



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:43 AM UTC

PDB ID : 9GHH / pdb_00009ghh
EMDB ID : EMD-51357
Title : Staphylococcus aureus FusB bound to the large subunit of the S. aureus 70S ribosome (FusB-Sa70S:LSU)
Authors : Gonzalez-Lopez, A.; Selmer, M.
Deposited on : 2024-08-15
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

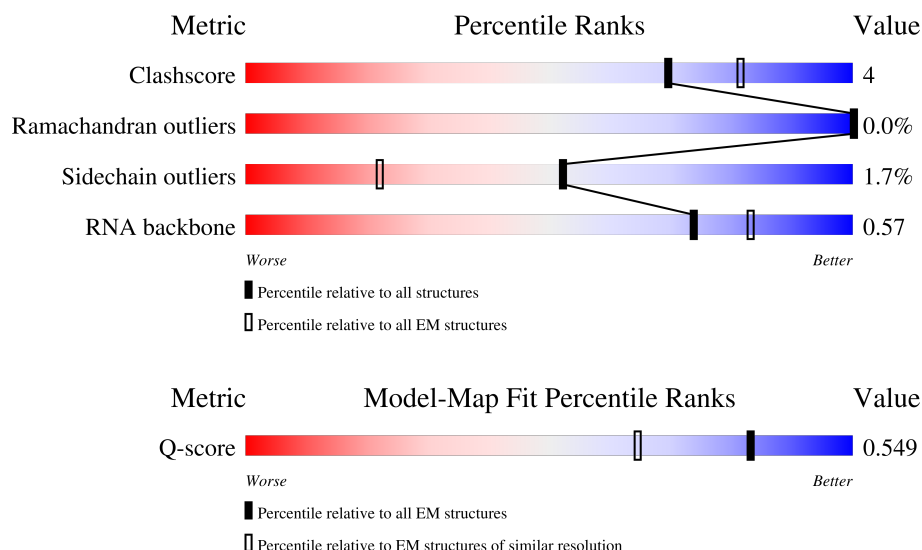
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

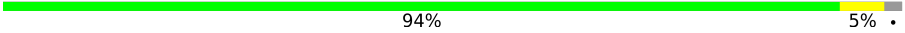
The reported resolution of this entry is 2.70 Å.

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.



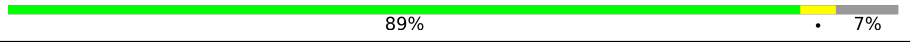
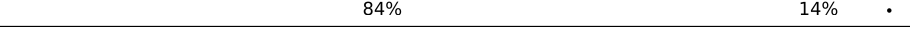
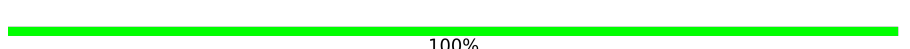
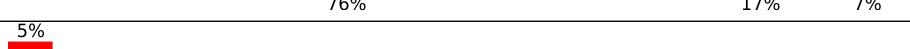
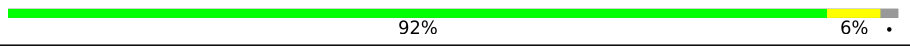
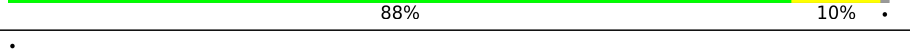
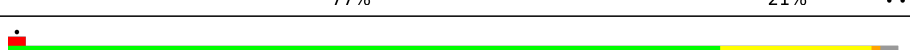
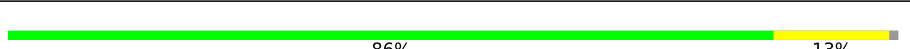
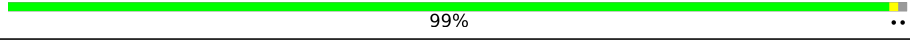
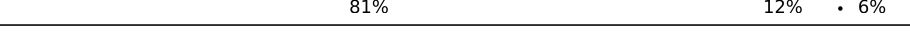
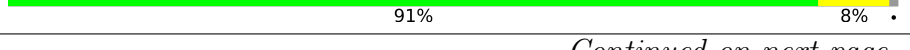
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	1	62	 94% 5%
2	2	69	 86% 9% 6%
3	3	59	 83% 12% 5%

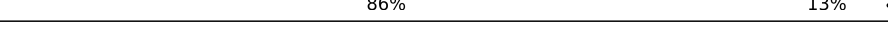
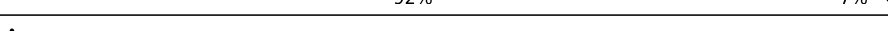
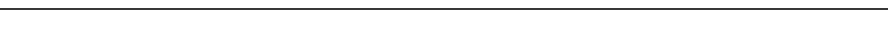
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Mol	Chain	Length	Quality of chain
4	4	84	
5	5	57	
6	6	49	
7	7	45	
8	8	66	
9	9	37	
10	A	2923	
11	B	115	
12	C	213	
13	D	77	
13	F	77	
14	G	277	
15	H	220	
16	I	207	
17	J	179	
18	K	178	
19	M	145	
20	N	122	
21	O	146	
22	P	144	
23	Q	122	
24	R	119	
25	S	116	
26	T	118	
27	U	102	

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Mol	Chain	Length	Quality of chain
28	V	117	
29	W	91	
30	X	105	
31	Y	217	
32	Z	94	
33	a	1555	
34	b	24	
35	c	255	
36	d	217	
37	e	200	
38	f	166	
39	g	98	
40	h	156	
41	i	132	
42	j	132	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	87	
51	s	80	
52	t	92	

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Mol	Chain	Length	Quality of chain
53	u	83	88% 8%
54	v	58	59% 74% 17% 9%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144758 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 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	61	Total	C	N	O	S	0	0
			481	298	104	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	80	Total	C	N	O	S	0	0
			654	417	111	123	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 6 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2848	Total	C	N	O	P	0	0
			61064	27267	11166	19783	2848		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 12 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	198	Total	C	N	O	S	1	0
			1659	1075	271	306	7		

- Molecule 13 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
13	F	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	178	Total	C	N	O	S	0	0
			1412	897	244	264	7		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	174	Total	C	N	O	S	0	0
			1361	846	249	263	3		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	144	Total	C	N	O	S	0	0
			1146	715	210	218	3		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	114	Total	C	N	O	0	0
			922	580	185	157		

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

- Molecule 31 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	82	Total	C	N	O	0	0
			626	386	122	118		

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1526	Total	C	N	O	P	0	0
			32707	14608	5975	10598	1526		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	10	Total	C	N	O	P	0	0
			218	98	45	65	10		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1612	1015	302	293	2		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	146	Total	C	N	O	S	0	0
			1165	727	222	212	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	128	Total	C	N	O	S	0	0
			1016	629	203	183	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	99	Total	C	N	O	S	0	0
			792	499	145	147	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			662	419	120	122	1		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	80	Total	C	N	O	S	0	0
			651	419	117	113	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	v	53	Total	C	N	O	0	0
			446	275	93	78		

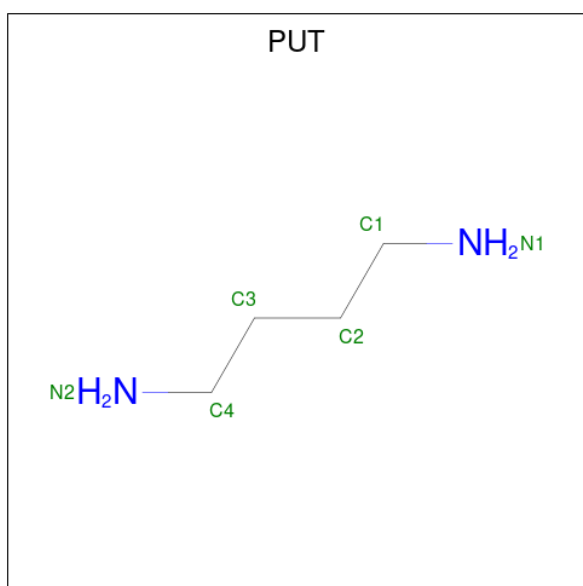
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	5	1	Total	Zn	0
			1	1	
55	9	1	Total	Zn	0
			1	1	
55	C	1	Total	Zn	0
			1	1	
55	o	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
56	A	119	Total	Mg	0
			119	119	
56	F	1	Total	Mg	0
			1	1	
56	G	1	Total	Mg	0
			1	1	
56	a	24	Total	Mg	0
			24	24	

- Molecule 57 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).

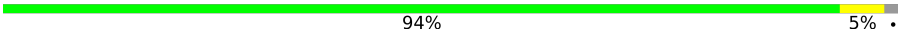


Mol	Chain	Residues	Atoms			AltConf
57	A	1	Total	C	N	0
			6	4	2	
57	A	1	Total	C	N	0
			6	4	2	

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: 50S ribosomal protein L28

Chain 1: 



- Molecule 2: 50S ribosomal protein L29

Chain 2: 



- Molecule 3: 50S ribosomal protein L30

Chain 3: 



- Molecule 4: 50S ribosomal protein L31 type B

Chain 4: 

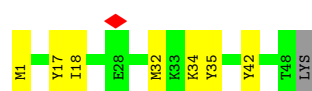
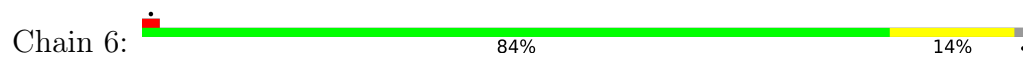


- Molecule 5: Large ribosomal subunit protein bL32

Chain 5: 



- Molecule 6: Large ribosomal subunit protein bL33A



- Molecule 7: 50S ribosomal protein L34



- Molecule 8: 50S ribosomal protein L35

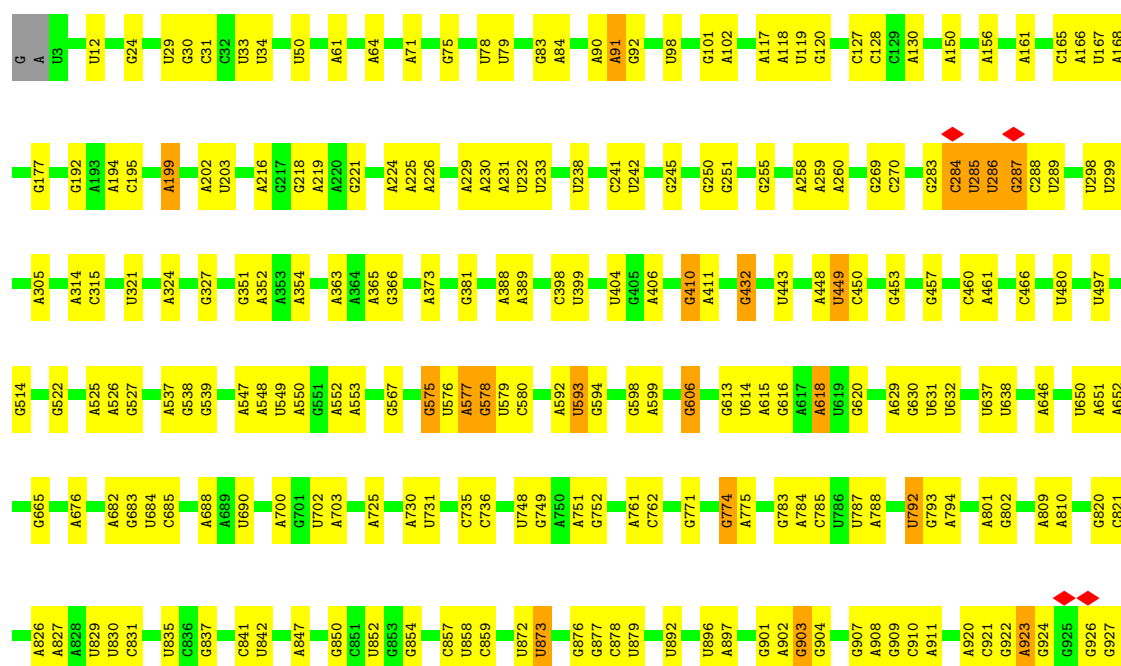
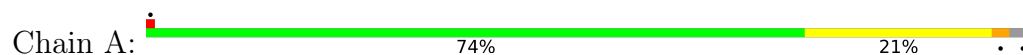


- Molecule 9: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

- Molecule 10: 23S rRNA



U2820	G2657	A2486	G2372	G2230	U	A2057	A1880	C1692	C1536	G1375	G1175	G1086	C929
U2821	U2501	U2502	A2372	A2235	G	A2058	A1881	C1696	A1537	U1176	U1176	A1070	C930
C2823	C2502	C2501	A2374	A2236	A	G2059	U1891	G1697	C1382	A1071	C1177	A1072	C
U2824	G2513	G2512	C2377	U2238	A	A2060	U1897	G1718	U1552	U1394	C1179	U1077	C
U2825	C2526	C2525	C2382	A2239	G	G2065	U1898	U1732	A1553	U1395	A1186		U
U2826	C2529	C2528	C2386	A2252	U	C2070	C1898	U1740	A1560	A1402	U1209	C1088	C935
U2827	U2531	U2530	A2387	A2254	G	G2078	G1900	G1740	A1567	U1210	U1209	C1089	G936
U2828	U2532	U2531	C2391	G2285	C	A2078	G1909	A1744	U1568	G1405	U1210	A1090	G937
C2836	G2535	G2534	A2396	G2286	G	C2082	A1927	U1756	G1569	C1407	U1216	G1091	G938
U2852	U2557	U2556	C2408	A2294	U	G2096	A1954	U1757	G1570	G1218	U1217	G1100	U940
G2869	C2561	C2560	G2409	A2295	C	G2097	A1955	G1767	G1571	A1415	U1217		A941
G2872	U2581	U2580	G2410	A2296	A	G2098	A1956	G1772	A1578	C1221	C1221	C1108	C942
C2873	U2582	U2581	A2405	U2270	G	G2099	A1957	G1783	C1579	A1222	A1222	U1109	C943
U2705	C2584	C2583	A2406	U2271	C	G2100	A1958	G1789	A1580	A1223	A1223	U1110	C944
A2706	A2544	A2543	C2408	A2294	U	G2101	A1959	G1791	A1581	U1238	U1238	A1111	A945
U2716	U2555	U2554	G2409	A2295	A	U2102	A1960	G1795	U1582	U1262	U1262	A1112	A955
A2717	U2556	U2555	A2411	U2298	G	G2109	A1961	G1799	U1583	A1275	A1275	A1113	A956
C2718	U2557	U2556	C2412	G2298	U	G2110	A1962	G1803	U1584	G1276	G1276	A1114	A969
A2740	C2561	C2560	U2429	A2300	C	G2111	A1963	U1806	G1585	A1430	A1430	G1115	U970
G2741	U2581	U2580	C2430	A2301	A	U2102	A1964	U1809	C1606	U1455	U1455	A1116	A971
U2753	U2582	U2581	C2433	A2305	G	G2128	A1965	A1810	A1616	A1456	A1456	A1117	A972
G2758	C2584	C2583	A2437	U2310	C	G2129	A1966	A1811	A1617	G1294	G1294	A1118	A977
C2759	U2585	U2584	A2438	C2312	U	G2136	A1967	U1818	A1618	A1306	A1306	A1119	A985
A2760	A2589	A2588	G2440	A2314	C	U2137	A1968	U1823	A1630	G1307	G1307	A1120	C988
G2762	C2594	C2593	U2446	A2315	G	U2137	A1969	U1824	A1631	A1457	A1457	A1121	C989
U2769	U2595	U2594	U2446	A2316	U	U2137	A1970	U1827	A1632	G1308	G1308	A1122	G990
U2770	U2611	U2610	U2450	G2317	G	U2137	A1971	U1828	A1633	A1310	A1310	U1123	A991
G2771	C2612	C2611	C2451	U2318	C	U2137	A1972	U1829	A1634	A1311	A1311	U1124	A992
A2774	A2614	A2613	A2452	U2319	A	U2137	A1973	U1830	U1625	A1312	A1312	U1125	A992
U2775	C2617	C2616	G2455	U2332	U	U2137	A1974	U1831	A1630	G1313	G1313	A1126	G1005
A2776	G2619	G2618	G2456	U2333	A	U2137	A1975	U1832	A1631	A1314	A1314	A1127	U1014
G2777	U2620	U2619	A2457	G2334	C	U2137	A1976	U1833	A1632	C1315	C1315	G1131	A1017
C2779	C2621	C2620	A2462	G2335	U	U2137	A1977	U1834	A1633	G1316	G1316	A1132	A1018
U2782	A2629	A2628	C2468	U2339	A	U2137	A1978	U1835	U1652	U1325	U1325	U1133	
C2783	G2630	G2629	G2472	A2347	C	U2137	A1979	U1836	A1653	G1329	G1329	U1134	A1027
A2784	U2631	U2630	A2475	G2348	G	U2137	A1980	U1837	A1654	U1330	U1330	G1135	G1028
U2785	U2632	U2631	U2476	A2349	U	U2137	A1981	U1838	A1655	C1331	C1331	C1136	C1029
A2791	C2636	C2635	U2477	A2354	A	U2137	A1982	U1839	A1656	A1337	A1337	U1138	C1038
U2792	U2637	U2636	G2482	A2355	G	U2137	A1983	U1840	A1657	C1351	C1351	A1139	C1039
G2793	U2640	U2639	A2486	G2357	C	U2137	A1984	U1841	G1675	C1352	C1352	A1140	A1040
A2805	U2641	U2640	U2361	G2358	C	U2137	A1985	U1842	A1679	G1357	G1357	U1141	A1044
U2806	C2642	C2641	C2494	U2361	U	U2137	A1986	U1843	A1690	A1366	A1366	A1148	A1045
G2807	C2644	C2643	A2495	A2362	U	U2137	A1987	U1844	G1691	U1367	U1367	U1149	A1052
						U2137	A1988	U1845				A1150	U1066
						U2137	A1989	U1846				G1154	A1057
						U2137	A1990	U1847				G1155	
						U2137	A1991	U1848				G1156	
						U2137	A1992	U1849				G1157	
						U2137	A1993	U1850				G1158	
						U2137	A1994	U1851				G1159	
						U2137	A1995	U1852				U1174	
						U2137	A1996	U1853					
						U2137	A1997	U1854					
						U2137	A1998	U1855					
						U2137	A1999	U1856					
						U2137	A2000	U1857					
						U2137	A2001	U1858					
						U2137	A2002	U1859					
						U2137	A2003	U1860					
						U2137	A2004	U1861					
						U2137	A2005	U1862					
						U2137	A2006	U1863					
						U2137	A2007	U1864					
						U2137	A2008	U1865					
						U2137	A2009	U1866					
						U2137	A2010	U1867					
						U2137	A2011	U1868					
						U2137	A2012	U1869					
						U2137	A2013	U1870					
						U2137	A2014	U1871					
						U2137	A2015	U1872					
						U2137	A2016	U1873					
						U2137	A2017	U1874					
						U2137	A2018	U1875					
						U2137	A2019	U1876					
						U2137	A2020	U1877					
						U2137	A2021	U1878					
						U2137	A2022	U1879					
						U2137	A2023	U1880					
						U2137	A2024	U1881					
						U2137	A2025	U1882					
						U2137	A2026	U1883					
						U2137	A2027	U1884					
						U2137	A2028	U1885					
						U2137	A2029	U1886					
						U2137	A2030	U1887					
						U2137	A2031	U1888					
						U2137	A2032	U1889					
						U2137	A2033	U1890					
						U2137	A2034	U1891					
						U2137	A2035	U1892					
						U2137	A2036	U1893					
						U2137	A2037	U1894					
						U2137	A2038	U1895					
						U2137	A2039	U1896					
						U2137	A2040	U1897					
						U2137	A2041	U1898					
						U2137	A2042	U1899					
						U2137	A2043	U1900					
						U2137	A2044	U1901					
						U2137	A2045	U1902					
						U2137	A2046	U1903					
						U2137	A2047	U1904					
						U2137	A2048	U1905					
						U2137	A2049	U1906					
						U2137	A2050	U1907					
						U2137	A2051	U1908					
						U2137	A2052	U1909					
						U2137	A2053	U1910					
						U2137	A2054	U1911					
						U2137	A2055	U1912					
						U2137	A2056	U1913					
						U2137	A2057	U1914					
						U2137	A2058	U1915					
						U2137	A2059	U1916					
						U2137	A2060	U1917					
						U2137	A2061	U1918					
						U2137	A2062	U1919					
						U2137	A2063	U1920					
						U2137	A2064	U1921					
						U2137	A2065	U1922					
						U2137	A2066	U1923					
						U2137	A2067	U1924					
						U2137	A2068	U1925					
						U2137	A2069	U1926					
						U2137	A2070	U1927					
						U2137	A2071	U1928					
						U2137	A2072	U1929					
						U2137	A2073	U1930					
					</								

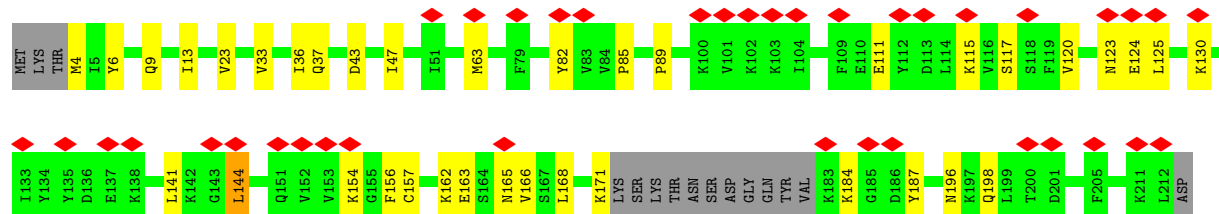
- Molecule 11: 5S rRNA

Chain B: 



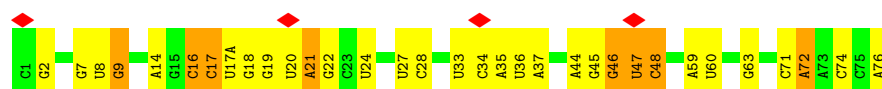
- Molecule 12: Far1

Chain C: 



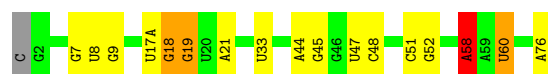
- Molecule 13: E-site tRNA

Chain D: 



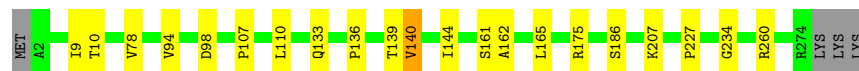
- Molecule 13: E-site tRNA

Chain F: 

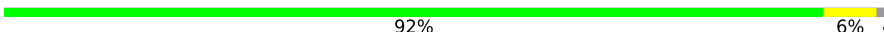


- Molecule 14: 50S ribosomal protein L2

Chain G: 



- Molecule 15: 50S ribosomal protein L3

Chain H: 



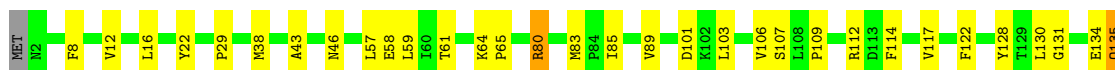
- Molecule 16: 50S ribosomal protein L4

Chain I: 



- Molecule 17: 50S ribosomal protein L5

Chain J: 77% 21% ..



- Molecule 18: 50S ribosomal protein L6

Chain K: 80% 17% ..



- Molecule 19: 50S ribosomal protein L13

Chain M: 86% 13% .



- Molecule 20: 50S ribosomal protein L14

Chain N: 89% 10% .



