD13	1.99	0.45
11:d:184:ARG:NH2	22:p:11:GLU:OE1	2.34	0.45
17:k:2:ILE:HD12	17:k:8:LEU:HD21	1.99	0.45
18:l:23:ILE:HG12	24:r:82:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1683:U:H2'	32:b:1684:G:C8	2.52	0.45
10:c:44:ASN:OD1	10:c:46:ASN:N	2.49	0.45
11:d:35:THR:HG22	11:d:73:VAL:HG21	1.99	0.45
13:f:134:GLU:HG2	13:f:149:VAL:HB	1.99	0.45
30:z:162:ARG:NH1	32:b:2505:G:C6	2.85	0.45
32:b:1394:U:H5'	32:b:1603:A:H4'	1.99	0.45
1:0:66:THR:O	1:0:70:GLU:HG3	2.17	0.44
13:f:4:LEU:HD13	13:f:101:GLU:HB2	1.98	0.44
14:g:45:HIS:HA	14:g:50:LEU:HD23	1.99	0.44
31:v:9:G:C8	31:v:46:G:H2'	2.52	0.44
32:b:371:A:H61	32:b:401:A:H3'	1.82	0.44
32:b:2331:G:H21	32:b:2336:A:H8	1.66	0.44
32:b:2789:C:H2'	32:b:2893:A:N7	2.31	0.44
8:8:33:HIS:O	8:8:35:GLN:HG3	2.17	0.44
27:u:74:ASN:HA	27:u:96:PHE:CE2	2.52	0.44
32:b:106:C:H2'	32:b:107:G:H8	1.82	0.44
4:3:5:GLN:NE2	32:b:2056:G:H4'	2.33	0.44
10:c:145:GLU:HG2	10:c:151:GLY:C	2.42	0.44
23:q:7:GLY:O	23:q:11:ARG:HG2	2.18	0.44
29:y:8:GLY:H	31:v:2:G:H4'	1.82	0.44
30:z:159[A]:TRP:HZ3	32:b:2058:A:C2	2.35	0.44
32:b:593:U:H3	32:b:664:G:H1	1.65	0.44
32:b:2096:C:H2'	32:b:2097:A:C8	2.53	0.44
15:h:18:GLN:HE22	15:h:39:ALA:HB2	1.82	0.44
17:k:41:ILE:HD11	17:k:86:LEU:CD2	2.48	0.44
20:n:12:ARG:HD3	20:n:16:HIS:HD2	1.77	0.44
25:s:49:LYS:HE3	32:b:488:G:H4'	1.99	0.44
29:y:70:GLU:CD	29:y:72:LYS:HE2	2.43	0.44
32:b:2428:G:H5''	32:b:2429:G:H5'	1.98	0.44
32:b:2788:C:H2'	32:b:2789:C:C6	2.52	0.44
14:g:18:LYS:NZ	14:g:20:ASN:OD1	2.51	0.44
31:v:52:A:O2'	31:v:53:G:H8	2.00	0.44
32:b:1306:C:H5''	32:b:1606:C:N4	2.33	0.44
32:b:2327:A:H2'	32:b:2328:A:C8	2.53	0.44
10:c:100:GLU:OE2	10:c:102:ARG:NE	2.48	0.44
17:k:109:SER:C	17:k:111:LYS:H	2.24	0.44
30:z:149:GLU:HG3	30:z:149:GLU:O	2.18	0.44
11:d:151:THR:HB	11:d:152:PRO:HD3	1.98	0.44
14:g:3:ARG:HA	14:g:6:LYS:HG2	2.00	0.44
15:h:8:LYS:HZ3	15:h:14:SER:HA	1.82	0.44
31:v:51:G:O2'	31:v:52:A:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:62:LYS:NZ	32:b:2810:A:H5'	2.32	0.44
19:m:41:LEU:HA	19:m:45:GLN:NE2	2.29	0.44
24:r:55:ASP:C	24:r:57:GLY:N	2.76	0.44
30:z:166:PRO:C	31:v:77:A:C3'	2.91	0.44
32:b:167:A:H2	32:b:2209:G:H4'	1.82	0.44
32:b:829:A:N7	32:b:2248:C:H5'	2.31	0.44
32:b:832:U:H2'	32:b:833:A:C8	2.53	0.44
32:b:2036:C:H2'	32:b:2037:A:H8	1.82	0.44
9:a:106:G:H2'	9:a:107:G:O4'	2.18	0.44
12:e:189:THR:O	12:e:193:VAL:HG23	2.17	0.44
13:f:29:PRO:HB2	13:f:169:LEU:HD22	2.00	0.44
13:f:80:ARG:CG	13:f:83:TYR:OH	2.65	0.44
13:f:123:ASP:OD2	13:f:127:ASN:HB2	2.18	0.44
14:g:12:PRO:HD2	14:g:15:VAL:HG11	1.99	0.44
17:k:35:VAL:HG11	17:k:104:THR:HG21	2.00	0.44
26:t:69:ARG:HG2	26:t:74:ILE:HD13	1.99	0.44
32:b:875:G:C8	32:b:875:G:C3'	3.01	0.44
4:3:26:THR:CG2	32:b:2814:A:O2'	2.66	0.43
4:3:28:LEU:HD22	25:s:38:TYR:CZ	2.53	0.43
18:l:19:LEU:HD12	18:l:27:LEU:HD13	2.00	0.43
22:p:100:LEU:HD11	22:p:110:ILE:HD11	2.00	0.43
32:b:521:U:H2'	32:b:522:A:C8	2.53	0.43
3:2:47:MET:HE3	32:b:850:U:O2'	2.16	0.43
21:o:4:LYS:O	21:o:8:ILE:HG12	2.18	0.43
25:s:90:LYS:HA	32:b:751:A:H5'	2.00	0.43
27:u:8:ASP:OD1	27:u:24:LYS:NZ	2.51	0.43
32:b:1426:G:H2'	32:b:1427:A:C8	2.53	0.43
32:b:2233:U:H2'	32:b:2234:G:H8	1.81	0.43
10:c:98:ASP:HB3	32:b:1490:A:H8	1.83	0.43
17:k:14:SER:OG	17:k:86:LEU:HD12	2.19	0.43
31:v:66:U:O2'	31:v:67:A:H8	2.02	0.43
32:b:767:U:H2'	32:b:768:G:H8	1.84	0.43
32:b:813:U:H2'	32:b:814:C:C6	2.53	0.43
32:b:2313:C:H2'	32:b:2314:A:C8	2.52	0.43
30:z:157:ILE:HD11	32:b:2058:A:H2	1.83	0.43
32:b:885:C:H2'	32:b:886:A:C8	2.54	0.43
13:f:134:GLU:CD	13:f:136:ILE:H	2.26	0.43
14:g:86:LYS:HG2	14:g:132:VAL:HG22	2.01	0.43
32:b:222:A:H61	32:b:232:G:H1'	1.83	0.43
32:b:1013:C:H2'	32:b:1014:A:H8	1.83	0.43
32:b:1508:A:H5'	32:b:1509:A:C4	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1700:A:H3'	32:b:1701:A:H8	1.83	0.43
13:f:16:LEU:HD22	13:f:20:PHE:HE2	1.84	0.43
22:p:100:LEU:HD23	22:p:100:LEU:HA	1.84	0.43
31:v:70:A:H2'	31:v:71:C:C6	2.54	0.43
3:2:12:SER:HB2	3:2:32:ILE:HD11	2.00	0.43
31:v:30:U:H2'	31:v:31:C:H6	1.83	0.43
32:b:1915:U:H3'	32:b:1916:A:H8	1.84	0.43
32:b:2765:A:N3	32:b:2765:A:C2'	2.82	0.43
10:c:107:PRO:HD2	10:c:110:LEU:HD22	2.00	0.43
14:g:24:ILE:HD12	14:g:43:VAL:HG21	2.00	0.43
16:j:13:ARG:NH1	16:j:49:ASP:O	2.52	0.43
19:m:9:PHE:CE2	32:b:911:A:C8	3.07	0.43
32:b:576:U:H2'	32:b:577:G:C8	2.53	0.43
32:b:874:G:O2'	32:b:875:G:C5'	2.66	0.43
21:o:82:ALA:HB1	21:o:87:ILE:HB	2.01	0.43
21:o:83:LEU:HD23	21:o:83:LEU:HA	1.76	0.43
27:u:15:THR:HG22	32:b:310:A:H5''	2.00	0.43
32:b:1047:G:O2'	32:b:1048:A:H8	2.00	0.43
32:b:1494:A:HO2'	32:b:1495:A:H8	1.63	0.43
32:b:1869:G:H22	32:b:1872:A:H1'	1.83	0.43
32:b:2099:U:H3	32:b:2190:G:H1	1.65	0.43
5:4:37:LYS:HG2	5:4:48:ILE:HD13	2.00	0.43
12:e:170:ARG:HH12	12:e:179:SER:HG	1.66	0.43
29:y:77:ARG:HG3	29:y:77:ARG:NH1	2.34	0.43
12:e:64:GLY:O	32:b:2059:A:C5'	2.61	0.42
27:u:15:THR:OG1	27:u:69:ASN:ND2	2.50	0.42
27:u:92:LYS:HB3	27:u:92:LYS:HE3	1.78	0.42
32:b:1381:G:H3'	32:b:1382:G:H21	1.83	0.42
13:f:175:PHE:HA	13:f:176:PRO:HD3	1.87	0.42
16:j:98:GLU:H	16:j:98:GLU:CD	2.26	0.42
32:b:222:A:N6	32:b:232:G:H1'	2.34	0.42
32:b:272:A:N1	32:b:273:G:C6	2.87	0.42
32:b:608:A:H2'	32:b:609:A:C8	2.54	0.42
32:b:2075:U:H1'	32:b:2597:G:H21	1.84	0.42
32:b:2114:A:H5''	32:b:2146:C:H41	1.84	0.42
9:a:49:C:H2'	9:a:50:A:C8	2.54	0.42
12:e:46:GLN:HB2	12:e:86:ALA:HB1	1.99	0.42
13:f:88:LYS:HD3	32:b:2313:C:H5''	2.01	0.42
19:m:58:LYS:HB2	19:m:58:LYS:HE2	1.47	0.42
20:n:96:ARG:O	20:n:113:ILE:HA	2.19	0.42
32:b:588:U:H2'	32:b:589:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:2863:C:H2'	32:b:2864:G:C8	2.54	0.42
1:0:32:ASN:HB2	32:b:397:U:H5''	2.01	0.42
3:2:11:ARG:HB2	3:2:54:MET:HB2	2.01	0.42
12:e:191:ASP:O	12:e:195:GLN:HG3	2.19	0.42
24:r:40:MET:CG	24:r:48:LYS:HA	2.49	0.42
32:b:281:C:H2'	32:b:282:A:H8	1.81	0.42
32:b:696:G:H1	32:b:766:U:H3	1.67	0.42
32:b:1004:U:H2'	32:b:1011:G:H2'	2.02	0.42
10:c:204:VAL:HG13	32:b:1792:G:H5'	2.00	0.42
13:f:78:LYS:HD2	13:f:78:LYS:HA	1.54	0.42
13:f:106:ILE:HG21	13:f:139:PRO:HG3	2.02	0.42
21:o:24:THR:HG23	21:o:90:VAL:HG12	2.02	0.42
29:y:16:SER:HB3	32:b:2261:C:C5	2.54	0.42
31:v:30:U:H2'	31:v:31:C:C6	2.55	0.42
32:b:318:C:H2'	32:b:319:G:H8	1.85	0.42
32:b:351:C:H2'	32:b:352:A:C8	2.55	0.42
32:b:611:C:O2'	32:b:612:G:H5'	2.19	0.42
32:b:892:A:H8	32:b:893:C:C5	2.37	0.42
32:b:1013:C:H2'	32:b:1014:A:C8	2.55	0.42
32:b:1049:C:H1'	32:b:1113:U:H4'	2.02	0.42
14:g:5:ALA:HB2	14:g:66:GLY:HA2	2.00	0.42
27:u:49:VAL:CG1	27:u:53:ASN:HB3	2.50	0.42
32:b:302:C:H2'	32:b:303:G:C8	2.54	0.42
32:b:1884:G:H5''	32:b:1884:G:C8	2.53	0.42
2:1:5:GLU:H	2:1:5:GLU:CD	2.27	0.42
4:3:27:SER:OG	32:b:2886:A:N6	2.52	0.42
9:a:50:A:H5''	21:o:67:ASN:HD21	1.85	0.42
27:u:81:ASP:OD2	27:u:96:PHE:HB3	2.20	0.42
29:y:41:ARG:HA	29:y:41:ARG:HD3	1.78	0.42
31:v:28:C:C2	31:v:29:U:C5	3.08	0.42
32:b:851:C:H2'	32:b:852:U:H5'	1.92	0.42
11:d:184:ARG:NH2	22:p:7:GLN:OE1	2.53	0.42
14:g:47:ASP:O	14:g:49:THR:N	2.53	0.42
17:k:64:ARG:HD2	17:k:79:PHE:CD2	2.55	0.42
28:w:80:HIS:CE1	28:w:83:LYS:HD2	2.55	0.42
31:v:75:C:P	32:b:2602:A:C5'	3.08	0.42
32:b:100:U:O2	32:b:100:U:O4'	2.37	0.42
32:b:367:G:H2'	32:b:368:A:H5'	2.02	0.42
32:b:1054:A:H1'	32:b:1106:G:H22	1.85	0.42
32:b:1432:G:H2'	32:b:1433:A:C8	2.55	0.42
32:b:2739:U:H5''	32:b:2763:G:O6	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:41:ALA:O	20:n:42:LYS:HB2	2.19	0.42
25:s:11:ARG:HA	25:s:11:ARG:HD2	1.89	0.42
32:b:1704:C:H2'	32:b:1705:A:C8	2.55	0.42
32:b:2062:A:H2'	32:b:2062:A:N3	2.35	0.42
9:a:70:C:H2'	9:a:71:C:H6	1.85	0.42
11:d:25:THR:HG21	11:d:193:VAL:HG22	2.01	0.42
13:f:72:LYS:HE2	13:f:72:LYS:HB3	1.70	0.42
23:q:92:ARG:HG3	23:q:92:ARG:NH1	2.34	0.42
27:u:50:PRO:O	27:u:51:ALA:C	2.63	0.42
32:b:49:A:H61	32:b:177:G:H2'	1.85	0.42
32:b:109:C:H5'	32:b:348:A:H4'	2.02	0.42
32:b:2334:U:H5	32:b:2335:A:H4'	1.84	0.42
32:b:2809:A:H2'	32:b:2810:A:C8	2.55	0.42
10:c:207:LYS:HB2	32:b:729:G:C6	2.55	0.41
32:b:220:G:H1'	32:b:234:U:H1'	2.01	0.41
7:7:14:PHE:O	7:7:15:LYS:HD3	2.20	0.41
14:g:87:LEU:HB2	14:g:131:ILE:HB	2.01	0.41
32:b:20:C:H2'	32:b:21:A:C8	2.55	0.41
32:b:558:U:H2'	32:b:559:G:C8	2.54	0.41
32:b:1744:A:H3'	32:b:1745:A:H8	1.84	0.41
15:h:30:LEU:HA	15:h:35:LYS:HB2	2.03	0.41
16:j:116:ARG:NH2	32:b:528:A:H8	2.17	0.41
20:n:41:ALA:HB1	20:n:97:ILE:HD13	2.01	0.41
27:u:86:ARG:HG2	27:u:95:PHE:CD1	2.55	0.41
29:y:53:CYS:HA	29:y:59:LEU:HD23	2.02	0.41
32:b:107:G:H21	32:b:346:A:H62	1.68	0.41
32:b:2116:G:H1'	32:b:2148:G:H21	1.85	0.41
32:b:2377:A:H2'	32:b:2378:A:C8	2.55	0.41
3:2:7:ILE:HD11	3:2:48:ILE:HD11	2.02	0.41
9:a:66:A:H4'	9:a:67:G:OP1	2.19	0.41
14:g:148:LEU:HD23	14:g:148:LEU:HA	1.93	0.41
32:b:128:C:H2'	32:b:129:C:C6	2.56	0.41
32:b:181:A:H1'	32:b:435:C:H5'	2.02	0.41
32:b:1808:A:H3'	32:b:1809:A:C8	2.55	0.41
32:b:1972:G:H2'	32:b:1973:G:C8	2.55	0.41
32:b:2125:G:C6	32:b:2126:A:H1'	2.55	0.41
32:b:2302:U:H2'	32:b:2303:G:C8	2.55	0.41
12:e:170:ARG:NH2	12:e:174:GLY:O	2.53	0.41
13:f:14:LYS:HE3	13:f:14:LYS:HB3	1.95	0.41
19:m:111:GLU:HG2	19:m:112:LEU:N	2.36	0.41
27:u:54:GLN:C	27:u:56:GLY:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:308:G:H2'	32:b:309:A:C8	2.56	0.41
32:b:1060:U:H4'	32:b:1061:U:H4'	2.03	0.41
32:b:2301:C:H2'	32:b:2302:U:C6	2.56	0.41
12:e:4:VAL:HA	12:e:11:ALA:HA	2.02	0.41
12:e:171:ASP:C	12:e:173:THR:H	2.29	0.41
25:s:99:ARG:HG2	25:s:99:ARG:HH11	1.85	0.41
32:b:1026:G:H2'	32:b:1027:A:H8	1.85	0.41
12:e:122:GLU:OE1	12:e:122:GLU:N	2.47	0.41
21:o:76:LYS:HG2	21:o:80:GLU:OE1	2.20	0.41
26:t:33:LYS:HG2	26:t:80:TRP:CZ3	2.56	0.41
27:u:7:ARG:NH1	27:u:27:ASN:HA	2.36	0.41
32:b:1069:A:C2	32:b:1095:A:H5''	2.54	0.41
32:b:1364:G:H5'	32:b:1809:A:H1'	2.01	0.41
32:b:1386:C:H2'	32:b:1387:A:C8	2.56	0.41
32:b:2663:G:N2	32:b:2664:G:H1'	2.36	0.41
32:b:2680:U:H2'	32:b:2681:C:C6	2.56	0.41
13:f:73:SER:OG	13:f:81:GLN:N	2.47	0.41
18:l:131:ALA:O	18:l:135:ILE:HG13	2.21	0.41
24:r:49:ILE:HD13	24:r:49:ILE:HA	1.52	0.41
31:v:27:A:C5	31:v:28:C:C5	3.08	0.41
32:b:2678:C:H2'	32:b:2679:A:C8	2.55	0.41
10:c:142:HIS:ND1	10:c:193:GLY:O	2.29	0.41
12:e:155:GLU:HG2	12:e:156:ASN:N	2.35	0.41
13:f:38:MET:CE	13:f:57:LEU:HB2	2.51	0.41
13:f:74:VAL:HB	13:f:79:ILE:HD11	2.03	0.41
21:o:11:ALA:HB1	21:o:15:ARG:HE	1.85	0.41
26:t:6:ARG:O	26:t:10:VAL:HG13	2.20	0.41
27:u:6:ARG:N	27:u:9:ASP:OD2	2.39	0.41
32:b:1083:U:H2'	32:b:1084:A:H2'	2.02	0.41
32:b:1986:C:H2'	32:b:1987:A:O5'	2.20	0.41
32:b:2173:A:H5''	32:b:2174:C:C5	2.56	0.41
32:b:2300:C:H2'	32:b:2301:C:C6	2.56	0.41
32:b:2696:U:H2'	32:b:2697:G:C8	2.56	0.41
2:1:11:VAL:HG12	2:1:15:ASN:HD21	1.86	0.41
4:3:40:ARG:HH12	32:b:2884:U:H2'	1.86	0.41
7:7:8:ARG:HA	7:7:8:ARG:HD2	1.90	0.41
10:c:241:GLY:HA3	32:b:2597:G:H5'	2.03	0.41
14:g:126:PRO:HD2	14:g:130:GLU:HB3	2.03	0.41
15:h:26:ALA:C	15:h:28:ASN:N	2.79	0.41
20:n:56:LYS:HE2	20:n:87:PHE:O	2.21	0.41
22:p:27:GLU:OE1	22:p:29:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:1938:A:C6	32:b:2590:A:H1'	2.56	0.41
32:b:1965:C:H2'	32:b:1966:A:C8	2.56	0.41
2:1:12:GLU:HA	2:1:15:ASN:HD22	1.86	0.40
4:3:50:ARG:O	4:3:50:ARG:HG2	2.21	0.40
13:f:8:TYR:HB2	13:f:173:PHE:CZ	2.56	0.40
17:k:7:MET:SD	17:k:20:MET:HB2	2.61	0.40
28:w:43:ASP:OD1	28:w:43:ASP:C	2.64	0.40
32:b:1366:A:H3'	32:b:1367:A:H8	1.86	0.40
32:b:1998:A:C2'	32:b:1999:C:O5'	2.70	0.40
32:b:2824:C:H2'	32:b:2825:G:O4'	2.20	0.40
12:e:142:ALA:O	12:e:143:LEU:HD23	2.20	0.40
16:j:32:LEU:HD22	16:j:54:ILE:HG21	2.03	0.40
16:j:45:THR:HB	16:j:48:VAL:CG1	2.51	0.40
28:w:48:MET:O	28:w:51:GLN:NE2	2.47	0.40
32:b:2115:G:N2	32:b:2119:A:H62	2.18	0.40
32:b:2783:U:H2'	32:b:2784:U:C5	2.55	0.40
11:d:19:GLY:HA2	22:p:79:PRO:HG2	2.03	0.40
11:d:48:ILE:HG12	11:d:84:LEU:HD11	2.03	0.40
19:m:133:LYS:HB3	19:m:133:LYS:HE2	1.79	0.40
28:w:58:SER:O	28:w:73:LYS:NZ	2.55	0.40
4:3:16:ARG:HE	4:3:16:ARG:HB3	1.32	0.40
12:e:16:GLU:HA	12:e:16:GLU:OE1	2.21	0.40
14:g:19:ILE:HG22	14:g:21:GLY:H	1.86	0.40
16:j:31:GLU:CG	16:j:142:ILE:HD12	2.51	0.40
32:b:360:U:H2'	32:b:361:G:C4	2.56	0.40
32:b:2829:A:H2'	32:b:2830:C:O4'	2.20	0.40
9:a:24:G:N7	9:a:56:G:H2'	2.37	0.40
10:c:44:ASN:OD1	10:c:44:ASN:C	2.64	0.40
10:c:243:HIS:HA	10:c:244:PRO:HD3	1.97	0.40
23:q:49:ASP:HA	23:q:52:GLN:HB2	2.04	0.40
23:q:109:LEU:HD23	23:q:109:LEU:HA	1.93	0.40
27:u:6:ARG:HG3	32:b:84:A:H5''	2.02	0.40
31:v:8:U:C5	31:v:15:G:N7	2.88	0.40
31:v:29:U:H2'	31:v:30:U:C6	2.57	0.40
32:b:452:G:H2'	32:b:453:A:C8	2.56	0.40
32:b:1447:C:H2'	32:b:1448:G:C8	2.56	0.40
32:b:1494:A:H1'	32:b:1495:A:H5'	2.04	0.40
32:b:1518:C:H2'	32:b:1519:G:C8	2.57	0.40
32:b:2368:C:H2'	32:b:2369:A:C8	2.57	0.40
32:b:2645:G:H5'	32:b:2732:G:H8	1.87	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	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
3	2	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
4	3	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
5	4	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
6	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
7	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
10	c	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	49
11	d	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
12	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
13	f	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	38
14	g	173/177 (98%)	159 (92%)	13 (8%)	1 (1%)	21	38
15	h	37/149 (25%)	33 (89%)	2 (5%)	2 (5%)	1	1
16	j	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
17	k	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
18	l	141/144 (98%)	130 (92%)	10 (7%)	1 (1%)	18	34
19	m	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
20	n	118/127 (93%)	112 (95%)	5 (4%)	1 (1%)	16	31
21	o	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
22	p	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
23	q	115/118 (98%)	115 (100%)	0	0	100	100
24	r	100/103 (97%)	92 (92%)	5 (5%)	3 (3%)	3	5
25	s	107/110 (97%)	100 (94%)	6 (6%)	1 (1%)	14	27
26	t	91/100 (91%)	88 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	u	100/104 (96%)	84 (84%)	13 (13%)	3 (3%)	3	5
28	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
29	y	78/85 (92%)	74 (95%)	3 (4%)	1 (1%)	9	18
30	z	17/161 (11%)	15 (88%)	2 (12%)	0	100	100
All	All	3070/3428 (90%)	2929 (95%)	126 (4%)	15 (0%)	26	43

