



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:42 PM UTC

PDB ID : 6YS3 / pdb_00006ys3
EMDB ID : EMD-10891
Title : Cryo-EM structure of the 50S ribosomal subunit at 2.58 Angstroms with modeled GBC SecM peptide
Authors : Schulte, L.; Reitz, J.; Kudlinzki, D.; Hodirnau, V.V.; Frangakis, A.; Schwalbe, H.
Deposited on : 2020-04-20
Resolution : 2.58 Å (reported)
Based on initial model : 3JBU

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

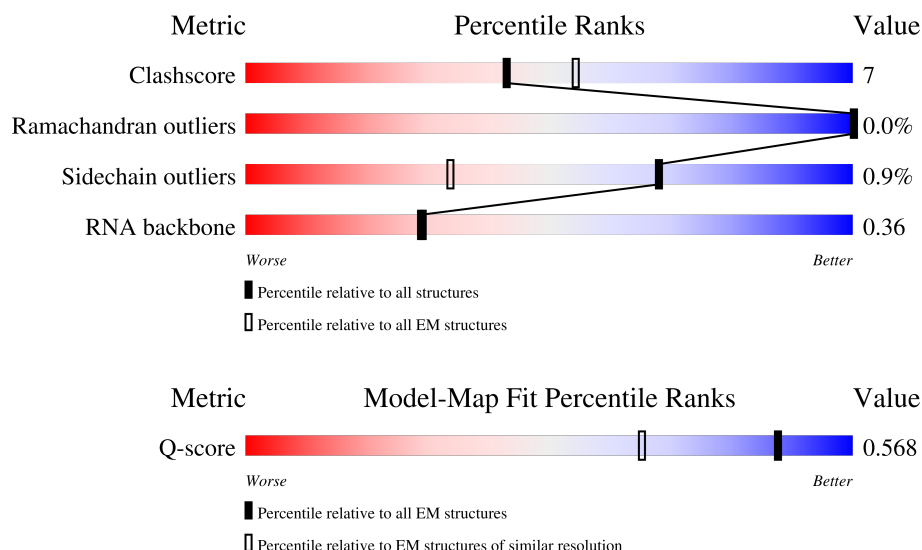
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.58 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.



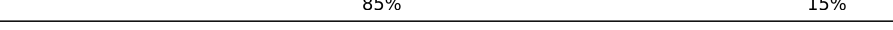
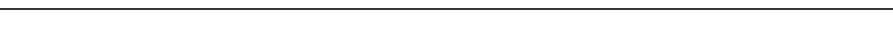
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

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

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

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Mol	Chain	Length	Quality of chain
4	3	57	 77% 19% .
5	4	55	 82% 9% 9%
6	6	46	 83% 17%
7	7	65	 85% 12% . .
8	8	38	 92% 8%
9	a	120	 58% 30% 10% .
10	b	2906	 61% 32% 6% .
11	c	273	 82% 18% .
12	d	209	 89% 11% .
13	e	201	 87% 12% .
14	f	179	 72% 26% . .
15	g	177	 86% 12% . .
16	h	149	 20% 5% . 74%
17	j	142	 85% 15%
18	k	123	 77% 22% .
19	l	144	 78% 21% .
20	m	136	 79% 21%
21	n	127	 84% 10% 6%
22	o	117	 77% 21% . .
23	p	115	 87% 11% .
24	q	118	 90% 9% .
25	r	103	 82% 15% .
26	s	110	 70% 29% .
27	t	100	 75% 17% . 7%
28	u	104	 85% 13% .

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Mol	Chain	Length	Quality of chain
29	v	75	8% 32% 52% 16%
30	w	94	86% 13%
31	y	85	71% 15% 13%
32	z	61	10% 39% 7% 43%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90553 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	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

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

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

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

- Molecule 4 is a protein called 50S ribosomal protein L32.

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

- Molecule 5 is a protein called 50S ribosomal protein L33.

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

- Molecule 6 is a protein called 50S ribosomal protein L34.

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

- Molecule 7 is a protein called 50S ribosomal protein L35.

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

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2888	Total	C	N	O	P	0	0
			62008	27660	11413	20047	2888		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

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

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1042	648	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	99	Total	C	N	O	S	0	0
			791	500	149	140	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	75	Total	C	N	O	P	0	0
			1583	707	270	531	75		

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	74	Total	C	N	O	S	0	0
			559	348	112	98	1		

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	35	Total	C	N	O	S	0	0
			275	172	48	51	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-12	MET	-	initiating methionine	UNP P02526
z	-11	GLY	-	expression tag	UNP P02526
z	-10	HIS	-	expression tag	UNP P02526
z	-9	HIS	-	expression tag	UNP P02526
z	-8	HIS	-	expression tag	UNP P02526
z	-7	HIS	-	expression tag	UNP P02526
z	-6	HIS	-	expression tag	UNP P02526
z	-5	HIS	-	expression tag	UNP P02526
z	-4	HIS	-	expression tag	UNP P02526
z	-3	HIS	-	expression tag	UNP P02526
z	-2	HIS	-	expression tag	UNP P02526
z	-1	HIS	-	expression tag	UNP P02526

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Chain	Residue	Modelled	Actual	Comment	Reference
z	150	PHE	ASN	conflict	UNP P02526
z	152	THR	ILE	conflict	UNP P02526
z	153	PRO	ARG	conflict	UNP P02526
z	155	TRP	-	expression tag	UNP P02526
z	156	ILE	-	expression tag	UNP P02526
z	157	SER	-	expression tag	UNP P02526
z	158	GLN	-	expression tag	UNP P02526
z	159	ALA	-	expression tag	UNP P02526
z	160	GLN	-	expression tag	UNP P02526
z	161	GLY	-	expression tag	UNP P02526
z	162	ILE	-	expression tag	UNP P02526
z	163	ARG	-	expression tag	UNP P02526
z	164	ALA	-	expression tag	UNP P02526
z	165	GLY	-	expression tag	UNP P02526

3 Residue-property plots

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

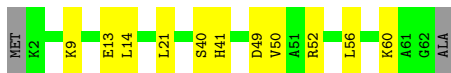
- Molecule 1: 50S ribosomal protein L28

Chain 0: 



- Molecule 2: 50S ribosomal protein L29

Chain 1: 



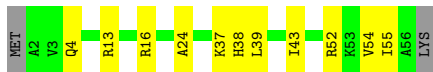
- Molecule 3: 50S ribosomal protein L30

Chain 2: 



- Molecule 4: 50S ribosomal protein L32

Chain 3: 



- Molecule 5: 50S ribosomal protein L33

Chain 4: 



- Molecule 6: 50S ribosomal protein L34

Chain 6:  83% 17%



- Molecule 7: 50S ribosomal protein L35

Chain 7:  85% 12% ..



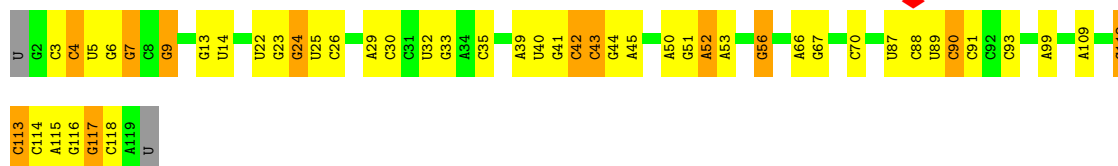
- Molecule 8: 50S ribosomal protein L36

Chain 8:  92% 8%



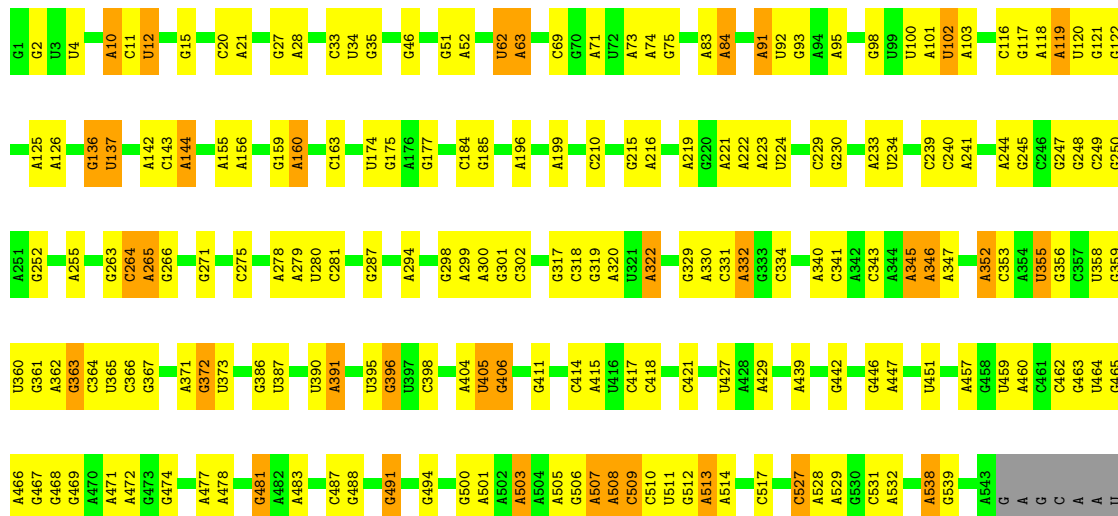
- Molecule 9: 5S rRNA

Chain a:  58% 30% 10% .

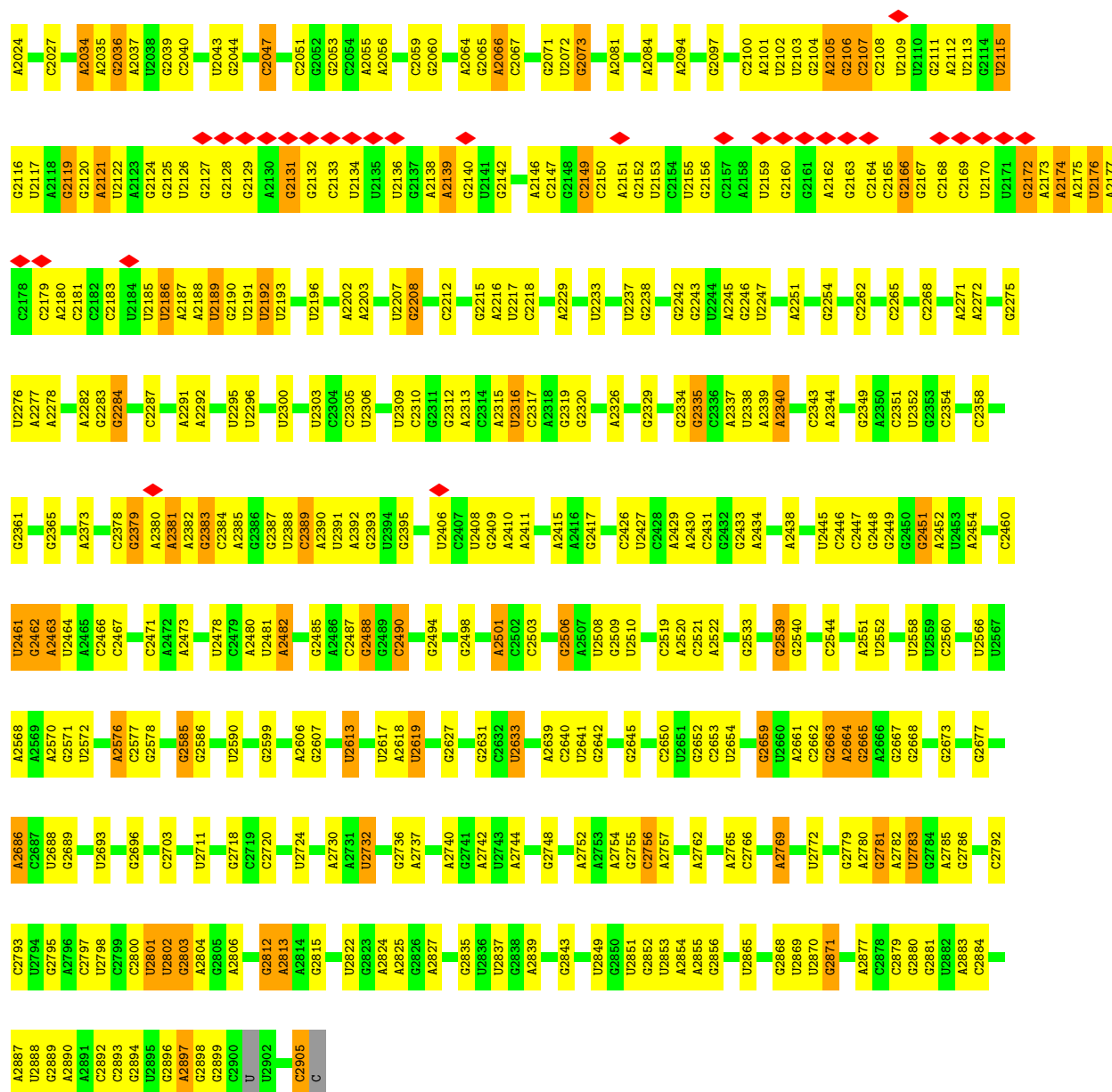


- Molecule 10: 23S rRNA

Chain b:  61% 32% 6% .