- Molecule 21: 50S ribosomal protein L15

Chain O: 99% ..



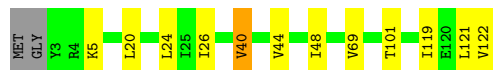
- Molecule 22: 50S ribosomal protein L16

Chain P: 81% 12% 6% ..



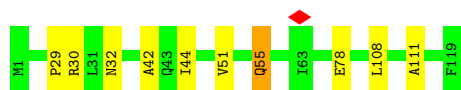
- Molecule 23: 50S ribosomal protein L17

Chain Q: 89% 9% ..



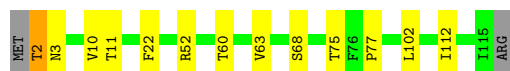
- Molecule 24: 50S ribosomal protein L18

Chain R: 92% 8% .



- Molecule 25: 50S ribosomal protein L19

Chain S: 87% 10% ..



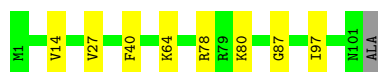
- Molecule 26: 50S ribosomal protein L20

Chain T: 86% 12% .



- Molecule 27: 50S ribosomal protein L21

Chain U: 91% 8% .



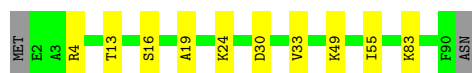
- Molecule 28: 50S ribosomal protein L22

Chain V: 79% 15% 5%

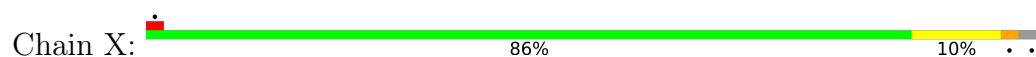


- Molecule 29: 50S ribosomal protein L23

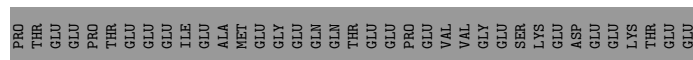
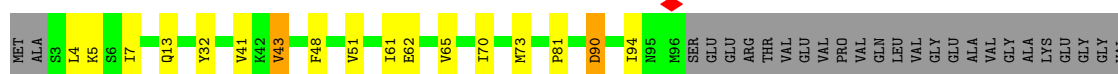
Chain W: 87% 11% .



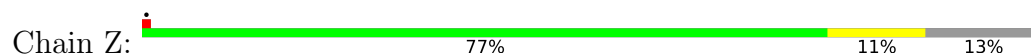
- Molecule 30: 50S ribosomal protein L24



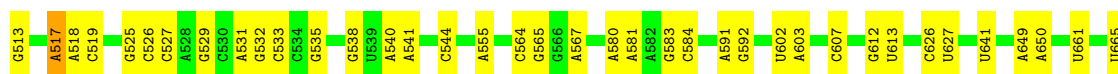
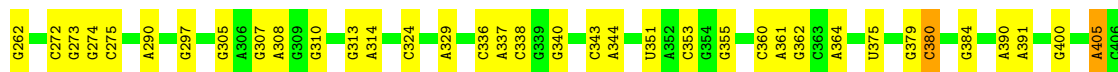
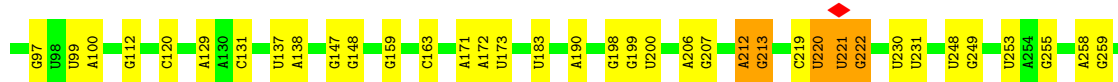
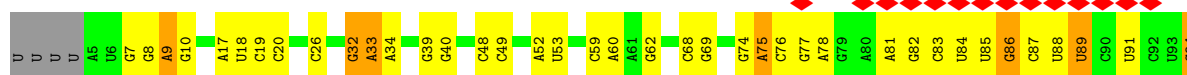
- Molecule 31: 50S ribosomal protein L25

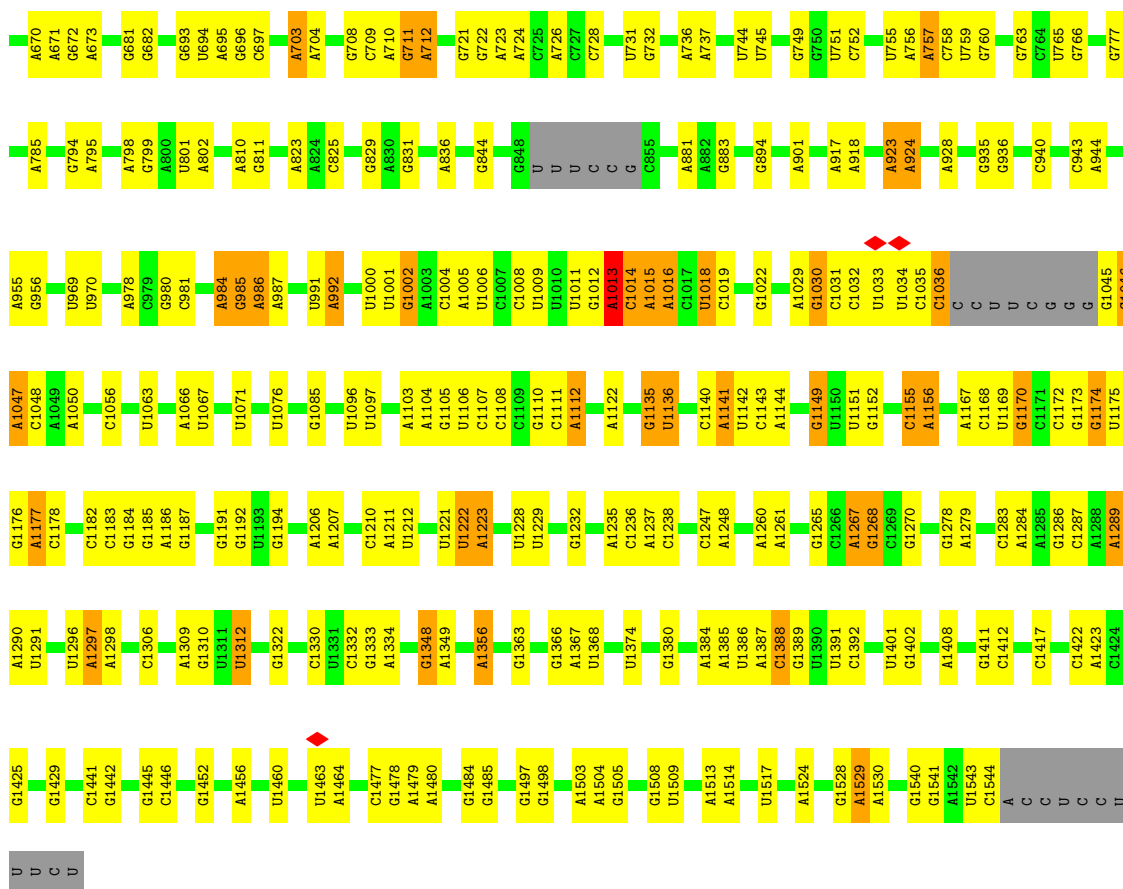


- Molecule 32: 50S ribosomal protein L27



- Molecule 33: 16S rRNA

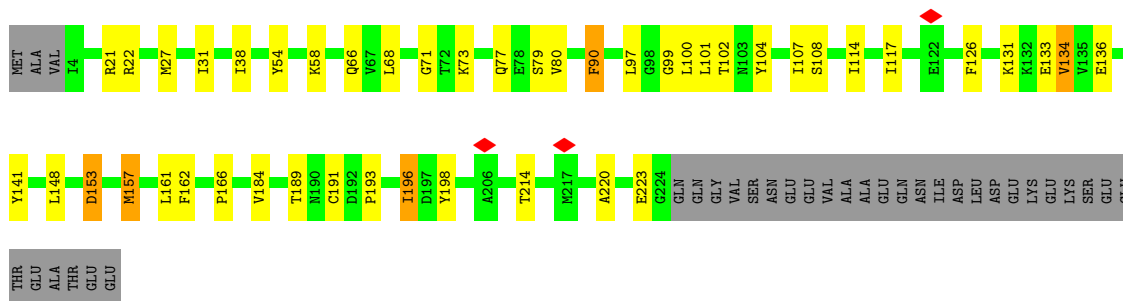




• Molecule 34: mRNA

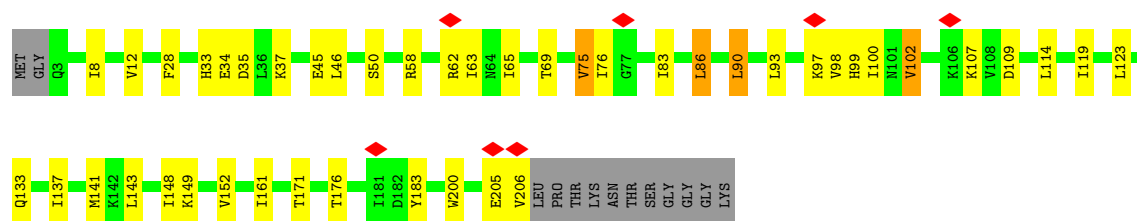


• Molecule 35: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S3





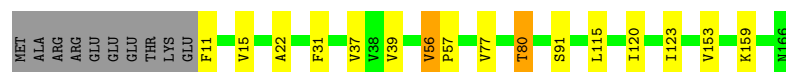
- Molecule 37: 30S ribosomal protein S4

Chain e: 86% 14%



- Molecule 38: 30S ribosomal protein S5

Chain f: 84% 8% 6%



- Molecule 39: 30S ribosomal protein S6

Chain g: 81% 12% 5%



- Molecule 40: 30S ribosomal protein S7

Chain h: 79% 13% 6%



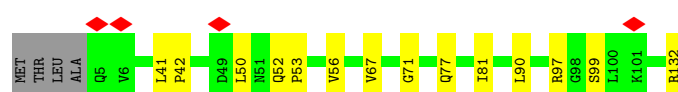
- Molecule 41: 30S ribosomal protein S8

Chain i: 86% 13%

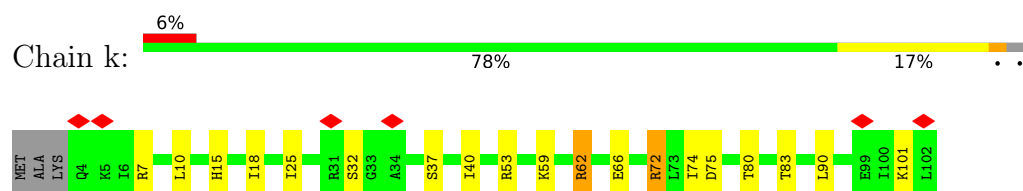


- Molecule 42: 30S ribosomal protein S9

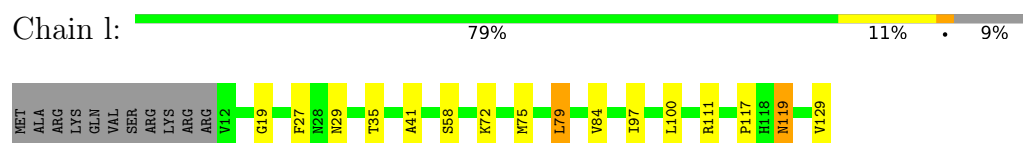
Chain j: 86% 11%



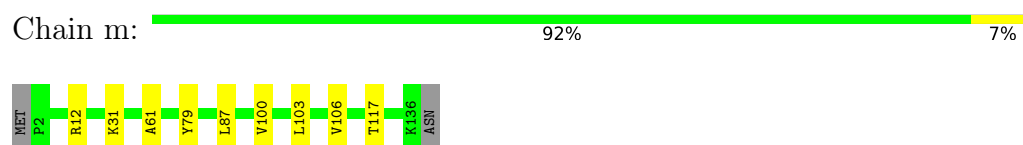
- Molecule 43: Small ribosomal subunit protein uS10



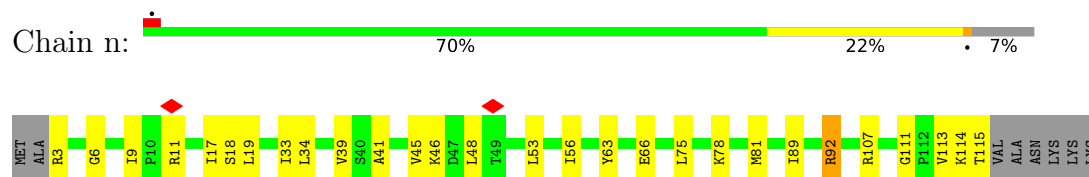
- Molecule 44: 30S ribosomal protein S11



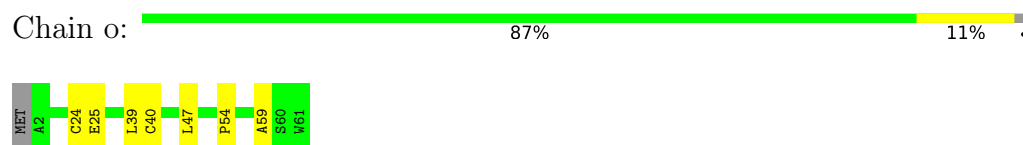
- Molecule 45: 30S ribosomal protein S12



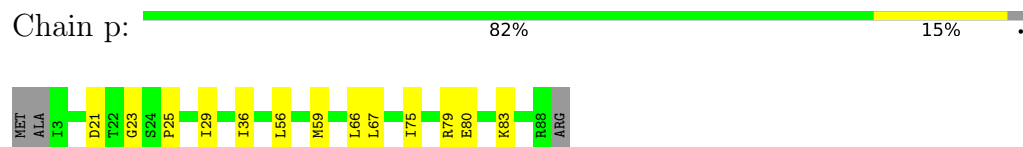
- Molecule 46: 30S ribosomal protein S13



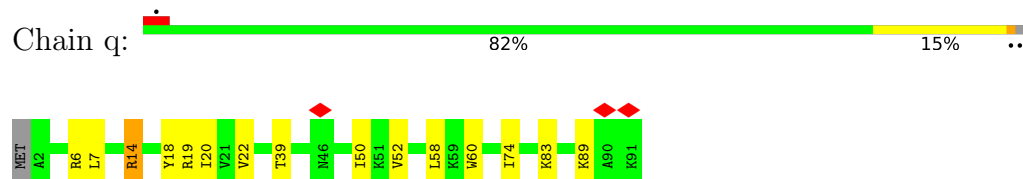
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17

Chain r:  80% 11% 8%



- Molecule 51: 30S ribosomal protein S18

Chain s:  71% 5% 21%



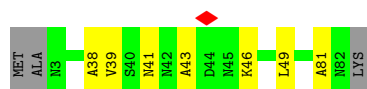
- Molecule 52: 30S ribosomal protein S19

Chain t:  5% 70% 16% 13%



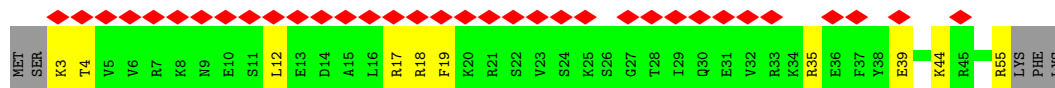
- Molecule 53: 30S ribosomal protein S20

Chain u:  88% 8%



- Molecule 54: 30S ribosomal protein S21

Chain v:  59% 74% 17% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15167	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 ($e^-/\text{\AA}^2$)	28.14	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.665	Depositor
Minimum map value	-0.406	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	436.8, 436.8, 436.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.728, 0.728, 0.728	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 2MG, 4OC, H2U, ZN, 5MU, 5MC, OMG, 3TD, PUT, MG, UR3, 2MA, MA6

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	1	0.47	0/487	0.76	0/649
2	2	0.41	0/536	0.91	0/713
3	3	0.44	0/438	0.86	0/590
4	4	0.47	0/671	0.83	0/900
5	5	0.48	0/429	0.82	0/571
6	6	0.44	0/407	0.79	0/545
7	7	0.48	0/371	0.90	0/484
8	8	0.46	0/526	0.86	0/690
9	9	0.49	0/299	0.77	0/393
10	A	0.52	0/68213	0.79	7/106380 (0.0%)
11	B	0.54	0/2692	0.76	0/4193
12	C	0.44	0/1693	0.86	0/2274
13	D	0.54	0/1832	0.81	1/2855 (0.0%)
13	F	0.55	0/1813	0.80	1/2825 (0.0%)
14	G	0.48	0/2120	0.81	0/2847
15	H	0.47	0/1661	0.80	0/2227
16	I	0.46	0/1587	0.87	0/2143
17	J	0.44	0/1430	0.88	0/1918
18	K	0.46	0/1379	0.83	0/1855
19	M	0.46	0/1168	0.80	0/1573
20	N	0.46	0/927	0.84	0/1243
21	O	0.47	0/1104	0.82	0/1471
22	P	0.46	0/1113	0.81	0/1493
23	Q	0.44	0/956	0.87	0/1277
24	R	0.46	0/931	0.84	0/1244
25	S	0.46	0/934	0.75	0/1249
26	T	0.44	0/955	0.92	0/1265
27	U	0.45	0/803	0.76	0/1073
28	V	0.47	0/861	0.83	0/1159
29	W	0.44	0/733	0.82	0/978
30	X	0.47	0/796	0.82	0/1063
31	Y	0.45	0/746	0.80	0/1000

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.46	0/632	0.80	0/838
33	a	0.53	1/36440 (0.0%)	0.76	1/56820 (0.0%)
34	b	0.55	0/245	0.80	0/380
35	c	0.44	0/1808	0.92	0/2426
36	d	0.45	0/1634	0.83	0/2195
37	e	0.46	0/1647	0.87	0/2211
38	f	0.47	0/1174	0.84	0/1583
39	g	0.43	0/784	0.83	0/1052
40	h	0.45	0/1181	0.93	1/1587 (0.1%)
41	i	0.46	0/1044	0.84	0/1401
42	j	0.47	0/1032	0.86	0/1386
43	k	0.47	0/804	0.87	0/1083
44	l	0.51	0/891	0.85	0/1203
45	m	0.48	0/1075	0.78	0/1439
46	n	0.45	0/909	0.93	0/1218
47	o	0.46	0/511	0.81	0/678
48	p	0.44	0/730	0.90	0/975
49	q	0.48	0/723	0.86	0/971
50	r	0.45	0/670	0.79	0/895
51	s	0.45	0/525	0.91	0/704
52	t	0.47	0/668	0.90	0/896
53	u	0.45	0/606	0.97	0/810
54	v	0.45	0/449	0.95	0/589
All	All	0.51	1/156793 (0.0%)	0.80	11/234480 (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
5	5	0	1
22	P	0	1
26	T	0	1
30	X	0	1
37	e	0	1
39	g	0	1
41	i	0	1
43	k	0	2
45	m	0	1
46	n	0	1
49	q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
50	r	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	535	G7M	O3'-P	5.08	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2078	A	O3'-P-O5'	-6.21	94.69	104.00
10	A	2673	C	O3'-P-O5'	-5.82	95.27	104.00
13	F	58	A	O3'-P-O5'	-5.60	95.59	104.00
10	A	1641	G	O3'-P-O5'	-5.43	95.86	104.00
10	A	480	U	O3'-P-O5'	-5.40	95.90	104.00
13	D	24	U	O3'-P-O5'	-5.33	96.00	104.00
40	h	71	PRO	N-CA-CB	-5.29	97.69	103.25
33	a	1013	A	O3'-P-O5'	-5.25	96.12	104.00
10	A	1275	A	O3'-P-O5'	-5.18	96.23	104.00
10	A	826	A	O3'-P-O5'	-5.15	96.28	104.00
10	A	1065	A	O3'-P-O5'	-5.01	96.48	104.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	5	6	ARG	Sidechain
22	P	56	ARG	Sidechain
26	T	48	ARG	Sidechain
30	X	92	ARG	Sidechain
37	e	105	ARG	Sidechain
39	g	88	ARG	Sidechain
41	i	61	ARG	Sidechain
43	k	62	ARG	Sidechain
43	k	72	ARG	Sidechain
45	m	12	ARG	Sidechain
46	n	92	ARG	Sidechain
49	q	14	ARG	Sidechain
50	r	7	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	1	481	0	523	2	0
2	2	535	0	566	5	0
3	3	436	0	473	5	0
4	4	654	0	631	19	0
5	5	422	0	426	1	0
6	6	402	0	413	4	0
7	7	367	0	415	3	0
8	8	521	0	586	3	0
9	9	296	0	339	0	0
10	A	61064	0	30708	250	0
11	B	2408	0	1218	11	0
12	C	1659	0	1689	20	0
13	D	1640	0	837	11	0
13	F	1623	0	825	5	0
14	G	2085	0	2192	12	0
15	H	1637	0	1680	8	0
16	I	1564	0	1611	13	0
17	J	1412	0	1470	29	0
18	K	1361	0	1392	18	0
19	M	1146	0	1142	10	0
20	N	920	0	981	9	0
21	O	1090	0	1131	1	0
22	P	1089	0	1155	11	0
23	Q	952	0	999	8	0
24	R	922	0	968	6	0
25	S	922	0	994	7	0
26	T	943	0	1014	12	0
27	U	793	0	831	6	0
28	V	853	0	914	11	0
29	W	725	0	761	6	0
30	X	787	0	853	5	0
31	Y	738	0	787	11	0
32	Z	626	0	645	6	0
33	a	32707	0	16479	206	0
34	b	218	0	110	3	0
35	c	1781	0	1844	27	0
36	d	1612	0	1674	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	e	1617	0	1646	14	0
38	f	1160	0	1223	11	0
39	g	773	0	772	9	0
40	h	1165	0	1204	11	0
41	i	1032	0	1082	9	0
42	j	1016	0	1039	8	0
43	k	792	0	833	13	0
44	l	876	0	895	12	0
45	m	1058	0	1130	5	0
46	n	902	0	950	17	0
47	o	501	0	523	5	0
48	p	721	0	751	9	0
49	q	712	0	744	10	0
50	r	662	0	702	6	0
51	s	516	0	548	4	0
52	t	651	0	658	10	0
53	u	606	0	650	4	0
54	v	446	0	487	8	0
55	5	1	0	0	0	0
55	9	1	0	0	0	0
55	C	1	0	0	0	0
55	o	1	0	0	0	0
56	A	119	0	0	0	0
56	F	1	0	0	0	0
56	G	1	0	0	0	0
56	a	24	0	0	0	0
57	A	12	0	24	1	0
All	All	144758	0	97137	853	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 4.