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	g	48	ASN
15	h	13	GLY
24	r	52	PRO
25	s	66	ILE
27	u	52	LEU
27	u	55	PRO
24	r	48	LYS
13	f	71	ARG
15	h	27	ARG
29	y	44	LYS
27	u	53	ASN
10	c	233	GLY
20	n	118	ARG
18	l	87	GLY
24	r	47	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	67 (100%)	0	100	100
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	47 (100%)	0	100	100
4	3	46/48 (96%)	43 (94%)	3 (6%)	15	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	45/49 (92%)	41 (91%)	4 (9%)	9	20
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	50 (98%)	1 (2%)	48	75
8	8	34/34 (100%)	34 (100%)	0	100	100
10	c	216/218 (99%)	216 (100%)	0	100	100
11	d	164/164 (100%)	160 (98%)	4 (2%)	43	70
12	e	165/165 (100%)	165 (100%)	0	100	100
13	f	148/150 (99%)	142 (96%)	6 (4%)	27	53
14	g	136/138 (99%)	132 (97%)	4 (3%)	37	65
15	h	30/114 (26%)	28 (93%)	2 (7%)	15	31
16	j	116/116 (100%)	116 (100%)	0	100	100
17	k	103/104 (99%)	101 (98%)	2 (2%)	50	76
18	l	102/103 (99%)	94 (92%)	8 (8%)	11	24
19	m	109/109 (100%)	108 (99%)	1 (1%)	70	87
20	n	100/103 (97%)	99 (99%)	1 (1%)	68	86
21	o	86/87 (99%)	82 (95%)	4 (5%)	23	47
22	p	98/100 (98%)	98 (100%)	0	100	100
23	q	89/90 (99%)	89 (100%)	0	100	100
24	r	84/84 (100%)	75 (89%)	9 (11%)	6	13
25	s	92/93 (99%)	91 (99%)	1 (1%)	65	84
26	t	80/84 (95%)	77 (96%)	3 (4%)	29	56
27	u	83/85 (98%)	79 (95%)	4 (5%)	23	46
28	w	78/78 (100%)	78 (100%)	0	100	100
29	y	58/63 (92%)	58 (100%)	0	100	100
30	z	18/130 (14%)	18 (100%)	0	100	100
All	All	2537/2771 (92%)	2480 (98%)	57 (2%)	45	73