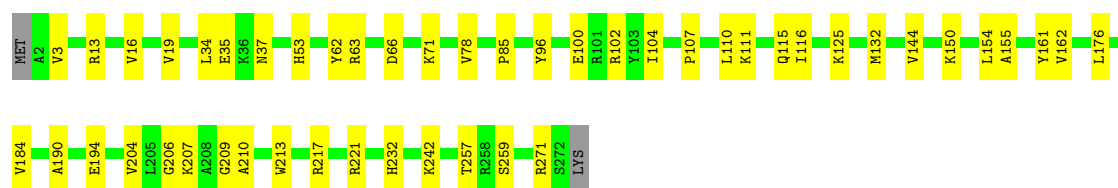


C1999	G1910	G1911	C1912	G1913	G1914	G1915	A1916	A1917	C1918	U1921	A1922	C1923	C1924	A1931	A1932	G1933	G1934	U1935	A1940	A1941	A1942	U1943	U1944	U1959	C1962	U1967	C1971	A1974	U1975	G1976	G1977	C1978	G1979	G1984	A1985	U1986	U1995	G1996	U1997	C1998	C2001	A2009	G2014	A2023										
A1782	U1783	U1784	A1785	A1786	A1787	A1788	A1791	C1792	A1793	G1794	G1799	U1800	C1801	C1802	A1803	A1810	G1813	C1818	G1819	U1820	G1830	A1831	C1835	G1844	G1851	A1856	G1859	A1741	G1740	A1741	C1750	A1616	G1755	A1756	A1757	G1758	A1759	U1760	G1765	C1766	U1771	U1775	A1786	U1887	G1888	G1892								
C1559	C1463	U1469	U1470	A1471	A1472	G1473	G1477	U1478	A1479	G1480	G1484	U1488	C1495	A1496	A1497	U1498	U1499	C1500	A1505	A1506	A1507	A1510	A1511	U1525	G1526	A1530	G1531	G1532	C1533	A1534	C1535	C1538	G1539	G1540	U1541	G1542	C1543	U1544	G1545	C1549	C1552	A1553	A1554	A1555	U1556	G1557	C1558							
A1361	G1366	A1367	A1368	A1369	G1370	A1380	U1381	G1382	A1385	C1388	A1394	A1395	U1396	A1397	U1398	U1402	U1411	U1412	U1413	U1417	G1418	A1421	A1422	G1423	G1428	A1429	C1430	G1431	G1432	A1433	G1434	A1435	A1436	A1441	U1442	G1443	U1444	U1445	G1452	C1453	G1454	A1455	C1456	G1457	G1461									
G1250	U1251	G1252	A1255	A1256	U1257	G1258	C1259	U1260	A1267	G1268	G1273	A1274	U1275	A1276	A1277	A1278	G1281	A1286	A1289	G1290	C1291	G1301	A1302	A1303	A1304	C1313	C1317	G1321	C1322	A1323	A1324	U1328	A1329	A1330	U1331	C1332	G1333	G1334	G1335	G1336	U1342	U1346	C1353	U1354	A1355									
A1135	A1136	C1137	G1138	U1143	A1144	G1165	G1170	A1171	C1172	G1173	C1174	U1175	U1176	A1177	U1178	G1179	G1187	G1188	G1189	U1190	G1197	U1201	A1206	A1207	G1208	C1209	G1212	U1213	G1214	G1218	U1226	G1229	G1234	G1237	G1238	A1239	G1240	U1242	A1243	U1244	G1245	A1246	G1247	A1248	A1249									
C1066	U1067	U1068	A1069	G1070	A1071	A1072	G1073	C1074	A1075	C1076	C1077	C1078	A1079	C1081	A1082	U1083	U1085	A1086	A1087	A1088	G1089	A1090	A1091	A1092	U1096	A1097	U1098	U1099	A1100	G1101	C1102	U1103	C1104	A1105	C1106	U1107	G1108	C1111	G1112	A1113	G1114	U1115	C1116	G1117	G1118	C1119	C1120	U1121	G1127	A1128	U1132	U1133	U1134	
A990	G991	A992	C997	A998	G999	C1000	U1001	A1002	A1003	G1004	G1005	U1006	C1007	C1008	C1009	A1012	G1013	U1014	C1015	U1021	A1022	A1023	G1024	U1025	G1028	A1029	A1030	U1035	G1036	U1037	G	G1039	G1040	A1041	A1042	G1043	G1044	C	G1046	C1047	A1048	G1049	U1055	A1056	G1057	G1058	A1059	G976	U1060	G1061	U1062	U1063	G1064	G1065
A879	A880	G881	G882	G883	A884	G885	U886	C887	A888	U889	C890	C891	C892	G893	A894	C895	U896	U897	A898	C899	A902	G909	A912	A913	C914	U921	A922	U933	A943	G944	A947	C948	A949	C950	G954	C963	G964	U965	C966	A974	A975	G976	G950	A985	A986	C989								
A763	U764	G765	U766	A767	C767	G777	G778	A783	A784	A785	G786	G787	A791	U792	C793	A794	A795	A796	C807	C808	G809	G811	U812	U813	C814	A821	U829	U830	A831	G832	A835	G836	G858	G859	G860	G861	A868	G871	U874	C875	G876	G877	C878											
G649	G653	U654	U655	A656	A657	G658	U659	U660	G661	G665	A670	G671	A672	C673	C674	G686	A687	U688	C689	A695	C700	U704	U705	G706	U712	U715	C719	A720	A723	C725	A729	G730	G731	A732	G735	A736	G740	U749	G750	A754	G759													
C	U	G553	A558	C559	A565	U568	U569	U570	U571	G572	U575	A576	A577	U578	C579	G580	U581	C583	A584	G587	A588	C589	U590	A604	A605	G606	G607	U608	A615	A616	U617	A623	G624	A629	G630	G631	C636	C637	G638	A639	U641	C642	U644	A645	U648									



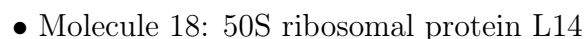
• Molecule 11: 50S ribosomal protein L2

Chain c: 82% 18%

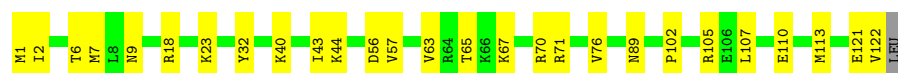


• Molecule 12: 50S ribosomal protein L3

Chain d: 89% 11%

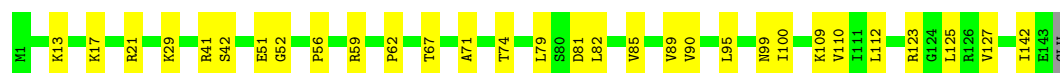


Chain k:  77% 22%



- Molecule 19: 50S ribosomal protein L15

Chain l:  78% 21%



- Molecule 20: 50S ribosomal protein L16

Chain m:  79% 21%



- Molecule 21: 50S ribosomal protein L17

Chain n:  84% 10% 6%



- Molecule 22: 50S ribosomal protein L18

Chain o:  77% 21%



- Molecule 23: 50S ribosomal protein L19

Chain p:  87% 11%



- Molecule 24: 50S ribosomal protein L20

Chain q:  90% 9%



- Molecule 25: 50S ribosomal protein L21

Chain r:  82% 15%



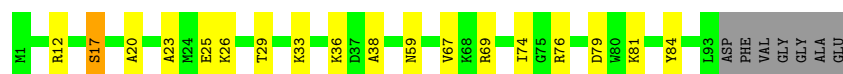
- Molecule 26: 50S ribosomal protein L22

Chain s:  70% 29%



- Molecule 27: 50S ribosomal protein L23

Chain t:  75% 17% 7%



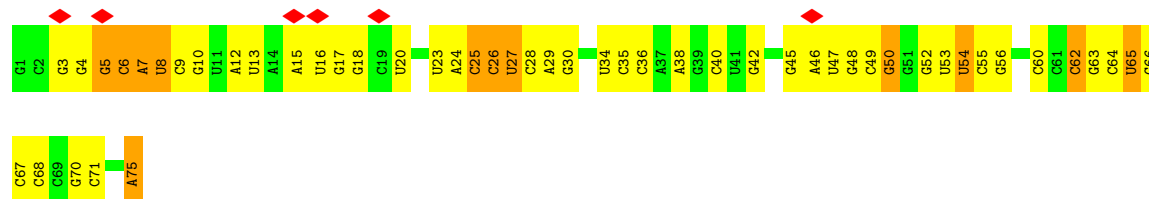
- Molecule 28: 50S ribosomal protein L24

Chain u:  85% 13%



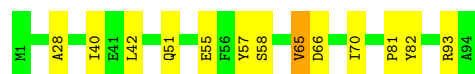
- Molecule 29: glycine-tRNA glyT

Chain v:  8% 32% 52% 16%



- Molecule 30: 50S ribosomal protein L25

Chain w:  86% 13%

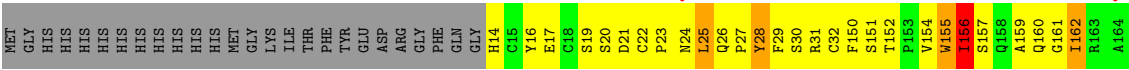


- Molecule 31: 50S ribosomal protein L27

Chain y:  71% 15% 13%



● Molecule 32: Gamma-crystallin B



G165

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00741	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.60	0/635	0.63	0/848
2	1	0.45	0/496	0.57	0/660
3	2	0.56	0/443	0.73	1/593 (0.2%)
4	3	0.67	0/440	0.62	0/588
5	4	0.42	0/416	0.65	1/554 (0.2%)
6	6	0.73	0/380	0.60	0/498
7	7	0.65	0/513	0.60	0/676
8	8	0.66	0/303	0.71	0/397
9	a	0.50	0/2824	0.52	0/4402
10	b	0.67	0/69446	0.53	6/108330 (0.0%)
11	c	0.63	0/2121	0.62	0/2852
12	d	0.63	0/1586	0.65	0/2134
13	e	0.57	0/1571	0.72	3/2113 (0.1%)
14	f	0.38	0/1434	0.73	1/1926 (0.1%)
15	g	0.41	0/1343	0.91	4/1816 (0.2%)
16	h	0.40	0/290	0.74	0/392
17	j	0.59	0/1152	0.56	0/1551
18	k	0.58	0/947	0.62	0/1268
19	l	0.60	0/1051	0.66	2/1400 (0.1%)
20	m	0.59	0/1093	0.58	0/1460
21	n	0.65	0/973	0.69	0/1301
22	o	0.42	0/902	0.69	0/1209
23	p	0.54	0/920	0.56	0/1231
24	q	0.70	0/960	0.61	0/1278
25	r	0.56	0/803	0.61	0/1070
26	s	0.61	0/852	0.57	0/1142
27	t	0.51	0/744	0.62	2/994 (0.2%)
28	u	0.45	0/787	0.75	0/1051
29	v	0.33	0/1764	0.56	0/2744
30	w	0.46	0/766	0.61	2/1025 (0.2%)
31	y	0.63	0/566	0.70	0/750
32	z	0.47	0/284	2.03	15/386 (3.9%)
All	All	0.64	0/98805	0.57	37/148639 (0.0%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	45	HIS	N-CA-C	-23.77	77.55	110.35
32	z	159	ALA	N-CA-C	-17.06	79.94	108.26
32	z	156	ILE	N-CA-C	13.27	136.93	109.34
32	z	28	TYR	N-CA-C	-10.72	86.76	107.44
15	g	46	ALA	N-CA-C	-10.34	88.78	110.80
32	z	151	SER	N-CA-C	10.11	127.03	111.56
13	e	124	PHE	N-CA-C	-9.60	92.33	108.26
32	z	155	TRP	N-CA-C	-9.31	90.98	110.80
32	z	162	ILE	N-CA-C	7.92	125.82	109.34
32	z	160	GLN	N-CA-C	7.75	123.80	113.72
32	z	152	THR	N-CA-C	-7.58	99.46	108.25
5	4	5	ILE	N-CA-C	-7.45	105.09	112.17
15	g	77	ILE	N-CA-C	-7.11	105.61	112.29
13	e	125	SER	N-CA-C	-7.00	98.08	108.79
32	z	161	GLY	N-CA-C	6.95	126.99	115.66
10	b	1301	G	C2'-C3'-O3'	6.86	123.99	113.70
32	z	19	SER	N-CA-C	6.74	120.31	109.86
32	z	151	SER	CB-CA-C	-6.74	98.43	111.03
3	2	44	ILE	N-CA-C	-6.52	106.44	112.96
27	t	17	SER	CA-C-N	6.44	133.83	121.54
27	t	17	SER	C-N-CA	6.44	133.83	121.54
32	z	27	PRO	CA-C-N	-6.38	112.90	122.47
32	z	27	PRO	C-N-CA	-6.38	112.90	122.47
32	z	156	ILE	N-CA-CB	-6.35	100.75	111.23
30	w	65	VAL	CA-C-N	6.25	131.01	122.07
30	w	65	VAL	C-N-CA	6.25	131.01	122.07
15	g	45	HIS	N-CA-CB	6.09	118.79	110.38
19	l	52	GLY	CA-C-N	-5.64	112.68	122.83
19	l	52	GLY	C-N-CA	-5.64	112.68	122.83
14	f	171	ALA	N-CA-C	-5.53	105.79	112.54
10	b	705	U	C2'-C3'-O3'	5.35	121.73	113.70
32	z	159	ALA	CB-CA-C	5.28	118.28	110.14
10	b	2462	G	O4'-C1'-N9	5.27	116.11	108.20
10	b	2539	G	C2'-C3'-O3'	5.16	121.44	113.70
13	e	124	PHE	CB-CA-C	5.13	118.05	110.14
10	b	2868	G	C2'-C3'-O3'	5.03	121.25	113.70
10	b	1597	C	C2'-C3'-O3'	5.03	121.25	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	5	0
2	1	495	0	526	8	0
3	2	439	0	482	2	0
4	3	434	0	445	9	0
5	4	409	0	440	2	0
6	6	377	0	418	10	0
7	7	504	0	572	10	0
8	8	302	0	341	3	0
9	a	2528	0	1283	49	0
10	b	62008	0	31185	478	0
11	c	2082	0	2154	33	0
12	d	1565	0	1616	16	0
13	e	1552	0	1619	26	0
14	f	1410	0	1444	48	0
15	g	1323	0	1371	12	0
16	h	287	0	307	6	0
17	j	1129	0	1162	15	0
18	k	938	0	1012	15	0
19	l	1042	0	1121	21	0
20	m	1074	0	1157	20	0
21	n	960	0	1000	10	0
22	o	892	0	923	20	0
23	p	908	0	956	9	0
24	q	947	0	1019	9	0
25	r	791	0	811	11	0
26	s	845	0	908	39	0
27	t	738	0	807	11	0
28	u	779	0	831	9	0
29	v	1583	0	807	38	0
30	w	753	0	780	10	0
31	y	559	0	575	11	0
32	z	275	0	247	79	0
All	All	90553	0	58971	875	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 7.