All (853) 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:Y:7:ILE:HD11	31:Y:65:VAL:HA	1.63	0.81
45:m:79:TYR:HB2	45:m:106:VAL:HG11	1.64	0.79
10:A:1571:G:H22	10:A:1593:G:H1	1.29	0.78
33:a:693:G:O2'	33:a:694:U:H5'	1.86	0.76
4:4:12:VAL:HG12	4:4:44:PRO:HG2	1.69	0.74
43:k:10:LEU:HB3	43:k:18:ILE:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:40:THR:HA	32:Z:72:ASP:OD1	1.88	0.73
10:A:942:C:H3'	10:A:943:C:H5''	1.72	0.71
38:f:15:VAL:HG12	38:f:37:VAL:HG22	1.72	0.71
33:a:1191:G:O2'	33:a:1192:G:N7	2.24	0.70
33:a:777:G:H4'	33:a:1524:A:H4'	1.73	0.70
4:4:71:VAL:HG23	52:t:42:PRO:HB3	1.74	0.69
33:a:831:G:HO2'	41:i:2:THR:N	1.89	0.69
23:Q:26:ILE:HD11	23:Q:69:VAL:HG21	1.74	0.69
43:k:80:THR:HB	43:k:83:THR:HG23	1.75	0.68
53:u:39:VAL:HA	53:u:46:LYS:HD3	1.75	0.68
33:a:665:U:H3	33:a:757:A:H62	1.41	0.68
36:d:76:ILE:HA	36:d:83:ILE:HB	1.74	0.68
12:C:13:ILE:HD11	12:C:47:ILE:HG21	1.76	0.68
53:u:39:VAL:HG11	53:u:81:ALA:HB1	1.76	0.67
33:a:1011:U:H2'	33:a:1012:G:C8	2.30	0.67
26:T:91:ASN:OD1	26:T:94:MET:HG2	1.95	0.67
18:K:121:ILE:HG21	18:K:144:LEU:HD12	1.78	0.66
17:J:8:PHE:HA	17:J:12:VAL:HB	1.78	0.66
12:C:154:LYS:HA	12:C:165:ASN:HA	1.78	0.66
33:a:984:A:H4'	33:a:985:G:H5''	1.79	0.65
18:K:16:THR:HG23	18:K:27:LYS:HB2	1.78	0.65
4:4:70:ARG:HG3	52:t:65:ASP:HA	1.79	0.65
33:a:726:A:H5'	44:l:119:ASN:HB2	1.79	0.65
10:A:1513:A:H2'	10:A:1514:A:C8	2.32	0.65
50:r:26:LEU:HD11	50:r:43:SER:HB3	1.78	0.64
14:G:140:VAL:HG13	14:G:161:SER:HB2	1.79	0.64
33:a:759:U:O2'	33:a:760:G:H5'	1.98	0.64
10:A:688:A:N1	10:A:2396:A:O2'	2.29	0.64
33:a:1155:C:H4'	33:a:1156:A:H5'	1.80	0.63
33:a:411:C:H5''	37:e:129:PRO:HD2	1.81	0.63
31:Y:5:LYS:HE3	31:Y:61:ILE:HG21	1.79	0.63
33:a:1122:A:N1	36:d:176:THR:HG22	2.14	0.63
48:p:29:ILE:HD11	48:p:66:LEU:HB2	1.80	0.63
10:A:923:A:N6	10:A:944:G:N7	2.46	0.62
31:Y:73:MET:HB2	31:Y:94:ILE:HD11	1.81	0.62
33:a:923:A:H2'	33:a:924:A:H5''	1.81	0.62
12:C:85:PRO:HA	12:C:115:LYS:HA	1.81	0.62
33:a:68:C:H2'	33:a:69:G:C8	2.35	0.62
10:A:1357:G:C2	10:A:1366:U:H5''	2.35	0.61
10:A:955:A:H2'	10:A:956:A:C8	2.34	0.61
10:A:2339:U:H5'	17:J:85:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:31:LEU:HB2	26:T:34:VAL:HG12	1.84	0.60
10:A:1806:U:H5	10:A:1811:A:N7	2.00	0.59
33:a:413:U:H1'	33:a:506:A:H2'	1.84	0.59
16:I:17:ILE:HD12	16:I:196:GLU:HG3	1.84	0.59
10:A:631:U:H2'	10:A:632:U:C6	2.36	0.59
19:M:18:VAL:HG23	19:M:138:PRO:HB2	1.84	0.59
10:A:921:C:H2'	10:A:922:G:C8	2.38	0.59
49:q:50:ILE:HG21	49:q:74:ILE:HG23	1.85	0.59
10:A:2611:U:H2'	10:A:2612:U:H2'	1.83	0.59
14:G:9:ILE:HG22	14:G:10:THR:HG23	1.85	0.59
10:A:2216:U:H3'	10:A:2217:G:H5''	1.85	0.59
37:e:88:ILE:HG22	37:e:185:LEU:HD11	1.85	0.58
4:4:1:MET:HG2	11:B:41:C:H5''	1.84	0.58
38:f:56:VAL:HG23	38:f:57:PRO:HD3	1.85	0.58
10:A:1100:G:H4'	10:A:1130:A:C8	2.37	0.58
20:N:35:ILE:HG21	20:N:103:ALA:HB3	1.84	0.58
4:4:51:SER:H	4:4:54:SER:HB3	1.68	0.58
10:A:892:U:H5	10:A:977:A:N1	2.01	0.58
10:A:1449:A:H8	10:A:1634:A:H62	1.52	0.58
18:K:9:ILE:HD11	18:K:69:ARG:HG2	1.85	0.58
33:a:444:C:O2'	33:a:445:U:H5'	2.03	0.58
12:C:37:GLN:NE2	12:C:63:MET:O	2.37	0.57
36:d:45:GLU:HG2	36:d:86:LEU:HG	1.86	0.57
50:r:13:LYS:HE3	50:r:58:GLY:HA2	1.85	0.57
33:a:721:G:H2'	33:a:722:G:C8	2.39	0.57
14:G:107:PRO:HD2	14:G:110:LEU:HD22	1.85	0.57
17:J:61:THR:HB	17:J:89:VAL:HG11	1.87	0.57
33:a:219:C:H3'	33:a:220:U:H6	1.69	0.57
10:A:1533:A:H2'	14:G:98:ASP:HB3	1.85	0.57
18:K:8:ILE:HD12	18:K:49:THR:HG21	1.86	0.57
33:a:1289:A:H4'	33:a:1291:U:H5	1.69	0.57
33:a:759:U:C2'	33:a:760:G:H5'	2.35	0.57
10:A:942:C:H3'	10:A:943:C:C5'	2.35	0.57
33:a:1014:C:H5'	33:a:1050:A:O4'	2.05	0.56
33:a:1015:A:H2'	33:a:1016:A:C8	2.40	0.56
33:a:1029:A:H3'	33:a:1030:G:H5''	1.87	0.56
7:7:40:ARG:NH2	10:A:514:G:N7	2.43	0.56
29:W:19:ALA:HB1	29:W:24:LYS:HB2	1.87	0.56
33:a:75:A:OP2	33:a:94:G:N2	2.35	0.56
33:a:199:G:O2'	33:a:200:U:H5'	2.05	0.56
33:a:955:A:H2'	33:a:956:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:117:VAL:HG22	17:J:176:PRO:O	2.06	0.56
38:f:159:LYS:NZ	41:i:42:SER:O	2.35	0.56
33:a:756:A:H1'	33:a:757:A:H2	1.70	0.56
42:j:67:VAL:HG11	42:j:81:ILE:HG12	1.88	0.56
10:A:2776:A:H1'	18:K:63:THR:HG22	1.87	0.56
33:a:99:U:H2'	33:a:100:A:C8	2.41	0.56
36:d:76:ILE:CG2	36:d:102:VAL:HG11	2.36	0.56
22:P:77:LYS:HE2	22:P:78:PRO:HD2	1.88	0.56
16:I:81:PRO:HB3	16:I:89:VAL:HG23	1.87	0.55
46:n:114:LYS:O	46:n:115:THR:C	2.48	0.55
10:A:1756:U:H2'	10:A:1757:U:O4'	2.06	0.55
33:a:1306:C:H4'	33:a:1312:U:O4	2.06	0.55
13:D:16:C:H3'	13:D:17:C:C6	2.42	0.55
22:P:35:GLN:HE22	31:Y:81:PRO:HB2	1.70	0.55
33:a:53:U:H1'	45:m:31:LYS:HE3	1.89	0.55
37:e:15:LEU:HD13	37:e:56:LYS:HA	1.88	0.55
33:a:986:A:H1'	33:a:991:U:O4	2.06	0.55
10:A:351:G:H2'	10:A:352:A:C8	2.41	0.55
10:A:1091:G:N2	10:A:1154:G:O2'	2.40	0.55
10:A:2354:A:H2'	10:A:2355:A:C8	2.41	0.55
40:h:70:MET:HB3	40:h:96:ARG:HG2	1.88	0.55
41:i:121:ARG:HB2	41:i:123:VAL:HG22	1.88	0.55
12:C:123:ASN:HA	12:C:130:LYS:HA	1.87	0.55
5:5:9:SER:HB3	10:A:2047:A:H5'	1.88	0.55
10:A:165:C:H2'	10:A:166:A:H5'	1.87	0.55
49:q:22:VAL:HG21	49:q:60:TRP:CD1	2.42	0.55
38:f:115:LEU:HD13	38:f:123:ILE:HG21	1.89	0.55
6:6:18:ILE:HD13	10:A:2446:U:H5''	1.88	0.55
39:g:31:ALA:HB2	39:g:37:VAL:HG23	1.89	0.55
18:K:9:ILE:HD13	18:K:72:LEU:HD23	1.89	0.54
33:a:464:A:O2'	33:a:465:U:H5'	2.08	0.54
33:a:1247:C:H3'	33:a:1248:A:H5'	1.88	0.54
35:c:162:PHE:HA	35:c:184:VAL:O	2.07	0.54
42:j:52:GLN:N	42:j:53:PRO:HD2	2.23	0.54
51:s:18:PHE:HA	51:s:23:ILE:HG23	1.89	0.54
33:a:1484:G:H2'	33:a:1485:G:C8	2.43	0.54
10:A:194:A:H2'	10:A:195:C:C6	2.42	0.54
33:a:26:C:H5'	33:a:532:G:H1'	1.90	0.54
36:d:34:GLU:HG3	36:d:37:LYS:HE2	1.88	0.54
4:4:14:PHE:HD2	4:4:48:LEU:HD21	1.72	0.54
33:a:756:A:H1'	33:a:757:A:C2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:26:PHE:HA	39:g:29:ILE:HD12	1.90	0.54
23:Q:121:LEU:O	23:Q:122:VAL:HB	2.08	0.54
33:a:18:U:H2'	33:a:19:C:C6	2.42	0.54
46:n:45:VAL:HA	46:n:48:LEU:HD12	1.89	0.54
33:a:765:U:H2'	33:a:766:G:O4'	2.08	0.54
41:i:43:GLU:HG3	41:i:103:ILE:HD13	1.90	0.54
11:B:50:A:O2'	11:B:51:A:OP2	2.26	0.53
13:D:36:U:H2'	13:D:37:A:O4'	2.08	0.53
36:d:8:ILE:HD11	36:d:183:TYR:H	1.73	0.53
26:T:107:ALA:O	26:T:111:THR:HG23	2.08	0.53
10:A:2555:U:H2'	10:A:2557:U:H5''	1.89	0.53
10:A:830:U:H2'	10:A:831:C:C6	2.44	0.53
10:A:1262:U:H4'	27:U:87:GLY:O	2.09	0.53
13:D:21:A:N1	13:D:46:G:H2'	2.24	0.53
10:A:1072:A:N6	10:A:1169:G:H2'	2.24	0.53
10:A:2404:A:H2'	10:A:2405:A:C8	2.44	0.53
33:a:923:A:C2'	33:a:924:A:H5''	2.38	0.53
33:a:1143:C:H2'	33:a:1144:A:C8	2.43	0.53
10:A:285:U:H4'	10:A:286:U:C5	2.43	0.53
10:A:787:U:H2'	10:A:788:A:C8	2.43	0.53
10:A:2294:A:H5''	10:A:2295:A:H5''	1.91	0.53
33:a:262:G:OP1	50:r:72:THR:HG22	2.09	0.53
33:a:390:A:H2'	33:a:391:A:C8	2.44	0.53
10:A:1827:C:OP1	14:G:260:ARG:NH2	2.42	0.52
35:c:66:GLN:HB3	35:c:90:PHE:HE2	1.74	0.52
44:l:84:VAL:HG11	44:l:97:ILE:HG12	1.90	0.52
10:A:29:U:H2'	10:A:30:G:C8	2.45	0.52
10:A:2758:G:H2'	10:A:2759:G:C8	2.44	0.52
7:7:2:VAL:N	10:A:1663:G:HO2'	2.07	0.52
33:a:1391:U:O2'	33:a:1392:C:H5'	2.10	0.52
18:K:23:HIS:HA	18:K:36:THR:HA	1.91	0.52
33:a:491:C:O2'	49:q:14:ARG:NH2	2.43	0.52
39:g:62:ILE:HD13	51:s:29:LYS:HD2	1.92	0.52
33:a:384:G:H5''	49:q:6:ARG:HB2	1.92	0.52
33:a:1184:G:O2'	33:a:1185:G:H5'	2.10	0.52
17:J:59:LEU:HB3	17:J:140:GLU:HG2	1.91	0.52
18:K:164:TYR:HB2	18:K:167:GLU:HB2	1.92	0.52
41:i:89:ALA:HB2	41:i:127:ILE:HD11	1.90	0.52
44:l:97:ILE:HG22	54:v:12:LEU:HD11	1.92	0.52
10:A:1880:A:H2'	10:A:1881:A:C8	2.45	0.51
24:R:78:GLU:HG3	24:R:111:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2683:U:H3	10:A:2692:A:H2	1.57	0.51
33:a:1097:U:H3	33:a:1110:G:H22	1.59	0.51
19:M:76:TYR:HB3	19:M:85:ILE:HD11	1.93	0.51
23:Q:101:THR:HG22	23:Q:121:LEU:HD23	1.92	0.51
33:a:1388:C:OP2	40:h:3:ARG:NH2	2.43	0.51
35:c:131:LYS:O	35:c:134:VAL:HG22	2.10	0.51
40:h:27:ILE:HG13	40:h:43:LEU:HD23	1.91	0.51
11:B:10:U:H3'	11:B:11:A:H5''	1.93	0.51
19:M:7:ALA:HB1	19:M:12:ILE:HD11	1.93	0.51
36:d:137:ILE:O	36:d:141:MET:HG2	2.11	0.51
17:J:80:ARG:HB3	17:J:83:MET:HG3	1.93	0.51
33:a:1366:G:H2'	33:a:1367:A:C8	2.46	0.51
33:a:1477:C:H2'	33:a:1478:G:O4'	2.10	0.51
40:h:113:GLU:HB2	40:h:119:ARG:HG2	1.92	0.51
36:d:62:ARG:HG2	36:d:97:LYS:HB2	1.92	0.51
32:Z:92:VAL:O	32:Z:93:ALA:C	2.53	0.51
37:e:101:LEU:HD21	37:e:165:LEU:HD22	1.93	0.51
10:A:903:G:N3	10:A:2295:A:H2'	2.25	0.51
33:a:343:C:H2'	33:a:344:A:C8	2.46	0.51
47:o:39:LEU:HD13	47:o:47:LEU:HD12	1.93	0.51
10:A:684:U:H2'	10:A:685:C:C6	2.46	0.51
36:d:50:SER:HB3	36:d:114:LEU:HD22	1.92	0.51
42:j:90:LEU:HD21	42:j:97:ARG:HA	1.92	0.51
42:j:77:GLN:O	42:j:81:ILE:HG13	2.11	0.50
10:A:2109:A:H2'	10:A:2110:G:O4'	2.11	0.50
19:M:46:THR:HB	19:M:49:VAL:HG22	1.92	0.50
22:P:104:PHE:HE1	22:P:125:LEU:HD11	1.76	0.50
33:a:1508:G:H1'	33:a:1529:MA6:H2	1.92	0.50
10:A:751:A:H2'	10:A:752:G:O4'	2.11	0.50
10:A:2672:G:H4'	10:A:2759:G:O2'	2.11	0.50
36:d:109:ASP:HB2	36:d:143:LEU:HD12	1.93	0.50
37:e:83:GLY:HA3	37:e:191:GLU:HB2	1.92	0.50
37:e:101:LEU:HD22	37:e:167:PHE:HB2	1.93	0.50
10:A:1238:U:H1'	26:T:4:VAL:HG22	1.92	0.50
35:c:126:PHE:CZ	35:c:134:VAL:HB	2.46	0.50
6:6:1:MET:HG2	10:A:2312:C:C5	2.47	0.50
10:A:12:U:O2	10:A:12:U:H2'	2.10	0.50
10:A:651:A:H2'	10:A:652:A:C8	2.47	0.50
3:3:6:ILE:HG23	3:3:56:VAL:HG22	1.93	0.50
10:A:120:G:H4'	10:A:150:A:H5'	1.93	0.50
10:A:539:G:H4'	28:V:6:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2335:G:N3	10:A:2335:G:H2'	2.25	0.50
33:a:1312:U:C5	46:n:17:ILE:HG13	2.47	0.50
33:a:429:U:H5'	33:a:430:C:H5	1.77	0.50
43:k:15:HIS:O	43:k:18:ILE:HG22	2.11	0.50
46:n:39:VAL:HG11	46:n:56:ILE:HD11	1.94	0.50
4:4:13:ILE:HG13	4:4:43:TYR:HB2	1.92	0.50
10:A:250:G:H4'	10:A:432:G:C5	2.47	0.50
11:B:3:U:H2'	11:B:4:G:C8	2.47	0.50
20:N:90:ASP:O	20:N:91:LYS:HB2	2.12	0.50
28:V:14:PRO:HG2	28:V:78:GLU:HG2	1.92	0.50
38:f:153:VAL:HG21	41:i:101:LEU:HD23	1.94	0.50
48:p:29:ILE:HD12	48:p:67:LEU:HG	1.94	0.50
12:C:144:LEU:HB2	12:C:171:LYS:HE3	1.94	0.49
23:Q:20:LEU:HB3	23:Q:40:VAL:HG21	1.93	0.49
29:W:30:ASP:HB3	29:W:33:VAL:HG13	1.94	0.49
33:a:9:A:C5	37:e:200:ARG:HB3	2.47	0.49
33:a:1141:A:O2'	33:a:1142:U:H5'	2.12	0.49
33:a:1238:C:H5'	46:n:113:VAL:HG13	1.92	0.49
10:A:1352:C:O2'	10:A:1429:G:N3	2.45	0.49
33:a:112:G:N3	33:a:361:A:O2'	2.44	0.49
33:a:137:U:O2'	33:a:138:A:H5'	2.12	0.49
30:X:12:ILE:HG12	30:X:67:ASN:O	2.12	0.49
33:a:39:G:H22	33:a:405:A:H5'	1.76	0.49
33:a:1222:U:H5'	33:a:1223:A:C8	2.48	0.49
10:A:2209:G:H2'	10:A:2210:C:O4'	2.13	0.49
15:H:15:VAL:HG21	15:H:186:VAL:HG11	1.93	0.49
10:A:575:G:N3	10:A:575:G:H2'	2.27	0.49
10:A:1836:A:H2'	10:A:1837:A:C8	2.48	0.49
32:Z:80:LYS:O	32:Z:84:LYS:HB2	2.12	0.49
10:A:522:G:H4'	10:A:547:A:N1	2.27	0.49
12:C:117:SER:HA	12:C:196:ASN:HB3	1.94	0.49
33:a:78:A:N3	33:a:78:A:H2'	2.27	0.49
52:t:11:VAL:HG21	52:t:16:MET:HE2	1.95	0.49
14:G:144:ILE:HD11	14:G:162:ALA:HB3	1.94	0.49
10:A:12:U:O2	10:A:12:U:C2'	2.60	0.49
10:A:2268:A:H2'	10:A:2269:G:C8	2.48	0.49
10:A:2372:G:N3	10:A:2408:C:H2'	2.28	0.49
15:H:131:ILE:HD12	15:H:149:ARG:HA	1.95	0.49
29:W:30:ASP:O	29:W:33:VAL:HG22	2.13	0.49
2:2:26:PHE:CG	29:W:4:ARG:HD2	2.48	0.49
4:4:2:LYS:HE3	11:B:38:U:H2'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:156:PHE:HA	12:C:163:GLU:HA	1.94	0.49
6:6:17:TYR:CE2	6:6:34:LYS:HB3	2.47	0.49
10:A:1115:G:H2'	10:A:1116:C:C6	2.48	0.49
10:A:2355:A:H2'	10:A:2356:A:C8	2.48	0.49
15:H:131:ILE:CD1	15:H:149:ARG:HA	2.43	0.49
33:a:1422:C:H2'	33:a:1423:A:C8	2.48	0.49
36:d:34:GLU:HG2	36:d:58:ARG:HH22	1.77	0.49
40:h:75:VAL:HB	40:h:86:GLN:HB3	1.94	0.49
17:J:29:PRO:HB3	17:J:160:ALA:HB2	1.94	0.48
31:Y:32:TYR:HE2	31:Y:90:ASP:HB3	1.78	0.48
33:a:1497:G:H2'	33:a:1498:G:C8	2.48	0.48
35:c:58:LYS:HE2	35:c:223:GLU:HB3	1.95	0.48
10:A:1959:A:H2'	10:A:1960:G:O4'	2.13	0.48
2:2:1:MET:HE3	2:2:6:ILE:HG12	1.94	0.48
4:4:78:PHE:CD2	52:t:9:PRO:HG3	2.49	0.48
10:A:1675:G:H1'	10:A:1679:A:N6	2.28	0.48
18:K:125:VAL:HG22	18:K:131:VAL:HG22	1.95	0.48
10:A:1766:C:H2'	10:A:1767:G:O4'	2.13	0.48
28:V:3:ALA:HB1	28:V:57:ASN:OD1	2.14	0.48
31:Y:65:VAL:HB	31:Y:70:ILE:HD13	1.96	0.48
38:f:77:VAL:O	38:f:80:THR:HG22	2.13	0.48
46:n:89:ILE:HG12	46:n:92:ARG:NH2	2.28	0.48
52:t:2:ALA:HB3	52:t:7:LYS:HD2	1.95	0.48
54:v:39:GLU:HG3	54:v:44:LYS:HG2	1.94	0.48
12:C:157:CYS:HB2	12:C:166:VAL:HG11	1.96	0.48
22:P:40:SER:HB3	22:P:127:VAL:HG13	1.95	0.48
33:a:1002:G:H2'	33:a:1004:C:H41	1.78	0.48
33:a:1228:U:H2'	33:a:1229:U:C6	2.47	0.48
36:d:63:ILE:HG22	36:d:65:ILE:HG13	1.95	0.48
10:A:858:U:H2'	10:A:859:C:C6	2.49	0.48
17:J:38:MET:HE2	17:J:57:LEU:HB2	1.94	0.48
33:a:1107:C:O2'	33:a:1108:C:H5'	2.14	0.48
33:a:1312:U:C6	46:n:17:ILE:HG21	2.49	0.48
36:d:69:THR:HG21	36:d:75:VAL:HG11	1.96	0.48
10:A:1038:C:OP1	26:T:53:ARG:NH2	2.47	0.48
22:P:34:LEU:HB2	22:P:118:LEU:HD22	1.96	0.48
41:i:21:ARG:NH1	41:i:70:ASP:O	2.47	0.48
44:l:117:PRO:HG2	54:v:35:ARG:HH11	1.78	0.48
48:p:36:ILE:HG23	48:p:56:LEU:HD11	1.94	0.48
10:A:1939:A:N1	33:a:1417:C:O2'	2.44	0.48
35:c:27:MET:HG2	35:c:193:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:90:LEU:HB3	36:d:98:VAL:HG11	1.95	0.48
12:C:111:GLU:O	12:C:115:LYS:HG3	2.14	0.48
36:d:149:LYS:HB3	36:d:200:TRP:HB2	1.96	0.48
48:p:75:ILE:HG22	48:p:79:ARG:HE	1.79	0.48
10:A:305:A:N6	10:A:410:G:H22	2.12	0.47
20:N:76:TYR:HB2	25:S:75:THR:HB	1.96	0.47
33:a:507:A:H4'	33:a:508:G:H5'	1.95	0.47
33:a:627:U:H5	37:e:127:ASP:HB3	1.78	0.47
33:a:672:G:H22	33:a:749:G:H1	1.62	0.47
13:F:58:A:O2'	13:F:60:U:OP2	2.26	0.47
33:a:86:G:H1'	33:a:87:C:C6	2.50	0.47
33:a:757:A:H2'	33:a:758:C:O4'	2.14	0.47
36:d:33:HIS:NE2	47:o:25:GLU:HB2	2.30	0.47
10:A:725:A:OP1	10:A:821:C:N4	2.46	0.47
10:A:1039:C:O2'	26:T:93:LYS:NZ	2.46	0.47
10:A:2048:G:H2'	10:A:2048:G:N3	2.30	0.47
16:I:148:GLN:HB3	16:I:152:VAL:HG21	1.95	0.47
8:8:15:LYS:HE3	10:A:676:A:H5''	1.97	0.47
10:A:2386:C:H2'	10:A:2387:A:C8	2.49	0.47
33:a:221:U:H4'	33:a:222:G:O5'	2.14	0.47
44:l:35:THR:HG22	44:l:41:ALA:HA	1.96	0.47
54:v:4:THR:HG21	54:v:19:PHE:HA	1.97	0.47
18:K:28:GLY:HA3	18:K:79:VAL:HB	1.97	0.47
33:a:1401:U:H2'	33:a:1402:G:C8	2.50	0.47
35:c:157:MET:HE2	35:c:157:MET:HA	1.95	0.47
10:A:2332:U:H5''	17:J:131:GLY:HA3	1.97	0.47
10:A:2785:A:C2	18:K:71:LEU:HD11	2.49	0.47
20:N:15:GLY:HA3	20:N:50:GLY:HA3	1.96	0.47
25:S:10:VAL:HG23	25:S:11:THR:HG23	1.97	0.47
33:a:694:U:O4	33:a:711:G:H1'	2.14	0.47
33:a:711:G:H4'	33:a:712:A:H5'	1.96	0.47
10:A:84:A:N1	10:A:98:U:O2'	2.42	0.47
10:A:618:A:OP2	10:A:2526:C:O2'	2.33	0.47
10:A:1312:A:N1	10:A:1332:C:O2'	2.47	0.47
33:a:1265:G:H2'	33:a:1289:A:H61	1.79	0.47
53:u:38:ALA:HB2	53:u:49:LEU:HD12	1.97	0.47
4:4:11:GLN:HB3	4:4:24:LEU:HD11	1.96	0.47
10:A:1222:A:H2'	10:A:1223:A:C8	2.50	0.47
10:A:1658:A:C2	28:V:93:ALA:HB2	2.50	0.47
28:V:10:ILE:HG21	28:V:46:VAL:HG11	1.97	0.47
33:a:307:G:H2'	33:a:308:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1386:U:O2'	33:a:1387:A:H5'	2.15	0.47
10:A:1764:A:H2'	10:A:1765:A:O4'	2.15	0.47
33:a:1151:U:H2'	33:a:1152:G:H8	1.80	0.47
35:c:97:LEU:HD12	35:c:148:LEU:HD21	1.97	0.47
37:e:182:ARG:HA	37:e:185:LEU:HD12	1.96	0.47
4:4:31:SER:HB2	4:4:46:ILE:HD13	1.96	0.46
10:A:2687:A:H2'	10:A:2688:G:O4'	2.15	0.46
12:C:4:MET:HA	12:C:82:TYR:O	2.15	0.46
33:a:32:G:H3'	33:a:33:A:H5''	1.97	0.46
33:a:1172:C:H2'	33:a:1173:G:H8	1.80	0.46
36:d:107:LYS:HB3	36:d:143:LEU:HD13	1.97	0.46
10:A:2300:A:H2'	10:A:2301:A:C8	2.50	0.46
10:A:2777:A:H1'	10:A:2779:C:N4	2.29	0.46
11:B:92:C:H2'	11:B:93:G:C8	2.50	0.46
33:a:744:U:H2'	33:a:745:U:C6	2.50	0.46
33:a:1286:G:H2'	33:a:1287:C:O4'	2.15	0.46
10:A:83:G:N2	10:A:101:G:H1'	2.30	0.46
10:A:992:A:H1'	10:A:1028:G:C8	2.50	0.46
10:A:285:U:H3'	10:A:287:G:H8	1.80	0.46
10:A:878:C:H2'	10:A:879:U:C6	2.50	0.46
10:A:2265:G:N3	10:A:2265:G:H2'	2.30	0.46
10:A:2439:A:H2'	10:A:2440:G:O4'	2.15	0.46
10:A:2664:U:H2'	10:A:2665:G:O4'	2.14	0.46
18:K:86:VAL:HG13	18:K:130:VAL:HG13	1.97	0.46
39:g:29:ILE:HD13	39:g:79:LEU:HD12	1.98	0.46
45:m:100:VAL:HG12	45:m:103:LEU:H	1.81	0.46
2:2:1:MET:HE1	2:2:17:GLN:HG2	1.98	0.46
10:A:365:A:OP1	16:I:168:ARG:HD2	2.15	0.46
10:A:2064:A:H2'	10:A:2065:G:C8	2.50	0.46
13:D:71:C:H2'	13:D:72:A:C8	2.51	0.46
33:a:1186:A:H2'	33:a:1187:G:C8	2.50	0.46
10:A:2774:G:O6	10:A:2782:C:H5''	2.16	0.46
16:I:200:LYS:O	16:I:204:GLU:HG3	2.16	0.46
33:a:1002:G:H2'	33:a:1002:G:N3	2.31	0.46
53:u:41:ASN:HD22	53:u:43:ALA:HB2	1.80	0.46
1:1:14:THR:HG21	10:A:192:G:OP2	2.15	0.46
19:M:126:TYR:OH	19:M:133:HIS:NE2	2.44	0.46
30:X:70:LEU:HD11	30:X:92:ARG:NH2	2.30	0.46
46:n:33:ILE:HG22	46:n:63:TYR:CE1	2.51	0.46
49:q:7:LEU:HB3	49:q:18:TYR:HB3	1.98	0.46
3:3:20:ARG:HH22	10:A:1014:U:P	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:83:G:H21	10:A:102:A:H2	1.62	0.46
10:A:922:G:H22	10:A:944:G:P	2.38	0.46
33:a:641:U:H2'	33:a:641:U:O2	2.16	0.46
44:l:19:GLY:HA3	44:l:79:LEU:HD11	1.98	0.46
33:a:1509:UR3:H6	33:a:1509:UR3:O5'	2.16	0.46
10:A:2050:A:H5'	10:A:2644:C:H4'	1.98	0.46
17:J:80:ARG:H	17:J:83:MET:HE2	1.80	0.46
33:a:986:A:H2'	33:a:987:A:H5''	1.98	0.46
36:d:119:ILE:O	36:d:123:LEU:HG	2.16	0.46
4:4:70:ARG:HA	4:4:73:ARG:HG2	1.98	0.45
10:A:1897:U:H2'	10:A:1898:C:C6	2.51	0.45
10:A:1979:A:C2	20:N:22:ILE:HG23	2.50	0.45
27:U:14:VAL:HB	27:U:97:ILE:HG13	1.98	0.45
33:a:1260:A:O3'	42:j:71:GLY:HA2	2.16	0.45
33:a:343:C:H2'	33:a:344:A:H8	1.81	0.45
39:g:11:ARG:HG3	39:g:14:ILE:HB	1.97	0.45
40:h:87:VAL:HG23	40:h:152:ALA:HA	1.98	0.45
44:l:111:ARG:HD3	54:v:3:LYS:HE2	1.98	0.45
10:A:1072:A:N3	10:A:2513:G:O2'	2.45	0.45
14:G:227:PRO:HG3	14:G:234:GLY:HA3	1.98	0.45
37:e:98:VAL:HG13	37:e:103:LEU:HB2	1.98	0.45
45:m:87:LEU:HD21	45:m:117:THR:HA	1.97	0.45
10:A:1473:G:H2'	10:A:1474:C:C6	2.51	0.45
13:D:71:C:H2'	13:D:72:A:H8	1.81	0.45
15:H:159:ASP:O	15:H:160:ALA:HB3	2.16	0.45
17:J:22:TYR:CE2	17:J:29:PRO:HD3	2.51	0.45
33:a:1135:G:H1'	33:a:1136:U:H5	1.81	0.45
10:A:1809:C:H1'	10:A:2636:U:H5''	1.99	0.45
10:A:1954:A:H2'	10:A:1955:A:C8	2.51	0.45
11:B:64:A:N6	11:B:104:A:H2'	2.31	0.45
16:I:77:THR:HG23	16:I:80:ALA:HB2	1.99	0.45
17:J:16:LEU:HD13	17:J:29:PRO:HD2	1.99	0.45
30:X:1:MET:HE1	30:X:26:THR:HB	1.98	0.45
30:X:84:LYS:HE2	30:X:93:ILE:HG13	1.98	0.45
33:a:305:G:H4'	33:a:565:G:H4'	1.99	0.45
33:a:1008:C:H2'	33:a:1009:U:C6	2.51	0.45
33:a:1033:U:C2	33:a:1034:U:H5	2.35	0.45
37:e:145:SER:HA	37:e:148:LEU:HG	1.98	0.45
10:A:1630:A:H1'	10:A:1631:G:H1'	1.98	0.45
18:K:89:LEU:HG	18:K:162:ILE:HG12	1.98	0.45
33:a:736:A:H2'	33:a:737:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:166:PRO:HG2	35:c:191:CYS:HB3	1.99	0.45
10:A:1044:A:H2'	10:A:1045:A:C8	2.52	0.45
10:A:2298:G:OP1	32:Z:26:SER:HB3	2.17	0.45
17:J:135:GLN:HG3	17:J:150:ARG:O	2.16	0.45
33:a:505:A:N3	33:a:505:A:H2'	2.31	0.45
33:a:681:G:H2'	33:a:682:G:C8	2.52	0.45
40:h:63:GLU:O	40:h:67:ASN:ND2	2.49	0.45
44:l:117:PRO:HD2	54:v:35:ARG:HD3	1.98	0.45
10:A:735:C:H2'	10:A:736:C:O4'	2.17	0.45
13:D:14:A:N1	13:D:21:A:O2'	2.50	0.45
33:a:147:G:H2'	33:a:148:G:C8	2.52	0.45
50:r:47:LYS:HG3	50:r:72:THR:HG23	1.99	0.45
54:v:17:ARG:NH2	54:v:18:ARG:HG2	2.31	0.45
10:A:852:U:O2	16:I:74:ARG:NH2	2.46	0.45
10:A:901:G:H2'	10:A:902:A:C8	2.52	0.45
23:Q:40:VAL:HG12	23:Q:119:ILE:HD13	1.98	0.45
10:A:287:G:H2'	10:A:287:G:N3	2.32	0.45
10:A:579:U:H2'	10:A:580:C:C6	2.52	0.45
10:A:1174:U:O2	10:A:2052:C:H5''	2.17	0.45
14:G:165:LEU:HD11	14:G:175:ARG:HB2	1.98	0.45
17:J:128:TYR:CE2	17:J:130:LEU:HB2	2.52	0.45
33:a:1085:G:O2'	33:a:1112:A:N1	2.46	0.45
44:l:72:LYS:HA	44:l:75:MET:HE2	1.99	0.45
46:n:81:MET:HE3	46:n:92:ARG:HG2	1.99	0.45
10:A:2253:C:H2'	10:A:2254:A:O4'	2.17	0.44
12:C:166:VAL:CG2	12:C:187:TYR:HB3	2.46	0.44
19:M:60:ALA:HB3	19:M:127:GLY:HA2	1.99	0.44
33:a:199:G:H2'	33:a:200:U:O4'	2.17	0.44
33:a:924:A:H8	33:a:924:A:H5'	1.82	0.44
10:A:91:A:H8	10:A:92:G:C8	2.35	0.44
33:a:1176:G:C3'	33:a:1177:A:H5''	2.47	0.44
33:a:1278:G:H2'	33:a:1279:A:C8	2.52	0.44
10:A:538:G:H2'	10:A:539:G:O4'	2.17	0.44
10:A:1450:A:N1	10:A:1633:A:H8	2.15	0.44
10:A:1582:U:O2'	10:A:1583:G:O5'	2.35	0.44
10:A:1592:A:H2'	10:A:1593:G:C8	2.52	0.44
11:B:61:C:H2'	11:B:62:U:C6	2.52	0.44