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3	16	ARG
4	3	18	SER
4	3	25	VAL

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Mol	Chain	Res	Type
5	4	42	VAL
5	4	50	LYS
5	4	51	GLU
5	4	53	LYS
7	7	19	LYS
11	d	88	GLU
11	d	99	GLU
11	d	103	ASP
11	d	105	LYS
13	f	9	LYS
13	f	11	GLU
13	f	24	SER
13	f	26	MET
13	f	72	LYS
13	f	78	LYS
14	g	47	ASP
14	g	81	GLU
14	g	130	GLU
14	g	176	LYS
15	h	15	LEU
15	h	27	ARG
17	k	25	LEU
17	k	67	LYS
18	l	69	ARG
18	l	70	LYS
18	l	73	ILE
18	l	77	ILE
18	l	85	VAL
18	l	92	LEU
18	l	103	ILE
18	l	104	GLN
19	m	58	LYS
20	n	118	ARG
21	o	15	ARG
21	o	67	ASN
21	o	68	LYS
21	o	69	ASP
24	r	40	MET
24	r	43	ASN
24	r	47	VAL
24	r	48	LYS
24	r	49	ILE

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Mol	Chain	Res	Type
24	r	51	VAL
24	r	52	PRO
24	r	54	VAL
24	r	55	ASP
25	s	62	ASP
26	t	1	MET
26	t	2	ILE
26	t	89	GLU
27	u	15	THR
27	u	39	ILE
27	u	52	LEU
27	u	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	34	HIS
2	1	15	ASN
2	1	27	ASN
2	1	36	GLN
4	3	19	HIS
5	4	45	GLN
6	6	26	ASN
7	7	43	HIS
10	c	117	GLN
10	c	153	GLN
10	c	163	GLN
10	c	200	HIS
10	c	243	HIS
11	d	150	GLN
12	e	29	HIS
12	e	92	HIS
12	e	136	GLN
12	e	163	ASN
13	f	52	ASN
14	g	38	ASN
14	g	48	ASN
15	h	18	GLN
15	h	33	GLN
16	j	76	HIS
16	j	136	GLN
17	k	29	HIS

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Mol	Chain	Res	Type
17	k	93	GLN
19	m	13	HIS
19	m	45	GLN
19	m	60	GLN
20	n	9	GLN
21	o	67	ASN
21	o	98	GLN
21	o	116	GLN
22	p	10	GLN
22	p	12	GLN
22	p	66	ASN
23	q	44	GLN
23	q	72	ASN
23	q	81	ASN
24	r	11	GLN
25	s	7	HIS
26	t	28	ASN
26	t	70	HIS
27	u	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	v	75/77 (97%)	16 (21%)	0
32	b	2898/2904 (99%)	1199 (41%)	0
9	a	117/120 (97%)	21 (17%)	0
All	All	3090/3101 (99%)	1236 (40%)	0

All (1236) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	25	U
9	a	26	C
9	a	30	C
9	a	32	U
9	a	35	C
9	a	41	G
9	a	42	C
9	a	43	C
9	a	44	G
9	a	50	A

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Mol	Chain	Res	Type
9	a	56	G
9	a	59	A
9	a	67	G
9	a	88	C
9	a	89	U
9	a	99	A
9	a	108	A
9	a	109	A
9	a	112	G
9	a	114	C
9	a	116	G
31	v	8	U
31	v	9	G
31	v	10	G
31	v	13	C
31	v	14	A
31	v	15	G
31	v	17	C
31	v	18	U
31	v	19	G
31	v	21	U
31	v	38	G
31	v	47	G
31	v	48	U
31	v	49	C
31	v	67	A
31	v	77	A
32	b	5	A
32	b	10	A
32	b	11	C
32	b	13	A
32	b	16	C
32	b	23	G
32	b	24	G
32	b	28	A
32	b	33	C
32	b	34	U
32	b	35	G
32	b	36	G
32	b	43	G
32	b	45	G
32	b	46	G

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Mol	Chain	Res	Type
32	b	49	A
32	b	50	U
32	b	51	G
32	b	55	G
32	b	60	G
32	b	62	U
32	b	63	A
32	b	64	A
32	b	65	U
32	b	69	C
32	b	70	G
32	b	71	A
32	b	73	A
32	b	74	A
32	b	75	G
32	b	84	A
32	b	87	U
32	b	91	A
32	b	93	G
32	b	96	C
32	b	99	U
32	b	100	U
32	b	101	A
32	b	102	U
32	b	114	U
32	b	116	C
32	b	118	A
32	b	119	A
32	b	120	U
32	b	122	G
32	b	124	G
32	b	125	A
32	b	126	A
32	b	127	A
32	b	128	C
32	b	131	A
32	b	134	G
32	b	135	U
32	b	136	G
32	b	139	U
32	b	140	C
32	b	141	G

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Mol	Chain	Res	Type
32	b	142	A
32	b	146	A
32	b	159	G
32	b	160	A
32	b	162	U
32	b	163	C
32	b	165	A
32	b	166	U
32	b	168	G
32	b	169	G
32	b	171	U
32	b	175	G
32	b	176	A
32	b	177	G
32	b	178	G
32	b	181	A
32	b	182	A
32	b	188	G
32	b	189	G
32	b	196	A
32	b	197	A
32	b	198	C
32	b	199	A
32	b	201	C
32	b	206	U
32	b	213	A
32	b	215	G
32	b	216	A
32	b	221	A
32	b	222	A
32	b	223	A
32	b	224	U
32	b	228	C
32	b	229	C
32	b	230	G
32	b	232	G
32	b	233	A
32	b	245	G
32	b	246	C
32	b	248	G
32	b	250	G
32	b	252	G

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Mol	Chain	Res	Type
32	b	255	A
32	b	257	C
32	b	261	G
32	b	265	A
32	b	266	G
32	b	268	C
32	b	271	G
32	b	277	G
32	b	278	A
32	b	279	A
32	b	280	U
32	b	281	C
32	b	286	U
32	b	287	G
32	b	288	U
32	b	289	G
32	b	291	G
32	b	298	G
32	b	300	A
32	b	303	G
32	b	311	A
32	b	312	G
32	b	313	G
32	b	317	G
32	b	321	U
32	b	322	A
32	b	323	C
32	b	324	A
32	b	325	G
32	b	326	G
32	b	327	G
32	b	329	G
32	b	330	A
32	b	332	A
32	b	334	C
32	b	338	G
32	b	340	A
32	b	343	C
32	b	345	A
32	b	347	A
32	b	348	A
32	b	350	G

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Mol	Chain	Res	Type
32	b	354	A
32	b	356	G
32	b	359	G
32	b	367	G
32	b	368	A
32	b	369	U
32	b	370	G
32	b	371	A
32	b	372	G
32	b	376	G
32	b	380	G
32	b	383	C
32	b	385	C
32	b	386	G
32	b	387	U
32	b	389	G
32	b	390	U
32	b	391	A
32	b	395	U
32	b	396	G
32	b	397	U
32	b	403	U
32	b	404	A
32	b	405	U
32	b	406	G
32	b	411	G
32	b	412	A
32	b	417	C
32	b	420	C
32	b	422	A
32	b	428	A
32	b	429	A
32	b	433	C
32	b	437	U
32	b	442	G
32	b	443	A
32	b	451	U
32	b	454	A
32	b	455	C
32	b	456	C
32	b	457	A
32	b	462	C

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Mol	Chain	Res	Type
32	b	471	A
32	b	474	G
32	b	475	C
32	b	479	A
32	b	480	A
32	b	481	G
32	b	482	A
32	b	489	G
32	b	490	C
32	b	491	G
32	b	496	G
32	b	504	A
32	b	505	A
32	b	508	A
32	b	509	C
32	b	512	G
32	b	513	A
32	b	520	G
32	b	527	C
32	b	528	A
32	b	529	A
32	b	530	G
32	b	531	C
32	b	532	A
32	b	536	G
32	b	538	A
32	b	542	C
32	b	543	G
32	b	547	A
32	b	548	G
32	b	554	U
32	b	555	G
32	b	562	U
32	b	563	A
32	b	573	U
32	b	574	A
32	b	575	A
32	b	576	U
32	b	586	A
32	b	587	C
32	b	597	G
32	b	603	A

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Mol	Chain	Res	Type
32	b	604	G
32	b	614	A
32	b	615	U
32	b	620	G
32	b	621	A
32	b	622	G
32	b	627	A
32	b	630	G
32	b	634	C
32	b	636	G
32	b	637	A
32	b	642	U
32	b	644	A
32	b	645	C
32	b	647	G
32	b	651	G
32	b	652	U
32	b	653	U
32	b	654	A
32	b	655	A
32	b	662	G
32	b	664	G
32	b	668	A
32	b	669	G
32	b	670	A
32	b	674	G
32	b	678	C
32	b	686	U
32	b	693	A
32	b	694	U
32	b	711	G
32	b	714	U
32	b	717	C
32	b	718	A
32	b	719	C
32	b	726	G
32	b	728	G
32	b	730	A
32	b	731	C
32	b	734	A
32	b	740	C
32	b	746	U

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Mol	Chain	Res	Type
32	b	747	U
32	b	757	G
32	b	764	A
32	b	769	U
32	b	774	G
32	b	775	G
32	b	776	G
32	b	777	G
32	b	781	A
32	b	782	A
32	b	783	A
32	b	784	G
32	b	785	G
32	b	789	A
32	b	791	C
32	b	792	A
32	b	793	A
32	b	794	A
32	b	805	G
32	b	806	C
32	b	811	U
32	b	812	C
32	b	819	A
32	b	827	U
32	b	828	U
32	b	829	A
32	b	830	G
32	b	831	G
32	b	841	G
32	b	842	U
32	b	845	A
32	b	846	U
32	b	847	U
32	b	848	C
32	b	851	C
32	b	852	U
32	b	853	C
32	b	854	C
32	b	855	G
32	b	859	G
32	b	860	U
32	b	864	G

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Mol	Chain	Res	Type
32	b	866	A
32	b	868	U
32	b	869	G
32	b	872	U
32	b	873	C
32	b	875	G
32	b	876	C
32	b	877	A
32	b	878	A
32	b	879	G
32	b	880	G
32	b	881	G
32	b	883	G
32	b	884	U
32	b	885	C
32	b	887	U
32	b	889	C
32	b	891	G
32	b	892	A
32	b	893	C
32	b	895	U
32	b	896	A
32	b	897	C
32	b	898	C
32	b	900	A
32	b	903	C
32	b	904	G
32	b	907	G
32	b	908	C
32	b	910	A
32	b	911	A
32	b	912	C
32	b	913	U
32	b	914	G
32	b	915	C
32	b	923	G
32	b	924	G
32	b	926	G
32	b	928	A
32	b	931	U
32	b	932	U
32	b	934	U

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Mol	Chain	Res	Type
32	b	937	C
32	b	938	G
32	b	941	A
32	b	946	C
32	b	958	U
32	b	961	C
32	b	965	C
32	b	968	C
32	b	969	G
32	b	974	G
32	b	975	A
32	b	980	A
32	b	982	C
32	b	983	A
32	b	985	C
32	b	988	A
32	b	989	G
32	b	990	A
32	b	991	C
32	b	996	A
32	b	1003	G
32	b	1005	C
32	b	1009	A
32	b	1012	U
32	b	1013	C
32	b	1016	G
32	b	1017	G
32	b	1018	U
32	b	1019	U
32	b	1020	A
32	b	1021	A
32	b	1022	G
32	b	1023	U
32	b	1024	G
32	b	1025	G
32	b	1026	G
32	b	1028	A
32	b	1030	C
32	b	1031	G
32	b	1032	A
32	b	1033	U
32	b	1034	G