All (875) 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)
32:z:23:PRO:HD2	32:z:32:CYS:SG	1.60	1.40
10:b:462:C:C5'	32:z:24:ASN:HB3	1.61	1.27
10:b:462:C:H4'	32:z:24:ASN:O	1.43	1.17
29:v:53:U:H2'	29:v:54:U:H5'	1.25	1.16
26:s:91:GLY:HA3	32:z:155:TRP:CH2	1.81	1.14
32:z:22:CYS:SG	32:z:23:PRO:HD2	1.88	1.13
26:s:91:GLY:HA3	32:z:155:TRP:HH2	0.96	1.11
32:z:26:GLN:OE1	32:z:32:CYS:HA	1.52	1.09
29:v:26:C:H2'	29:v:27:U:C5	1.88	1.08
10:b:2066:A:N7	32:z:162:ILE:HD11	1.66	1.07
29:v:75:A:O3'	32:z:165:GLY:C	1.97	1.07
10:b:52:A:N7	10:b:119:A:N6	2.03	1.06
26:s:90:LYS:O	32:z:155:TRP:HZ3	1.40	1.04
10:b:2271:A:N6	10:b:2276:U:H3	1.55	1.04
10:b:462:C:H5'	32:z:24:ASN:CB	1.89	1.03
10:b:462:C:C5'	32:z:24:ASN:CB	2.37	1.02
26:s:83:LYS:HB2	32:z:20:SER:HB3	1.42	1.02
30:w:65:VAL:O	30:w:66:ASP:OD1	1.75	1.02
26:s:85:ILE:HD11	32:z:22:CYS:HA	1.43	1.01
29:v:53:U:C2'	29:v:54:U:H5'	1.91	0.99
32:z:26:GLN:OE1	32:z:32:CYS:CA	2.11	0.98
10:b:2066:A:C5	32:z:162:ILE:HD11	1.98	0.97
26:s:90:LYS:O	32:z:155:TRP:CZ3	2.18	0.97
13:e:134:LEU:HA	13:e:137:LYS:HB2	1.46	0.96
10:b:588:A:N1	10:b:811:G:O2'	1.97	0.96
32:z:23:PRO:CD	32:z:32:CYS:SG	2.53	0.95
10:b:462:C:H5'	32:z:24:ASN:HB3	0.97	0.95
26:s:91:GLY:CA	32:z:155:TRP:HH2	1.79	0.95
10:b:2271:A:H62	10:b:2276:U:H3	0.98	0.94
32:z:22:CYS:SG	32:z:23:PRO:CD	2.55	0.94
10:b:1668:G:N2	10:b:1998:C:O2	2.01	0.93
10:b:463:G:N2	10:b:466:A:OP2	2.03	0.91
10:b:1021:U:HO2'	10:b:1023:A:H2	1.00	0.91
10:b:976:G:H8	10:b:992:A:H62	1.11	0.91
10:b:2271:A:N6	10:b:2276:U:O2	2.03	0.90
14:f:158:THR:OG1	14:f:169:LEU:HD21	1.72	0.90
32:z:162:ILE:HD12	32:z:162:ILE:O	1.70	0.90
14:f:29:PRO:HB2	14:f:169:LEU:HD22	1.51	0.89
32:z:26:GLN:OE1	32:z:31:ARG:C	2.17	0.87
10:b:2664:A:O2'	10:b:2665:G:O4'	1.91	0.87
10:b:2073:G:N2	10:b:2446:C:O2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2271:A:N6	10:b:2276:U:N3	2.21	0.87
29:v:53:U:H2'	29:v:54:U:C5'	2.05	0.86
10:b:462:C:H5''	32:z:24:ASN:CB	2.06	0.85
10:b:1412:G:N2	10:b:1594:C:O2	2.09	0.85
10:b:2271:A:N6	10:b:2276:U:C2	2.45	0.84
10:b:462:C:C4'	32:z:24:ASN:O	2.24	0.84
9:a:9:G:C6	9:a:112:G:O6	2.32	0.83
29:v:26:C:H2'	29:v:27:U:C6	2.15	0.82
10:b:2382:A:C4	10:b:2383:G:C8	2.69	0.81
32:z:26:GLN:OE1	32:z:31:ARG:O	2.00	0.80
32:z:17:GLU:O	32:z:17:GLU:OE1	2.00	0.79
31:y:51:VAL:HG21	31:y:80:ILE:O	1.83	0.78
14:f:169:LEU:HD12	14:f:169:LEU:O	1.83	0.78
10:b:2835:G:OP2	12:d:59:ARG:NH1	2.16	0.77
13:e:67:ARG:HD3	32:z:31:ARG:HD2	1.65	0.77
32:z:17:GLU:O	32:z:17:GLU:CD	2.28	0.76
13:e:67:ARG:HH21	32:z:31:ARG:HG3	1.50	0.76
6:6:3:ARG:NH2	10:b:791:A:C2	2.54	0.76
10:b:829:U:O2'	10:b:2072:U:N3	2.19	0.76
10:b:949:A:C2'	10:b:986:A:H2	1.98	0.75
9:a:33:G:N3	9:a:50:A:C2	2.55	0.74
10:b:275:C:H1'	10:b:363:G:H22	1.51	0.74
32:z:26:GLN:OE1	32:z:32:CYS:N	2.20	0.74
13:e:73:ILE:HD12	32:z:28:TYR:HE1	1.53	0.74
9:a:113:C:H6	22:o:46:GLU:OE2	1.71	0.74
10:b:27:G:H1'	10:b:513:A:N6	2.03	0.73
26:s:85:ILE:CD1	32:z:23:PRO:HD3	2.18	0.73
29:v:23:U:O4	29:v:24:A:N6	2.21	0.73
10:b:2066:A:C5	32:z:162:ILE:CD1	2.72	0.73
13:e:138:LEU:HB3	13:e:143:LEU:HB2	1.72	0.71
32:z:25:LEU:N	32:z:25:LEU:HD12	2.05	0.71
26:s:85:ILE:HD13	32:z:23:PRO:HD3	1.73	0.71
10:b:2382:A:C4	10:b:2383:G:H8	2.07	0.71
10:b:1781:U:H5	10:b:1786:A:N7	1.86	0.71
10:b:1488:U:H3	10:b:1505:A:H61	1.38	0.71
14:f:158:THR:HG21	14:f:169:LEU:HD23	1.73	0.71
9:a:42:C:O2	14:f:90:THR:HG22	1.90	0.71
15:g:44:LYS:C	15:g:45:HIS:O	2.12	0.71
29:v:26:C:C2'	29:v:27:U:C5	2.71	0.71
10:b:1171:A:H2'	10:b:1172:C:O4'	1.91	0.71
10:b:949:A:HO2'	10:b:986:A:H2	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2379:G:C6	10:b:2383:G:O6	2.45	0.70
10:b:462:C:H5''	32:z:24:ASN:HB2	1.73	0.70
10:b:839:C:N4	10:b:943:A:N6	2.39	0.70
10:b:247:G:OP2	10:b:249:C:N4	2.23	0.70
29:v:10:G:H1	29:v:23:U:H3	1.40	0.69
10:b:949:A:H2'	10:b:986:A:H2	1.56	0.69
7:7:12:LYS:NZ	10:b:247:G:O6	2.22	0.69
10:b:1021:U:H3	10:b:1144:A:H62	1.41	0.69
26:s:85:ILE:CD1	32:z:22:CYS:HA	2.21	0.69
16:h:4:ILE:HG13	16:h:18:GLN:HB3	1.74	0.69
10:b:964:G:H21	10:b:2254:G:H1	1.41	0.68
10:b:462:C:C5'	32:z:24:ASN:O	2.41	0.68
10:b:1441:A:H62	10:b:1554:A:H8	1.41	0.68
29:v:53:U:C3'	29:v:54:U:H5'	2.22	0.68
9:a:43:C:H5''	9:a:43:C:H6	1.58	0.68
10:b:2662:C:H2'	10:b:2663:G:H5'	1.76	0.67
32:z:156:ILE:HD12	32:z:156:ILE:O	1.94	0.67
10:b:715:G:H21	10:b:720:A:H2	1.42	0.67
10:b:2662:C:C2'	10:b:2663:G:H5'	2.24	0.67
9:a:113:C:C6	22:o:46:GLU:OE2	2.47	0.66
10:b:1722:U:H2'	10:b:1723:G:O4'	1.94	0.66
10:b:1040:G:H1	10:b:1118:G:H22	1.41	0.66
10:b:2383:G:N3	10:b:2383:G:H2'	2.10	0.66
9:a:3:C:H42	9:a:117:G:H1	1.44	0.66
10:b:1799:G:HO2'	11:c:257:THR:HG1	1.40	0.66
13:e:58:LYS:HG3	13:e:71:GLY:HA2	1.78	0.66
30:w:65:VAL:C	30:w:66:ASP:OD1	2.38	0.66
10:b:949:A:O2'	10:b:986:A:C2	2.48	0.66
10:b:1801:G:N2	10:b:1820:U:O2'	2.29	0.66
10:b:1584:C:O2'	10:b:1587:C:N3	2.28	0.65
10:b:2460:C:C2'	10:b:2461:U:H5'	2.26	0.65
10:b:2462:G:H8	10:b:2463:A:H62	1.45	0.65
10:b:1791:A:OP2	11:c:221:ARG:NH1	2.29	0.65
10:b:2382:A:C8	10:b:2383:G:N7	2.64	0.65
10:b:2686:A:H61	10:b:2732:U:H1'	1.61	0.65
26:s:83:LYS:CB	32:z:20:SER:HB3	2.24	0.65
10:b:136:G:C5	10:b:137:U:C4	2.84	0.65
11:c:232:HIS:HA	11:c:242:LYS:HE3	1.78	0.65
10:b:2382:A:C5	10:b:2383:G:C8	2.85	0.65
10:b:1616:A:H1'	32:z:25:LEU:HD11	1.79	0.65
10:b:2104:G:C6	10:b:2105:A:C5	2.85	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:10:A:H2'	10:b:11:C:H5'	1.78	0.64
26:s:85:ILE:HG12	32:z:150:PHE:CE2	2.33	0.64
10:b:1584:C:O2'	10:b:1587:C:N4	2.29	0.64
10:b:528:A:C2	10:b:2047:C:H4'	2.33	0.64
27:t:25:GLU:HG3	27:t:26:LYS:HG2	1.80	0.64
10:b:807:G:O6	10:b:2072:U:H5	1.81	0.63
20:m:17:ASN:O	20:m:38:ARG:NH1	2.31	0.63
10:b:2843:G:N2	21:n:91:ALA:O	2.31	0.63
10:b:839:C:N4	10:b:943:A:H62	1.97	0.63
10:b:1530:A:N6	10:b:1545:G:O2'	2.32	0.63
10:b:976:G:C8	10:b:992:A:N6	2.57	0.62
10:b:1173:G:H21	10:b:1174:C:H41	1.46	0.62
9:a:51:G:O2'	9:a:52:A:O5'	2.17	0.62
13:e:73:ILE:CD1	32:z:28:TYR:HE1	2.12	0.62
10:b:1800:U:OP2	11:c:271:ARG:NH2	2.33	0.62
18:k:43:ILE:HD12	18:k:56:ASP:HB2	1.82	0.62
10:b:2106:G:C2	10:b:2192:U:N3	2.68	0.62
10:b:2316:U:OP1	14:f:70:ALA:O	2.18	0.62
10:b:527:C:N4	10:b:2783:U:OP2	2.33	0.61
9:a:9:G:C6	9:a:112:G:C6	2.88	0.61
10:b:2769:A:H2'	10:b:2769:A:N3	2.13	0.61
10:b:1723:G:O2'	10:b:1741:A:N6	2.34	0.61
13:e:73:ILE:HD12	32:z:28:TYR:CE1	2.33	0.61
29:v:50:G:H1	29:v:62:C:H42	1.46	0.61
4:3:16:ARG:NE	10:b:1268:G:OP1	2.33	0.61
10:b:579:G:OP1	10:b:2506:G:O2'	2.19	0.61
26:s:83:LYS:HB2	32:z:20:SER:CB	2.25	0.61
14:f:158:THR:HG21	14:f:169:LEU:CD2	2.30	0.61
3:2:19:LYS:NZ	10:b:922:A:OP1	2.33	0.61
10:b:2585:G:OP2	10:b:2585:G:N2	2.31	0.61
29:v:23:U:H2'	29:v:24:A:C8	2.35	0.61
29:v:8:U:O2'	29:v:10:G:N7	2.33	0.61
14:f:158:THR:OG1	14:f:169:LEU:CD2	2.47	0.60
10:b:2108:C:N3	10:b:2188:A:N6	2.48	0.60
7:7:19:LYS:HG2	10:b:653:G:H5'	1.84	0.60
10:b:1411:U:O2	10:b:1595:A:N1	2.33	0.60
22:o:69:ASP:OD1	22:o:69:ASP:N	2.33	0.60
29:v:28:C:N3	29:v:29:A:C2	2.69	0.60
10:b:2014:G:H5''	26:s:42:LYS:HB2	1.83	0.60
10:b:2117:U:OP1	10:b:2149:C:N4	2.35	0.60
10:b:27:G:H1'	10:b:513:A:H61	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:34:GLU:HG3	25:r:60:LYS:HG2	1.84	0.60
10:b:1044:G:H1	10:b:1114:G:H1	1.49	0.60
26:s:6:LYS:HG2	26:s:104:THR:HG23	1.82	0.60
10:b:2105:A:C2	10:b:2193:U:C2	2.89	0.60
10:b:2138:A:H3'	10:b:2139:A:H8	1.67	0.60
6:6:1:MET:SD	6:6:1:MET:N	2.74	0.59
10:b:301:G:OP2	28:u:82:ARG:NH1	2.35	0.59
14:f:158:THR:CB	14:f:169:LEU:HD21	2.31	0.59
26:s:85:ILE:HG12	32:z:150:PHE:HE2	1.65	0.59
9:a:113:C:C6	9:a:113:C:C5'	2.86	0.59
10:b:2378:C:N4	10:b:2379:G:O6	2.35	0.59
10:b:949:A:O2'	10:b:986:A:H2	1.81	0.59
20:m:38:ARG:HB2	20:m:98:PRO:HD3	1.84	0.59
14:f:117:LEU:HB2	14:f:177:PHE:HA	1.85	0.59
10:b:807:G:O6	10:b:2072:U:C5	2.56	0.59
10:b:2382:A:C8	10:b:2383:G:C8	2.91	0.59
10:b:2462:G:O2'	10:b:2464:U:O4	2.21	0.59
14:f:34:ILE:HG12	14:f:96:MET:HE3	1.85	0.59
10:b:2460:C:H2'	10:b:2461:U:H5'	1.83	0.59
14:f:63:GLN:NE2	14:f:90:THR:O	2.36	0.59
10:b:491:G:O6	26:s:49:LYS:NZ	2.33	0.58
9:a:112:G:C8	9:a:112:G:C5'	2.87	0.58
14:f:135:GLN:HE21	14:f:149:VAL:HA	1.66	0.58
13:e:67:ARG:HD3	32:z:31:ARG:CD	2.31	0.58
14:f:165:GLU:O	14:f:169:LEU:CB	2.51	0.58
26:s:4:ILE:HG12	26:s:106:VAL:HG22	1.84	0.58
10:b:275:C:H1'	10:b:363:G:N2	2.18	0.58
32:z:154:VAL:HG12	32:z:154:VAL:O	2.02	0.58
10:b:117:G:OP2	10:b:119:A:O2'	2.20	0.58
10:b:488:G:O2'	26:s:49:LYS:NZ	2.31	0.58
10:b:1096:U:N3	10:b:1098:A:OP2	2.36	0.58
10:b:263:G:O2'	10:b:429:A:N3	2.34	0.58
10:b:506:G:H4'	10:b:507:A:H5'	1.86	0.58
29:v:30:G:N2	29:v:40:C:O2	2.36	0.58
11:c:107:PRO:HD2	11:c:110:LEU:HD22	1.85	0.58
12:d:46:ARG:NH2	12:d:88:GLU:O	2.36	0.58
10:b:1412:G:C5'	10:b:1412:G:C8	2.87	0.58
13:e:61:ARG:NH1	32:z:155:TRP:O	2.37	0.58
29:v:53:U:C2'	29:v:54:U:C5'	2.72	0.58
10:b:1085:U:H2'	10:b:1086:A:H2'	1.85	0.58
10:b:2382:A:N9	10:b:2383:G:C8	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:46:ILE:HD12	20:m:69:PRO:HG3	1.85	0.58
10:b:954:G:H21	10:b:2271:A:H2	1.51	0.58
15:g:155:GLU:HG3	15:g:157:TYR:H	1.69	0.57
10:b:12:U:H2'	10:b:12:U:O2	2.04	0.57
10:b:2552:U:O2	18:k:23:LYS:NZ	2.37	0.57
24:q:97:ASP:OD1	25:r:13:ARG:NH1	2.33	0.57
10:b:2066:A:C8	32:z:162:ILE:HD11	2.37	0.57
10:b:1056:A:H1'	10:b:1108:G:H22	1.70	0.56
13:e:138:LEU:CB	13:e:143:LEU:HB2	2.35	0.56
9:a:33:G:C2	9:a:50:A:C2	2.93	0.56
10:b:483:A:O2'	28:u:56:GLY:O	2.22	0.56
10:b:2487:C:O2'	20:m:51:ARG:NH1	2.38	0.56
10:b:712:U:H3	10:b:723:A:H61	1.53	0.56
14:f:29:PRO:O	14:f:169:LEU:HD13	2.05	0.56
10:b:265:A:N6	10:b:427:U:O2'	2.31	0.56
10:b:1412:G:O5'	10:b:1412:G:H8	1.88	0.56
10:b:1633:G:N1	10:b:1636:A:OP2	2.32	0.56
3:2:12:SER:HB3	3:2:32:ILE:HD11	1.88	0.56
10:b:631:G:N3	10:b:641:U:O2'	2.39	0.56
17:j:96:ARG:HH21	17:j:99:ARG:HG2	1.71	0.56
14:f:116:GLY:HA3	14:f:178:ARG:HD3	1.87	0.56
22:o:29:HIS:HB3	22:o:36:TYR:HB2	1.87	0.56
20:m:66:ARG:NH1	20:m:104:GLU:OE1	2.37	0.55
10:b:1856:A:H62	10:b:1892:G:H8	1.54	0.55
21:n:19:ALA:O	21:n:23:ASN:ND2	2.40	0.55
10:b:508:A:C8	32:z:16:TYR:HE1	2.23	0.55