11:B:110:C:H4'	24:R:51:VAL:HG12	1.99	0.44
19:M:1:MET:O	26:T:93:LYS:NZ	2.33	0.44
33:a:1411:G:H2'	33:a:1412:4OC:O4'	2.18	0.44
43:k:59:LYS:HE2	43:k:62:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2783:U:H1'	10:A:2784:A:H5''	1.99	0.44
10:A:2912:A:H4'	10:A:2913:G:N3	2.32	0.44
20:N:104:ARG:HG2	20:N:121:VAL:HG12	1.99	0.44
26:T:78:ARG:HA	26:T:78:ARG:HD3	1.74	0.44
33:a:681:G:O3'	39:g:88:ARG:NH2	2.51	0.44
3:3:52:HIS:CD2	3:3:53:LEU:HG	2.52	0.44
10:A:283:G:H3'	10:A:284:C:C5'	2.48	0.44
10:A:363:A:H4'	10:A:365:A:C8	2.53	0.44
20:N:100:GLY:HA2	25:S:68:SER:HB2	2.00	0.44
33:a:591:A:H2'	33:a:592:G:O4'	2.18	0.44
33:a:1103:A:H2'	33:a:1104:A:C8	2.52	0.44
42:j:56:VAL:HG12	42:j:99:SER:HB3	1.99	0.44
10:A:629:A:N1	10:A:854:G:O2'	2.44	0.44
23:Q:44:VAL:O	23:Q:48:ILE:HG12	2.18	0.44
33:a:290:A:H2'	33:a:290:A:N3	2.32	0.44
33:a:429:U:H5'	33:a:430:C:C5	2.52	0.44
33:a:1036:C:O2	33:a:1036:C:H2'	2.17	0.44
38:f:56:VAL:N	38:f:57:PRO:CD	2.81	0.44
46:n:107:ARG:O	46:n:111:GLY:N	2.51	0.44
10:A:1964:A:H1'	10:A:1966:5MU:H72	1.99	0.44
33:a:171:A:H2'	33:a:172:A:C8	2.53	0.44
33:a:436:G:H5''	37:e:10:LYS:HG3	2.00	0.44
33:a:532:G:H2'	33:a:533:C:C6	2.52	0.44
35:c:117:ILE:HG21	35:c:141:TYR:HB2	1.99	0.44
49:q:19:ARG:HG2	49:q:39:THR:HG22	2.00	0.44
4:4:16:ASP:O	4:4:20:ASN:N	2.51	0.44
10:A:2052:C:H2'	10:A:2053:U:C6	2.53	0.44
10:A:2101:U:H2'	10:A:2102:U:C6	2.53	0.44
17:J:12:VAL:HG22	17:J:172:ASN:HB3	2.00	0.44
33:a:489:G:O2'	33:a:491:C:N4	2.48	0.44
33:a:1046:G:H4'	33:a:1047:A:H5'	1.99	0.44
10:A:873:U:H4'	10:A:876:G:N1	2.33	0.44
10:A:926:G:H2'	10:A:926:G:N3	2.32	0.44
10:A:1115:G:H1'	10:A:1133:G:H2'	2.00	0.44
10:A:2594:G:H2'	10:A:2595:C:C6	2.53	0.44
12:C:124:GLU:O	12:C:125:LEU:HB3	2.17	0.44
17:J:135:GLN:HE22	17:J:146:VAL:HG11	1.83	0.44
22:P:118:LEU:HD12	22:P:131:PHE:CD1	2.53	0.44
33:a:1385:A:H2'	33:a:1386:U:O4'	2.18	0.44
35:c:100:LEU:HA	35:c:107:ILE:HG13	1.99	0.44
46:n:9:ILE:HB	46:n:18:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:221:G:H22	10:A:238:U:H4'	1.82	0.43
10:A:928:C:H2'	10:A:929:C:C6	2.53	0.43
10:A:1617:A:H2'	10:A:1618:A:C8	2.53	0.43
17:J:158:THR:HG22	17:J:160:ALA:H	1.83	0.43
33:a:697:C:OP1	44:l:29:ASN:ND2	2.51	0.43
40:h:51:GLU:HB2	40:h:58:ALA:HB2	2.00	0.43
50:r:32:THR:HA	50:r:39:ARG:HA	2.00	0.43
10:A:577:A:H4'	10:A:578:G:C8	2.52	0.43
10:A:748:U:H2'	10:A:749:G:O4'	2.18	0.43
10:A:774:G:C6	14:G:207:LYS:HB2	2.53	0.43
10:A:1966:5MU:OP1	10:A:2631:U:O2'	2.36	0.43
13:D:21:A:H61	13:D:46:G:H3'	1.83	0.43
25:S:102:LEU:HD21	25:S:112:ILE:HD11	1.99	0.43
33:a:351:U:H2'	33:a:353:C:C5	2.53	0.43
42:j:41:LEU:HA	42:j:42:PRO:HD3	1.88	0.43
43:k:25:ILE:HG22	43:k:90:LEU:HD23	2.00	0.43
48:p:25:PRO:O	48:p:29:ILE:HG12	2.18	0.43
10:A:1697:G:C6	23:Q:5:LYS:HB2	2.53	0.43
10:A:2494:C:H2'	10:A:2495:A:O4'	2.18	0.43
17:J:103:LEU:HA	17:J:107:SER:HB3	2.00	0.43
33:a:602:U:H2'	33:a:603:A:O4'	2.17	0.43
33:a:1168:C:C5	33:a:1170:G:H1'	2.53	0.43
43:k:7:ARG:HB2	43:k:101:LYS:HB2	2.00	0.43
4:4:55:HIS:NE2	17:J:114:PHE:HB3	2.34	0.43
10:A:2391:C:H4'	32:Z:64:ASP:OD1	2.19	0.43
11:B:111:C:O2'	24:R:55:GLN:HG3	2.17	0.43
35:c:66:GLN:HB3	35:c:90:PHE:CE2	2.52	0.43
2:2:6:ILE:HD12	2:2:52:ARG:HB3	2.00	0.43
10:A:2778:G:N3	10:A:2778:G:H2'	2.34	0.43
12:C:168:LEU:HA	12:C:187:TYR:HA	1.99	0.43
33:a:9:A:N6	37:e:196:GLU:O	2.50	0.43
33:a:1031:C:H2'	33:a:1032:C:C6	2.52	0.43
10:A:398:C:H2'	10:A:399:U:O4'	2.19	0.43
10:A:877:G:N3	21:O:52:GLY:HA3	2.34	0.43
10:A:2348:G:H3'	10:A:2348:G:N3	2.33	0.43
12:C:6:TYR:HB2	12:C:9:GLN:HG3	2.00	0.43
14:G:133:GLN:HB3	14:G:186:SER:HB2	1.99	0.43
17:J:43:ALA:HA	17:J:46:ASN:O	2.18	0.43
33:a:212:A:H4'	33:a:213:G:OP1	2.19	0.43
33:a:1191:G:O2'	33:a:1192:G:C8	2.66	0.43
34:b:19:G:HO2'	34:b:20:C:P	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:54:TYR:CD2	35:c:220:ALA:HB2	2.54	0.43
35:c:68:LEU:HB3	35:c:161:LEU:HD12	1.99	0.43
46:n:19:LEU:HD13	46:n:33:ILE:HD11	2.00	0.43
48:p:29:ILE:HD11	48:p:66:LEU:CB	2.46	0.43
10:A:702:U:H2'	10:A:703:A:C8	2.54	0.43
10:A:1732:U:O2	10:A:1744:A:H8	2.01	0.43
13:D:47:U:H5'	13:D:48:C:H5'	2.01	0.43
17:J:112:ARG:NH2	46:n:66:GLU:OE1	2.51	0.43
20:N:15:GLY:HA2	20:N:47:THR:HG23	2.01	0.43
33:a:76:C:H2'	33:a:77:G:O4'	2.19	0.43
33:a:755:U:H2'	33:a:756:A:O4'	2.18	0.43
33:a:1514:A:N6	33:a:1543:U:H1'	2.33	0.43
10:A:2051:C:H2'	10:A:2052:C:C6	2.54	0.43
26:T:105:ALA:HB1	27:U:40:PHE:HZ	1.84	0.43
10:A:226:A:N1	10:A:453:G:O2'	2.43	0.43
10:A:537:A:H2'	10:A:538:G:O4'	2.19	0.43
10:A:2705:U:H2'	10:A:2706:A:C8	2.54	0.43
33:a:722:G:H2'	33:a:723:A:C8	2.53	0.43
33:a:985:G:H5'	33:a:1368:U:O2'	2.19	0.43
33:a:1267:A:H4'	33:a:1268:G:H5'	2.01	0.43
8:8:16:ARG:NH2	8:8:62:LEU:O	2.52	0.43
10:A:460:C:H2'	10:A:461:A:C8	2.54	0.43
10:A:2535:G:O6	57:A:3102:PUT:N2	2.51	0.43
33:a:272:C:H2'	33:a:273:G:O4'	2.19	0.43
33:a:1071:U:H5''	43:k:53:ARG:HG2	2.01	0.43
35:c:104:TYR:O	35:c:108:SER:N	2.43	0.43
36:d:90:LEU:HD12	36:d:93:LEU:HD12	2.00	0.43
4:4:35:MET:HB2	4:4:45:VAL:HG21	2.00	0.42
10:A:259:A:H2'	10:A:260:A:C8	2.54	0.42
10:A:1312:A:N3	10:A:1313:G:H1'	2.33	0.42
10:A:2098:A:H2'	10:A:2099:G:C8	2.54	0.42
20:N:115:VAL:HG13	20:N:121:VAL:HG21	2.00	0.42
25:S:60:THR:HG22	25:S:77:PRO:HA	2.00	0.42
33:a:75:A:H2'	33:a:75:A:N3	2.34	0.42
33:a:75:A:N6	33:a:94:G:O2'	2.52	0.42
33:a:310:G:N3	33:a:564:C:H4'	2.34	0.42
33:a:917:A:H2'	33:a:918:A:C8	2.53	0.42
39:g:9:ILE:HD12	39:g:88:ARG:HB2	2.01	0.42
10:A:525:A:H1'	10:A:526:A:H5''	2.00	0.42
10:A:892:U:C5	10:A:977:A:N1	2.85	0.42
10:A:1155:A:H1'	10:A:1156:G:H1'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1306:A:H2'	10:A:1307:G:O4'	2.19	0.42
10:A:2642:U:H2'	10:A:2643:C:C6	2.54	0.42
11:B:60:C:O2'	11:B:61:C:H5'	2.19	0.42
24:R:30:ARG:NH1	24:R:32:ASN:HD22	2.17	0.42
25:S:2:THR:OG1	25:S:3:ASN:O	2.37	0.42
33:a:1005:A:H2'	33:a:1006:U:C6	2.54	0.42
33:a:1283:C:H2'	33:a:1284:A:O4'	2.19	0.42
33:a:1332:C:P	52:t:78:ARG:HH12	2.41	0.42
10:A:1017:A:H5''	27:U:80:LYS:HD2	2.01	0.42
10:A:1088:C:O2'	10:A:1155:A:N1	2.50	0.42
10:A:2058:A:N3	10:A:2482:G:O2'	2.47	0.42
10:A:2618:C:H2'	10:A:2619:G:C8	2.55	0.42
17:J:106:VAL:C	17:J:109:PRO:HD2	2.44	0.42
25:S:22:PHE:O	25:S:52:ARG:NH1	2.48	0.42
28:V:58:ALA:HA	28:V:62:TYR:HD2	1.84	0.42
29:W:13:THR:H	29:W:16:SER:HB3	1.84	0.42
29:W:49:LYS:HB3	29:W:83:LYS:HE3	2.01	0.42
33:a:607:C:H4'	41:i:124:GLY:C	2.45	0.42
33:a:758:C:O2	48:p:23:GLY:HA3	2.20	0.42
33:a:1167:A:H1'	33:a:1191:G:N2	2.34	0.42
35:c:31:ILE:HD11	35:c:189:THR:HG22	2.02	0.42
3:3:42:ALA:O	10:A:896:U:O2'	2.37	0.42
4:4:10:HIS:CE1	4:4:30:THR:HG22	2.54	0.42
10:A:127:C:H2'	10:A:128:C:C6	2.54	0.42
10:A:195:C:O2'	10:A:847:A:N3	2.51	0.42
10:A:606:G:OP2	27:U:78:ARG:NH1	2.52	0.42
10:A:1512:U:H2'	10:A:1567:A:N6	2.34	0.42
10:A:2382:C:H1'	32:Z:47:ARG:HH21	1.83	0.42
16:I:46:GLN:HG2	16:I:48:THR:HG23	2.01	0.42
31:Y:4:LEU:HA	31:Y:62:GLU:O	2.20	0.42
33:a:272:C:O2'	50:r:68:PRO:O	2.28	0.42
33:a:1045:G:H2'	33:a:1046:G:C8	2.53	0.42
34:b:19:G:H2'	34:b:20:C:C6	2.54	0.42
40:h:27:ILE:HD13	40:h:40:GLN:HG2	2.01	0.42
52:t:18:LYS:HD2	52:t:31:ILE:HG23	1.99	0.42
10:A:613:G:H2'	10:A:2057:A:N7	2.34	0.42
10:A:637:U:H2'	10:A:638:U:C6	2.54	0.42
10:A:794:A:H4'	10:A:1309:G:N3	2.33	0.42
10:A:909:G:N7	22:P:22:LYS:NZ	2.59	0.42
12:C:162:LYS:HG3	12:C:198:GLN:HB3	2.02	0.42
18:K:69:ARG:HD3	18:K:69:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:48:GLU:O	28:V:52:MET:HG2	2.19	0.42
33:a:59:C:H2'	33:a:60:A:H8	1.84	0.42
33:a:810:A:H2'	33:a:811:G:O4'	2.19	0.42
33:a:1348:G:H2'	33:a:1349:A:C8	2.55	0.42
35:c:71:GLY:HA3	35:c:80:VAL:HG21	2.01	0.42
10:A:784:A:H1'	10:A:785:C:H5	1.84	0.42
10:A:841:C:H2'	10:A:842:U:C6	2.55	0.42
10:A:2347:A:H2'	10:A:2347:A:N3	2.35	0.42
33:a:480:G:N3	49:q:89:LYS:NZ	2.68	0.42
33:a:502:C:O2'	33:a:504:G:H1'	2.18	0.42
33:a:728:C:O2'	51:s:61:THR:HG21	2.20	0.42
33:a:1174:G:H2'	33:a:1174:G:N3	2.34	0.42
36:d:28:PHE:CZ	47:o:54:PRO:HD2	2.54	0.42
36:d:35:ASP:OD1	36:d:58:ARG:NH2	2.49	0.42
43:k:32:SER:HB2	43:k:83:THR:HG22	2.02	0.42
10:A:199:A:H2'	10:A:199:A:N3	2.35	0.42
10:A:1221:C:O2'	10:A:1222:A:O5'	2.34	0.42
26:T:91:ASN:OD1	26:T:94:MET:CG	2.67	0.42
33:a:456:A:H2'	33:a:457:A:O4'	2.20	0.42
10:A:2584:G:H2'	10:A:2585:C:C6	2.55	0.42
10:A:2617:A:H2'	10:A:2618:C:C6	2.55	0.42
13:D:44:A:H2'	13:D:45:G:C8	2.55	0.42
13:F:44:A:H2'	13:F:45:G:C8	2.55	0.42
19:M:113:THR:O	19:M:117:GLU:HG2	2.18	0.42
33:a:88:U:H2'	33:a:89:U:C6	2.55	0.42
33:a:407:G:H2'	33:a:408:C:C6	2.55	0.42
33:a:525:G:H4'	33:a:527:C:C2	2.55	0.42
33:a:1045:G:C8	33:a:1046:G:H2'	2.54	0.42
33:a:1297:A:H2'	33:a:1298:A:C8	2.54	0.42
41:i:15:ARG:HG2	41:i:19:MET:HE3	2.01	0.42
43:k:32:SER:CB	43:k:83:THR:HG22	2.50	0.42
43:k:80:THR:O	43:k:83:THR:OG1	2.33	0.42
44:l:27:PHE:O	44:l:58:SER:HB3	2.20	0.42
49:q:58:LEU:HD11	49:q:83:LYS:HE2	2.01	0.42
6:6:35:TYR:HA	6:6:42:TYR:HA	2.02	0.42
10:A:1325:U:O2'	10:A:1691:G:N2	2.53	0.42
10:A:2793:G:N3	10:A:2793:G:H2'	2.34	0.42
13:F:18:G:N2	13:F:58:A:OP2	2.52	0.42
28:V:7:ALA:HB2	28:V:50:VAL:HG22	2.02	0.42
33:a:1149:G:C2	33:a:1151:U:C5	3.08	0.42
36:d:137:ILE:HA	36:d:148:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:37:SER:OG	43:k:75:ASP:HB2	2.20	0.42
3:3:45:GLY:HA3	10:A:897:A:H5'	2.02	0.42
10:A:1329:G:H2'	10:A:1330:U:C6	2.55	0.42
10:A:1351:C:O2	10:A:1351:C:H2'	2.18	0.42
10:A:2053:U:H2'	10:A:2054:G:O4'	2.20	0.42
10:A:2206:C:H2'	10:A:2207:U:O4'	2.19	0.42
10:A:2872:G:H2'	10:A:2873:C:O4'	2.19	0.42
13:F:19:G:H1	17:J:80:ARG:HH22	1.68	0.42
17:J:134:GLU:HG3	17:J:137:ILE:HG23	2.02	0.42
18:K:26:VAL:HG11	18:K:76:VAL:HA	2.02	0.42
19:M:79:SER:O	19:M:80:ASN:HB2	2.20	0.42
22:P:32:PHE:HD1	22:P:133:LYS:HG2	1.85	0.42
30:X:10:LYS:HB2	30:X:71:LEU:HD21	2.02	0.42
33:a:20:C:H5''	38:f:91:SER:HB2	2.01	0.42
33:a:583:G:O2'	33:a:829:G:H5'	2.20	0.42
35:c:184:VAL:HG22	35:c:198:TYR:HB2	2.01	0.42
36:d:62:ARG:HH22	36:d:99:HIS:CB	2.33	0.42
36:d:90:LEU:HD22	36:d:100:ILE:HD11	2.01	0.42
38:f:11:PHE:HB3	38:f:39:VAL:HG13	2.02	0.42
10:A:1696:C:H2'	10:A:1697:G:O4'	2.20	0.41
10:A:2836:C:O2	10:A:2903:A:O2'	2.36	0.41
14:G:136:PRO:HD2	14:G:139:THR:HG21	2.02	0.41
15:H:139:GLY:HA3	15:H:147:PHE:HD1	1.85	0.41
35:c:79:SER:HB3	35:c:214:THR:HG21	2.02	0.41
10:A:24:G:O2'	28:V:78:GLU:O	2.35	0.41
10:A:78:U:H2'	10:A:79:U:C6	2.55	0.41
10:A:1394:U:H2'	10:A:1395:G:O4'	2.20	0.41
10:A:2539:C:H2'	10:A:2540:A:O4'	2.20	0.41
13:D:33:U:H3'	13:D:35:A:OP2	2.20	0.41
13:F:33:U:OP2	42:j:132:ARG:NH2	2.46	0.41
26:T:90:ILE:CG2	26:T:94:MET:HB2	2.50	0.41
33:a:17:A:N1	33:a:928:A:H2	2.19	0.41
33:a:1013:A:HO2'	33:a:1034:U:H3	1.68	0.41
35:c:153:ASP:OD1	35:c:153:ASP:N	2.47	0.41
10:A:1115:G:O5'	10:A:1115:G:H8	2.03	0.41
10:A:1209:U:H2'	10:A:1210:U:C6	2.56	0.41
10:A:1602:U:H2'	10:A:1603:U:C6	2.55	0.41
10:A:1757:U:O2'	10:A:1758:A:H5''	2.20	0.41
10:A:2692:A:H2'	10:A:2693:C:O4'	2.20	0.41
10:A:2716:U:H5''	10:A:2740:A:C2	2.55	0.41
22:P:11:ARG:HG2	22:P:75:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:64:VAL:HG22	22:P:106:VAL:HG12	2.01	0.41
28:V:44:SER:HB2	28:V:45:PRO:HD3	2.01	0.41
33:a:413:U:H3'	33:a:414:G:H5'	2.02	0.41
33:a:1356:A:N1	33:a:1384:A:H5''	2.35	0.41
33:a:1479:A:H2'	33:a:1480:A:O4'	2.20	0.41
35:c:101:LEU:HA	35:c:157:MET:HE1	2.02	0.41
38:f:22:ALA:HB2	38:f:31:PHE:CD1	2.55	0.41
49:q:22:VAL:HG21	49:q:60:TRP:CG	2.55	0.41
10:A:229:A:O2'	10:A:231:A:N1	2.53	0.41
10:A:593:U:OP2	27:U:64:LYS:NZ	2.53	0.41
10:A:1315:C:H2'	10:A:1316:G:C8	2.56	0.41
10:A:1424:A:H5'	10:A:1513:A:H1'	2.02	0.41
10:A:1810:A:N1	10:A:2614:A:H2'	2.36	0.41
18:K:76:VAL:O	18:K:80:SER:OG	2.36	0.41
33:a:459:A:H4'	33:a:460:A:O5'	2.20	0.41
33:a:1260:A:O2'	33:a:1261:A:H5'	2.21	0.41
36:d:133:GLN:OE1	36:d:152:VAL:HG12	2.21	0.41
4:4:5:ILE:HD12	17:J:64:LYS:HE2	2.02	0.41
4:4:7:PRO:HG3	17:J:58:GLU:HG2	2.02	0.41
16:I:3:ASN:HD21	16:I:16:SER:HB2	1.85	0.41
17:J:122:PHE:CE2	17:J:128:TYR:HB2	2.55	0.41
19:M:119:GLN:HA	19:M:122:LYS:HE2	2.01	0.41
33:a:496:C:O2'	33:a:497:C:H5'	2.21	0.41
33:a:751:U:H2'	33:a:752:C:C6	2.55	0.41
33:a:1386:U:H2'	33:a:1387:A:C8	2.55	0.41
38:f:115:LEU:HD22	38:f:120:ILE:HD12	2.02	0.41
10:A:226:A:O2'	10:A:466:C:O2	2.38	0.41
10:A:792:5MU:H4'	28:V:92:ARG:HH22	1.85	0.41
10:A:2210:C:H2'	10:A:2211:U:O4'	2.20	0.41
10:A:2270:U:H2'	10:A:2271:U:C6	2.55	0.41
10:A:2869:G:O2'	10:A:2886:G:N2	2.54	0.41
17:J:128:TYR:HE2	17:J:130:LEU:HB2	1.86	0.41
24:R:42:ALA:HB2	24:R:108:LEU:HD11	2.02	0.41
31:Y:5:LYS:HB3	31:Y:51:VAL:HG21	2.02	0.41
31:Y:7:ILE:HD13	31:Y:41:VAL:HB	2.03	0.41
33:a:497:C:O2'	33:a:498:U:H5'	2.20	0.41
33:a:704:A:H1'	33:a:794:G:O2'	2.20	0.41
33:a:723:A:H2'	33:a:724:A:C8	2.56	0.41
33:a:1013:A:O2'	33:a:1034:U:N3	2.53	0.41
33:a:1297:A:H8	33:a:1297:A:H5''	1.86	0.41
36:d:62:ARG:HH22	36:d:99:HIS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:64:TYR:CD1	10:A:245:G:H5'	2.56	0.41
10:A:448:A:H2'	10:A:449:U:O4'	2.20	0.41
10:A:620:G:O2'	10:A:1292:A:OP1	2.36	0.41
33:a:33:A:H2'	33:a:34:A:C8	2.56	0.41
33:a:230:U:H2'	33:a:231:U:C6	2.55	0.41
33:a:476:C:O2	33:a:476:C:O4'	2.38	0.41
35:c:97:LEU:HB2	35:c:100:LEU:HD13	2.02	0.41
46:n:34:LEU:HD13	46:n:41:ALA:HA	2.03	0.41
46:n:75:LEU:HA	46:n:78:LYS:HD2	2.03	0.41
10:A:229:A:H2'	10:A:230:A:C8	2.56	0.41
10:A:2820:U:H2'	10:A:2822:C:C5	2.55	0.41
16:I:51:VAL:HG21	16:I:91:GLY:HA3	2.03	0.41
33:a:693:G:O2'	33:a:694:U:C5'	2.65	0.41
33:a:708:G:H2'	33:a:709:C:C6	2.54	0.41
36:d:205:GLU:O	36:d:206:VAL:C	2.63	0.41
43:k:66:GLU:HB3	47:o:59:ALA:HB2	2.03	0.41
44:l:111:ARG:HB3	54:v:3:LYS:HG3	2.03	0.41
1:1:10:ARG:HD3	10:A:443:U:OP2	2.21	0.41
4:4:2:LYS:HD2	4:4:5:ILE:HD13	2.02	0.41
7:7:12:LYS:NZ	10:A:730:A:OP1	2.50	0.41
10:A:31:C:O2'	10:A:1276:G:OP1	2.37	0.41
10:A:749:G:N3	10:A:771:G:C2	2.89	0.41
10:A:801:A:H2'	10:A:802:G:O4'	2.21	0.41
10:A:1375:G:O2'	10:A:1430:A:N1	2.52	0.41
10:A:1891:U:OP1	10:A:2437:G:O2'	2.35	0.41
10:A:1941:C:H2'	10:A:1942:3TD:H6	2.02	0.41
10:A:2128:G:H2'	10:A:2129:C:O4'	2.21	0.41
10:A:2318:U:H2'	10:A:2319:U:C6	2.56	0.41
12:C:33:VAL:O	12:C:37:GLN:HG3	2.20	0.41
12:C:89:PRO:HB3	12:C:141:LEU:HD22	2.02	0.41
16:I:32:VAL:HG21	16:I:108:LEU:HD23	2.01	0.41
17:J:57:LEU:HD23	17:J:65:PRO:HB3	2.02	0.41
18:K:104:ILE:HG23	18:K:114:GLU:HG2	2.03	0.41
33:a:517:A:H2'	33:a:518:A:C8	2.55	0.41
33:a:612:G:H2'	33:a:613:U:O4'	2.21	0.41
33:a:670:A:H2'	33:a:671:A:C8	2.56	0.41
33:a:798:A:H2'	33:a:799:G:C8	2.56	0.41
33:a:992:A:H2	33:a:1232:G:H22	1.69	0.41
33:a:1172:C:H2'	33:a:1173:G:C8	2.56	0.41
33:a:1182:C:H2'	33:a:1183:C:C6	2.55	0.41
39:g:11:ARG:HG2	39:g:85:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:15:ASP:O	40:h:19:ASN:N	2.51	0.41
51:s:37:PHE:HB3	51:s:60:LEU:HD21	2.03	0.41
52:t:15:LEU:O	52:t:19:VAL:HG23	2.20	0.41
10:A:1149:U:H2'	10:A:1150:A:H8	1.86	0.41
15:H:71:LYS:N	15:H:72:PRO:CD	2.84	0.41
31:Y:7:ILE:HG22	31:Y:43:VAL:HB	2.03	0.41
33:a:1445:G:H2'	33:a:1446:C:C6	2.55	0.41
39:g:29:ILE:HA	39:g:32:THR:HG23	2.03	0.41
10:A:665:G:H2'	10:A:665:G:N3	2.37	0.40
10:A:1630:A:H1'	10:A:1631:G:C1'	2.51	0.40
10:A:1823:U:H2'	10:A:1824:C:C6	2.56	0.40
12:C:43:ASP:O	12:C:47:ILE:HG12	2.21	0.40
16:I:21:ASP:O	16:I:25:GLY:N	2.54	0.40
18:K:144:LEU:O	18:K:148:ILE:HG13	2.21	0.40
23:Q:24:LEU:HD23	23:Q:44:VAL:HG21	2.03	0.40
33:a:1018:U:O2	33:a:1018:U:H2'	2.21	0.40
40:h:51:GLU:HG3	40:h:56:ARG:O	2.21	0.40
10:A:161:A:N3	10:A:2235:A:O2'	2.54	0.40
10:A:2472:2MG:P	16:I:74:ARG:HH12	2.44	0.40
24:R:29:PRO:HB2	24:R:44:ILE:HG22	2.03	0.40
31:Y:5:LYS:HE2	31:Y:48:PHE:HD1	1.87	0.40
33:a:379:G:H2'	33:a:380:C:O4'	2.21	0.40
33:a:477:U:H2'	33:a:478:G:O4'	2.20	0.40
33:a:525:G:N2	33:a:538:G:OP1	2.54	0.40
33:a:531:A:N6	45:m:100:VAL:HG13	2.36	0.40
33:a:1063:U:O4	33:a:1210:C:O2'	2.33	0.40
35:c:21:ARG:HG3	35:c:22:ARG:HG3	2.02	0.40
35:c:99:GLY:HA2	35:c:102:THR:OG1	2.21	0.40
35:c:133:GLU:O	35:c:136:GLU:HG2	2.20	0.40
37:e:152:VAL:O	37:e:156:GLU:HG2	2.20	0.40
49:q:20:ILE:HD12	49:q:52:VAL:HG22	2.03	0.40
2:2:40:THR:HB	10:A:61:A:O4'	2.20	0.40
10:A:2620:U:H2'	10:A:2621:C:C6	2.56	0.40
10:A:2911:A:H2'	10:A:2912:A:O4'	2.22	0.40
13:D:9:G:H1'	13:D:45:G:H2'	2.04	0.40
33:a:206:A:H2'	33:a:207:G:C8	2.56	0.40
33:a:703:A:H2'	33:a:704:A:C8	2.57	0.40
33:a:1333:G:H2'	33:a:1334:A:C8	2.57	0.40
35:c:73:LYS:O	35:c:77:GLN:HG3	2.21	0.40
10:A:305:A:H61	10:A:410:G:H22	1.68	0.40
10:A:783:G:H2'	10:A:784:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1423:C:H2'	10:A:1424:A:C8	2.56	0.40
10:A:1580:A:C2	10:A:1583:G:H2'	2.55	0.40
12:C:23:VAL:HG21	12:C:36:ILE:HG21	2.03	0.40
15:H:116:ILE:HD12	15:H:211:ILE:HG23	2.04	0.40
33:a:495:A:H2'	33:a:496:C:O4'	2.22	0.40
33:a:1015:A:H2'	33:a:1016:A:N7	2.37	0.40
33:a:1508:G:H1'	33:a:1529:MA6:C2	2.52	0.40
34:b:21:A:O2'	34:b:22:A:O5'	2.37	0.40
43:k:25:ILE:HD11	43:k:74:ILE:HD13	2.03	0.40
47:o:24:CYS:HB2	47:o:40:CYS:HB3	2.04	0.40
48:p:56:LEU:HA	48:p:59:MET:HE2	2.04	0.40
52:t:63:THR:HG22	52:t:66:MET:HG3	2.03	0.40
10:A:221:G:N2	10:A:238:U:H4'	2.36	0.40
10:A:241:C:H2'	10:A:242:U:O4'	2.21	0.40
10:A:907:G:H2'	10:A:908:A:O4'	2.22	0.40
10:A:1039:C:C5	26:T:57:PHE:CZ	3.09	0.40
10:A:2496:A:H4'	22:P:56:ARG:NH1	2.36	0.40
14:G:78:VAL:HG22	14:G:94:VAL:HG12	2.04	0.40
15:H:4:GLY:HA2	15:H:211:ILE:O	2.22	0.40
33:a:794:G:H2'	33:a:795:A:O4'	2.22	0.40
33:a:901:A:O2'	33:a:1425:G:H4'	2.21	0.40
33:a:1441:C:H2'	33:a:1442:G:O4'	2.21	0.40
35:c:196:ILE:H	35:c:196:ILE:HD12	1.86	0.40
46:n:3:ARG:HE	46:n:6:GLY:HA2	1.87	0.40
46:n:11:ARG:HB3	46:n:46:LYS:HB3	2.04	0.40
48:p:80:GLU:HA	48:p:83:LYS:HE3	2.03	0.40
52:t:23:GLU:OE2	52:t:43:ASN:ND2	2.55	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	1	59/62 (95%)	59 (100%)	0	0	100	100
2	2	63/69 (91%)	63 (100%)	0	0	100	100
3	3	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
4	4	78/84 (93%)	78 (100%)	0	0	100	100
5	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
6	6	46/49 (94%)	46 (100%)	0	0	100	100
7	7	41/45 (91%)	41 (100%)	0	0	100	100
8	8	62/66 (94%)	62 (100%)	0	0	100	100
9	9	35/37 (95%)	35 (100%)	0	0	100	100
12	C	195/213 (92%)	193 (99%)	2 (1%)	0	100	100
14	G	271/277 (98%)	268 (99%)	3 (1%)	0	100	100
15	H	214/220 (97%)	206 (96%)	8 (4%)	0	100	100
16	I	202/207 (98%)	201 (100%)	1 (0%)	0	100	100
17	J	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
18	K	172/178 (97%)	171 (99%)	1 (1%)	0	100	100
19	M	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
20	N	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
21	O	143/146 (98%)	138 (96%)	5 (4%)	0	100	100
22	P	134/144 (93%)	133 (99%)	1 (1%)	0	100	100
23	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	R	117/119 (98%)	117 (100%)	0	0	100	100
25	S	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
26	T	114/118 (97%)	114 (100%)	0	0	100	100
27	U	99/102 (97%)	99 (100%)	0	0	100	100
28	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
29	W	87/91 (96%)	86 (99%)	1 (1%)	0	100	100
30	X	100/105 (95%)	100 (100%)	0	0	100	100
31	Y	92/217 (42%)	92 (100%)	0	0	100	100
32	Z	80/94 (85%)	77 (96%)	3 (4%)	0	100	100
35	c	219/255 (86%)	217 (99%)	2 (1%)	0	100	100
36	d	202/217 (93%)	198 (98%)	4 (2%)	0	100	100
37	e	197/200 (98%)	196 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	f	154/166 (93%)	153 (99%)	1 (1%)	0	100	100
39	g	91/98 (93%)	91 (100%)	0	0	100	100
40	h	142/156 (91%)	140 (99%)	2 (1%)	0	100	100
41	i	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
42	j	126/132 (96%)	124 (98%)	2 (2%)	0	100	100
43	k	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
44	l	116/129 (90%)	113 (97%)	3 (3%)	0	100	100
45	m	133/137 (97%)	129 (97%)	3 (2%)	1 (1%)	16	37
46	n	111/121 (92%)	109 (98%)	2 (2%)	0	100	100
47	o	58/61 (95%)	58 (100%)	0	0	100	100
48	p	84/89 (94%)	84 (100%)	0	0	100	100
49	q	88/91 (97%)	88 (100%)	0	0	100	100
50	r	78/87 (90%)	77 (99%)	1 (1%)	0	100	100
51	s	61/80 (76%)	61 (100%)	0	0	100	100
52	t	78/92 (85%)	77 (99%)	1 (1%)	0	100	100
53	u	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
54	v	51/58 (88%)	51 (100%)	0	0	100	100
All	All	5579/6046 (92%)	5511 (99%)	67 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	m	61	ALA