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Mol	Chain	Res	Type
32	b	1035	U
32	b	1037	G
32	b	1040	A
32	b	1042	G
32	b	1045	C
32	b	1046	A
32	b	1047	G
32	b	1048	A
32	b	1050	A
32	b	1051	G
32	b	1052	C
32	b	1053	C
32	b	1054	A
32	b	1055	G
32	b	1056	G
32	b	1057	A
32	b	1058	U
32	b	1060	U
32	b	1061	U
32	b	1062	G
32	b	1063	G
32	b	1064	C
32	b	1066	U
32	b	1067	A
32	b	1068	G
32	b	1069	A
32	b	1070	A
32	b	1071	G
32	b	1072	C
32	b	1073	A
32	b	1074	G
32	b	1076	C
32	b	1077	A
32	b	1078	U
32	b	1079	C
32	b	1080	A
32	b	1083	U
32	b	1084	A
32	b	1085	A
32	b	1086	A
32	b	1087	G
32	b	1088	A

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Mol	Chain	Res	Type
32	b	1089	A
32	b	1090	A
32	b	1091	G
32	b	1093	G
32	b	1094	U
32	b	1095	A
32	b	1097	U
32	b	1098	A
32	b	1099	G
32	b	1101	U
32	b	1102	C
32	b	1103	A
32	b	1104	C
32	b	1105	U
32	b	1106	G
32	b	1108	U
32	b	1109	C
32	b	1111	A
32	b	1112	G
32	b	1119	U
32	b	1126	A
32	b	1130	U
32	b	1131	G
32	b	1132	U
32	b	1133	A
32	b	1134	A
32	b	1135	C
32	b	1137	G
32	b	1141	U
32	b	1142	A
32	b	1144	A
32	b	1151	A
32	b	1154	G
32	b	1156	A
32	b	1157	G
32	b	1158	C
32	b	1163	G
32	b	1165	A
32	b	1166	G
32	b	1169	A
32	b	1171	G
32	b	1172	C

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Mol	Chain	Res	Type
32	b	1174	U
32	b	1175	A
32	b	1176	U
32	b	1177	G
32	b	1178	C
32	b	1182	G
32	b	1183	U
32	b	1185	G
32	b	1186	G
32	b	1195	G
32	b	1197	G
32	b	1198	U
32	b	1203	U
32	b	1204	A
32	b	1205	A
32	b	1206	G
32	b	1210	G
32	b	1211	C
32	b	1212	G
32	b	1216	G
32	b	1217	U
32	b	1218	G
32	b	1220	G
32	b	1223	G
32	b	1226	A
32	b	1227	G
32	b	1232	G
32	b	1236	G
32	b	1237	A
32	b	1238	G
32	b	1245	G
32	b	1247	A
32	b	1250	G
32	b	1251	C
32	b	1252	G
32	b	1253	A
32	b	1254	A
32	b	1256	G
32	b	1259	G
32	b	1262	A
32	b	1265	A
32	b	1266	G

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Mol	Chain	Res	Type
32	b	1267	U
32	b	1271	G
32	b	1272	A
32	b	1275	A
32	b	1276	A
32	b	1279	G
32	b	1280	G
32	b	1281	G
32	b	1285	A
32	b	1288	G
32	b	1289	C
32	b	1294	U
32	b	1299	G
32	b	1300	G
32	b	1301	A
32	b	1302	A
32	b	1303	G
32	b	1304	A
32	b	1305	C
32	b	1311	G
32	b	1312	U
32	b	1313	U
32	b	1315	C
32	b	1320	C
32	b	1321	A
32	b	1324	G
32	b	1325	U
32	b	1326	U
32	b	1329	U
32	b	1330	C
32	b	1332	G
32	b	1336	A
32	b	1338	G
32	b	1341	G
32	b	1342	A
32	b	1345	C
32	b	1346	G
32	b	1352	U
32	b	1354	A
32	b	1355	G
32	b	1359	A
32	b	1365	A

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Mol	Chain	Res	Type
32	b	1366	A
32	b	1368	G
32	b	1371	G
32	b	1374	G
32	b	1376	C
32	b	1378	A
32	b	1379	U
32	b	1380	G
32	b	1381	G
32	b	1383	A
32	b	1385	A
32	b	1387	A
32	b	1388	G
32	b	1392	A
32	b	1393	A
32	b	1394	U
32	b	1395	A
32	b	1396	U
32	b	1402	U
32	b	1403	A
32	b	1407	G
32	b	1409	U
32	b	1410	G
32	b	1413	A
32	b	1416	G
32	b	1419	A
32	b	1420	A
32	b	1421	G
32	b	1423	G
32	b	1427	A
32	b	1428	C
32	b	1429	G
32	b	1435	G
32	b	1436	G
32	b	1439	A
32	b	1441	G
32	b	1444	G
32	b	1449	G
32	b	1451	C
32	b	1452	G
32	b	1453	A
32	b	1454	C

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Mol	Chain	Res	Type
32	b	1455	G
32	b	1456	G
32	b	1457	U
32	b	1458	U
32	b	1459	G
32	b	1460	U
32	b	1461	C
32	b	1464	G
32	b	1466	U
32	b	1469	A
32	b	1474	U
32	b	1475	G
32	b	1476	U
32	b	1477	A
32	b	1478	G
32	b	1479	G
32	b	1482	G
32	b	1483	G
32	b	1486	U
32	b	1492	G
32	b	1493	C
32	b	1494	A
32	b	1495	A
32	b	1496	A
32	b	1498	C
32	b	1503	A
32	b	1508	A
32	b	1509	A
32	b	1510	G
32	b	1516	G
32	b	1517	G
32	b	1523	U
32	b	1524	G
32	b	1529	G
32	b	1530	G
32	b	1531	C
32	b	1532	A
32	b	1536	C
32	b	1537	G
32	b	1538	G
32	b	1539	U
32	b	1544	A

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Mol	Chain	Res	Type
32	b	1547	C
32	b	1552	A
32	b	1554	U
32	b	1555	G
32	b	1558	C
32	b	1559	U
32	b	1560	G
32	b	1563	U
32	b	1565	C
32	b	1566	A
32	b	1567	G
32	b	1568	G
32	b	1569	A
32	b	1571	A
32	b	1575	C
32	b	1576	U
32	b	1578	U
32	b	1581	G
32	b	1582	C
32	b	1583	A
32	b	1584	U
32	b	1585	C
32	b	1588	G
32	b	1589	U
32	b	1593	A
32	b	1595	C
32	b	1596	A
32	b	1607	C
32	b	1608	A
32	b	1610	A
32	b	1611	C
32	b	1613	G
32	b	1617	C
32	b	1618	A
32	b	1622	G
32	b	1627	G
32	b	1630	A
32	b	1634	A
32	b	1635	A
32	b	1642	G
32	b	1643	G
32	b	1647	U

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Mol	Chain	Res	Type
32	b	1648	U
32	b	1649	G
32	b	1664	A
32	b	1665	A
32	b	1666	G
32	b	1667	G
32	b	1669	A
32	b	1673	G
32	b	1674	G
32	b	1675	C
32	b	1681	G
32	b	1689	A
32	b	1693	U
32	b	1694	C
32	b	1699	G
32	b	1700	A
32	b	1701	A
32	b	1703	G
32	b	1706	C
32	b	1707	G
32	b	1713	A
32	b	1714	U
32	b	1715	G
32	b	1716	U
32	b	1721	G
32	b	1725	C
32	b	1726	G
32	b	1729	U
32	b	1731	G
32	b	1732	C
32	b	1733	U
32	b	1735	G
32	b	1736	U
32	b	1738	G
32	b	1740	G
32	b	1749	A
32	b	1750	G
32	b	1755	A
32	b	1756	G
32	b	1758	U
32	b	1759	A
32	b	1762	A

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Mol	Chain	Res	Type
32	b	1763	G
32	b	1764	C
32	b	1773	A
32	b	1776	G
32	b	1779	U
32	b	1782	U
32	b	1784	A
32	b	1786	A
32	b	1787	A
32	b	1792	G
32	b	1794	A
32	b	1800	C
32	b	1801	A
32	b	1805	A
32	b	1808	A
32	b	1809	A
32	b	1811	G
32	b	1816	C
32	b	1818	U
32	b	1821	A
32	b	1823	G
32	b	1827	U
32	b	1829	A
32	b	1833	C
32	b	1836	C
32	b	1848	A
32	b	1849	G
32	b	1853	A
32	b	1856	U
32	b	1857	G
32	b	1858	A
32	b	1862	G
32	b	1863	G
32	b	1864	U
32	b	1869	G
32	b	1871	A
32	b	1872	A
32	b	1873	G
32	b	1875	G
32	b	1876	A
32	b	1882	U
32	b	1884	G

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Mol	Chain	Res	Type
32	b	1887	C
32	b	1889	A
32	b	1890	A
32	b	1895	C
32	b	1899	A
32	b	1900	A
32	b	1906	G
32	b	1913	A
32	b	1917	U
32	b	1921	G
32	b	1922	G
32	b	1923	U
32	b	1924	C
32	b	1925	C
32	b	1927	A
32	b	1929	G
32	b	1930	G
32	b	1931	U
32	b	1937	A
32	b	1938	A
32	b	1939	U
32	b	1940	U
32	b	1944	U
32	b	1946	U
32	b	1952	A
32	b	1953	A
32	b	1954	G
32	b	1955	U
32	b	1956	U
32	b	1958	C
32	b	1961	C
32	b	1964	G
32	b	1965	C
32	b	1966	A
32	b	1967	C
32	b	1970	A
32	b	1971	U
32	b	1972	G
32	b	1975	G
32	b	1980	G
32	b	1981	A
32	b	1985	C

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Mol	Chain	Res	Type
32	b	1987	A
32	b	1991	U
32	b	1992	G
32	b	1993	U
32	b	1996	C
32	b	1997	C
32	b	1998	A
32	b	1999	C
32	b	2002	G
32	b	2020	A
32	b	2021	C
32	b	2022	U
32	b	2023	C
32	b	2024	G
32	b	2029	G
32	b	2030	A
32	b	2031	A
32	b	2032	G
32	b	2033	A
32	b	2034	U
32	b	2036	C
32	b	2039	U
32	b	2043	C
32	b	2051	A
32	b	2055	C
32	b	2056	G
32	b	2060	A
32	b	2061	G
32	b	2062	A
32	b	2063	C
32	b	2068	U
32	b	2069	G
32	b	2076	U
32	b	2077	A
32	b	2078	C
32	b	2080	A
32	b	2081	U
32	b	2085	U
32	b	2093	G
32	b	2095	A
32	b	2100	G
32	b	2101	A

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Mol	Chain	Res	Type
32	b	2102	G
32	b	2104	C
32	b	2105	U
32	b	2106	U
32	b	2107	G
32	b	2109	U
32	b	2110	G
32	b	2111	U
32	b	2112	G
32	b	2113	U
32	b	2114	A
32	b	2115	G
32	b	2116	G
32	b	2117	A
32	b	2118	U
32	b	2119	A
32	b	2120	G
32	b	2121	G
32	b	2123	G
32	b	2124	G
32	b	2126	A
32	b	2127	G
32	b	2128	G
32	b	2129	C
32	b	2130	U
32	b	2131	U
32	b	2133	G
32	b	2134	A
32	b	2135	A
32	b	2136	G
32	b	2137	U
32	b	2138	G
32	b	2139	U
32	b	2140	G
32	b	2142	A
32	b	2143	C
32	b	2144	G
32	b	2145	C
32	b	2146	C
32	b	2147	A
32	b	2148	G
32	b	2149	U

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Mol	Chain	Res	Type
32	b	2150	C
32	b	2151	U
32	b	2152	G
32	b	2153	C
32	b	2154	A
32	b	2155	U
32	b	2157	G
32	b	2158	A
32	b	2159	G
32	b	2160	C
32	b	2161	C
32	b	2162	G
32	b	2163	A
32	b	2164	C
32	b	2165	C
32	b	2166	U
32	b	2169	A
32	b	2170	A
32	b	2171	A
32	b	2172	U
32	b	2174	C
32	b	2175	C
32	b	2176	A
32	b	2177	C
32	b	2178	C
32	b	2180	U
32	b	2183	A
32	b	2186	G
32	b	2190	G
32	b	2192	U
32	b	2193	G
32	b	2197	U
32	b	2198	A
32	b	2199	A
32	b	2203	U
32	b	2204	G
32	b	2211	A
32	b	2212	A
32	b	2213	U
32	b	2214	C
32	b	2225	A
32	b	2228	G