10:b:2055:A:C2	10:b:2056:A:N6	2.74	0.55
14:f:135:GLN:NE2	14:f:148:ARG:O	2.40	0.55
9:a:9:G:N1	9:a:112:G:C6	2.74	0.55
14:f:34:ILE:HG22	14:f:156:ILE:HA	1.87	0.55
10:b:2379:G:C5	10:b:2383:G:O6	2.59	0.55
32:z:22:CYS:SG	32:z:23:PRO:HD3	2.45	0.55
10:b:835:A:H2'	10:b:836:G:C8	2.41	0.55
10:b:1023:A:H61	10:b:1144:A:H61	1.54	0.55
10:b:2639:A:O2'	12:d:49:GLN:NE2	2.40	0.55
10:b:2466:C:H2'	10:b:2467:C:C6	2.42	0.55
26:s:85:ILE:HD11	32:z:23:PRO:HD3	1.89	0.55
10:b:1267:A:OP1	10:b:1267:A:H8	1.90	0.55
10:b:2772:U:O3'	17:j:95:ARG:NH2	2.39	0.55
10:b:2802:U:O2'	10:b:2803:G:N2	2.34	0.55
26:s:73:LYS:HB2	26:s:106:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:106:ILE:HG21	14:f:139:PRO:HG3	1.89	0.55
21:n:42:LYS:HA	21:n:45:ARG:HE	1.72	0.55
31:y:49:ALA:O	31:y:51:VAL:HG22	2.07	0.55
9:a:113:C:H2'	9:a:113:C:O2	2.07	0.54
14:f:165:GLU:O	14:f:169:LEU:HB3	2.06	0.54
26:s:85:ILE:HD13	32:z:23:PRO:CD	2.36	0.54
10:b:950:C:H1'	10:b:986:A:N3	2.21	0.54
28:u:33:LYS:HB3	28:u:64:ALA:HB1	1.88	0.54
10:b:1165:G:OP1	25:r:24:LYS:NZ	2.41	0.54
22:o:88:LYS:HB2	22:o:116:GLN:HG2	1.90	0.54
9:a:32:U:H3	9:a:50:A:H61	1.53	0.54
13:e:46:GLN:O	13:e:88:ARG:NH1	2.39	0.54
14:f:164:GLU:HA	14:f:167:ARG:HB2	1.90	0.54
10:b:1260:U:OP1	32:z:30:SER:CB	2.55	0.54
10:b:1723:G:N2	10:b:1740:G:O2'	2.40	0.54
10:b:871:G:O3'	20:m:6:ARG:NH1	2.41	0.54
10:b:1660:C:H2'	10:b:1660:C:O2	2.08	0.54
10:b:1301:G:O2'	10:b:1302:G:OP2	2.15	0.53
10:b:1423:G:O2'	10:b:1496:A:N6	2.40	0.53
10:b:2343:C:H2'	10:b:2344:A:C8	2.43	0.53
11:c:3:VAL:HG12	11:c:19:VAL:HG12	1.90	0.53
1:0:29:PHE:HB3	10:b:396:G:H1'	1.90	0.53
9:a:32:U:H3	9:a:50:A:N6	2.07	0.53
10:b:674:C:OP2	19:l:42:SER:OG	2.23	0.53
9:a:33:G:C4	9:a:50:A:N1	2.77	0.53
10:b:1021:U:O2'	10:b:1023:A:H2	1.79	0.53
22:o:17:LYS:HA	22:o:20:GLU:HG2	1.88	0.53
22:o:52:SER:OG	22:o:53:THR:N	2.41	0.53
26:s:74:ILE:HD13	26:s:105:VAL:HG22	1.90	0.53
9:a:113:C:C6	9:a:113:C:H5''	2.44	0.53
18:k:7:MET:HE1	18:k:44:LYS:HG3	1.91	0.53
6:6:39:ARG:NH2	10:b:468:G:N7	2.42	0.53
18:k:65:THR:HG22	18:k:67:LYS:H	1.74	0.53
29:v:75:A:HO3'	32:z:165:GLY:C	2.12	0.53
10:b:2664:A:C6	10:b:2665:G:C2	2.96	0.53
2:1:14:LEU:HD11	2:1:56:LEU:HD23	1.90	0.53
11:c:66:ASP:OD1	11:c:102:ARG:NH1	2.41	0.53
25:r:58:VAL:H	25:r:102:SER:HB3	1.74	0.53
26:s:80:PRO:O	26:s:100:THR:OG1	2.26	0.53
13:e:138:LEU:HA	13:e:141:MET:HB2	1.90	0.53
10:b:1250:G:OP2	13:e:44:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:v:26:C:N3	29:v:27:U:O4	2.42	0.53
30:w:51:GLN:OE1	30:w:57:TYR:OH	2.26	0.52
10:b:287:G:O6	10:b:352:A:N6	2.41	0.52
10:b:508:A:OP1	32:z:16:TYR:OH	2.21	0.52
10:b:839:C:C4	10:b:943:A:N6	2.77	0.52
10:b:1301:G:C8	10:b:1301:G:H3'	2.45	0.52
10:b:1549:C:H5''	10:b:1549:C:H6	1.73	0.52
29:v:26:C:C4	29:v:27:U:O4	2.62	0.52
29:v:75:A:O2'	32:z:165:GLY:CA	2.58	0.52
10:b:27:G:H22	10:b:512:G:H1'	1.74	0.52
10:b:1453:C:H5	10:b:1461:G:H1	1.57	0.52
10:b:2106:G:N3	10:b:2192:U:N3	2.58	0.52
13:e:52:VAL:HG21	13:e:82:GLY:H	1.74	0.52
14:f:58:ALA:HB2	14:f:65:PRO:HD3	1.91	0.52
25:r:46:GLU:OE1	25:r:48:LYS:NZ	2.43	0.52
10:b:1201:U:H1'	24:q:4:VAL:HG22	1.92	0.52
10:b:1412:G:C5'	10:b:1412:G:H8	2.22	0.52
10:b:2105:A:C2	10:b:2193:U:O2	2.63	0.52
20:m:36:VAL:HG12	30:w:82:TYR:HB2	1.90	0.52
2:1:9:LYS:HE3	2:1:13:GLU:HG2	1.90	0.52
10:b:116:C:HO2'	10:b:126:A:H8	1.55	0.52
10:b:572:G:H2'	10:b:2034:A:N7	2.25	0.52
10:b:116:C:O2'	10:b:126:A:C8	2.63	0.52
10:b:2449:G:OP1	13:e:69:ARG:NH1	2.34	0.52
22:o:67:ASN:OD1	22:o:67:ASN:N	2.42	0.52
23:p:7:GLN:OE1	23:p:10:GLN:NE2	2.42	0.52
10:b:2812:G:O2'	10:b:2894:G:O6	2.24	0.52
25:r:5:PHE:HB3	25:r:59:ILE:HD12	1.92	0.52
27:t:23:ALA:HB1	27:t:29:THR:HB	1.91	0.52
29:v:7:A:N7	29:v:12:A:N6	2.57	0.52
32:z:162:ILE:O	32:z:162:ILE:CD1	2.51	0.52
10:b:1530:A:OP2	10:b:1545:G:N2	2.39	0.51
10:b:2724:U:OP1	23:p:53:ARG:NH2	2.43	0.51
27:t:67:VAL:O	27:t:69:ARG:NH1	2.42	0.51
10:b:883:G:N2	10:b:899:C:O2'	2.42	0.51
22:o:24:THR:HG22	22:o:90:VAL:HG13	1.91	0.51
31:y:59:LEU:HD12	31:y:80:ILE:HD12	1.91	0.51
10:b:1443:G:H2'	10:b:1444:U:C6	2.45	0.51
10:b:2640:C:O2'	12:d:45:TYR:OH	2.26	0.51
14:f:170:LEU:C	14:f:170:LEU:HD12	2.35	0.51
10:b:2305:C:O2'	10:b:2306:U:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:59:SER:OG	21:n:62:ASN:OD1	2.25	0.51
29:v:5:G:H2'	29:v:6:C:H4'	1.92	0.51
9:a:112:G:C8	9:a:112:G:H5''	2.46	0.51
10:b:2661:A:H62	10:b:2668:G:H21	1.57	0.51
18:k:9:ASN:OD1	18:k:18:ARG:NH1	2.43	0.51
10:b:240:C:OP2	10:b:241:A:O2'	2.25	0.51
10:b:1247:G:OP1	19:l:13:LYS:NZ	2.44	0.51
10:b:2104:G:O6	10:b:2105:A:C6	2.63	0.51
10:b:2802:U:O2	10:b:2803:G:N2	2.44	0.51
29:v:53:U:C3'	29:v:54:U:C5'	2.89	0.51
10:b:250:G:H4'	19:l:59:ARG:HD2	1.91	0.51
10:b:587:G:N7	24:q:6:ARG:NH1	2.49	0.51
29:v:25:C:H2'	29:v:26:C:O4'	2.11	0.51
32:z:25:LEU:N	32:z:25:LEU:CD1	2.73	0.51
2:1:49:ASP:OD1	2:1:52:ARG:NH2	2.43	0.51
7:7:8:ARG:NH2	10:b:244:A:OP2	2.42	0.51
10:b:1330:A:H2'	10:b:1332:C:C5	2.46	0.51
10:b:1444:U:H2'	10:b:1445:U:C6	2.46	0.51
10:b:2131:G:N2	10:b:2165:C:N3	2.57	0.51
10:b:2473:A:N6	10:b:2485:G:O2'	2.44	0.51
26:s:1:MET:N	26:s:109:ASP:OD1	2.44	0.51
6:6:4:THR:HG22	10:b:689:C:H1'	1.93	0.50
10:b:508:A:N7	32:z:16:TYR:CE1	2.79	0.50
10:b:839:C:H42	10:b:943:A:N6	2.10	0.50
10:b:2879:C:OP1	21:n:4:ARG:NH2	2.41	0.50
18:k:63:VAL:HG12	18:k:107:LEU:HD21	1.93	0.50
2:1:41:HIS:ND1	10:b:95:A:O2'	2.44	0.50
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.92	0.50
10:b:950:C:O4'	10:b:986:A:C2	2.65	0.50
10:b:1428:G:O2'	10:b:1574:A:N6	2.45	0.50
10:b:219:A:N3	10:b:234:U:O2'	2.39	0.50
10:b:1366:G:N2	10:b:1369:A:OP2	2.36	0.50
10:b:1584:C:O2'	10:b:1587:C:C4	2.64	0.50
10:b:2172:G:H1	10:b:2174:A:H3'	1.76	0.50
10:b:2792:C:H2'	10:b:2793:C:C6	2.46	0.50
22:o:40:ILE:HG12	22:o:47:VAL:HG12	1.92	0.50
10:b:27:G:N2	10:b:512:G:H1'	2.26	0.50
10:b:997:C:O2	17:j:3:THR:OG1	2.26	0.50
10:b:2451:G:N2	10:b:2454:A:OP2	2.39	0.50
31:y:40:GLN:NE2	31:y:57:HIS:O	2.45	0.50
8:8:4:ARG:NH2	10:b:2481:U:O2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:404:A:N6	10:b:421:C:O2'	2.44	0.50
10:b:2106:G:N2	10:b:2107:C:C2	2.80	0.50
15:g:28:GLY:HA3	15:g:79:VAL:HB	1.94	0.50
10:b:2131:G:O2'	10:b:2133:C:N4	2.41	0.50
14:f:29:PRO:HB2	14:f:169:LEU:CD2	2.32	0.50
28:u:27:ASN:N	28:u:27:ASN:OD1	2.45	0.50
10:b:244:A:H5''	19:l:67:THR:HG21	1.93	0.50
10:b:1660:C:OP1	12:d:140:HIS:NE2	2.45	0.50
10:b:2055:A:H2	10:b:2056:A:N6	2.10	0.50
10:b:2316:U:H2'	10:b:2317:C:C6	2.46	0.50
2:l:21:LEU:HB3	2:l:50:VAL:HG12	1.94	0.50
10:b:1471:A:H2'	10:b:1472:A:C8	2.47	0.50
10:b:2316:U:H2'	10:b:2317:C:H6	1.76	0.50
10:b:2641:U:C4	10:b:2642:G:C6	3.00	0.50
20:m:17:ASN:OD1	20:m:97:GLN:NE2	2.45	0.50
30:w:65:VAL:O	30:w:65:VAL:HG13	2.12	0.50
9:a:113:C:O4'	22:o:46:GLU:OE1	2.30	0.50
10:b:2115:U:O2	10:b:2147:C:O2'	2.29	0.50
20:m:15:GLY:O	20:m:16:ARG:NH1	2.36	0.50
5:4:37:LYS:HG2	5:4:48:ILE:HG13	1.93	0.49
7:7:25:LYS:HB3	19:l:62:PRO:HG2	1.94	0.49
17:j:102:GLU:HB3	17:j:119:PHE:HZ	1.77	0.49
19:l:85:VAL:HG11	19:l:90:VAL:HG22	1.94	0.49
10:b:1452:G:N2	10:b:1454:G:O6	2.44	0.49
10:b:2107:C:N4	10:b:2108:C:N3	2.61	0.49
10:b:2661:A:O3'	15:g:160:LYS:NZ	2.45	0.49
10:b:638:G:OP2	19:l:109:LYS:NZ	2.43	0.49
10:b:783:A:OP1	11:c:217:ARG:NH2	2.43	0.49
10:b:813:U:H2'	19:l:21:ARG:HA	1.94	0.49
10:b:1324:A:H5''	26:s:82:MET:HE1	1.94	0.49
19:l:79:LEU:HD11	19:l:112:LEU:HD12	1.94	0.49
22:o:99:TYR:HH	22:o:111:ARG:HH12	1.57	0.49
10:b:1412:G:C8	10:b:1412:G:H5''	2.47	0.49
10:b:1771:U:O2'	10:b:1962:C:OP1	2.30	0.49
29:v:26:C:C2	29:v:27:U:O4	2.65	0.49
10:b:2237:U:H2'	10:b:2238:G:C8	2.48	0.49
10:b:160:A:N3	10:b:2212:C:O2'	2.44	0.49
10:b:645:A:N6	10:b:2373:A:O2'	2.46	0.49
10:b:1030:A:N3	10:b:2490:C:O2'	2.43	0.49
10:b:1047:C:H4'	10:b:1048:A:H5''	1.95	0.49
10:b:2104:G:C6	10:b:2105:A:C6	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2305:C:H2'	10:b:2306:U:O4'	2.12	0.49
10:b:1021:U:H3	10:b:1144:A:N6	2.08	0.49
10:b:1334:G:N7	10:b:1611:A:O2'	2.38	0.49
10:b:1984:G:O2'	10:b:1986:U:OP2	2.31	0.49
10:b:2306:U:O2'	14:f:123:ASP:O	2.31	0.49
10:b:2798:U:H3	10:b:2806:A:H61	1.59	0.49
12:d:60:VAL:HG23	12:d:64:GLU:HG3	1.95	0.49
11:c:144:VAL:HB	11:c:154:LEU:HB2	1.95	0.49
11:c:161:TYR:HB3	11:c:194:GLU:HB2	1.95	0.49
10:b:2642:G:O2'	10:b:2779:G:N2	2.36	0.48
20:m:20:LEU:HD13	30:w:81:PRO:HG2	1.94	0.48
10:b:1000:C:OP1	24:q:92:ARG:NH2	2.44	0.48
10:b:2664:A:C6	10:b:2665:G:N2	2.81	0.48
12:d:37:VAL:HG12	12:d:48:ILE:HG22	1.95	0.48
13:e:67:ARG:CD	32:z:31:ARG:CD	2.91	0.48
9:a:24:G:C8	9:a:56:G:C8	3.02	0.48
10:b:579:G:O2'	10:b:1256:A:OP1	2.31	0.48
10:b:686:G:C2	10:b:796:A:C2	3.01	0.48
10:b:989:C:O2'	10:b:1002:A:N3	2.45	0.48
10:b:1042:A:H61	10:b:1116:C:H42	1.61	0.48
10:b:1793:A:N6	10:b:1830:G:O2'	2.40	0.48
23:p:10:GLN:HA	23:p:13:MET:HG3	1.94	0.48
30:w:40:ILE:HD12	30:w:42:LEU:HD21	1.95	0.48
11:c:115:GLN:O	11:c:125:LYS:NZ	2.46	0.48
26:s:77:ASP:HB2	26:s:102:HIS:HB2	1.95	0.48
9:a:42:C:C2	14:f:90:THR:HG22	2.49	0.48
10:b:263:G:H2'	10:b:264:C:O4'	2.14	0.48
10:b:364:C:O2'	10:b:365:U:H5'	2.14	0.48
10:b:508:A:C8	32:z:16:TYR:CE1	3.01	0.48
10:b:1317:C:O2'	10:b:1394:A:N3	2.46	0.48
19:l:82:LEU:HD22	19:l:90:VAL:HG21	1.95	0.48
24:q:99:ALA:O	24:q:103:LYS:NZ	2.46	0.48
27:t:76:ARG:NH2	27:t:79:ASP:OD1	2.46	0.48
9:a:112:G:O5'	9:a:112:G:H8	1.96	0.48
10:b:888:A:O2'	10:b:890:C:OP2	2.31	0.48
10:b:2664:A:C8	10:b:2664:A:H5'	2.48	0.48
4:3:24:ALA:HB2	26:s:23:LEU:HD22	1.95	0.48
10:b:83:A:N6	10:b:102:U:OP1	2.34	0.48
10:b:766:A:H5''	11:c:209:GLY:HA3	1.95	0.48
10:b:1653:G:H4'	21:n:39:PRO:HG2	1.96	0.48
10:b:2835:G:OP1	12:d:56:LYS:NZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:21:ARG:O	13:e:114:ARG:NH2	2.39	0.48
17:j:118:MET:HA	17:j:121:LYS:HE2	1.96	0.48
10:b:405:U:O2'	10:b:406:G:OP1	2.30	0.48
10:b:1755:G:N2	10:b:1758:G:OP2	2.40	0.48
28:u:74:ASN:ND2	28:u:81:ASP:OD2	2.44	0.48
9:a:6:G:H2'	9:a:7:G:C8	2.49	0.48
10:b:1443:G:O2'	10:b:1444:U:H5'	2.14	0.48
10:b:2880:G:OP1	23:p:2:SER:N	2.46	0.48
15:g:23:VAL:HG13	15:g:36:THR:HB	1.94	0.48
6:6:37:LYS:NZ	10:b:469:G:N7	2.62	0.48
10:b:511:U:H4'	10:b:1237:G:H4'	1.95	0.48