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	1	51/52 (98%)	50 (98%)	1 (2%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	59/62 (95%)	59 (100%)	0	100	100
3	3	51/53 (96%)	51 (100%)	0	100	100
4	4	71/75 (95%)	68 (96%)	3 (4%)	26	55
5	5	48/50 (96%)	48 (100%)	0	100	100
6	6	46/47 (98%)	45 (98%)	1 (2%)	45	74
7	7	39/40 (98%)	38 (97%)	1 (3%)	40	70
8	8	55/57 (96%)	53 (96%)	2 (4%)	31	60
9	9	35/35 (100%)	35 (100%)	0	100	100
12	C	191/204 (94%)	188 (98%)	3 (2%)	55	80
14	G	220/224 (98%)	219 (100%)	1 (0%)	81	92
15	H	174/177 (98%)	174 (100%)	0	100	100
16	I	168/169 (99%)	167 (99%)	1 (1%)	78	91
17	J	157/158 (99%)	153 (98%)	4 (2%)	42	71
18	K	152/155 (98%)	148 (97%)	4 (3%)	40	70
19	M	123/123 (100%)	123 (100%)	0	100	100
20	N	100/100 (100%)	99 (99%)	1 (1%)	68	86
21	O	111/112 (99%)	111 (100%)	0	100	100
22	P	113/119 (95%)	112 (99%)	1 (1%)	70	87
23	Q	101/102 (99%)	100 (99%)	1 (1%)	68	86
24	R	95/95 (100%)	94 (99%)	1 (1%)	65	85
25	S	100/102 (98%)	98 (98%)	2 (2%)	48	76
26	T	96/98 (98%)	96 (100%)	0	100	100
27	U	86/86 (100%)	85 (99%)	1 (1%)	63	84
28	V	90/94 (96%)	89 (99%)	1 (1%)	65	85
29	W	80/82 (98%)	79 (99%)	1 (1%)	61	83
30	X	87/90 (97%)	84 (97%)	3 (3%)	32	62
31	Y	83/190 (44%)	80 (96%)	3 (4%)	31	60
32	Z	64/75 (85%)	63 (98%)	1 (2%)	55	80
35	c	192/221 (87%)	185 (96%)	7 (4%)	31	60
36	d	166/175 (95%)	158 (95%)	8 (5%)	23	50
37	e	174/175 (99%)	169 (97%)	5 (3%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	f	122/131 (93%)	120 (98%)	2 (2%)	55	80
39	g	81/86 (94%)	78 (96%)	3 (4%)	30	59
40	h	124/132 (94%)	119 (96%)	5 (4%)	28	56
41	i	112/113 (99%)	110 (98%)	2 (2%)	51	78
42	j	106/109 (97%)	105 (99%)	1 (1%)	70	87
43	k	89/91 (98%)	87 (98%)	2 (2%)	45	74
44	l	94/104 (90%)	90 (96%)	4 (4%)	26	54
45	m	117/119 (98%)	117 (100%)	0	100	100
46	n	98/104 (94%)	97 (99%)	1 (1%)	68	86
47	o	52/53 (98%)	52 (100%)	0	100	100
48	p	79/81 (98%)	78 (99%)	1 (1%)	61	83
49	q	76/77 (99%)	76 (100%)	0	100	100
50	r	75/82 (92%)	75 (100%)	0	100	100
51	s	56/68 (82%)	54 (96%)	2 (4%)	31	60
52	t	70/80 (88%)	69 (99%)	1 (1%)	59	82
53	u	67/69 (97%)	67 (100%)	0	100	100
54	v	49/54 (91%)	48 (98%)	1 (2%)	48	76
All	All	4845/5150 (94%)	4763 (98%)	82 (2%)	52	79