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Mol	Chain	Res	Type
32	b	2234	G
32	b	2238	G
32	b	2239	G
32	b	2243	U
32	b	2249	U
32	b	2250	G
32	b	2258	C
32	b	2259	U
32	b	2261	C
32	b	2266	A
32	b	2268	A
32	b	2273	A
32	b	2278	A
32	b	2282	G
32	b	2283	C
32	b	2286	G
32	b	2287	A
32	b	2288	A
32	b	2295	C
32	b	2297	A
32	b	2298	A
32	b	2305	U
32	b	2307	G
32	b	2308	G
32	b	2309	A
32	b	2311	A
32	b	2312	U
32	b	2315	G
32	b	2316	G
32	b	2317	A
32	b	2319	G
32	b	2320	U
32	b	2321	U
32	b	2322	A
32	b	2325	G
32	b	2327	A
32	b	2333	A
32	b	2334	U
32	b	2336	A
32	b	2337	G
32	b	2340	A
32	b	2345	G

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Mol	Chain	Res	Type
32	b	2347	C
32	b	2350	C
32	b	2352	A
32	b	2354	C
32	b	2355	G
32	b	2361	G
32	b	2364	C
32	b	2367	G
32	b	2368	C
32	b	2379	G
32	b	2383	G
32	b	2385	C
32	b	2389	G
32	b	2391	G
32	b	2396	G
32	b	2397	G
32	b	2399	G
32	b	2402	U
32	b	2403	C
32	b	2405	G
32	b	2406	A
32	b	2407	A
32	b	2408	U
32	b	2410	G
32	b	2416	C
32	b	2419	U
32	b	2420	C
32	b	2422	C
32	b	2423	U
32	b	2424	C
32	b	2425	A
32	b	2427	C
32	b	2428	G
32	b	2429	G
32	b	2430	A
32	b	2431	U
32	b	2435	A
32	b	2441	U
32	b	2445	G
32	b	2447	G
32	b	2448	A
32	b	2454	G

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Mol	Chain	Res	Type
32	b	2457	U
32	b	2458	G
32	b	2459	A
32	b	2464	G
32	b	2468	A
32	b	2470	G
32	b	2471	A
32	b	2473	U
32	b	2474	U
32	b	2475	C
32	b	2476	A
32	b	2478	A
32	b	2480	C
32	b	2482	A
32	b	2484	G
32	b	2485	G
32	b	2486	C
32	b	2488	G
32	b	2490	G
32	b	2491	U
32	b	2492	U
32	b	2494	G
32	b	2497	A
32	b	2498	C
32	b	2499	C
32	b	2502	G
32	b	2503	A
32	b	2505	G
32	b	2506	U
32	b	2513	A
32	b	2518	A
32	b	2519	U
32	b	2520	C
32	b	2526	G
32	b	2528	U
32	b	2529	G
32	b	2533	U
32	b	2534	A
32	b	2535	G
32	b	2536	G
32	b	2537	U
32	b	2543	G

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Mol	Chain	Res	Type
32	b	2546	U
32	b	2547	G
32	b	2550	G
32	b	2554	U
32	b	2556	C
32	b	2560	A
32	b	2562	U
32	b	2564	A
32	b	2566	A
32	b	2567	G
32	b	2572	A
32	b	2573	C
32	b	2574	G
32	b	2579	C
32	b	2581	G
32	b	2582	G
32	b	2583	G
32	b	2585	U
32	b	2593	U
32	b	2603	G
32	b	2608	G
32	b	2609	U
32	b	2610	C
32	b	2611	C
32	b	2613	U
32	b	2614	A
32	b	2615	U
32	b	2618	G
32	b	2623	G
32	b	2625	G
32	b	2626	C
32	b	2629	U
32	b	2630	G
32	b	2634	A
32	b	2636	C
32	b	2639	A
32	b	2643	G
32	b	2646	C
32	b	2655	G
32	b	2656	U
32	b	2658	C
32	b	2660	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	b	2661	G
32	b	2663	G
32	b	2664	G
32	b	2668	G
32	b	2669	G
32	b	2673	G
32	b	2674	G
32	b	2676	C
32	b	2679	A
32	b	2681	C
32	b	2684	U
32	b	2688	G
32	b	2689	U
32	b	2690	U
32	b	2691	C
32	b	2692	G
32	b	2700	A
32	b	2702	G
32	b	2705	A
32	b	2713	U
32	b	2716	C
32	b	2718	G
32	b	2724	U
32	b	2725	A
32	b	2726	A
32	b	2731	G
32	b	2733	A
32	b	2736	A
32	b	2737	G
32	b	2744	G
32	b	2746	U
32	b	2748	A
32	b	2750	A
32	b	2751	G
32	b	2752	C
32	b	2754	U
32	b	2755	C
32	b	2757	A
32	b	2761	A
32	b	2762	C
32	b	2765	A
32	b	2768	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	b	2771	C
32	b	2773	C
32	b	2777	G
32	b	2778	A
32	b	2779	U
32	b	2780	G
32	b	2781	A
32	b	2783	U
32	b	2790	U
32	b	2796	U
32	b	2797	U
32	b	2798	U
32	b	2799	A
32	b	2800	A
32	b	2802	G
32	b	2803	G
32	b	2804	U
32	b	2807	U
32	b	2808	G
32	b	2818	U
32	b	2819	G
32	b	2820	A
32	b	2821	A
32	b	2822	G
32	b	2832	U
32	b	2833	U
32	b	2835	A
32	b	2836	U
32	b	2837	A
32	b	2843	G
32	b	2848	G
32	b	2849	U
32	b	2859	G
32	b	2861	U
32	b	2864	G
32	b	2865	U
32	b	2866	U
32	b	2867	G
32	b	2871	U
32	b	2879	A
32	b	2883	A
32	b	2884	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	b	2886	A
32	b	2887	A
32	b	2892	G
32	b	2893	A
32	b	2894	G
32	b	2895	G
32	b	2898	U
32	b	2900	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	b	4
31	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	2601:C	O3'	2602:A	P	4.74
1	b	2334:U	O3'	2335:A	P	4.39
1	b	2059:A	O3'	2060:A	P	1.99
1	b	2058:A	O3'	2059:A	P	1.92
1	v	1:C	O3'	2:G	P	0.75

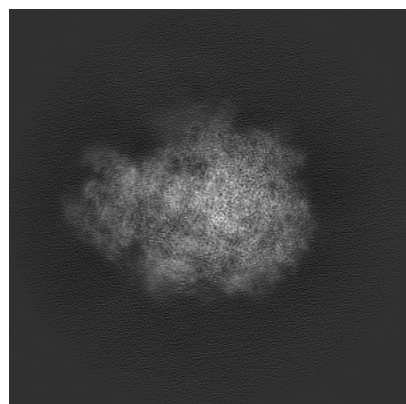
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52417. These allow visual inspection of the internal detail of the map and identification of artifacts.

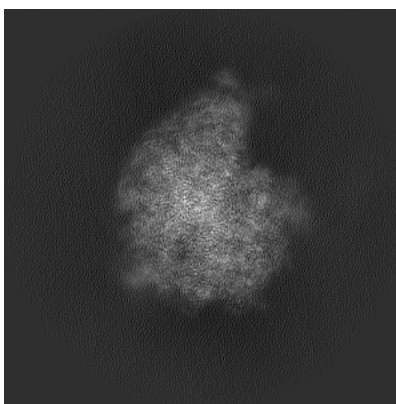
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

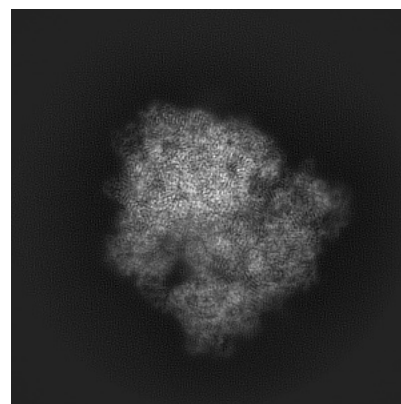
6.1.1 Primary map



X

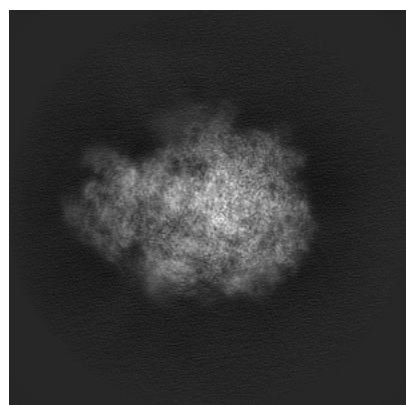


Y

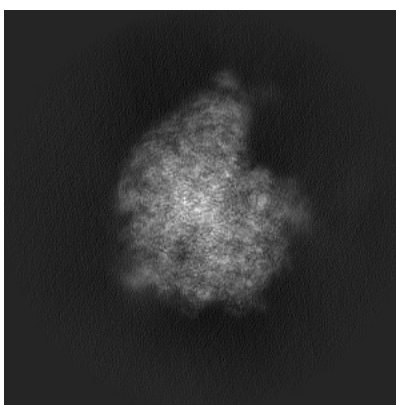


Z

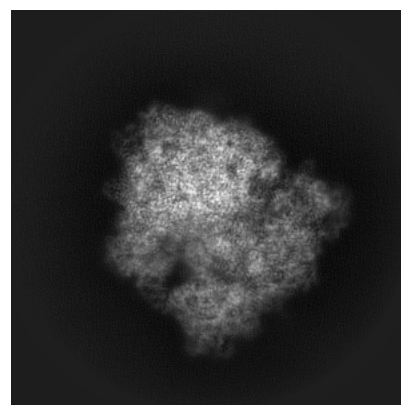
6.1.2 Raw map



X



Y

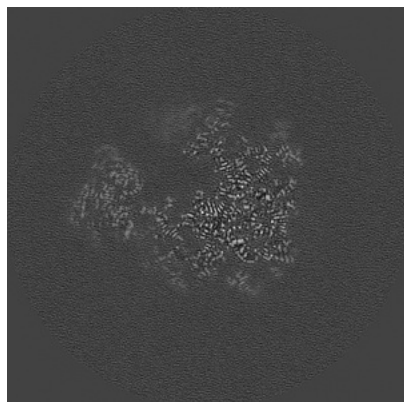


Z

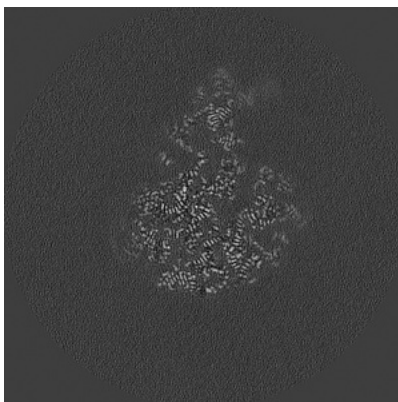
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

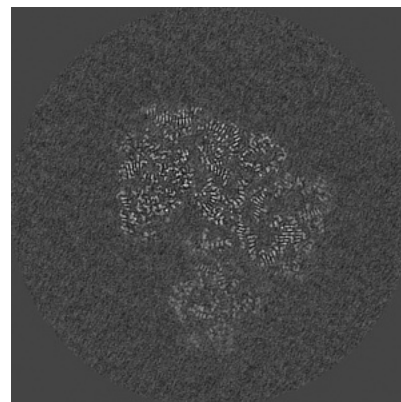
6.2.1 Primary map



X Index: 192

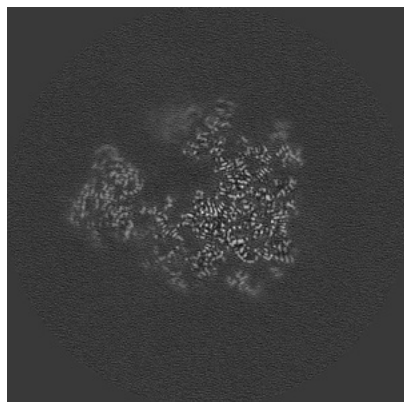


Y Index: 192

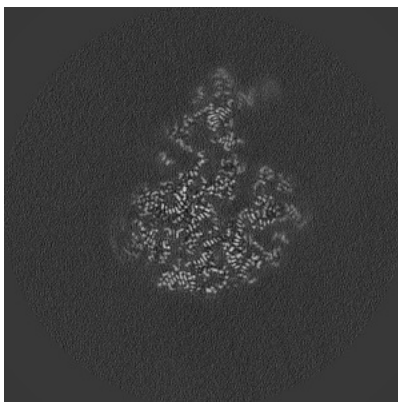


Z Index: 192

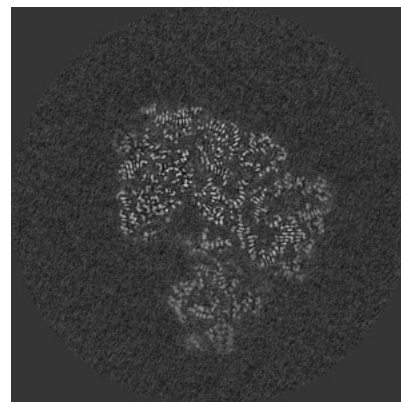
6.2.2 Raw map



X Index: 192



Y Index: 192

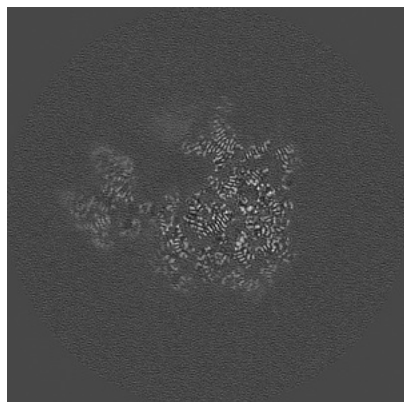


Z Index: 192

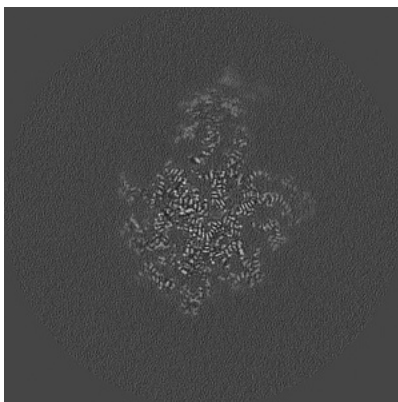
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