10:b:607:G:N3	10:b:659:U:O2'	2.47	0.48
14:f:170:LEU:HD11	14:f:177:PHE:HZ	1.79	0.48
29:v:10:G:C2	29:v:24:A:C2	3.02	0.48
9:a:90:C:H5''	20:m:18:ARG:HG2	1.94	0.47
10:b:62:U:H2'	10:b:63:A:H2	1.78	0.47
10:b:513:A:H5''	10:b:1218:G:O2'	2.13	0.47
10:b:1724:A:H2'	10:b:1725:G:C8	2.49	0.47
10:b:2391:U:OP1	31:y:55:ARG:NH2	2.47	0.47
29:v:24:A:C2'	29:v:25:C:H5'	2.44	0.47
29:v:55:C:N4	29:v:56:G:O6	2.47	0.47
17:j:45:THR:HB	24:q:64:ARG:HH21	1.79	0.47
10:b:1792:C:H2'	10:b:1793:A:C5	2.49	0.47
11:c:37:ASN:HB2	11:c:62:TYR:HB2	1.96	0.47
11:c:104:ILE:HD13	11:c:116:ILE:HD13	1.94	0.47
11:c:132:MET:HE3	11:c:190:ALA:HB2	1.96	0.47
14:f:29:PRO:HB2	14:f:169:LEU:HD13	1.96	0.47
10:b:884:G:H2'	10:b:885:G:C8	2.49	0.47
10:b:1173:G:C5'	10:b:1174:C:H5'	2.44	0.47
10:b:1323:A:O2'	26:s:11:ARG:NH2	2.47	0.47
10:b:2754:A:O2'	10:b:2756:C:N4	2.44	0.47
10:b:2769:A:N3	10:b:2769:A:C2'	2.77	0.47
10:b:2853:U:N3	10:b:2871:G:O4'	2.48	0.47
4:3:43:ILE:HG12	21:n:100:CYS:HA	1.96	0.47
10:b:665:G:H5''	19:l:17:LYS:HD2	1.97	0.47
10:b:1647:G:H5''	10:b:1648:C:H5'	1.97	0.47
28:u:13:VAL:HG21	28:u:39:ILE:HG21	1.96	0.47
9:a:24:G:C8	9:a:56:G:N7	2.83	0.47
9:a:115:A:H2'	9:a:116:G:H8	1.78	0.47
9:a:41:G:N2	10:b:2343:C:O2'	2.42	0.47
10:b:1173:G:H4'	10:b:1174:C:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1411:U:O2	10:b:1595:A:C2	2.68	0.47
10:b:1669:G:O2'	10:b:1995:U:O4	2.23	0.47
10:b:2262:C:O2'	10:b:2431:C:OP2	2.31	0.47
18:k:110:GLU:HA	18:k:113:MET:HG2	1.96	0.47
27:t:59:ASN:O	27:t:84:TYR:N	2.45	0.47
8:8:32:LYS:HE2	10:b:2482:A:H5'	1.96	0.47
10:b:33:C:O2	10:b:447:A:N6	2.46	0.47
10:b:355:U:H2'	10:b:356:G:C8	2.50	0.47
10:b:966:C:O2'	10:b:2277:A:N3	2.38	0.47
10:b:2277:A:H2'	10:b:2278:A:C8	2.49	0.47
19:l:51:GLU:HG3	19:l:56:PRO:HA	1.97	0.47
9:a:22:U:H2'	9:a:23:G:C8	2.50	0.47
9:a:112:G:H2'	22:o:46:GLU:OE2	2.14	0.47
10:b:807:G:H22	10:b:830:U:H5''	1.80	0.47
10:b:1023:A:C8	10:b:1023:A:H3'	2.50	0.47
18:k:121:GLU:HG2	18:k:122:VAL:HG23	1.97	0.47
10:b:2383:G:N3	10:b:2383:G:C2'	2.78	0.47
15:g:137:ASP:HB3	15:g:140:VAL:HB	1.97	0.47
6:6:29:GLN:NE2	10:b:210:C:OP1	2.47	0.46
10:b:2166:G:O2'	10:b:2176:U:O4	2.33	0.46
4:3:52:ARG:HH11	4:3:54:VAL:HA	1.80	0.46
10:b:976:G:H8	10:b:992:A:N6	1.95	0.46
10:b:1865:G:HO2'	10:b:2415:A:HO2'	1.60	0.46
10:b:2119:G:N3	10:b:2121:A:N6	2.63	0.46
10:b:494:G:H4'	26:s:6:LYS:HB2	1.97	0.46
10:b:831:A:N7	10:b:2251:A:O2'	2.44	0.46
10:b:1436:A:H62	10:b:1560:C:H42	1.62	0.46
10:b:345:A:H1'	10:b:346:A:H2	1.80	0.46
16:h:12:LEU:H	16:h:12:LEU:HG	1.57	0.46
16:h:30:LEU:HB3	16:h:36:ALA:HB3	1.98	0.46
10:b:572:G:OP1	10:b:974:A:O2'	2.24	0.46
10:b:2447:C:H2'	10:b:2448:G:C8	2.50	0.46
12:d:77:ARG:NH2	12:d:200:ASP:OD1	2.49	0.46
9:a:14:U:OP2	9:a:70:C:O2'	2.31	0.46
10:b:1066:C:H42	10:b:1075:A:H62	1.63	0.46
10:b:2631:G:O2'	10:b:2785:A:N1	2.38	0.46
14:f:44:ILE:HG21	14:f:79:ILE:HG22	1.97	0.46
19:l:81:ASP:HB3	19:l:100:ILE:HD13	1.96	0.46
9:a:50:A:H2'	9:a:51:G:H5'	1.97	0.46
10:b:1781:U:C5	10:b:1786:A:N7	2.76	0.46
10:b:2488:G:O2'	20:m:123:LYS:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2585:G:H2'	10:b:2585:G:N3	2.30	0.46
10:b:2659:G:O2'	10:b:2668:G:N1	2.46	0.46
25:r:41:ILE:HD11	25:r:57:GLY:HA3	1.97	0.46
29:v:28:C:C4	29:v:29:A:C6	3.03	0.46
7:7:32:ILE:HG22	7:7:32:ILE:O	2.16	0.46
10:b:459:U:H2'	10:b:460:A:H8	1.80	0.46
10:b:463:G:N2	10:b:465:G:H3'	2.31	0.46
10:b:623:A:OP2	19:l:99:ASN:OD1	2.33	0.46
10:b:1533:C:H42	10:b:1542:G:H1	1.64	0.46
13:e:141:MET:HE3	13:e:141:MET:HB3	1.78	0.46
19:l:127:VAL:HG21	19:l:142:ILE:HD13	1.98	0.46
29:v:7:A:H61	29:v:13:U:H5''	1.81	0.46
29:v:23:U:C4	29:v:24:A:N6	2.84	0.46
29:v:27:U:OP2	29:v:27:U:H6	1.98	0.46
9:a:33:G:C4	9:a:50:A:C2	3.04	0.46
10:b:10:A:H2	10:b:2633:U:H3	1.64	0.46
10:b:1570:G:OP1	11:c:63:ARG:NH2	2.39	0.46
10:b:2382:A:H4'	22:o:117:PHE:HB2	1.98	0.46
14:f:170:LEU:HD12	14:f:171:ALA:N	2.31	0.46
6:6:25:LYS:HB3	6:6:25:LYS:HE3	1.82	0.45
10:b:63:A:N6	10:b:91:A:H62	2.14	0.45
10:b:1654:A:C2	10:b:2009:A:N6	2.84	0.45
13:e:67:ARG:HH21	32:z:31:ARG:CG	2.25	0.45
26:s:95:ARG:NH2	32:z:20:SER:HB2	2.31	0.45
10:b:948:C:H2'	10:b:949:A:H8	1.81	0.45
10:b:1818:C:H41	11:c:35:GLU:CD	2.25	0.45
19:l:89:VAL:HG13	19:l:123:ARG:HD3	1.98	0.45
11:c:16:VAL:HG22	11:c:206:GLY:HA3	1.99	0.45
14:f:33:LYS:HG3	14:f:157:THR:HB	1.99	0.45
14:f:49:LEU:HA	14:f:52:ASN:HB2	1.98	0.45
14:f:171:ALA:HB2	14:f:177:PHE:HE2	1.81	0.45
19:l:110:VAL:HB	19:l:127:VAL:HG12	1.97	0.45
23:p:14:LYS:HG3	23:p:77:HIS:HA	1.99	0.45
4:3:38:HIS:ND1	4:3:39:LEU:O	2.37	0.45
10:b:481:G:H2'	10:b:507:A:N1	2.31	0.45
10:b:948:C:H2'	10:b:949:A:C8	2.52	0.45
10:b:1260:U:OP1	32:z:30:SER:OG	2.32	0.45
10:b:1940:A:H61	10:b:1967:U:H3	1.64	0.45
10:b:2066:A:C6	32:z:162:ILE:HG12	2.51	0.45
10:b:2382:A:N9	10:b:2383:G:H8	2.10	0.45
10:b:2466:C:H2'	10:b:2467:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2568:A:OP1	10:b:2652:G:O2'	2.29	0.45
7:7:18:GLY:N	10:b:631:G:OP1	2.50	0.45
10:b:239:C:HO2'	10:b:624:G:HO2'	1.56	0.45
10:b:1175:U:N3	10:b:1178:U:C4	2.84	0.45
10:b:1496:A:H2'	10:b:1497:A:C8	2.51	0.45
10:b:2576:A:OP1	10:b:2578:G:H4'	2.17	0.45
15:g:25:THR:HG23	15:g:34:THR:HB	1.98	0.45
22:o:41:ALA:HB2	22:o:48:LEU:HD21	1.99	0.45
29:v:26:C:C2	29:v:27:U:C4	3.05	0.45
10:b:462:C:OP1	32:z:24:ASN:ND2	2.50	0.45
10:b:604:A:HO2'	10:b:606:G:HO2'	1.57	0.45
10:b:1724:A:N6	10:b:1740:G:H1'	2.31	0.45
13:e:18:THR:HG23	13:e:106:LYS:HG2	1.99	0.45
17:j:19:ASP:O	17:j:23:LYS:NZ	2.34	0.45
20:m:47:GLU:OE2	20:m:50:ARG:NH1	2.38	0.45
32:z:29:PHE:HA	32:z:32:CYS:HB2	1.98	0.45
2:1:40:SER:O	2:1:40:SER:OG	2.34	0.45
10:b:1869:G:H1	10:b:1878:C:H42	1.64	0.45
2:1:14:LEU:HD21	2:1:56:LEU:HG	1.98	0.45
10:b:1063:U:H3	10:b:1070:G:H1'	1.82	0.45
10:b:2073:G:N1	10:b:2446:C:N3	2.47	0.45
16:h:12:LEU:HB2	16:h:19:VAL:HG21	1.98	0.45
8:8:4:ARG:O	8:8:38:GLY:N	2.49	0.45
10:b:876:G:OP1	20:m:62:LYS:NZ	2.42	0.45
10:b:1565:U:H2'	10:b:1566:C:C6	2.52	0.45
10:b:2245:A:H2'	10:b:2246:G:C8	2.52	0.45
14:f:29:PRO:O	14:f:169:LEU:CD1	2.65	0.45
6:6:3:ARG:CZ	10:b:791:A:C2	2.99	0.45
10:b:695:A:O2'	10:b:1355:A:N3	2.47	0.45
10:b:1028:G:H2'	10:b:1029:A:H8	1.81	0.45
10:b:2544:C:O2'	10:b:2744:A:N3	2.47	0.45
14:f:29:PRO:CB	14:f:169:LEU:HD22	2.36	0.45
10:b:500:G:N1	10:b:503:A:OP2	2.45	0.44
10:b:785:A:O2'	10:b:787:G:OP1	2.35	0.44
10:b:989:C:H2'	10:b:990:A:O4'	2.17	0.44
10:b:2106:G:C2	10:b:2192:U:C4	3.05	0.44
10:b:2390:A:H4'	31:y:56:ASP:HA	1.99	0.44
15:g:86:LYS:HG2	15:g:132:VAL:HG12	1.98	0.44
7:7:31:HIS:H	7:7:31:HIS:CD2	2.36	0.44
10:b:488:G:O2'	10:b:491:G:N7	2.36	0.44
10:b:2186:U:H2'	10:b:2187:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2305:C:H2'	10:b:2306:U:C6	2.52	0.44
10:b:2664:A:H5'	10:b:2664:A:H8	1.81	0.44
10:b:2843:G:O2'	21:n:49:GLU:OE1	2.29	0.44
18:k:71:ARG:HH22	18:k:105:ARG:HG2	1.83	0.44
10:b:481:G:O2'	10:b:506:G:N2	2.51	0.44
10:b:581:G:O2'	10:b:2023:A:OP1	2.34	0.44
10:b:1040:G:H22	10:b:1118:G:N2	2.15	0.44
10:b:1173:G:H5''	10:b:1174:C:H5'	1.99	0.44
10:b:1412:G:N2	10:b:1594:C:C2	2.66	0.44
10:b:2282:A:OP1	20:m:10:ARG:NH2	2.50	0.44
10:b:2576:A:N7	12:d:150:GLN:HB2	2.32	0.44
10:b:731:G:C6	11:c:207:LYS:HB2	2.53	0.44
10:b:943:A:H2'	10:b:944:G:O4'	2.17	0.44
10:b:2104:G:N1	10:b:2105:A:C4	2.86	0.44
10:b:2106:G:C8	10:b:2106:G:OP2	2.70	0.44
10:b:835:A:H2'	10:b:836:G:H8	1.81	0.44
10:b:1301:G:O5'	10:b:1301:G:H8	2.00	0.44
10:b:1353:C:H2'	10:b:1354:U:O4'	2.17	0.44
10:b:2043:U:H2'	10:b:2044:G:H8	1.82	0.44
10:b:2855:A:H2'	10:b:2856:G:O4'	2.17	0.44
11:c:34:LEU:HD23	11:c:34:LEU:HA	1.84	0.44
14:f:169:LEU:HD12	14:f:169:LEU:C	2.42	0.44
32:z:14:HIS:O	32:z:14:HIS:CG	2.70	0.44
10:b:136:G:C6	10:b:137:U:C4	3.06	0.44
11:c:154:LEU:HD22	11:c:176:LEU:HD22	1.99	0.44
18:k:102:PRO:HB3	18:k:121:GLU:HB3	2.00	0.44
20:m:21:ALA:HB1	20:m:100:LYS:HD3	1.99	0.44
9:a:43:C:H6	9:a:43:C:C5'	2.26	0.44
10:b:2208:G:OP2	11:c:150:LYS:NZ	2.36	0.44
12:d:13:ARG:HD2	12:d:21:SER:HB2	1.99	0.44
13:e:67:ARG:NH1	32:z:154:VAL:CG2	2.81	0.44
30:w:55:GLU:HA	30:w:58:SER:HB3	2.00	0.44
30:w:70:ILE:HG21	30:w:93:ARG:HE	1.82	0.44
1:0:3:ARG:CD	1:0:30:LEU:HD23	2.48	0.44
9:a:41:G:H3'	9:a:42:C:H5''	1.99	0.44
9:a:112:G:C8	9:a:112:G:O5'	2.70	0.44
9:a:113:C:C6	9:a:113:C:O5'	2.71	0.44
10:b:84:A:N1	10:b:98:G:O2'	2.47	0.44
10:b:2189:U:H2'	10:b:2190:G:H8	1.81	0.44
19:l:71:ALA:HA	19:l:74:THR:HG22	1.99	0.44
26:s:17:VAL:HB	26:s:76:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:v:27:U:C6	29:v:27:U:OP2	2.70	0.44
10:b:657:A:H4'	10:b:658:G:H5'	2.00	0.44
10:b:2641:U:O4	10:b:2642:G:C6	2.71	0.44
10:b:2896:G:H5''	10:b:2897:A:H5'	2.00	0.44
10:b:69:C:O2	10:b:73:A:O2'	2.28	0.43
10:b:155:A:H2'	10:b:156:A:C8	2.53	0.43
10:b:1396:U:H4'	10:b:1605:A:H4'	2.00	0.43
10:b:2319:G:H2'	10:b:2320:G:H8	1.83	0.43
11:c:259:SER:O	11:c:259:SER:OG	2.31	0.43
22:o:39:VAL:HB	22:o:49:VAL:HG22	2.00	0.43
10:b:1301:G:C8	10:b:1301:G:C3'	3.01	0.43
10:b:1443:G:C2'	10:b:1444:U:H5'	2.48	0.43
10:b:2335:G:H4'	31:y:43:THR:H	1.83	0.43
17:j:36:LEU:HD11	17:j:122:LEU:HD13	1.99	0.43
17:j:121:LYS:HB2	17:j:121:LYS:HE3	1.82	0.43
10:b:364:C:H2'	10:b:365:U:H6	1.83	0.43
10:b:568:U:H5''	19:l:29:LYS:HE3	2.00	0.43
10:b:1431:G:H2'	10:b:1432:G:H8	1.83	0.43
17:j:23:LYS:HE2	17:j:142:ILE:HB	2.00	0.43
20:m:53:MET:HG3	20:m:120:ALA:HB2	2.01	0.43
21:n:22:ARG:HE	21:n:22:ARG:HB2	1.66	0.43
29:v:65:U:H2'	29:v:66:G:C8	2.53	0.43
9:a:50:A:OP1	22:o:68:LYS:N	2.43	0.43
10:b:483:A:OP1	28:u:47:LYS:NZ	2.51	0.43
10:b:655:U:O2'	10:b:657:A:OP1	2.36	0.43
10:b:1187:G:H5''	10:b:1187:G:H8	1.84	0.43
10:b:2100:C:H2'	10:b:2101:A:C8	2.53	0.43
10:b:2335:G:H21	10:b:2340:A:H8	1.67	0.43
20:m:35:ALA:HA	20:m:128:THR:HG22	2.00	0.43
26:s:83:LYS:CB	32:z:20:SER:CB	2.91	0.43
29:v:25:C:C6	29:v:25:C:OP2	2.70	0.43
9:a:24:G:C5	9:a:56:G:C4	3.07	0.43
10:b:143:C:H2'	10:b:144:A:C8	2.53	0.43
10:b:184:C:H2'	10:b:185:G:C8	2.53	0.43
10:b:1672:C:O2	12:d:134:HIS:NE2	2.36	0.43
10:b:2382:A:H3'	10:b:2383:G:C8	2.53	0.43
26:s:55:ILE:HG23	26:s:66:ILE:HD12	2.00	0.43
9:a:24:G:N7	9:a:56:G:C4	2.86	0.43
9:a:40:U:C2	9:a:43:C:H5'	2.54	0.43