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	24	SER
4	4	49	ASP
4	4	53	ASP
4	4	76	LYS
6	6	32	MET
7	7	25	THR
8	8	2	PRO
8	8	55	MET
12	C	120	VAL
12	C	144	LEU
12	C	184	LYS
14	G	140	VAL
16	I	17	ILE
17	J	80	ARG

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Mol	Chain	Res	Type
17	J	101	ASP
17	J	135	GLN
17	J	146	VAL
18	K	16	THR
18	K	43	PHE
18	K	73	ASN
18	K	107	VAL
20	N	47	THR
22	P	7	VAL
23	Q	40	VAL
24	R	55	GLN
25	S	2	THR
25	S	63	VAL
27	U	27	VAL
28	V	86	ARG
29	W	55	ILE
30	X	12	ILE
30	X	24	ILE
30	X	75	THR
31	Y	13	GLN
31	Y	43	VAL
31	Y	90	ASP
32	Z	15	VAL
35	c	38	ILE
35	c	90	PHE
35	c	114	ILE
35	c	134	VAL
35	c	153	ASP
35	c	157	MET
35	c	196	ILE
36	d	12	VAL
36	d	46	LEU
36	d	75	VAL
36	d	86	LEU
36	d	90	LEU
36	d	102	VAL
36	d	161	ILE
36	d	171	THR
37	e	8	ASN
37	e	17	ILE
37	e	25	GLU
37	e	28	LYS

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Mol	Chain	Res	Type
37	e	64	THR
38	f	56	VAL
38	f	80	THR
39	g	32	THR
39	g	65	VAL
39	g	92	ILE
40	h	13	LEU
40	h	15	ASP
40	h	59	LEU
40	h	87	VAL
40	h	130	ASN
41	i	25	LEU
41	i	98	LEU
42	j	50	LEU
43	k	40	ILE
43	k	72	ARG
44	l	79	LEU
44	l	100	LEU
44	l	119	ASN
44	l	129	VAL
46	n	53	LEU
48	p	21	ASP
51	s	23	ILE
51	s	29	LYS
52	t	18	LYS
54	v	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
6	6	26	ASN
12	C	45	ASN
12	C	95	GLN
12	C	128	ASN
12	C	198	GLN
12	C	204	GLN
14	G	86	ASN
14	G	199	GLN
15	H	14	GLN
15	H	136	GLN
15	H	181	GLN
15	H	200	ASN

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Mol	Chain	Res	Type
16	I	3	ASN
16	I	53	ASN
16	I	162	ASN
16	I	174	GLN
16	I	188	ASN
17	J	52	ASN
18	K	38	ASN
18	K	73	ASN
18	K	99	GLN
19	M	81	HIS
19	M	119	GLN
20	N	45	ASN
22	P	13	HIS
22	P	35	GLN
22	P	123	HIS
23	Q	61	ASN
23	Q	79	GLN
24	R	32	ASN
27	U	81	ASN
30	X	39	ASN
31	Y	13	GLN
31	Y	38	ASN
31	Y	85	GLN
35	c	55	ASN
35	c	66	GLN
35	c	94	GLN
36	d	91	ASN
36	d	118	ASN
37	e	40	GLN
37	e	115	ASN
39	g	69	ASN
40	h	67	ASN
40	h	86	GLN
40	h	153	HIS
41	i	18	ASN
42	j	16	ASN
42	j	70	HIS
44	l	15	ASN
44	l	18	ASN
45	m	73	ASN
46	n	31	GLN
46	n	76	ASN

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Mol	Chain	Res	Type
49	q	62	ASN
52	t	14	HIS
52	t	47	HIS
53	u	41	ASN
53	u	82	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2845/2923 (97%)	349 (12%)	63 (2%)
11	B	112/115 (97%)	15 (13%)	5 (4%)
13	D	76/77 (98%)	23 (30%)	2 (2%)
13	F	75/77 (97%)	13 (17%)	2 (2%)
33	a	1523/1555 (97%)	213 (13%)	0
34	b	9/24 (37%)	4 (44%)	0
All	All	4640/4771 (97%)	617 (13%)	72 (1%)

All (617) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	33	U
10	A	34	U
10	A	64	A
10	A	71	A
10	A	75	G
10	A	90	A
10	A	91	A
10	A	117	A
10	A	118	A
10	A	119	U
10	A	130	A
10	A	156	A
10	A	167	U
10	A	168	A
10	A	177	G
10	A	199	A
10	A	202	A
10	A	203	U
10	A	216	A
10	A	218	G
10	A	219	A

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Mol	Chain	Res	Type
10	A	224	A
10	A	225	A
10	A	232	U
10	A	233	U
10	A	251	G
10	A	255	G
10	A	269	G
10	A	270	C
10	A	284	C
10	A	285	U
10	A	286	U
10	A	287	G
10	A	288	C
10	A	289	U
10	A	299	U
10	A	300	G
10	A	314	A
10	A	315	C
10	A	321	U
10	A	324	A
10	A	327	G
10	A	354	A
10	A	373	A
10	A	381	G
10	A	388	A
10	A	389	A
10	A	404	U
10	A	406	A
10	A	410	G
10	A	411	A
10	A	432	G
10	A	449	U
10	A	450	C
10	A	457	G
10	A	497	U
10	A	527	G
10	A	548	A
10	A	549	U
10	A	550	A
10	A	553	A
10	A	567	G
10	A	575	G

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Mol	Chain	Res	Type
10	A	576	U
10	A	577	A
10	A	578	G
10	A	592	A
10	A	593	U
10	A	594	G
10	A	598	G
10	A	599	A
10	A	606	G
10	A	614	U
10	A	615	A
10	A	616	G
10	A	618	A
10	A	630	G
10	A	646	A
10	A	650	U
10	A	682	A
10	A	683	G
10	A	690	U
10	A	700	A
10	A	731	U
10	A	762	C
10	A	774	G
10	A	775	A
10	A	792	5MU
10	A	809	A
10	A	810	A
10	A	820	G
10	A	827	A
10	A	829	U
10	A	835	U
10	A	837	G
10	A	850	G
10	A	857	C
10	A	872	U
10	A	873	U
10	A	903	G
10	A	904	G
10	A	910	C
10	A	911	A
10	A	920	A
10	A	923	A

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Mol	Chain	Res	Type
10	A	924	G
10	A	927	G
10	A	930	C
10	A	937	G
10	A	941	A
10	A	943	C
10	A	944	G
10	A	945	A
10	A	955	A
10	A	969	A
10	A	970	U
10	A	972	A
10	A	985	A
10	A	988	C
10	A	989	A
10	A	990	G
10	A	1005	G
10	A	1018	A
10	A	1027	A
10	A	1029	C
10	A	1040	A
10	A	1052	A
10	A	1056	U
10	A	1057	A
10	A	1066	G
10	A	1070	A
10	A	1077	U
10	A	1090	A
10	A	1091	G
10	A	1114	A
10	A	1126	U
10	A	1129	A
10	A	1131	G
10	A	1132	A
10	A	1141	U
10	A	1155	A
10	A	1156	G
10	A	1174	U
10	A	1176	U
10	A	1177	A
10	A	1178	C
10	A	1179	C

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Mol	Chain	Res	Type
10	A	1186	A
10	A	1218	G
10	A	1221	C
10	A	1222	A
10	A	1276	G
10	A	1291	A
10	A	1292	A
10	A	1294	G
10	A	1309	G
10	A	1310	A
10	A	1337	A
10	A	1358	A
10	A	1382	C
10	A	1402	A
10	A	1405	G
10	A	1415	A
10	A	1416	U
10	A	1421	A
10	A	1449	A
10	A	1455	U
10	A	1457	U
10	A	1458	A
10	A	1459	A
10	A	1463	A
10	A	1464	U
10	A	1471	A
10	A	1472	C
10	A	1490	G
10	A	1496	G
10	A	1497	A
10	A	1500	G
10	A	1510	U
10	A	1511	C
10	A	1526	G
10	A	1533	A
10	A	1536	C
10	A	1537	A
10	A	1553	A
10	A	1560	A
10	A	1569	G
10	A	1578	A
10	A	1580	A

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Mol	Chain	Res	Type
10	A	1581	U
10	A	1582	U
10	A	1583	G
10	A	1585	G
10	A	1606	C
10	A	1616	A
10	A	1625	U
10	A	1630	A
10	A	1631	G
10	A	1633	A
10	A	1634	A
10	A	1642	C
10	A	1652	A
10	A	1653	A
10	A	1658	A
10	A	1690	A
10	A	1691	G
10	A	1692	C
10	A	1718	G
10	A	1740	G
10	A	1758	A
10	A	1759	G
10	A	1772	G
10	A	1783	G
10	A	1789	A
10	A	1790	G
10	A	1791	G
10	A	1795	A
10	A	1800	A
10	A	1803	G
10	A	1809	C
10	A	1818	A
10	A	1827	C
10	A	1828	U
10	A	1843	U
10	A	1856	A
10	A	1874	A
10	A	1875	A
10	A	1899	U
10	A	1900	G
10	A	1909	C
10	A	1933	G

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Mol	Chain	Res	Type
10	A	1941	C
10	A	1956	G
10	A	1957	G
10	A	1963	A
10	A	1964	A
10	A	1965	A
10	A	1982	U
10	A	1994	C
10	A	1997	A
10	A	1998	A
10	A	1999	G
10	A	2018	U
10	A	2019	G
10	A	2020	U
10	A	2040	A
10	A	2050	A
10	A	2058	A
10	A	2059	G
10	A	2060	A
10	A	2070	C
10	A	2082	C
10	A	2083	G
10	A	2087	A
10	A	2088	G
10	A	2089	A
10	A	2096	G
10	A	2120	G
10	A	2136	U
10	A	2137	G
10	A	2205	C
10	A	2208	A
10	A	2209	G
10	A	2215	U
10	A	2217	G
10	A	2218	G
10	A	2225	A
10	A	2230	G
10	A	2238	U
10	A	2239	A
10	A	2252	A
10	A	2265	G
10	A	2266	G

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Mol	Chain	Res	Type
10	A	2295	A
10	A	2305	A
10	A	2310	C
10	A	2313	A
10	A	2314	A
10	A	2316	G
10	A	2333	U
10	A	2334	G
10	A	2335	G
10	A	2339	U
10	A	2347	A
10	A	2348	G
10	A	2349	A
10	A	2358	G
10	A	2361	U
10	A	2362	A
10	A	2374	C
10	A	2377	C
10	A	2410	G
10	A	2412	C
10	A	2429	U
10	A	2430	C
10	A	2433	C
10	A	2452	A
10	A	2455	G
10	A	2456	G
10	A	2457	A
10	A	2462	A
10	A	2468	C
10	A	2475	A
10	A	2476	H2U
10	A	2486	A
10	A	2495	A
10	A	2496	A
10	A	2502	C
10	A	2529	G
10	A	2532	G
10	A	2544	C
10	A	2545	A
10	A	2556	G
10	A	2557	U
10	A	2561	C

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Mol	Chain	Res	Type
10	A	2581	U
10	A	2593	A
10	A	2594	G
10	A	2629	A
10	A	2637	C
10	A	2640	U
10	A	2657	G
10	A	2666	A
10	A	2692	A
10	A	2716	U
10	A	2718	C
10	A	2741	G
10	A	2753	U
10	A	2760	A
10	A	2762	G
10	A	2769	G
10	A	2771	G
10	A	2777	A
10	A	2784	A
10	A	2791	A
10	A	2792	A
10	A	2805	A
10	A	2806	U
10	A	2807	G
10	A	2824	G
10	A	2825	U
10	A	2827	A
10	A	2828	U
10	A	2852	U
10	A	2887	G
10	A	2888	A
10	A	2892	G
10	A	2903	A
10	A	2913	G
11	B	10	U
11	B	23	U
11	B	27	A
11	B	32	U
11	B	33	U
11	B	49	G
11	B	51	A
11	B	54	U

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Mol	Chain	Res	Type
11	B	55	A
11	B	85	U
11	B	86	A
11	B	87	C
11	B	88	G
11	B	105	C
11	B	106	G
13	D	2	G
13	D	7	G
13	D	8	U
13	D	9	G
13	D	16	C
13	D	17	C
13	D	17(A)	U
13	D	18	G
13	D	19	G
13	D	20	U
13	D	21	A
13	D	22	G
13	D	27	U
13	D	28	C
13	D	34	C
13	D	46	G
13	D	47	U
13	D	48	C
13	D	59	A
13	D	63	G
13	D	72	A
13	D	74	C
13	D	76	A
13	F	7	G
13	F	8	U
13	F	9	G
13	F	17(A)	U
13	F	18	G
13	F	19	G
13	F	21	A
13	F	47	U
13	F	48	C
13	F	51	C
13	F	52	G
13	F	58	A

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Mol	Chain	Res	Type
13	F	76	A
33	a	7	G
33	a	8	G
33	a	9	A
33	a	10	G
33	a	32	G
33	a	33	A
33	a	40	G
33	a	48	C
33	a	49	C
33	a	52	A
33	a	62	G
33	a	74	G
33	a	75	A
33	a	81	A
33	a	82	G
33	a	83	C
33	a	84	U
33	a	85	U
33	a	86	G
33	a	89	U
33	a	91	U
33	a	94	G
33	a	97	G
33	a	120	C
33	a	129	A
33	a	131	C
33	a	159	G
33	a	163	C
33	a	173	U
33	a	183	U
33	a	190	A
33	a	198	G
33	a	212	A
33	a	213	G
33	a	220	U
33	a	221	U
33	a	222	G
33	a	248	U
33	a	249	G
33	a	253	U
33	a	255	G

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Mol	Chain	Res	Type
33	a	258	A
33	a	259	G
33	a	274	G
33	a	275	C
33	a	297	G
33	a	313	G
33	a	314	A
33	a	324	C
33	a	329	A
33	a	336	C
33	a	337	A
33	a	338	C
33	a	340	G
33	a	355	G
33	a	360	C
33	a	362	G
33	a	364	A
33	a	375	U
33	a	380	C
33	a	400	G
33	a	405	A
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G
33	a	429	U
33	a	432	G
33	a	437	U
33	a	447	U
33	a	456	A
33	a	461	C
33	a	492	G
33	a	493	G
33	a	505	A
33	a	513	G
33	a	517	A
33	a	519	C
33	a	526	C
33	a	529	G
33	a	540	A
33	a	541	A
33	a	544	C

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Mol	Chain	Res	Type
33	a	555	A
33	a	567	A
33	a	580	A
33	a	581	A
33	a	584	C
33	a	626	C
33	a	649	A
33	a	650	A
33	a	661	U
33	a	673	A
33	a	695	A
33	a	696	G
33	a	703	A
33	a	710	A
33	a	711	G
33	a	712	A
33	a	731	U
33	a	732	G
33	a	757	A
33	a	763	G
33	a	785	A
33	a	801	U
33	a	802	A
33	a	823	A
33	a	825	C
33	a	836	A
33	a	844	G
33	a	881	A
33	a	883	G
33	a	894	G
33	a	923	A
33	a	924	A
33	a	935	G
33	a	936	G
33	a	940	C
33	a	943	C
33	a	944	A
33	a	969	U
33	a	970	U
33	a	978	A
33	a	980	G
33	a	981	C

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Mol	Chain	Res	Type
33	a	984	A
33	a	985	G
33	a	986	A
33	a	992	A
33	a	1000	U
33	a	1001	U
33	a	1002	G
33	a	1013	A
33	a	1014	C
33	a	1015	A
33	a	1016	A
33	a	1018	U
33	a	1019	C
33	a	1022	G
33	a	1030	G
33	a	1035	C
33	a	1036	C
33	a	1046	G
33	a	1047	A
33	a	1048	C
33	a	1056	C
33	a	1066	A
33	a	1067	U
33	a	1076	U
33	a	1096	U
33	a	1105	G
33	a	1106	U
33	a	1111	C
33	a	1112	A
33	a	1135	G
33	a	1136	U
33	a	1140	C
33	a	1141	A
33	a	1149	G
33	a	1155	C
33	a	1156	A
33	a	1169	U
33	a	1170	G
33	a	1174	G
33	a	1175	U
33	a	1177	A
33	a	1178	C

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Mol	Chain	Res	Type
33	a	1194	G
33	a	1206	A
33	a	1207	A
33	a	1211	A
33	a	1212	U
33	a	1221	U
33	a	1222	U
33	a	1223	A
33	a	1235	A
33	a	1236	C
33	a	1237	A
33	a	1267	A
33	a	1268	G
33	a	1270	G
33	a	1289	A
33	a	1290	A
33	a	1296	U
33	a	1297	A
33	a	1309	A
33	a	1310	G
33	a	1312	U
33	a	1322	G
33	a	1330	C
33	a	1348	G
33	a	1356	A
33	a	1363	G
33	a	1374	U
33	a	1380	G
33	a	1388	C
33	a	1389	G
33	a	1408	A
33	a	1429	G
33	a	1452	G
33	a	1456	A
33	a	1460	U
33	a	1463	U
33	a	1464	A
33	a	1503	A
33	a	1504	A
33	a	1505	G
33	a	1513	A
33	a	1517	U

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Mol	Chain	Res	Type
33	a	1528	G
33	a	1540	G
33	a	1541	G
33	a	1544	C
34	b	19	G
34	b	20	C
34	b	21	A
34	b	22	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	33	U
10	A	50	U
10	A	90	A
10	A	202	A
10	A	232	U
10	A	258	A
10	A	298	U
10	A	299	U
10	A	366	G
10	A	388	A
10	A	449	U
10	A	548	A
10	A	552	A
10	A	598	G
10	A	614	U
10	A	761	A
10	A	793	G
10	A	809	A
10	A	872	U
10	A	903	G
10	A	910	C
10	A	911	A
10	A	923	A
10	A	969	A
10	A	988	C
10	A	1028	G
10	A	1090	A
10	A	1113	A
10	A	1135	G
10	A	1176	U

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Mol	Chain	Res	Type
10	A	1177	A
10	A	1186	A
10	A	1221	C
10	A	1291	A
10	A	1308	C
10	A	1357	G
10	A	1381	U
10	A	1407	C
10	A	1433	U
10	A	1457	U
10	A	1496	G
10	A	1510	U
10	A	1633	A
10	A	1652	A
10	A	1690	A
10	A	1691	G
10	A	1789	A
10	A	1874	A
10	A	1927	A
10	A	1940	A
10	A	2094	G
10	A	2313	A
10	A	2347	A
10	A	2409	G
10	A	2450	U
10	A	2457	A
10	A	2495	A
10	A	2501	U
10	A	2544	C
10	A	2783	U
10	A	2805	A
10	A	2887	G
10	A	2912	A
11	B	19	G
11	B	32	U
11	B	85	U
11	B	87	C
11	B	105	C
13	D	7	G
13	D	60	U
13	F	7	G
13	F	60	U