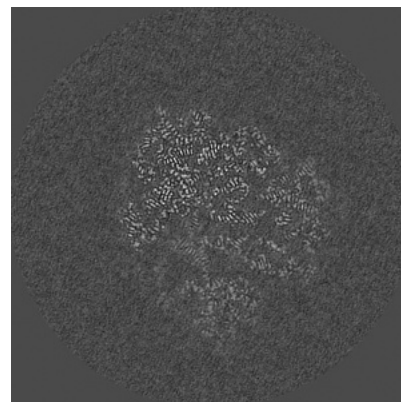
6.3.1 Primary map



X Index: 198

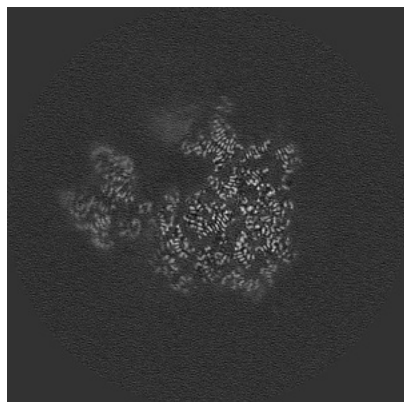


Y Index: 208

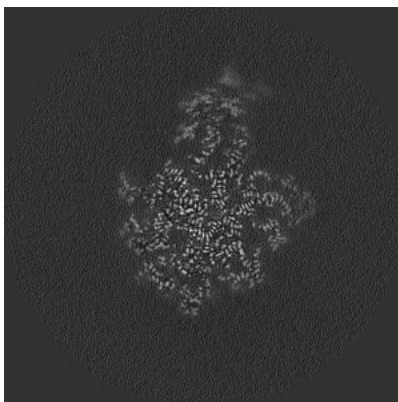


Z Index: 200

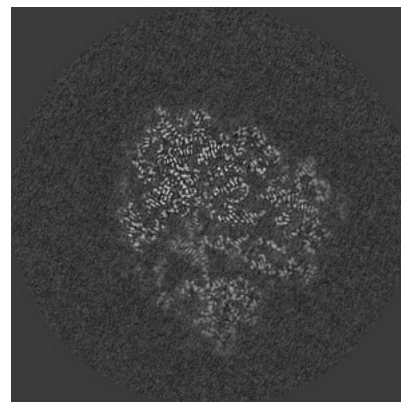
6.3.2 Raw map



X Index: 198



Y Index: 208

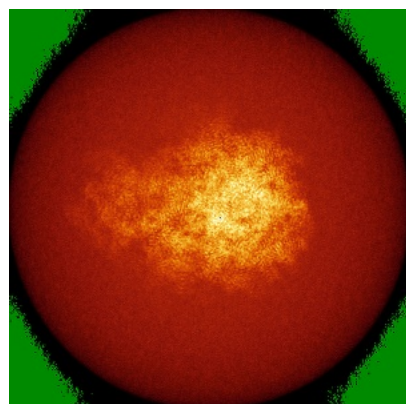


Z Index: 200

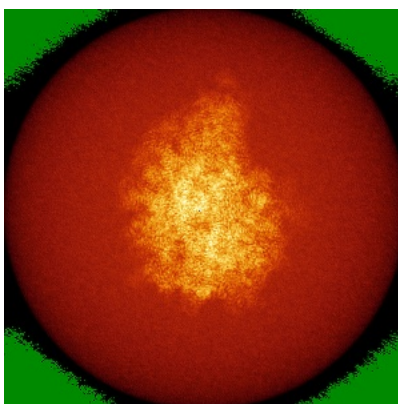
The images above show the largest variance slices of the map in three orthogonal directions.

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

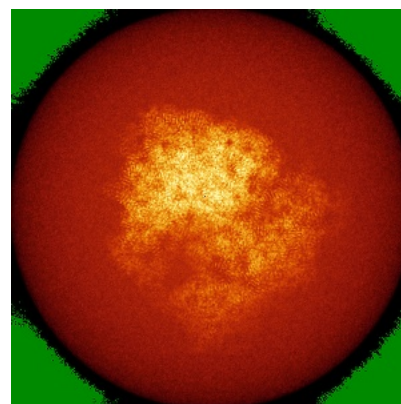
6.4.1 Primary map



X

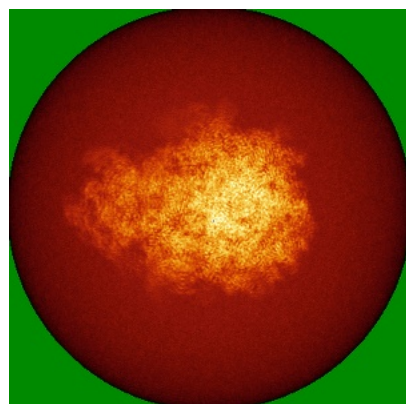


Y

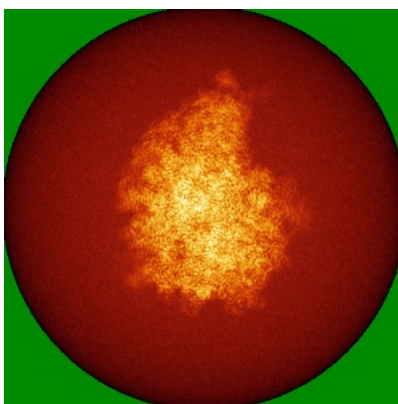


Z

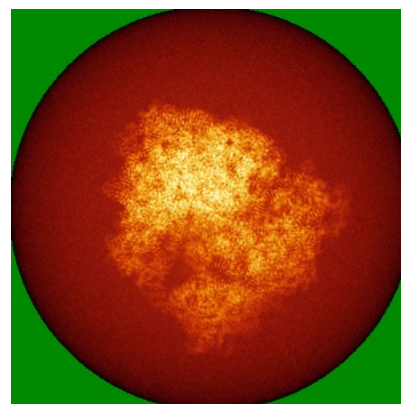
6.4.2 Raw map



X



Y

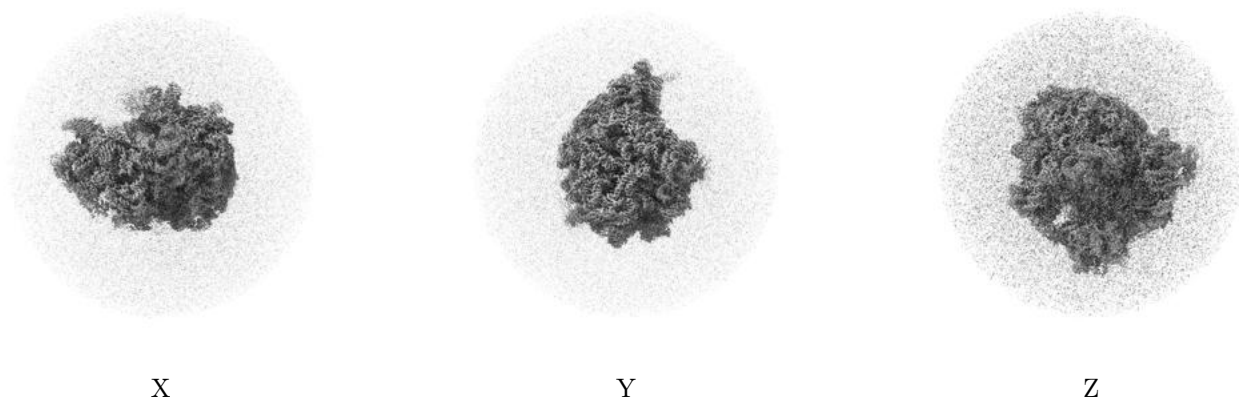


Z

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

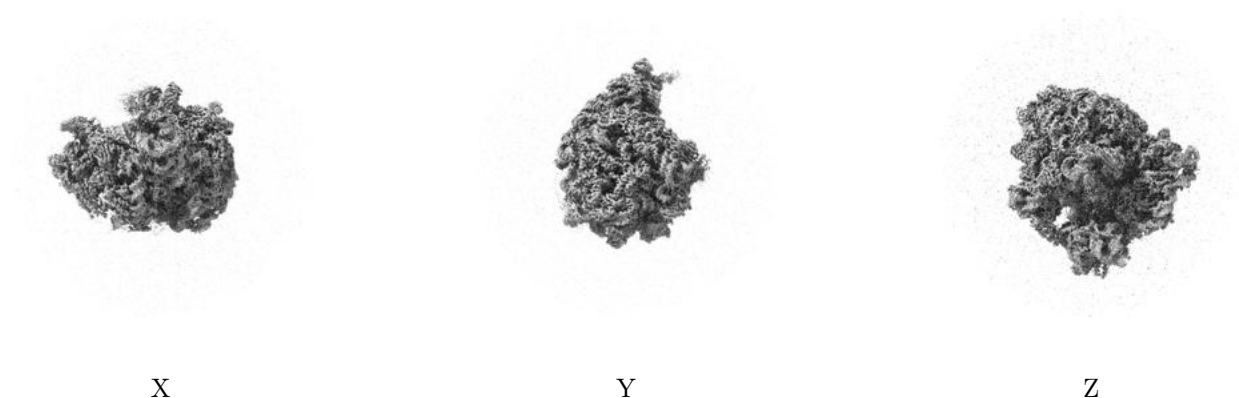
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

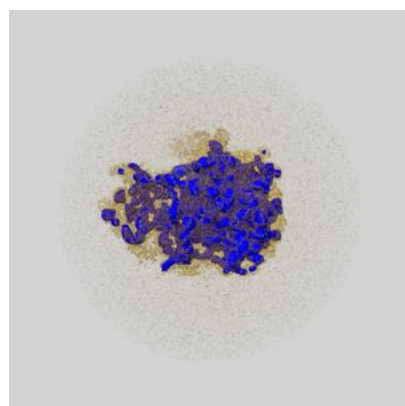
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

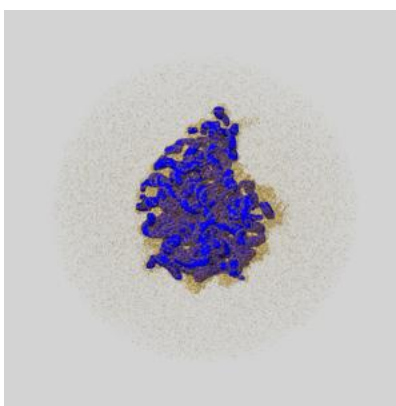
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

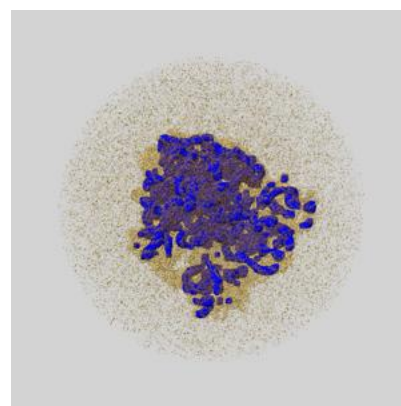
6.6.1 emd_52417_msk_1.map [i](#)