10:b:1021:U:O2'	10:b:1023:A:C2	2.61	0.43
10:b:1023:A:H3'	10:b:1023:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1330:A:H4'	10:b:1331:U:H5	1.83	0.43
26:s:3:THR:OG1	26:s:62:ASP:OD2	2.32	0.43
10:b:1143:U:H4'	10:b:1144:A:O4'	2.18	0.43
10:b:1479:A:N1	10:b:1559:C:O2'	2.51	0.43
17:j:92:MET:HE3	17:j:92:MET:HB3	1.86	0.43
27:t:38:ALA:O	27:t:81:LYS:NZ	2.46	0.43
14:f:158:THR:CG2	14:f:169:LEU:CD2	2.97	0.43
15:g:127:THR:OG1	15:g:130:GLU:OE1	2.32	0.43
26:s:85:ILE:HD12	32:z:21:ASP:O	2.19	0.43
10:b:700:C:O2'	10:b:736:A:N6	2.50	0.43
10:b:1009:C:OP1	17:j:37:ARG:NH2	2.51	0.43
10:b:1915:U:H3'	10:b:1922:A:H61	1.83	0.43
13:e:145:ASP:HA	13:e:166:LYS:HB3	2.00	0.43
14:f:8:TYR:OH	14:f:30:ARG:HG2	2.19	0.43
25:r:24:LYS:HE2	25:r:24:LYS:HB3	1.83	0.43
28:u:38:GLY:N	28:u:62:GLU:OE1	2.41	0.43
1:0:56:MET:HB3	1:0:56:MET:HE2	1.89	0.43
10:b:1756:A:O2'	23:p:103:ARG:NH1	2.50	0.43
10:b:2072:U:H5''	10:b:2072:U:H6	1.84	0.43
10:b:2471:C:O2	20:m:123:LYS:NZ	2.51	0.43
11:c:53:HIS:HA	11:c:217:ARG:HB2	2.01	0.43
14:f:64:LYS:HA	14:f:65:PRO:HD3	1.88	0.43
10:b:340:A:H2'	10:b:341:C:O4'	2.19	0.42
10:b:398:C:OP1	10:b:2094:A:O2'	2.35	0.42
10:b:1602:C:OP1	27:t:81:LYS:NZ	2.41	0.42
10:b:2051:C:O2'	10:b:2827:A:N1	2.44	0.42
10:b:2381:A:O2'	22:o:111:ARG:NH2	2.52	0.42
4:3:37:LYS:HB2	4:3:37:LYS:HE3	1.84	0.42
7:7:30:ARG:HD2	7:7:30:ARG:HA	1.75	0.42
9:a:4:C:H42	9:a:115:A:H61	1.66	0.42
9:a:6:G:H2'	9:a:7:G:H8	1.82	0.42
10:b:1434:G:H2'	10:b:1435:A:C8	2.53	0.42
10:b:2066:A:N6	32:z:162:ILE:HG12	2.34	0.42
10:b:2780:A:H4'	10:b:2781:G:H5''	2.00	0.42
12:d:33:ARG:NH1	12:d:75:ALA:O	2.52	0.42
16:h:3:VAL:HG12	16:h:38:PRO:HA	2.00	0.42
1:0:72:ARG:HG3	1:0:78:TYR:HE2	1.83	0.42
2:1:60:LYS:HB3	2:1:60:LYS:HE2	1.84	0.42
9:a:24:G:N7	9:a:56:G:C8	2.87	0.42
10:b:27:G:C2	10:b:512:G:N3	2.87	0.42
10:b:527:C:C5	10:b:2783:U:H2'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1127:G:OP2	10:b:1128:A:O2'	2.29	0.42
10:b:1552:C:OP1	10:b:1722:U:O2'	2.33	0.42
14:f:51:ASP:O	14:f:55:ALA:N	2.52	0.42
15:g:7:ALA:O	15:g:69:ARG:NE	2.51	0.42
17:j:11:VAL:HG21	17:j:50:THR:HA	2.01	0.42
23:p:106:LYS:HA	23:p:109:ARG:HG3	2.01	0.42
29:v:25:C:OP2	29:v:25:C:C5	2.71	0.42
32:z:25:LEU:HD12	32:z:25:LEU:H	1.82	0.42
10:b:514:A:N3	10:b:583:C:O2'	2.50	0.42
10:b:735:G:O6	10:b:763:A:C8	2.73	0.42
10:b:1591:U:H2'	10:b:1592:A:C8	2.54	0.42
10:b:1794:G:H5'	11:c:204:VAL:HG13	2.00	0.42
13:e:67:ARG:NH1	32:z:154:VAL:HG21	2.34	0.42
13:e:134:LEU:CA	13:e:137:LYS:HB2	2.33	0.42
9:a:4:C:N4	9:a:115:A:H61	2.16	0.42
10:b:391:A:H1'	10:b:411:G:O4'	2.20	0.42
10:b:1569:G:H3'	11:c:85:PRO:HG3	2.02	0.42
10:b:2319:G:H2'	10:b:2320:G:C8	2.54	0.42
10:b:1023:A:C8	10:b:1023:A:C3'	3.03	0.42
10:b:1342:U:OP1	27:t:84:TYR:OH	2.30	0.42
11:c:155:ALA:HB2	11:c:162:VAL:HG13	2.01	0.42
17:j:105:VAL:HG11	17:j:122:LEU:HD22	2.01	0.42
27:t:17:SER:HB3	27:t:20:ALA:H	1.85	0.42
6:6:3:ARG:NH1	10:b:754:A:OP1	2.48	0.42
10:b:299:A:N3	10:b:319:G:O2'	2.49	0.42
10:b:964:G:N2	10:b:2254:G:H1	2.14	0.42
10:b:2849:U:H5''	23:p:52:ASN:O	2.19	0.42
14:f:129:SER:HB2	14:f:155:THR:HG23	2.02	0.42
10:b:320:A:O2'	10:b:322:A:OP2	2.34	0.42
12:d:25:THR:HG21	12:d:193:VAL:HG22	2.02	0.42
12:d:121:THR:HB	12:d:127:PHE:CD2	2.55	0.42
18:k:2:ILE:HD12	18:k:6:THR:HG21	2.01	0.42
10:b:364:C:H2'	10:b:365:U:C6	2.54	0.42
10:b:1049:G:O2'	10:b:1112:G:N1	2.30	0.42
31:y:19:LYS:HA	31:y:19:LYS:HD3	1.79	0.42
31:y:50:ASN:HB2	31:y:82:ILE:HB	2.01	0.42
10:b:414:C:H2'	10:b:415:A:C8	2.54	0.42
10:b:2664:A:O2'	10:b:2665:G:C5'	2.68	0.42
11:c:71:LYS:NZ	11:c:100:GLU:OE1	2.40	0.42
11:c:210:ALA:HA	11:c:213:TRP:CE2	2.55	0.42
14:f:34:ILE:HG13	14:f:91:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:15:LYS:HE2	24:q:15:LYS:HB3	1.75	0.42
10:b:912:A:N3	10:b:2268:C:O2'	2.47	0.41
10:b:1330:A:H4'	10:b:1331:U:C5	2.55	0.41
10:b:2175:A:O2'	10:b:2176:U:O5'	2.37	0.41
10:b:2447:C:H2'	10:b:2448:G:H8	1.84	0.41
10:b:2792:C:O2'	10:b:2813:A:N3	2.52	0.41
10:b:1587:C:H3'	10:b:1588:A:H8	1.86	0.41
11:c:96:TYR:HE1	11:c:102:ARG:HG3	1.85	0.41
27:t:36:LYS:HA	27:t:36:LYS:HD2	1.86	0.41
10:b:2265:C:OP1	31:y:19:LYS:NZ	2.37	0.41
10:b:2284:G:O2'	10:b:2392:A:N1	2.52	0.41
10:b:2696:G:N3	10:b:2851:U:O2'	2.52	0.41
10:b:2801:U:H6	10:b:2801:U:H2'	1.68	0.41
24:q:17:ILE:HD13	24:q:17:ILE:HA	1.95	0.41
10:b:2640:C:H2'	10:b:2641:U:C6	2.55	0.41
14:f:37:ASN:HB3	14:f:153:ASP:HB2	2.02	0.41
16:h:8:LYS:O	16:h:8:LYS:NZ	2.42	0.41
21:n:20:MET:HE2	21:n:20:MET:HB3	1.80	0.41
26:s:90:LYS:O	32:z:155:TRP:CH2	2.69	0.41
10:b:2036:G:N2	12:d:151:THR:OG1	2.45	0.41
11:c:13:ARG:HD2	11:c:13:ARG:HA	1.86	0.41
11:c:111:LYS:HE3	11:c:111:LYS:HB3	1.88	0.41
17:j:32:LEU:HD22	17:j:54:ILE:HG21	2.01	0.41
19:l:95:LEU:HD11	19:l:125:LEU:HD21	2.02	0.41
9:a:45:A:O4'	14:f:92:ARG:NE	2.53	0.41
10:b:670:A:H2'	10:b:672:A:H62	1.85	0.41
10:b:1024:G:N2	10:b:1025:U:O4	2.45	0.41
10:b:1431:G:H2'	10:b:1432:G:C8	2.56	0.41
10:b:2303:U:OP2	14:f:71:ARG:NH1	2.52	0.41
10:b:2389:C:H2'	10:b:2390:A:C8	2.56	0.41
24:q:24:TYR:O	24:q:29:SER:OG	2.33	0.41
25:r:60:LYS:HB2	25:r:60:LYS:HE3	1.89	0.41
26:s:17:VAL:HG11	26:s:103:ILE:HG12	2.01	0.41
10:b:729:A:OP1	10:b:1433:A:O2'	2.28	0.41
10:b:1367:A:H8	10:b:1810:A:H61	1.66	0.41
13:e:138:LEU:O	13:e:142:ALA:N	2.54	0.41
22:o:18:LEU:HD13	22:o:25:ARG:HG2	2.02	0.41
9:a:3:C:N3	9:a:117:G:N2	2.67	0.41
10:b:583:C:H2'	10:b:584:A:C8	2.56	0.41
10:b:604:A:O2'	10:b:606:G:O2'	2.25	0.41
10:b:980:G:O2'	10:b:1004:G:O2'	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1921:U:H2'	10:b:1922:A:O4'	2.21	0.41
10:b:2519:C:H2'	10:b:2520:A:H8	1.85	0.41
11:c:78:VAL:HG21	11:c:110:LEU:HD11	2.01	0.41
14:f:125:ARG:HD3	14:f:125:ARG:HA	1.86	0.41
20:m:33:LEU:HD13	20:m:117:PHE:HB3	2.02	0.41
25:r:40:MET:HG3	25:r:48:LYS:HG2	2.02	0.41
5:4:9:ILE:HA	5:4:53:LYS:HB2	2.02	0.41
7:7:31:HIS:H	7:7:31:HIS:HD2	1.69	0.41
10:b:10:A:C2'	10:b:11:C:H5'	2.50	0.41
10:b:332:A:O2'	10:b:334:C:OP2	2.33	0.41
10:b:477:A:H2'	10:b:478:A:C8	2.55	0.41
10:b:507:A:O4'	10:b:509:C:C2	2.74	0.41
10:b:893:G:H4'	10:b:894:A:C4	2.55	0.41
18:k:1:MET:HA	18:k:32:TYR:HB3	2.02	0.41
18:k:70:ARG:HD2	18:k:76:VAL:HG22	2.02	0.41
22:o:52:SER:HB3	22:o:54:VAL:HG12	2.02	0.41
6:6:40:ALA:N	10:b:459:U:OP1	2.43	0.41
10:b:2:G:N2	10:b:2905:C:O2	2.53	0.41
10:b:1173:G:H5'	10:b:1174:C:H6	1.86	0.41
10:b:1175:U:C2	10:b:1178:U:C4	3.09	0.41
10:b:1784:U:H1'	10:b:2613:U:H5''	2.03	0.41
10:b:2454:A:OP1	10:b:2501:A:O2'	2.33	0.41
15:g:76:VAL:HA	15:g:79:VAL:HG22	2.03	0.41
26:s:83:LYS:O	26:s:84:ARG:NH2	2.49	0.41
10:b:538:A:H3'	10:b:539:G:H8	1.86	0.40
10:b:588:A:H2	10:b:811:G:N3	2.19	0.40
10:b:2034:A:C2	10:b:2503:C:H5''	2.57	0.40
10:b:2034:A:N3	10:b:2503:C:H5''	2.36	0.40
10:b:2519:C:H2'	10:b:2520:A:C8	2.56	0.40
10:b:2892:C:H2'	10:b:2893:C:C6	2.56	0.40
18:k:40:LYS:NZ	18:k:89:ASN:OD1	2.41	0.40
1:0:61:LYS:HD2	10:b:372:G:C8	2.57	0.40
29:v:4:G:H1	29:v:66:G:H1	1.69	0.40
10:b:20:C:H2'	10:b:21:A:C8	2.56	0.40
10:b:360:U:H3'	10:b:361:G:C8	2.56	0.40
14:f:170:LEU:HA	14:f:173:PHE:HD2	1.86	0.40
15:g:47:ASP:OD1	15:g:47:ASP:N	2.53	0.40
25:r:73:LYS:HD3	25:r:73:LYS:HA	1.86	0.40
27:t:12:ARG:HB2	27:t:33:LYS:HG2	2.02	0.40
28:u:86:ARG:NH1	28:u:100:SER:O	2.55	0.40
30:w:28:ALA:HB3	30:w:40:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:y:33:ALA:N	31:y:64:ASP:OD1	2.54	0.40
4:3:4:GLN:HA	10:b:2619:U:C2	2.57	0.40
4:3:13:ARG:NH1	10:b:517:C:OP1	2.49	0.40
7:7:8:ARG:HD2	7:7:8:ARG:HA	1.90	0.40
9:a:42:C:H3'	9:a:43:C:H5''	2.03	0.40
10:b:2295:U:H2'	10:b:2296:U:C6	2.57	0.40
32:z:157:SER:O	32:z:157:SER:OG	2.28	0.40
9:a:51:G:HO2'	9:a:52:A:P	2.45	0.40
10:b:778:G:N7	10:b:795:A:O2'	2.48	0.40
10:b:808:C:OP2	19:l:41:ARG:NH1	2.45	0.40
10:b:1940:A:N6	10:b:1967:U:H3	2.20	0.40
14:f:166:GLY:HA2	14:f:169:LEU:HB3	2.02	0.40
18:k:40:LYS:HE3	18:k:57:VAL:HG12	2.03	0.40
23:p:6:LYS:HB2	23:p:6:LYS:HE2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
14	f	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
15	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	21	39
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	33/61 (54%)	25 (76%)	8 (24%)	0	100	100
All	All	3076/3328 (92%)	2855 (93%)	220 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	g	47	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	66 (98%)	1 (2%)	57	78
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	46 (98%)	1 (2%)	47	71
4	3	46/48 (96%)	46 (100%)	0	100	100
5	4	45/49 (92%)	45 (100%)	0	100	100
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	49 (96%)	2 (4%)	28	53
8	8	34/34 (100%)	34 (100%)	0	100	100
11	c	216/218 (99%)	215 (100%)	1 (0%)	81	91
12	d	164/164 (100%)	162 (99%)	2 (1%)	63	82
13	e	165/165 (100%)	162 (98%)	3 (2%)	51	74
14	f	148/150 (99%)	146 (99%)	2 (1%)	59	79
15	g	137/138 (99%)	136 (99%)	1 (1%)	76	88
16	h	30/114 (26%)	29 (97%)	1 (3%)	33	59
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	102 (100%)	0	100	100
20	m	109/109 (100%)	108 (99%)	1 (1%)	70	85
21	n	100/103 (97%)	100 (100%)	0	100	100
22	o	86/87 (99%)	85 (99%)	1 (1%)	63	82
23	p	98/100 (98%)	97 (99%)	1 (1%)	68	84
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	82/84 (98%)	81 (99%)	1 (1%)	63	82
26	s	92/93 (99%)	91 (99%)	1 (1%)	65	83
27	t	80/84 (95%)	79 (99%)	1 (1%)	61	81
28	u	83/85 (98%)	83 (100%)	0	100	100
30	w	78/78 (100%)	78 (100%)	0	100	100
31	y	55/63 (87%)	54 (98%)	1 (2%)	51	74
32	z	31/53 (58%)	29 (94%)	2 (6%)	15	33
All	All	2546/2694 (94%)	2523 (99%)	23 (1%)	68	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
3	2	36	VAL
7	7	6	THR
7	7	30	ARG
11	c	184	VAL
12	d	121	THR
12	d	151	THR
13	e	121	VAL
13	e	137	LYS
13	e	138	LEU
14	f	146	VAL
14	f	169	LEU
15	g	43	VAL
16	h	12	LEU
20	m	75	GLU
22	o	67	ASN
23	p	92	VAL
25	r	72	VAL
26	s	29	VAL
27	t	74	ILE
31	y	51	VAL
32	z	25	LEU
32	z	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	20	HIS
2	1	25	GLN
5	4	26	ASN
11	c	163	GLN
13	e	9	GLN
13	e	90	GLN
14	f	27	GLN
14	f	135	GLN
15	g	73	ASN
15	g	115	HIS
17	j	80	HIS
19	l	104	GLN
20	m	13	HIS
20	m	97	GLN
21	n	73	ASN
22	o	98	GLN