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	3TD	A	1942	10	19,22,23	0.21	0	23,32,35	0.34	0
10	H2U	A	2476	10	18,21,22	0.26	0	19,30,33	0.49	0
10	5MU	A	1966	10	19,22,23	0.21	0	27,32,35	0.30	0
33	4OC	a	1412	56,33	20,23,24	0.20	0	25,32,35	0.41	0
10	2MA	A	2530	56,10	22,25,26	0.97	2 (9%)	32,37,40	1.28	3 (9%)
33	2MG	a	975	33	23,26,27	0.19	0	33,38,41	0.29	0
10	OMG	A	2278	10,13	23,26,27	0.22	0	32,38,41	0.29	0
10	5MU	A	792	10	19,22,23	0.14	0	27,32,35	0.25	0
33	UR3	a	1509	33	19,22,23	0.17	0	26,32,35	0.20	0
10	2MG	A	2472	10	23,26,27	0.18	0	33,38,41	0.34	0
33	G7M	a	535	33	23,26,27	0.20	0	34,39,42	0.43	0
33	5MC	a	976	33	19,22,23	0.14	0	26,32,35	0.35	0
33	MA6	a	1529	33	23,26,27	0.17	0	33,38,41	0.57	1 (3%)
33	MA6	a	1530	33	23,26,27	0.19	0	33,38,41	0.56	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3TD	A	1942	10	-	0/7/25/26	0/2/2/2
10	H2U	A	2476	10	-	2/7/38/39	0/2/2/2
10	5MU	A	1966	10	-	0/7/25/26	0/2/2/2
33	4OC	a	1412	56,33	-	0/9/29/30	0/2/2/2
10	2MA	A	2530	56,10	-	4/7/25/26	0/3/3/3
33	2MG	a	975	33	-	0/9/27/28	0/3/3/3
10	OMG	A	2278	10,13	-	1/9/27/28	0/3/3/3
10	5MU	A	792	10	-	0/7/25/26	0/2/2/2
33	UR3	a	1509	33	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	2MG	A	2472	10	-	0/9/27/28	0/3/3/3
33	G7M	a	535	33	-	2/7/25/26	0/3/3/3
33	5MC	a	976	33	-	0/7/25/26	0/2/2/2
33	MA6	a	1529	33	-	0/11/29/30	0/3/3/3
33	MA6	a	1530	33	-	2/11/29/30	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2530	2MA	C6-N6	-2.71	1.27	1.34
10	A	2530	2MA	C6-N1	2.32	1.38	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2530	2MA	N6-C6-N1	4.83	123.54	117.03
10	A	2530	2MA	C5-C6-N1	-3.43	113.57	118.90
10	A	2530	2MA	C2-N1-C6	3.22	123.06	118.10
33	a	1530	MA6	C2-N1-C6	2.31	117.47	111.83
33	a	1529	MA6	C2-N1-C6	2.24	117.31	111.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2278	OMG	C1'-C2'-O2'-CM2
33	a	1530	MA6	O4'-C4'-C5'-O5'
33	a	1530	MA6	C3'-C4'-C5'-O5'
33	a	535	G7M	C3'-C4'-C5'-O5'
10	A	2530	2MA	O4'-C4'-C5'-O5'
10	A	2476	H2U	O4'-C4'-C5'-O5'
10	A	2530	2MA	C4'-C5'-O5'-P
10	A	2530	2MA	C3'-C4'-C5'-O5'
33	a	535	G7M	C4'-C5'-O5'-P
10	A	2476	H2U	C4'-C5'-O5'-P
10	A	2530	2MA	O4'-C1'-N9-C8

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1942	3TD	1	0
10	A	1966	5MU	2	0
33	a	1412	4OC	1	0
10	A	792	5MU	1	0
33	a	1509	UR3	1	0
10	A	2472	2MG	1	0
33	a	1529	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 149 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PUT	A	3101	-	5,5,5	0.11	0	4,4,4	0.15	0
57	PUT	A	3102	-	5,5,5	0.10	0	4,4,4	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PUT	A	3101	-	-	0/3/3/3	-
57	PUT	A	3102	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	3102	PUT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

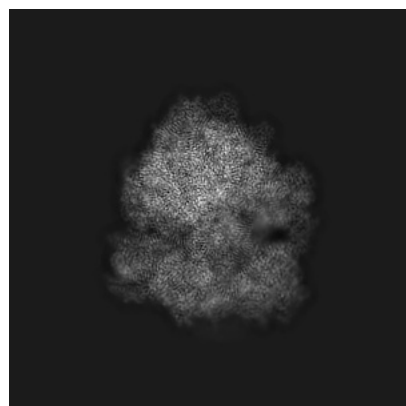
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51357. These allow visual inspection of the internal detail of the map and identification of artifacts.

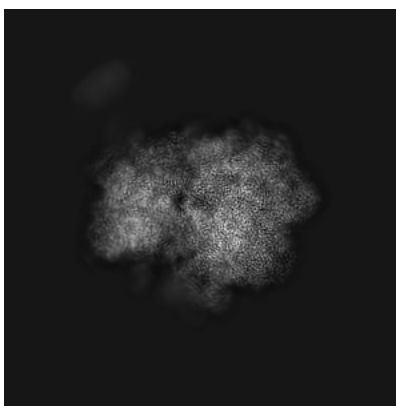
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

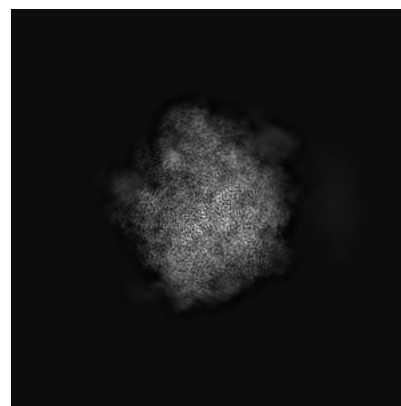
6.1.1 Primary map



X

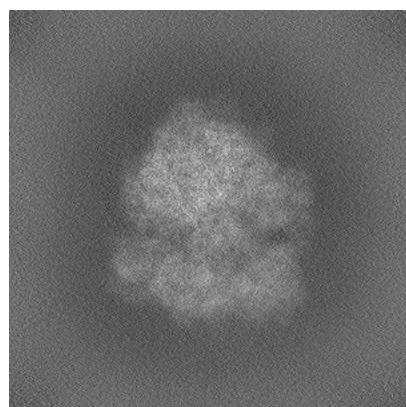


Y

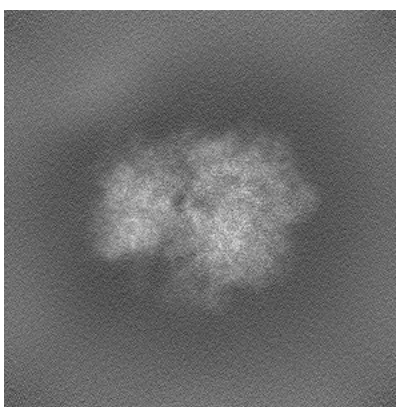


Z

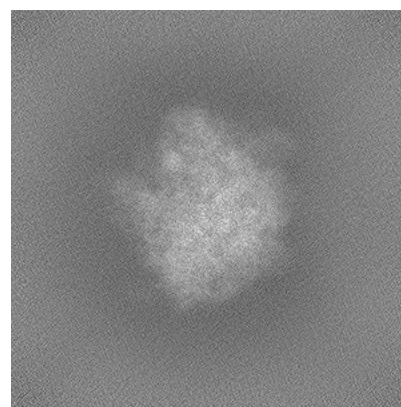
6.1.2 Raw map



X



Y

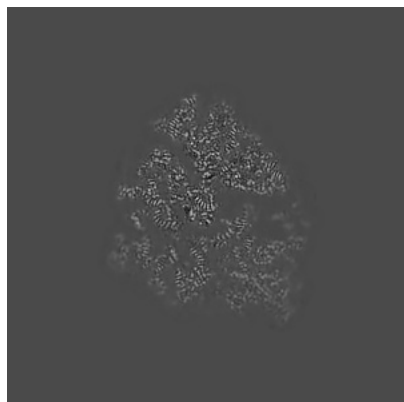


Z

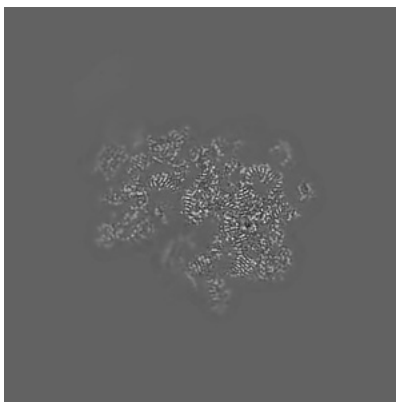
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

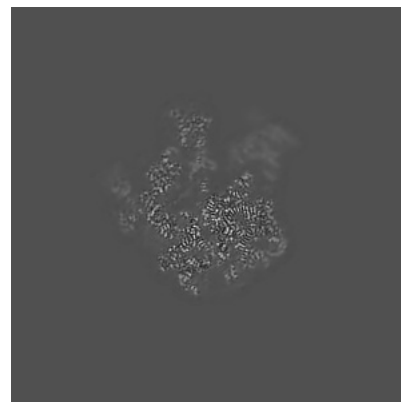
6.2.1 Primary map



X Index: 300

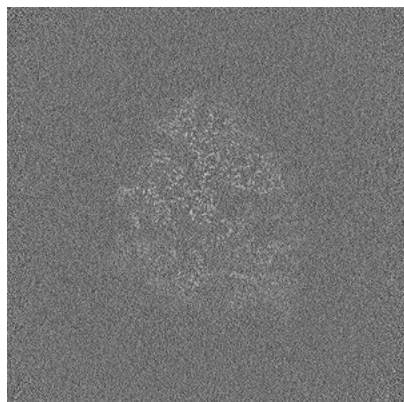


Y Index: 300

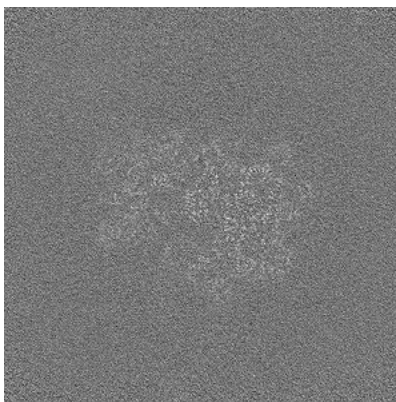


Z Index: 300

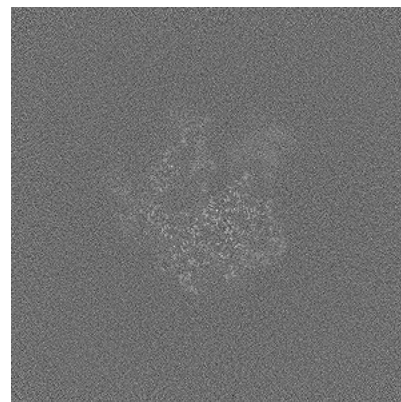
6.2.2 Raw map



X Index: 300



Y Index: 300

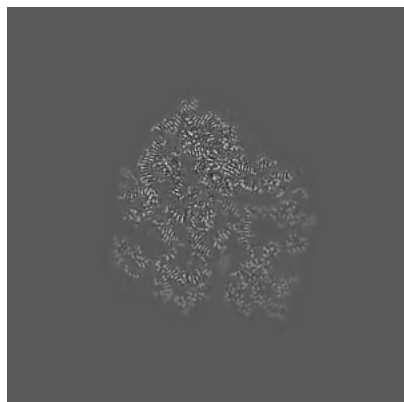


Z Index: 300

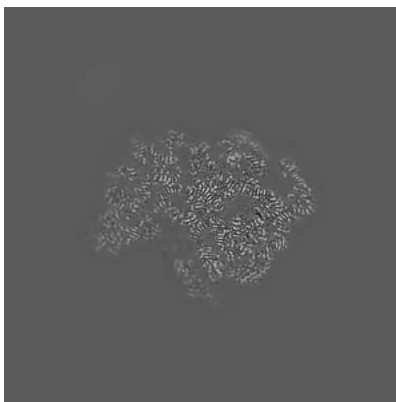
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

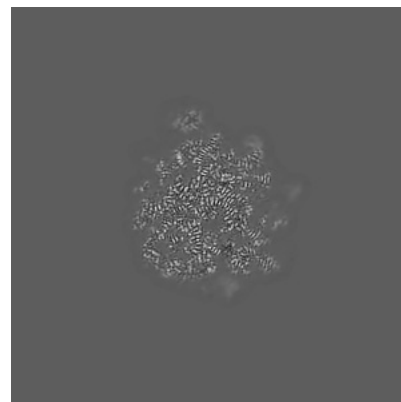
6.3.1 Primary map



X Index: 291

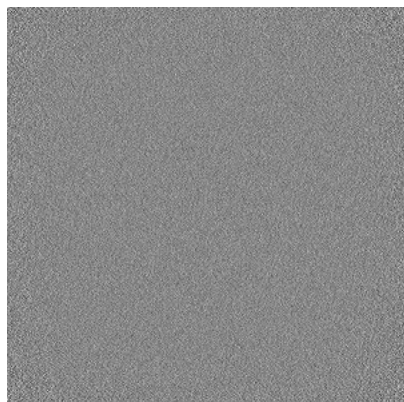


Y Index: 277

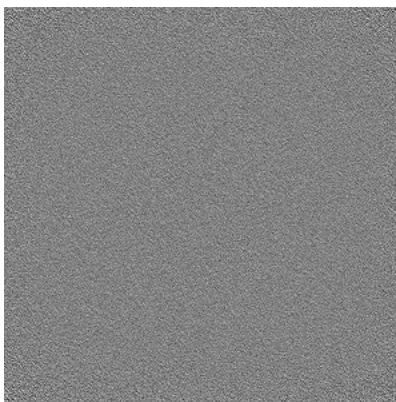


Z Index: 360

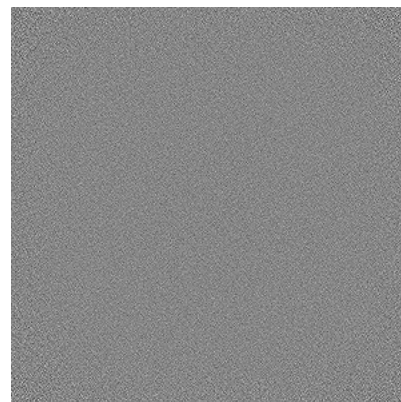
6.3.2 Raw map



X Index: 0



Y Index: 0

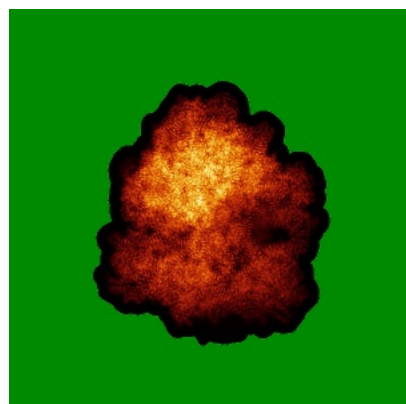


Z Index: 0

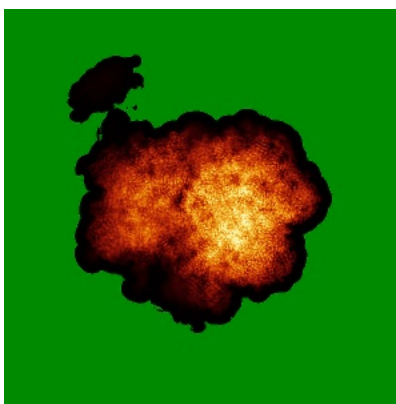
The images above show the largest variance slices of the map in three orthogonal directions.

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

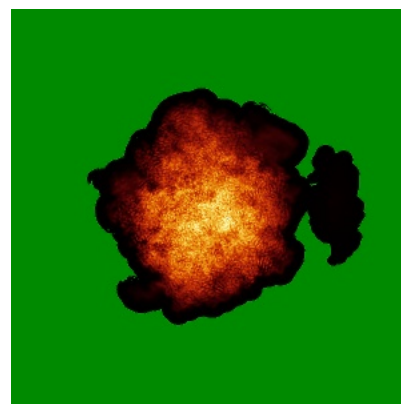
6.4.1 Primary map



X

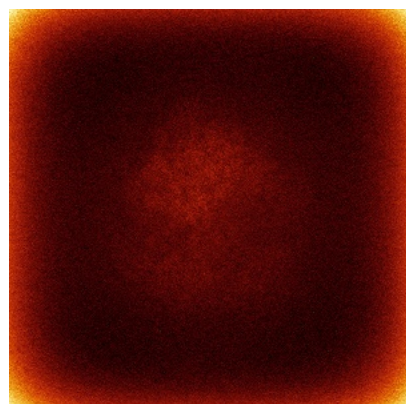


Y

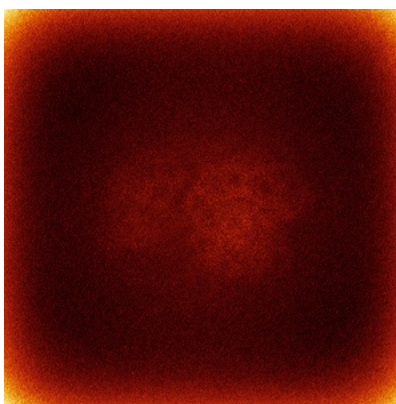


Z

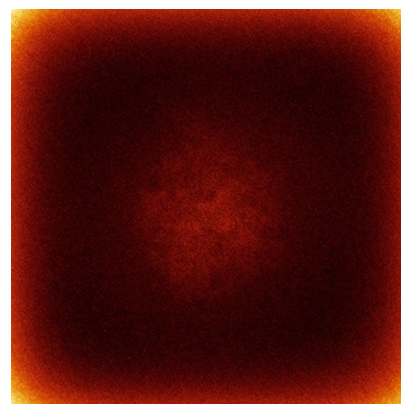
6.4.2 Raw map



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](#)

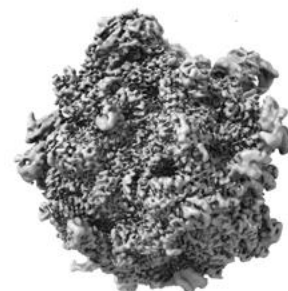
6.5.1 Primary map



X



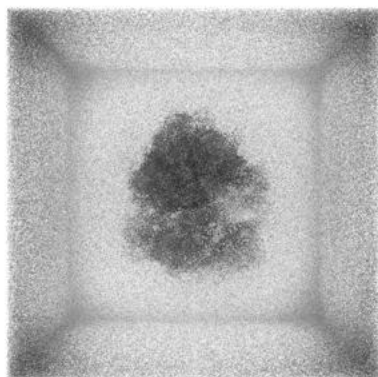
Y



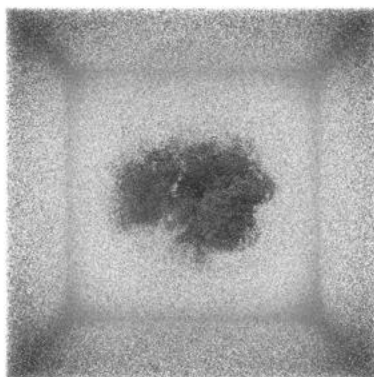
Z

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.

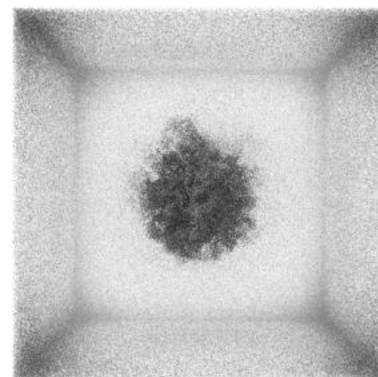
6.5.2 Raw map



X



Y



Z

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.

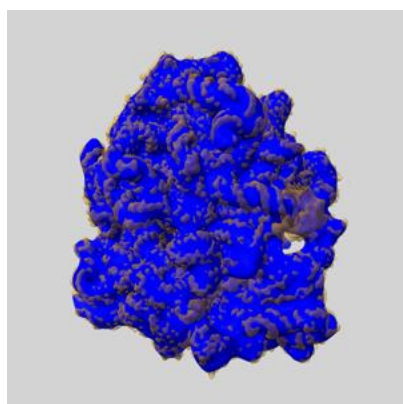
6.6 Mask visualisation [i](#)

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

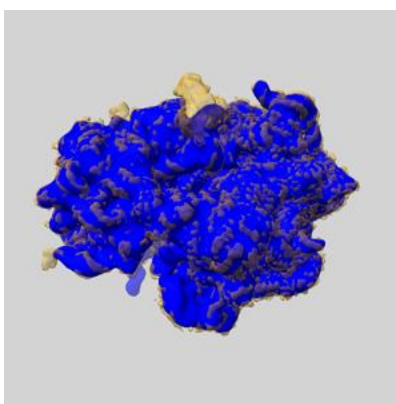
A mask typically either:

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

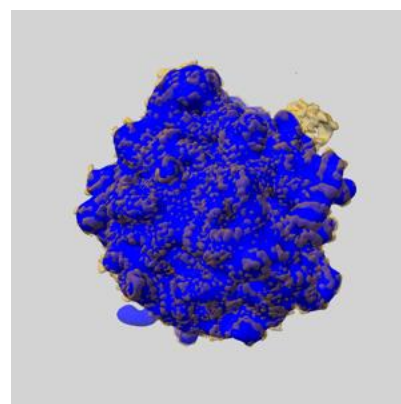
6.6.1 emd_51357_msk_1.map [i](#)