X



Y

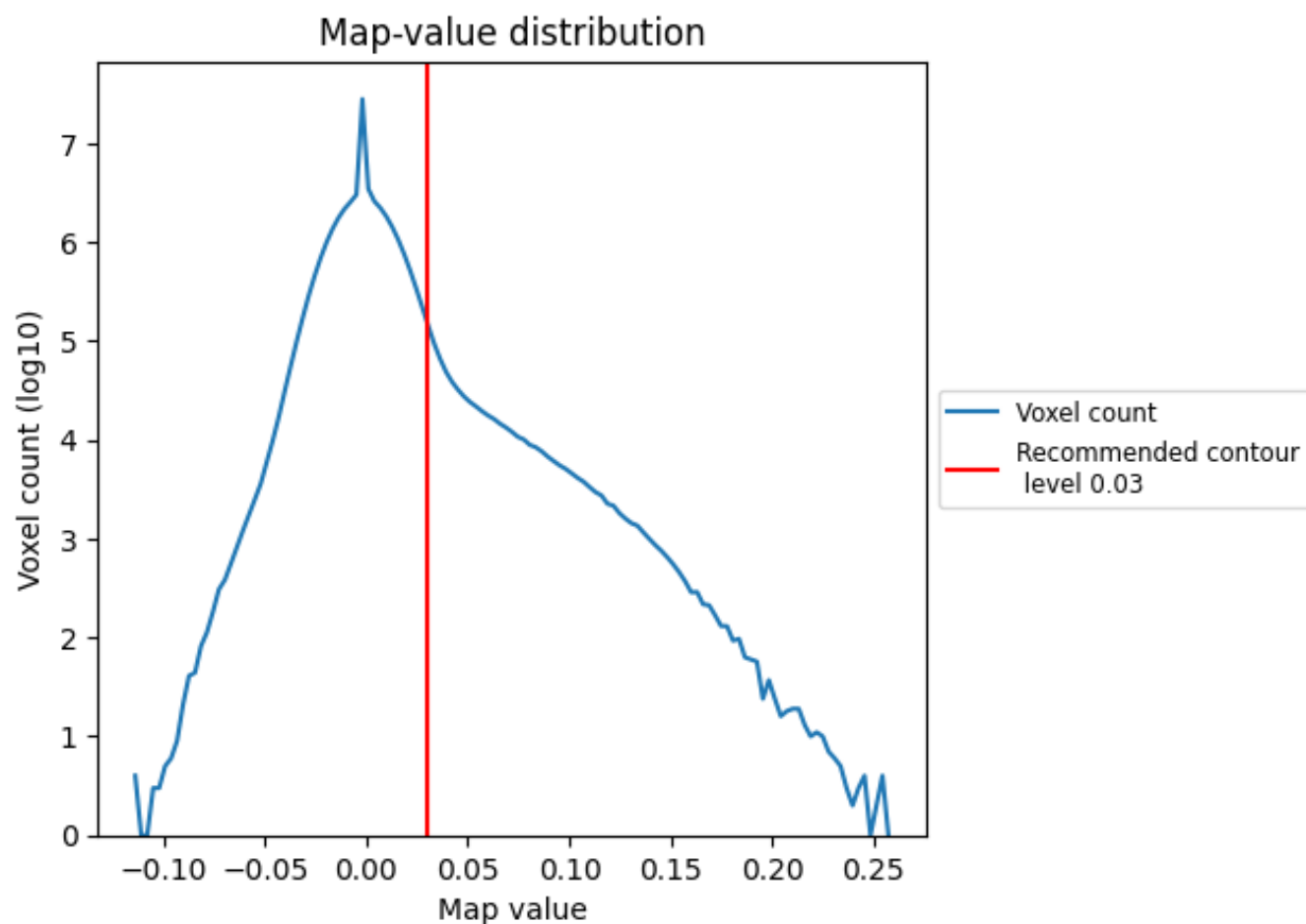


Z

7 Map analysis [i](#)

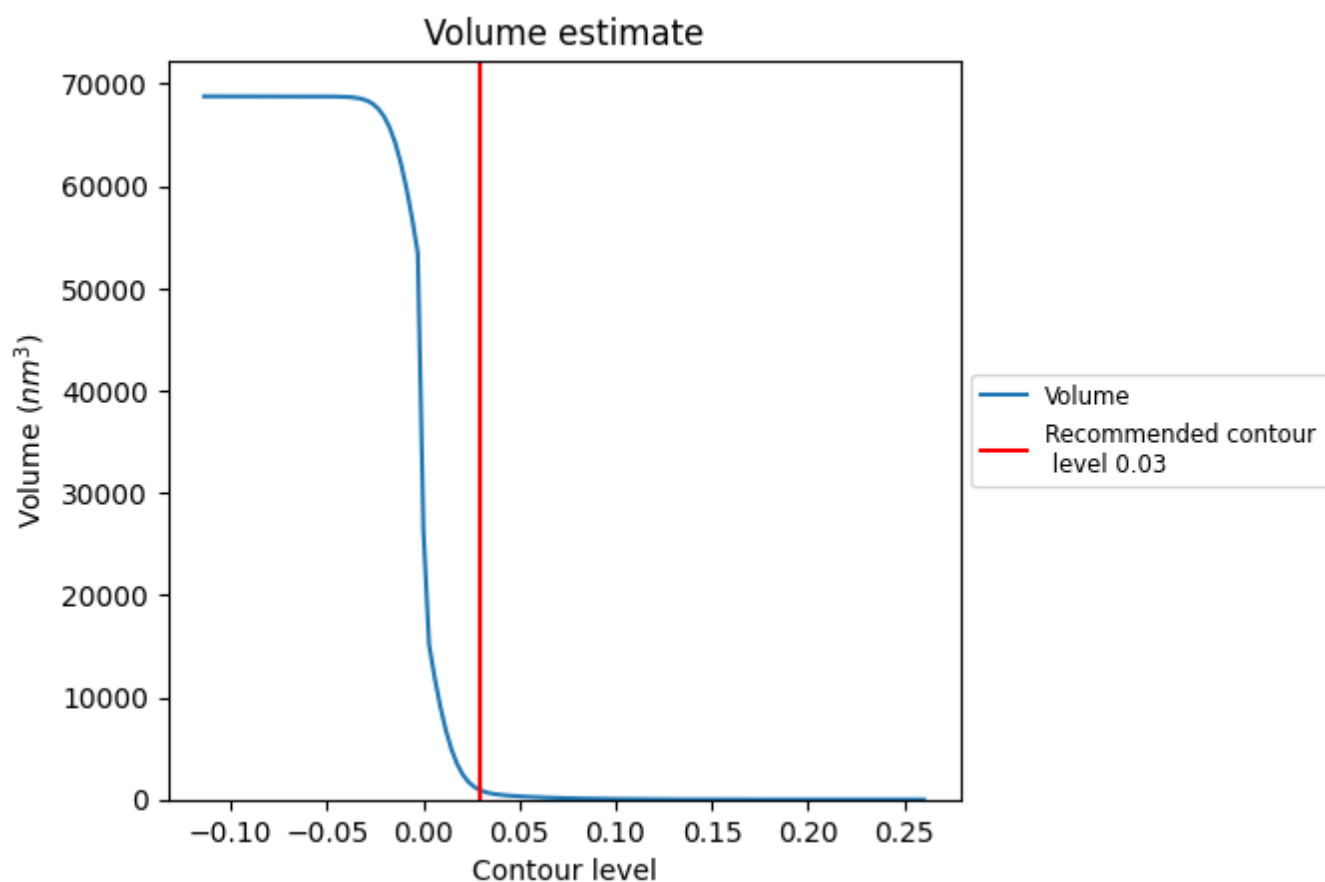
This section contains the results of statistical analysis of the map.

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.

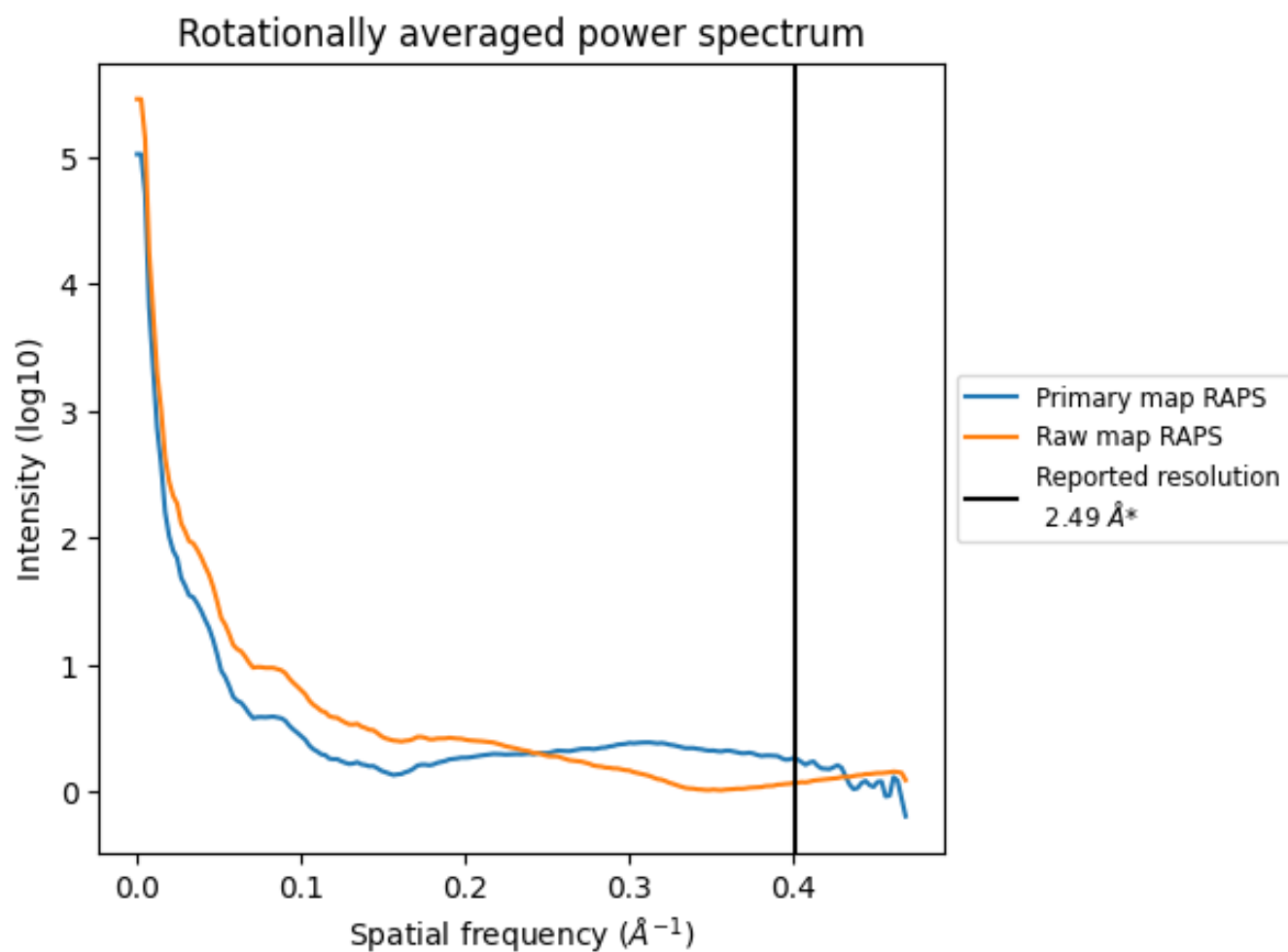
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 893 nm³; this corresponds to an approximate mass of 806 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 ⓘ