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Mol	Chain	Res	Type
23	p	56	HIS
23	p	66	ASN
24	q	71	GLN
25	r	12	HIS
26	s	7	HIS
27	t	15	HIS
27	t	59	ASN
32	z	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2882/2906 (99%)	767 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3072/3101 (99%)	837 (27%)	0

All (837) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G
9	a	24	G
9	a	25	U
9	a	26	C
9	a	29	A
9	a	30	C
9	a	35	C
9	a	39	A
9	a	42	C
9	a	43	C
9	a	44	G
9	a	52	A
9	a	53	A
9	a	56	G
9	a	66	A
9	a	67	G
9	a	87	U

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Mol	Chain	Res	Type
9	a	88	C
9	a	89	U
9	a	90	C
9	a	91	C
9	a	93	C
9	a	99	A
9	a	109	A
9	a	112	G
9	a	113	C
9	a	114	C
9	a	117	G
9	a	118	C
10	b	4	U
10	b	10	A
10	b	12	U
10	b	15	G
10	b	28	A
10	b	34	U
10	b	35	G
10	b	46	G
10	b	51	G
10	b	62	U
10	b	63	A
10	b	71	A
10	b	74	A
10	b	75	G
10	b	84	A
10	b	91	A
10	b	92	U
10	b	93	G
10	b	100	U
10	b	101	A
10	b	102	U
10	b	103	A
10	b	118	A
10	b	119	A
10	b	120	U
10	b	121	G
10	b	122	G
10	b	125	A
10	b	136	G
10	b	137	U