X



Y

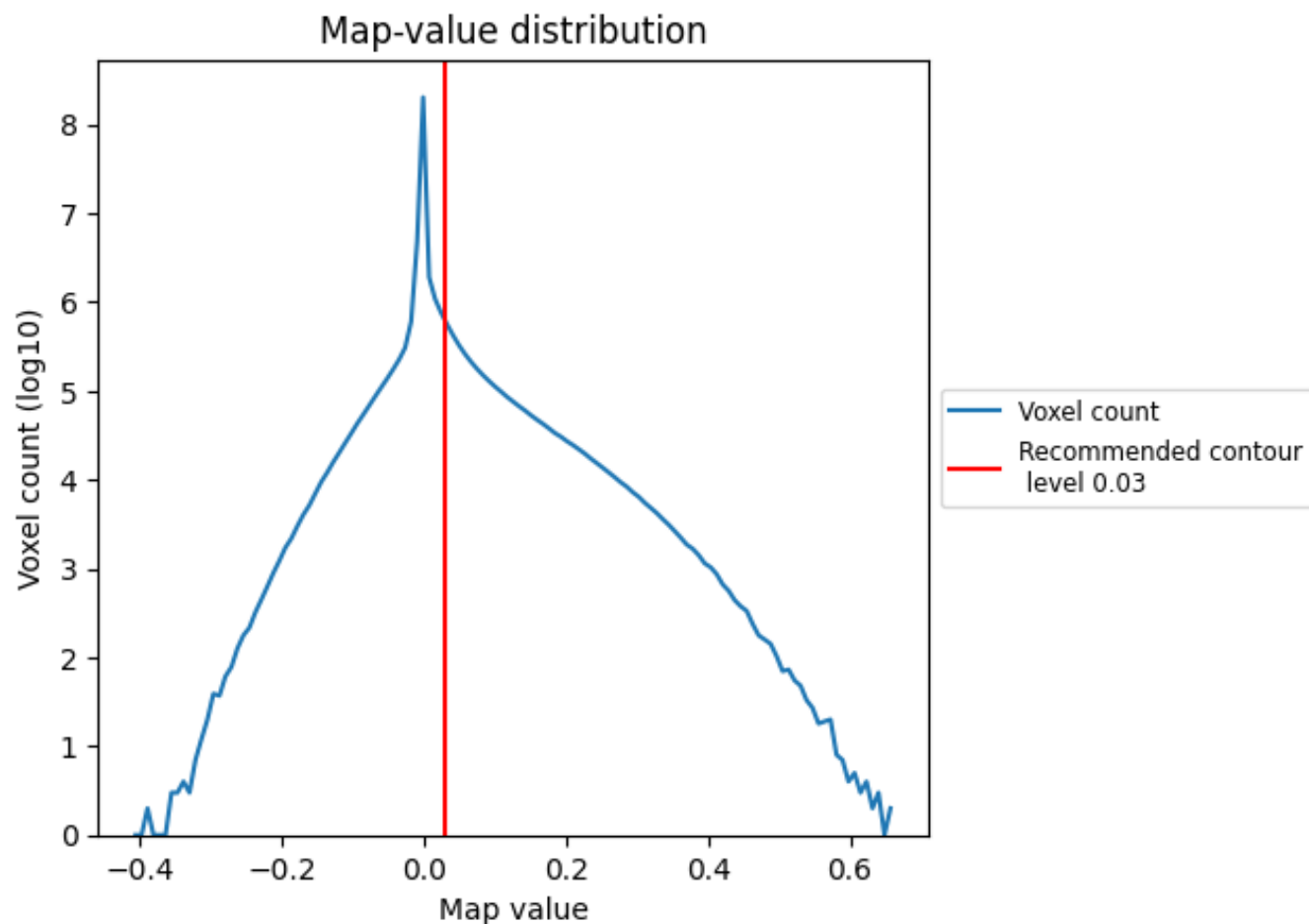


Z

7 Map analysis [i](#)

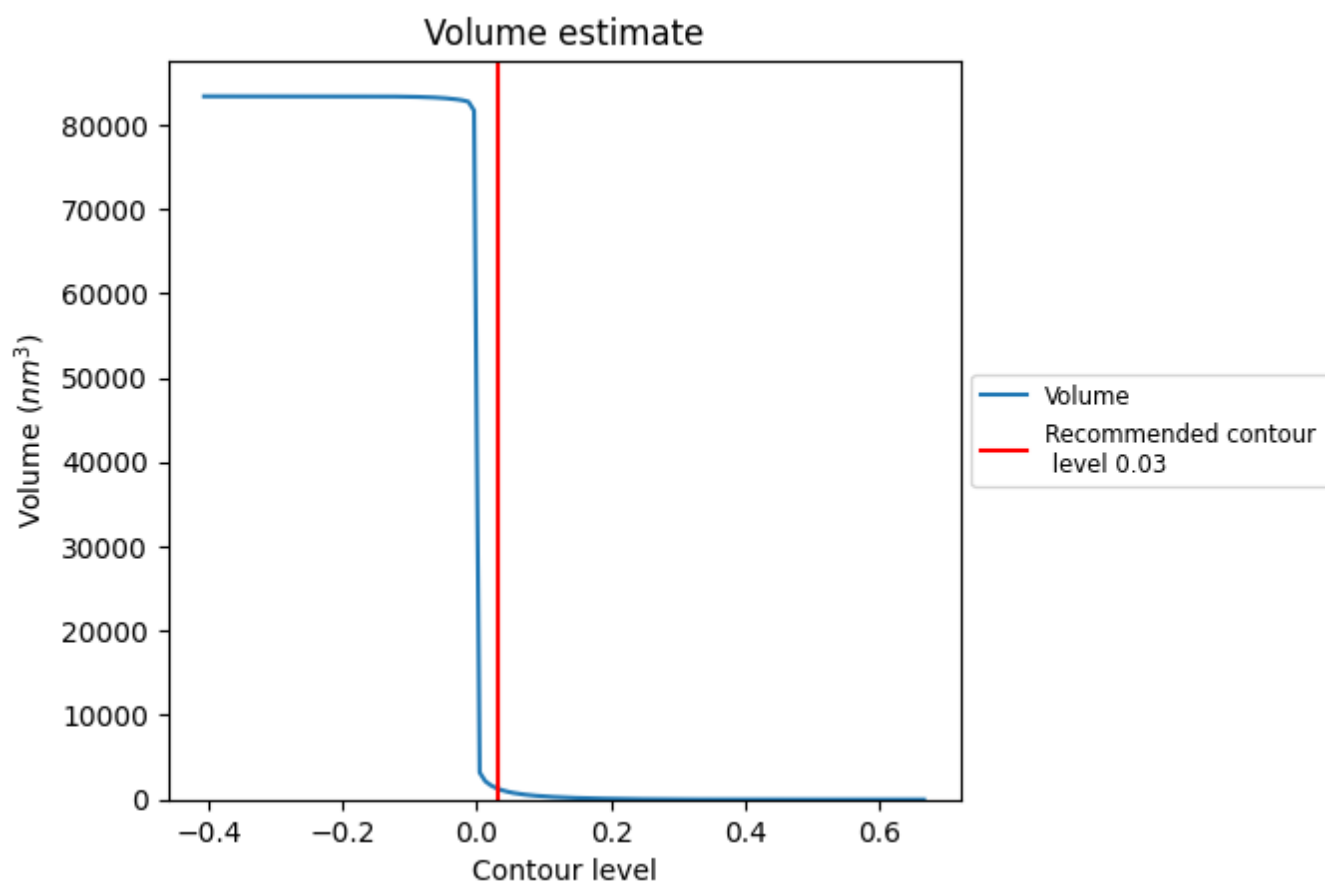
This section contains the results of statistical analysis of the map.

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.

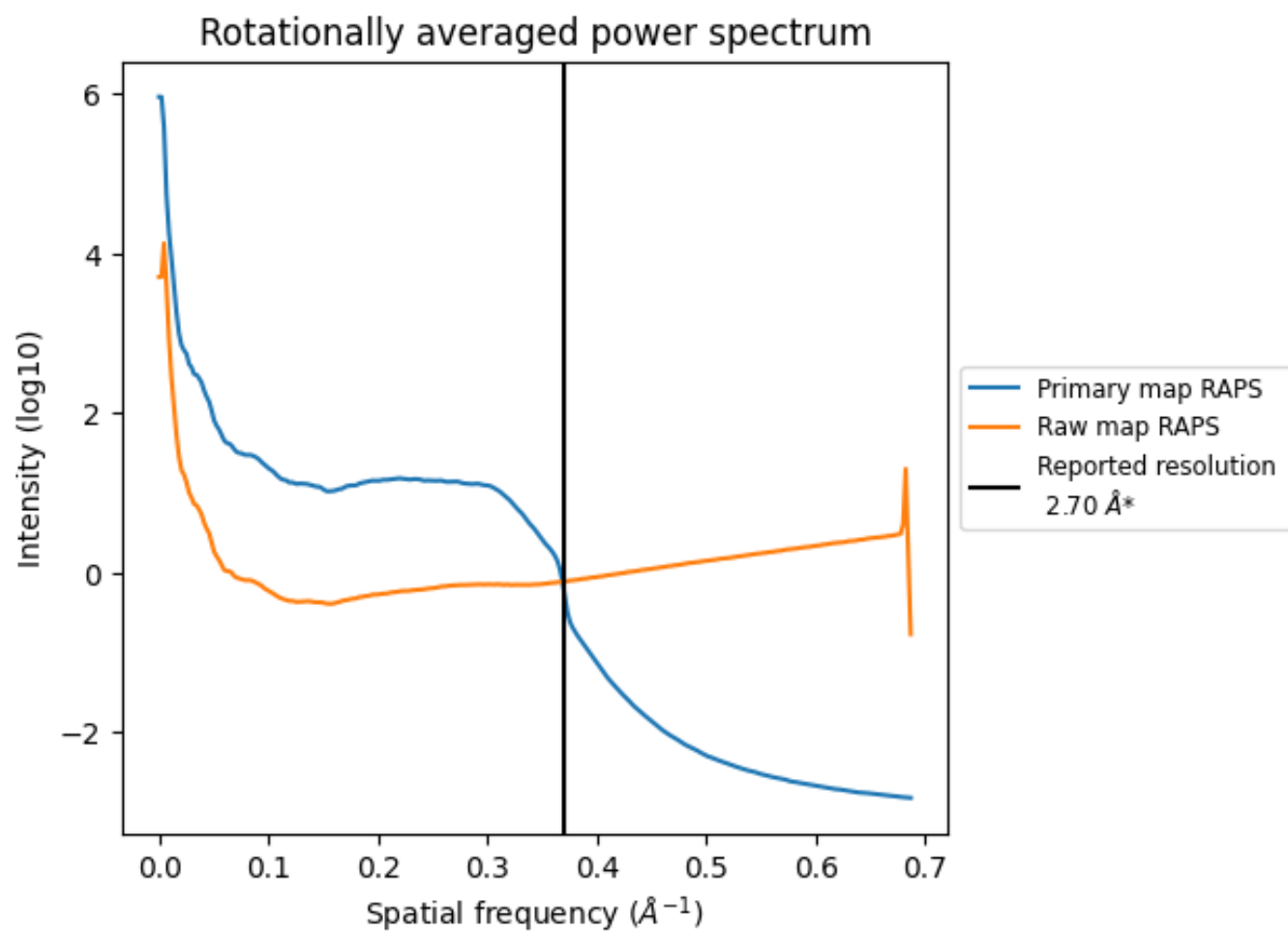
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1325 nm^3 ; this corresponds to an approximate mass of 1197 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 ⓘ

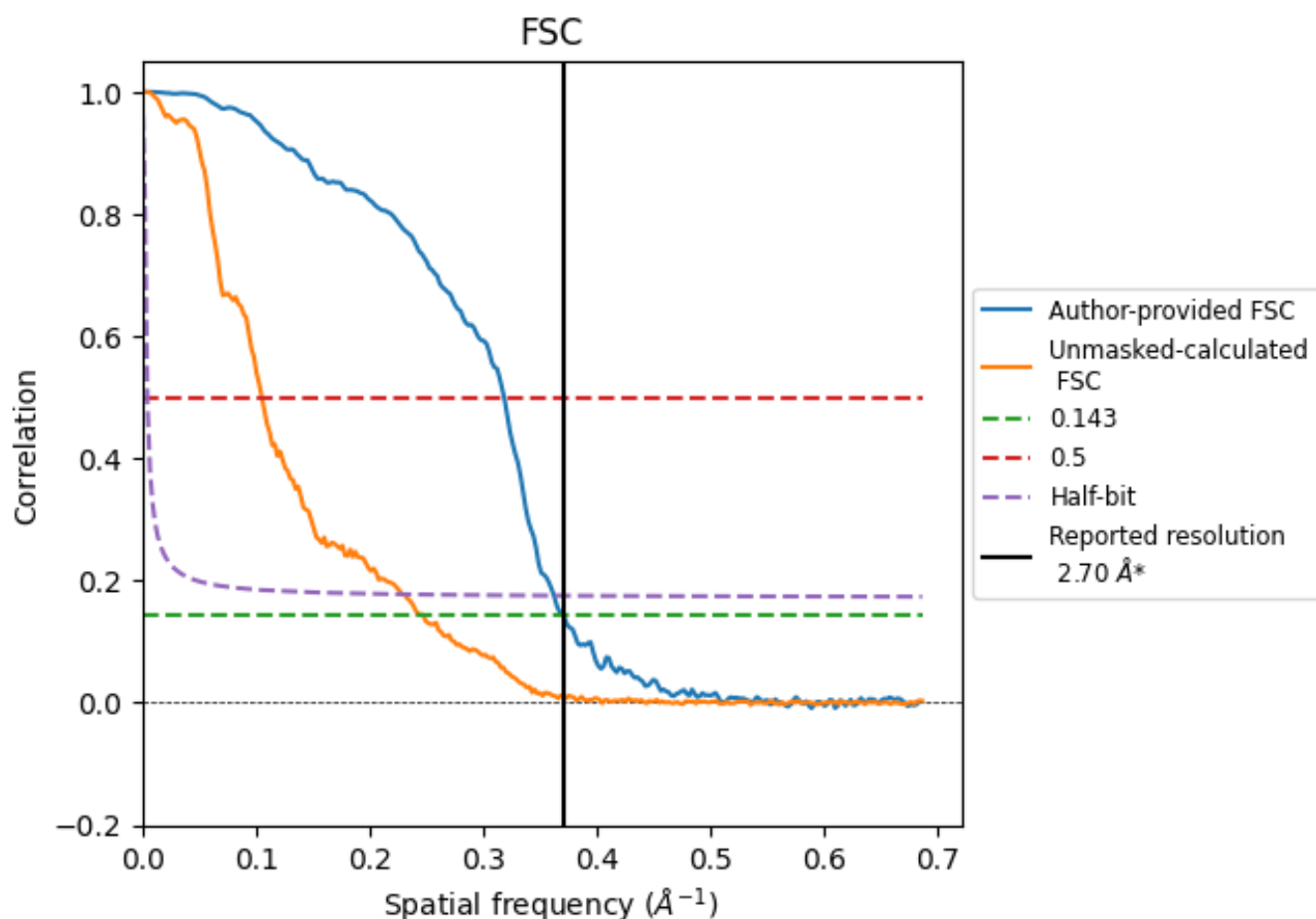


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates

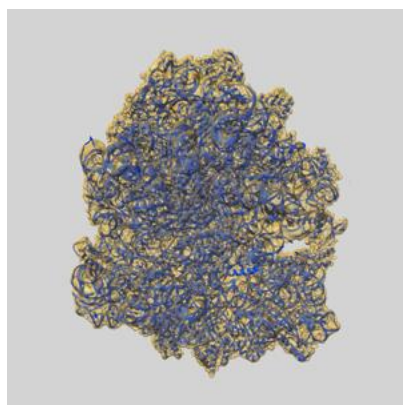
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.14	2.76
Unmasked-calculated*	4.04	9.50	4.37

*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 4.04 differs from the reported value 2.7 by more than 10 %

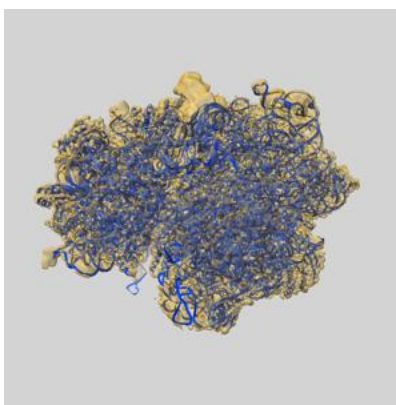
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51357 and PDB model 9GHH. Per-residue inclusion information can be found in section [3](#) on page [15](#).

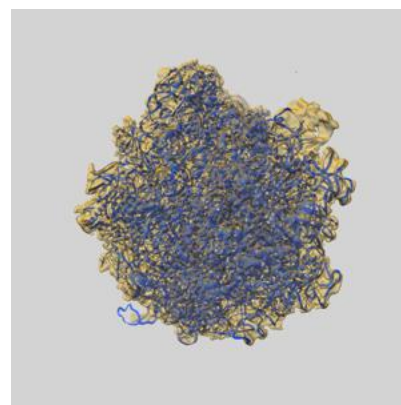
9.1 Map-model overlay [i](#)



X



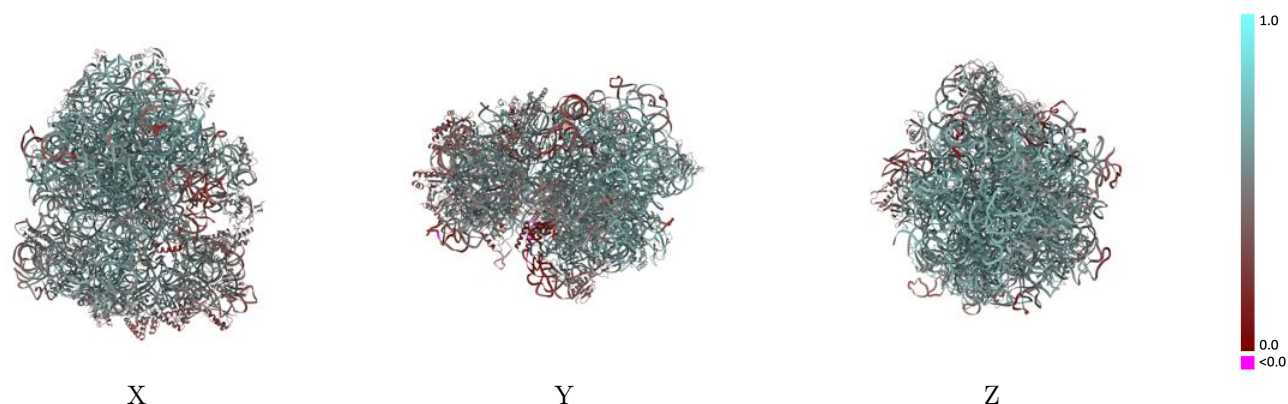
Y



Z

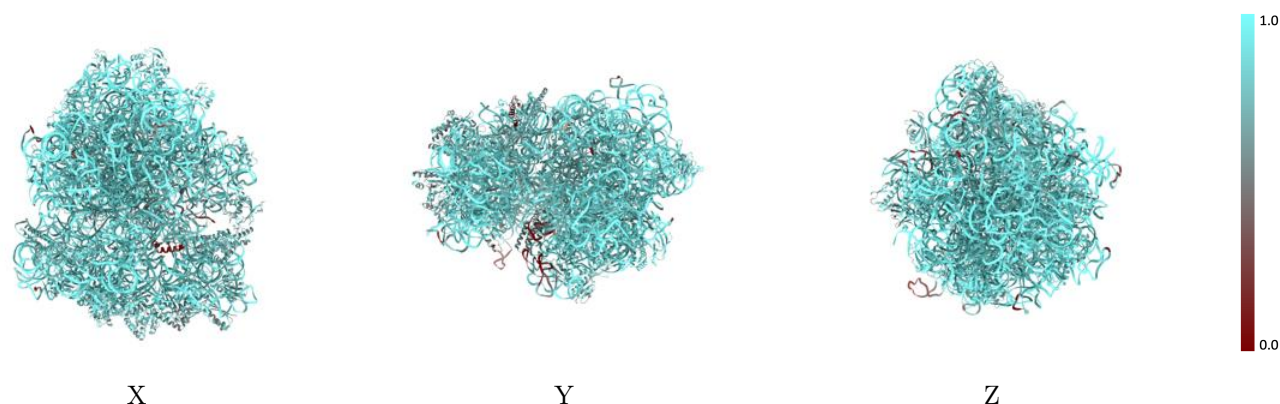
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



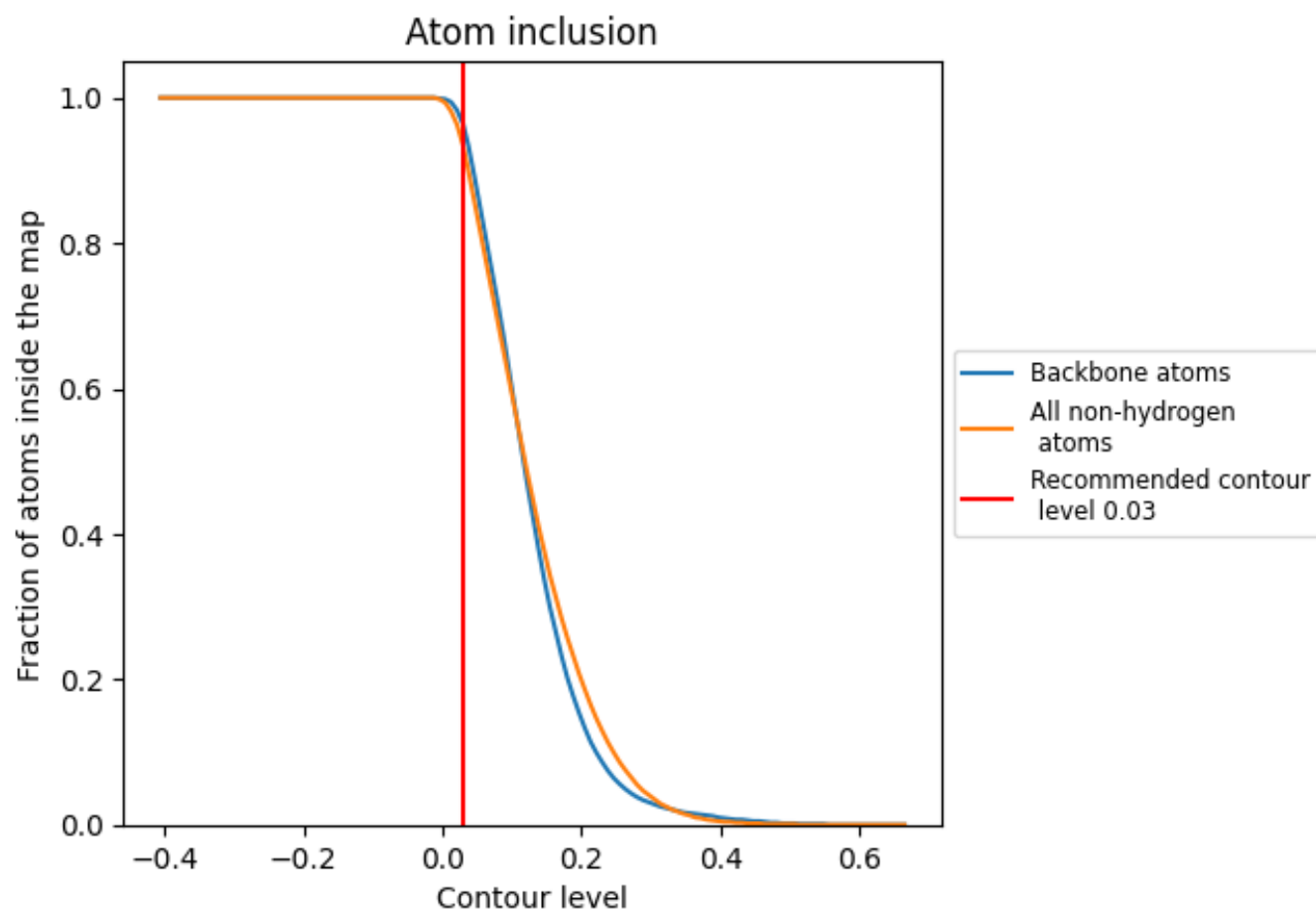
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 93% 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	 0.9330	 0.5490
1	 0.9270	 0.5690
2	 0.8820	 0.5150
3	 0.9580	 0.5970
4	 0.7490	 0.3960
5	 0.9360	 0.5960
6	 0.7830	 0.4800
7	 0.9880	 0.6520
8	 0.9800	 0.6400
9	 0.9210	 0.5660
A	 0.9730	 0.5950
B	 0.9770	 0.5380
C	 0.5350	 0.2210
D	 0.8040	 0.2620
F	 0.9310	 0.5280
G	 0.9620	 0.6190
H	 0.9550	 0.6130
I	 0.9280	 0.5860
J	 0.8100	 0.4490
K	 0.7860	 0.4070
M	 0.9490	 0.6040
N	 0.9540	 0.5970
O	 0.9380	 0.5860
P	 0.9280	 0.5780
Q	 0.9460	 0.5910
R	 0.8440	 0.4790
S	 0.9300	 0.5840
T	 0.9640	 0.6200
U	 0.9370	 0.5900
V	 0.9580	 0.6120
W	 0.9380	 0.5630
X	 0.8640	 0.5000
Y	 0.8120	 0.4410
Z	 0.9560	 0.5900
a	 0.9610	 0.5390



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Chain	Atom inclusion	Q-score
b	 0.8670	 0.4360
c	 0.7470	 0.3910
d	 0.7710	 0.4290
e	 0.8560	 0.4870
f	 0.9240	 0.5500
g	 0.8510	 0.5020
h	 0.7760	 0.4150
i	 0.8940	 0.5360
j	 0.8120	 0.4240
k	 0.7550	 0.3940
l	 0.8180	 0.4670
m	 0.8880	 0.5380
n	 0.8160	 0.4450
o	 0.8840	 0.4990
p	 0.8890	 0.5220
q	 0.8480	 0.4890
r	 0.8610	 0.5030
s	 0.8900	 0.5250
t	 0.7760	 0.4270
u	 0.8730	 0.5150
v	 0.3230	 0.2290