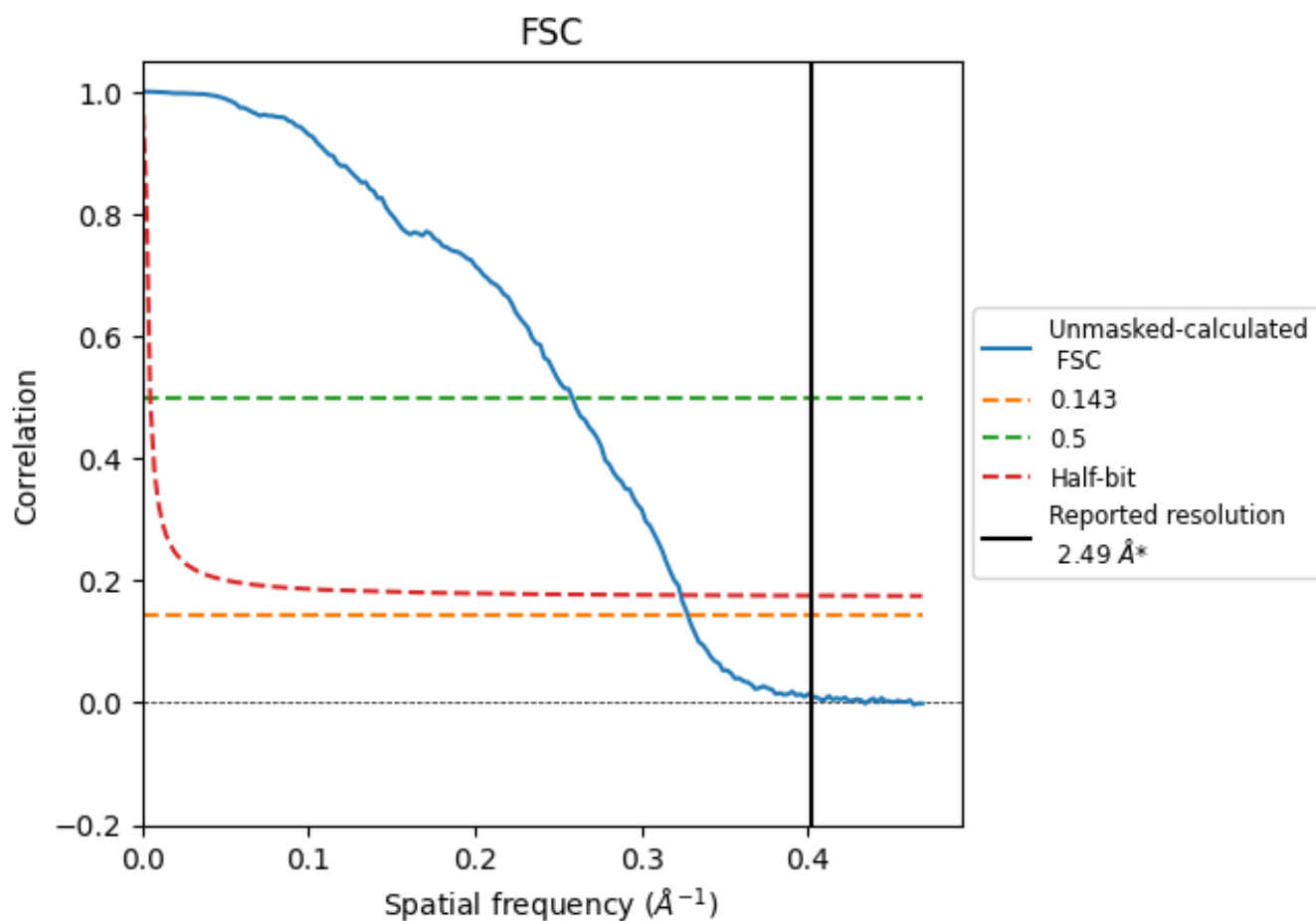


*Reported resolution corresponds to spatial frequency of 0.402 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.402 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

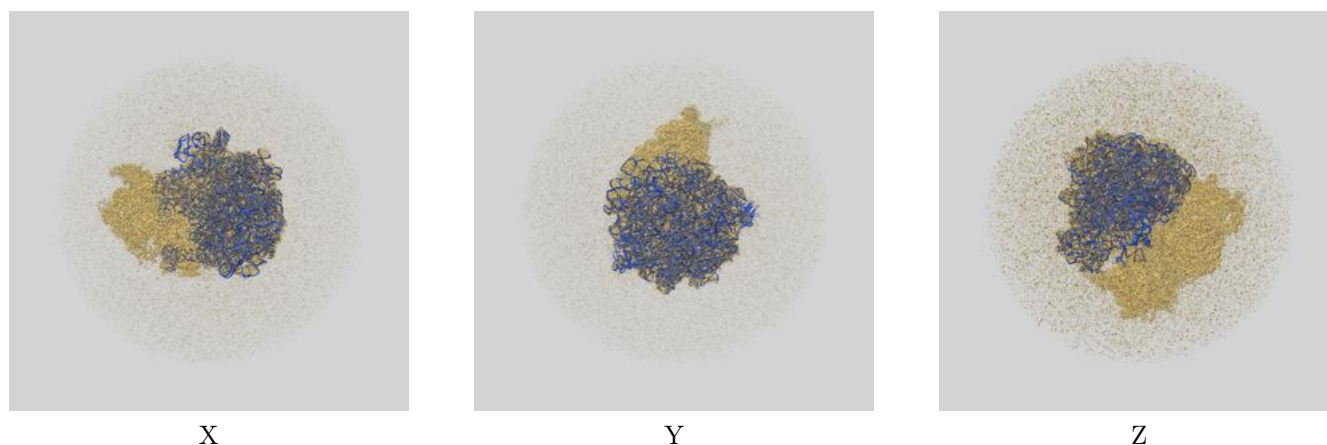
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.05	3.87	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.49 by more than 10 %

9 Map-model fit [i](#)

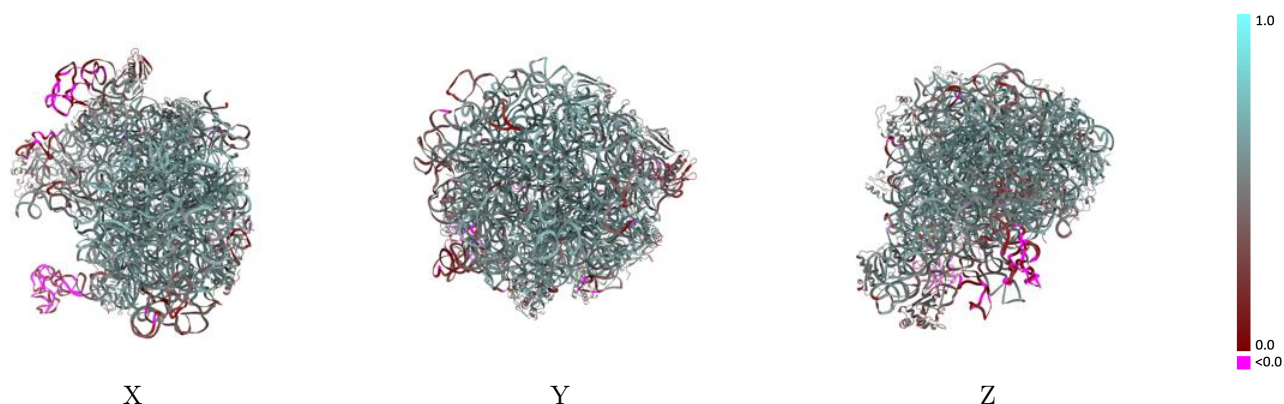
This section contains information regarding the fit between EMDB map EMD-52417 and PDB model 9HUQ. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



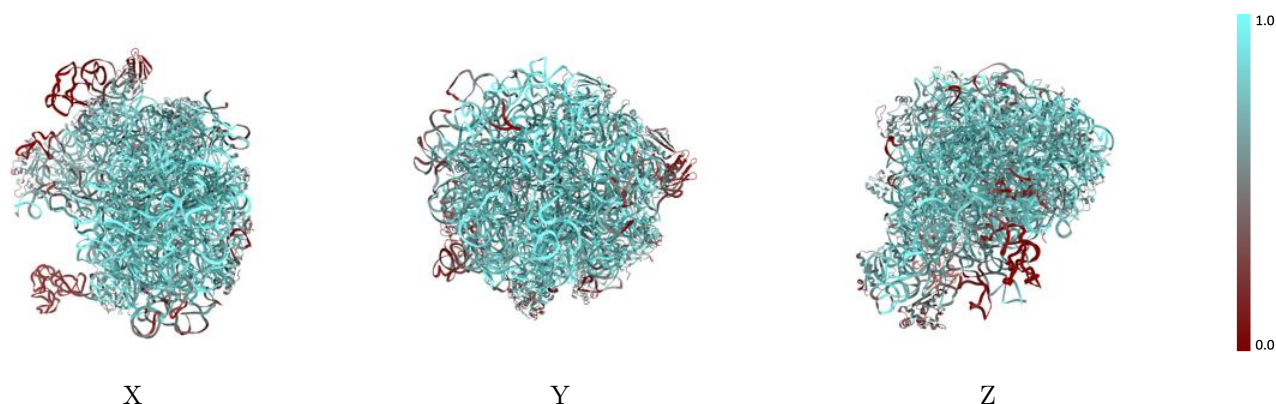
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



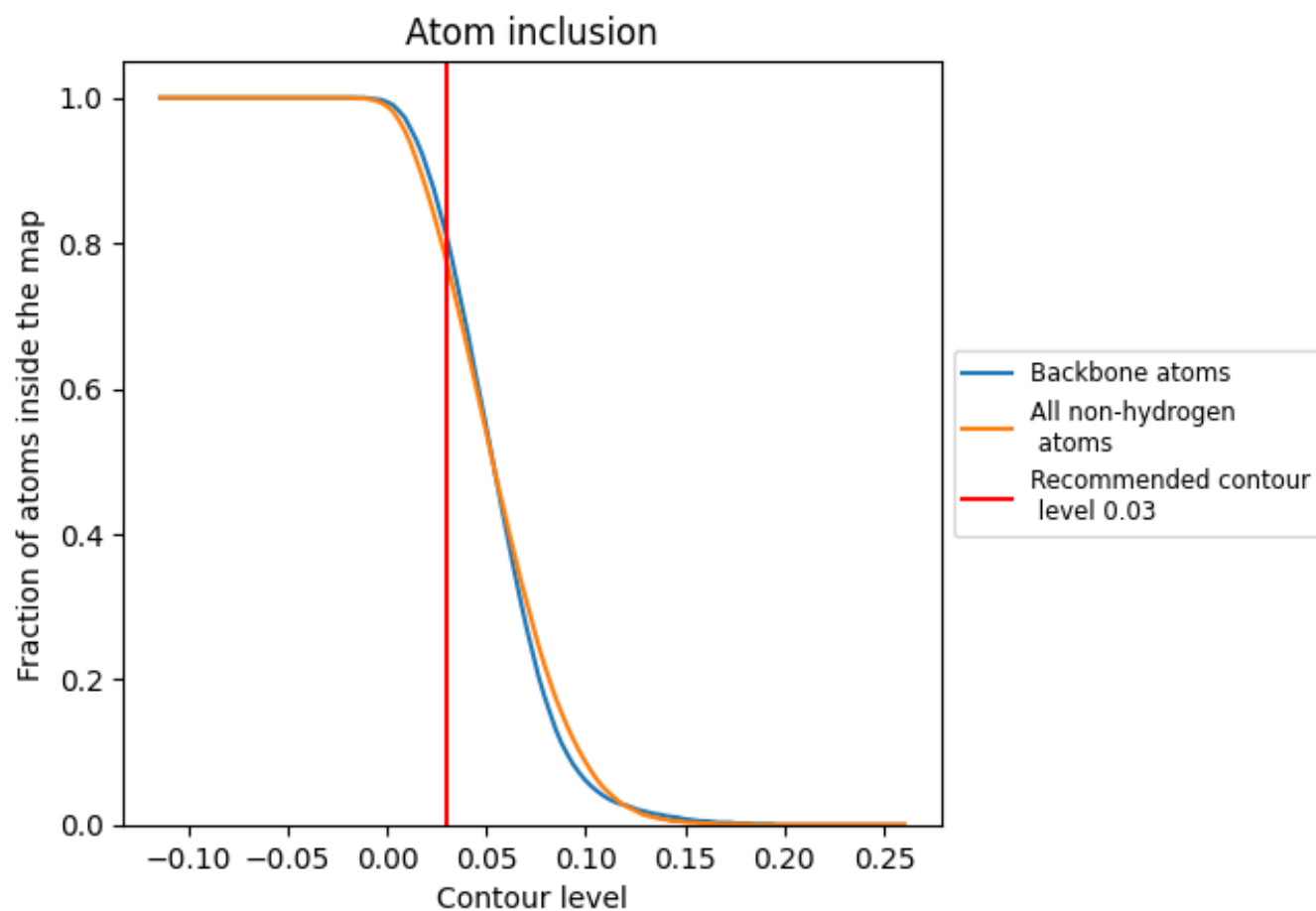
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.5270
0	 0.7920	 0.5840
1	 0.6170	 0.4850
2	 0.7700	 0.5750
3	 0.7940	 0.5770
4	 0.6830	 0.4990
6	 0.9350	 0.6500
7	 0.8960	 0.6230
8	 0.7460	 0.5640
a	 0.7880	 0.5190
b	 0.8020	 0.5270
c	 0.8420	 0.5920
d	 0.7940	 0.5810
e	 0.6860	 0.5300
f	 0.4280	 0.3820
g	 0.3510	 0.3780
h	 0.3520	 0.3600
j	 0.7820	 0.5710
k	 0.7860	 0.5740
l	 0.7750	 0.5640
m	 0.7670	 0.5530
n	 0.8710	 0.6120
o	 0.6290	 0.4790
p	 0.7520	 0.5560
q	 0.8390	 0.6110
r	 0.6850	 0.5250
s	 0.8310	 0.5930
t	 0.7050	 0.5290
u	 0.6140	 0.4730
v	 0.6000	 0.4330
w	 0.6170	 0.4910
y	 0.7980	 0.5800
z	 0.3020	 0.3170