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Mol	Chain	Res	Type
10	b	142	A
10	b	144	A
10	b	159	G
10	b	160	A
10	b	163	C
10	b	174	U
10	b	175	G
10	b	177	G
10	b	196	A
10	b	199	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A
10	b	223	A
10	b	224	U
10	b	229	C
10	b	230	G
10	b	233	A
10	b	245	G
10	b	248	G
10	b	252	G
10	b	255	A
10	b	264	C
10	b	265	A
10	b	266	G
10	b	271	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	294	A
10	b	298	G
10	b	300	A
10	b	302	C
10	b	317	G
10	b	318	C
10	b	322	A
10	b	329	G
10	b	330	A
10	b	331	C
10	b	332	A

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Mol	Chain	Res	Type
10	b	343	C
10	b	345	A
10	b	346	A
10	b	347	A
10	b	352	A
10	b	353	C
10	b	355	U
10	b	358	U
10	b	359	G
10	b	362	A
10	b	363	G
10	b	366	C
10	b	367	G
10	b	371	A
10	b	372	G
10	b	373	U
10	b	386	G
10	b	387	U
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G
10	b	405	U
10	b	406	G
10	b	417	C
10	b	418	C
10	b	439	A
10	b	442	G
10	b	446	G
10	b	451	U
10	b	457	A
10	b	464	U
10	b	467	G
10	b	471	A
10	b	472	A
10	b	474	G
10	b	481	G
10	b	487	C
10	b	491	G
10	b	501	A
10	b	503	A
10	b	505	A

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Mol	Chain	Res	Type
10	b	507	A
10	b	508	A
10	b	509	C
10	b	510	C
10	b	513	A
10	b	527	C
10	b	529	A
10	b	531	C
10	b	532	A
10	b	538	A
10	b	558	A
10	b	559	C
10	b	565	A
10	b	570	U
10	b	575	U
10	b	577	A
10	b	579	G
10	b	590	U
10	b	604	A
10	b	605	A
10	b	606	G
10	b	608	U
10	b	615	A
10	b	616	A
10	b	617	U
10	b	624	G
10	b	629	A
10	b	636	C
10	b	639	A
10	b	642	C
10	b	644	U
10	b	648	U
10	b	649	G
10	b	655	U
10	b	656	A
10	b	657	A
10	b	661	G
10	b	670	A
10	b	671	G
10	b	672	A
10	b	688	U
10	b	704	U

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Mol	Chain	Res	Type
10	b	706	G
10	b	719	C
10	b	720	A
10	b	725	C
10	b	729	A
10	b	732	A
10	b	740	G
10	b	749	U
10	b	750	G
10	b	754	A
10	b	759	G
10	b	764	U
10	b	766	A
10	b	767	C
10	b	777	G
10	b	778	G
10	b	784	A
10	b	786	G
10	b	787	G
10	b	791	A
10	b	793	C
10	b	807	G
10	b	808	C
10	b	811	G
10	b	813	U
10	b	814	C
10	b	821	A
10	b	829	U
10	b	832	G
10	b	848	U
10	b	849	U
10	b	858	G
10	b	860	G
10	b	861	G
10	b	868	A
10	b	871	G
10	b	874	U
10	b	875	C
10	b	878	C
10	b	879	A
10	b	880	A
10	b	882	G

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Mol	Chain	Res	Type
10	b	883	G
10	b	884	G
10	b	885	G
10	b	886	U
10	b	889	U
10	b	890	C
10	b	896	U
10	b	897	U
10	b	898	A
10	b	899	C
10	b	902	A
10	b	909	G
10	b	912	A
10	b	913	A
10	b	914	C
10	b	921	U
10	b	933	U
10	b	943	A
10	b	947	A
10	b	948	C
10	b	963	C
10	b	975	A
10	b	976	G
10	b	985	A
10	b	991	G
10	b	992	A
10	b	998	A
10	b	1005	G
10	b	1007	C
10	b	1012	A
10	b	1014	U
10	b	1015	C
10	b	1021	U
10	b	1024	G
10	b	1028	G
10	b	1035	U
10	b	1037	U
10	b	1040	G
10	b	1049	G
10	b	1055	C
10	b	1056	A
10	b	1058	G

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Mol	Chain	Res	Type
10	b	1059	A
10	b	1060	U
10	b	1061	G
10	b	1062	U
10	b	1063	U
10	b	1064	G
10	b	1066	C
10	b	1068	U
10	b	1069	A
10	b	1070	G
10	b	1071	A
10	b	1072	A
10	b	1073	G
10	b	1075	A
10	b	1076	G
10	b	1077	C
10	b	1078	C
10	b	1079	A
10	b	1080	U
10	b	1081	C
10	b	1082	A
10	b	1083	U
10	b	1086	A
10	b	1087	A
10	b	1088	A
10	b	1089	G
10	b	1090	A
10	b	1091	A
10	b	1092	A
10	b	1097	A
10	b	1099	U
10	b	1100	A
10	b	1101	G
10	b	1102	C
10	b	1103	U
10	b	1104	C
10	b	1106	C
10	b	1107	U
10	b	1108	G
10	b	1111	C
10	b	1113	A
10	b	1114	G

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Mol	Chain	Res	Type
10	b	1119	C
10	b	1121	U
10	b	1132	U
10	b	1134	U
10	b	1135	A
10	b	1136	A
10	b	1137	C
10	b	1138	G
10	b	1144	A
10	b	1170	G
10	b	1171	A
10	b	1172	C
10	b	1173	G
10	b	1174	C
10	b	1175	U
10	b	1177	A
10	b	1178	U
10	b	1179	G
10	b	1187	G
10	b	1189	G
10	b	1190	U
10	b	1197	G
10	b	1206	A
10	b	1207	A
10	b	1208	G
10	b	1209	C
10	b	1212	G
10	b	1214	G
10	b	1226	U
10	b	1229	G
10	b	1234	G
10	b	1238	G
10	b	1239	A
10	b	1240	G
10	b	1242	U
10	b	1243	A
10	b	1244	U
10	b	1246	A
10	b	1249	A
10	b	1251	U
10	b	1252	G
10	b	1255	A

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Mol	Chain	Res	Type
10	b	1257	U
10	b	1258	G
10	b	1268	G
10	b	1273	G
10	b	1274	A
10	b	1275	U
10	b	1277	A
10	b	1278	A
10	b	1281	G
10	b	1286	A
10	b	1289	A
10	b	1291	C
10	b	1302	G
10	b	1303	A
10	b	1304	A
10	b	1313	G
10	b	1321	C
10	b	1323	A
10	b	1328	U
10	b	1331	U
10	b	1336	G
10	b	1342	U
10	b	1346	U
10	b	1354	U
10	b	1361	A
10	b	1367	A
10	b	1370	G
10	b	1380	A
10	b	1381	U
10	b	1382	G
10	b	1385	A
10	b	1388	C
10	b	1397	A
10	b	1398	U
10	b	1402	U
10	b	1412	G
10	b	1413	U
10	b	1417	U
10	b	1418	G
10	b	1421	A
10	b	1422	A
10	b	1423	G

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Mol	Chain	Res	Type
10	b	1429	A
10	b	1430	C
10	b	1444	U
10	b	1453	C
10	b	1454	G
10	b	1455	A
10	b	1456	C
10	b	1457	G
10	b	1461	G
10	b	1462	U
10	b	1463	C
10	b	1469	U
10	b	1471	A
10	b	1473	G
10	b	1477	G
10	b	1478	U
10	b	1479	A
10	b	1480	G
10	b	1484	G
10	b	1495	C
10	b	1497	A
10	b	1498	A
10	b	1499	U
10	b	1500	C
10	b	1505	A
10	b	1507	A
10	b	1510	A
10	b	1511	A
10	b	1525	U
10	b	1526	G
10	b	1531	G
10	b	1534	A
10	b	1535	C
10	b	1538	C
10	b	1539	G
10	b	1540	G
10	b	1541	U
10	b	1542	G
10	b	1544	U
10	b	1545	G
10	b	1549	C
10	b	1554	A

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Mol	Chain	Res	Type
10	b	1556	U
10	b	1558	C
10	b	1561	U
10	b	1567	C
10	b	1568	A
10	b	1570	G
10	b	1571	A
10	b	1580	U
10	b	1583	G
10	b	1585	A
10	b	1586	U
10	b	1587	C
10	b	1598	A
10	b	1601	U
10	b	1609	C
10	b	1610	A
10	b	1612	A
10	b	1620	A
10	b	1621	G
10	b	1649	U
10	b	1650	U
10	b	1651	G
10	b	1662	G
10	b	1670	A
10	b	1676	G
10	b	1677	C
10	b	1680	A
10	b	1697	G
10	b	1705	G
10	b	1707	A
10	b	1708	C
10	b	1709	G
10	b	1717	G
10	b	1720	G
10	b	1723	G
10	b	1724	A
10	b	1732	C
10	b	1733	G
10	b	1735	G
10	b	1736	G
10	b	1740	G
10	b	1750	C

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Mol	Chain	Res	Type
10	b	1758	G
10	b	1759	A
10	b	1760	U
10	b	1765	G
10	b	1766	C
10	b	1775	A
10	b	1778	G
10	b	1783	U
10	b	1784	U
10	b	1786	A
10	b	1788	A
10	b	1793	A
10	b	1802	C
10	b	1803	A
10	b	1810	A
10	b	1813	G
10	b	1818	C
10	b	1831	A
10	b	1835	C
10	b	1844	G
10	b	1851	G
10	b	1859	G
10	b	1864	G
10	b	1870	C
10	b	1886	U
10	b	1888	G
10	b	1899	C
10	b	1910	G
10	b	1911	G
10	b	1912	C
10	b	1914	G
10	b	1917	A
10	b	1918	C
10	b	1922	A
10	b	1924	C
10	b	1931	A
10	b	1933	G
10	b	1934	G
10	b	1935	U
10	b	1941	A
10	b	1942	A
10	b	1944	U

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Mol	Chain	Res	Type
10	b	1959	U
10	b	1971	C
10	b	1974	A
10	b	1975	U
10	b	1976	G
10	b	1978	C
10	b	1979	G
10	b	1985	A
10	b	1986	U
10	b	1995	U
10	b	1996	G
10	b	1997	U
10	b	2001	C
10	b	2024	A
10	b	2027	C
10	b	2034	A
10	b	2035	A
10	b	2036	G
10	b	2037	A
10	b	2039	G
10	b	2040	C
10	b	2047	C
10	b	2053	G
10	b	2059	C
10	b	2060	G
10	b	2064	A
10	b	2065	G
10	b	2066	A
10	b	2067	C
10	b	2071	G
10	b	2073	G
10	b	2081	A
10	b	2084	A
10	b	2097	G
10	b	2102	U
10	b	2103	U
10	b	2105	A
10	b	2106	G
10	b	2107	C
10	b	2109	U
10	b	2111	G
10	b	2112	A

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Mol	Chain	Res	Type
10	b	2113	U
10	b	2115	U
10	b	2116	G
10	b	2119	G
10	b	2120	G
10	b	2121	A
10	b	2122	U
10	b	2124	G
10	b	2125	G
10	b	2126	U
10	b	2127	G
10	b	2128	G
10	b	2129	G
10	b	2131	G
10	b	2132	G
10	b	2134	U
10	b	2136	U
10	b	2139	A
10	b	2140	G
10	b	2142	G
10	b	2146	A
10	b	2149	C
10	b	2150	C
10	b	2151	A
10	b	2152	G
10	b	2153	U
10	b	2155	U
10	b	2156	G
10	b	2159	U
10	b	2160	G
10	b	2162	A
10	b	2163	G
10	b	2164	C
10	b	2166	G
10	b	2167	G
10	b	2168	C
10	b	2169	C
10	b	2170	U
10	b	2172	G
10	b	2173	A
10	b	2174	A
10	b	2176	U

Continued on next page...

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Mol	Chain	Res	Type
10	b	2177	A
10	b	2179	C
10	b	2180	A
10	b	2181	C
10	b	2183	C
10	b	2185	U
10	b	2186	U
10	b	2189	U
10	b	2191	U
10	b	2192	U
10	b	2196	U
10	b	2202	A
10	b	2203	A
10	b	2207	U
10	b	2208	G
10	b	2215	G
10	b	2216	A
10	b	2217	U
10	b	2218	C
10	b	2229	A
10	b	2233	U
10	b	2242	G
10	b	2243	G
10	b	2247	U
10	b	2272	A
10	b	2275	G
10	b	2283	G
10	b	2284	G
10	b	2287	C
10	b	2291	A
10	b	2292	A
10	b	2300	U
10	b	2309	U
10	b	2310	C
10	b	2312	G
10	b	2313	A
10	b	2315	A
10	b	2316	U
10	b	2326	A
10	b	2329	G
10	b	2334	G
10	b	2335	G

Continued on next page...

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Mol	Chain	Res	Type
10	b	2337	A
10	b	2338	U
10	b	2339	A
10	b	2340	A
10	b	2349	G
10	b	2351	C
10	b	2352	U
10	b	2354	C
10	b	2358	C
10	b	2361	G
10	b	2365	G
10	b	2379	G
10	b	2380	A
10	b	2381	A
10	b	2383	G
10	b	2384	C
10	b	2385	A
10	b	2387	G
10	b	2388	U
10	b	2389	C
10	b	2393	G
10	b	2395	G
10	b	2406	U
10	b	2408	U
10	b	2409	G
10	b	2410	A
10	b	2411	A
10	b	2417	G
10	b	2426	C
10	b	2427	U
10	b	2429	A
10	b	2430	A
10	b	2433	G
10	b	2434	A
10	b	2438	A
10	b	2445	U
10	b	2451	G
10	b	2452	A
10	b	2461	U
10	b	2463	A
10	b	2478	U
10	b	2480	A

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Mol	Chain	Res	Type
10	b	2482	A
10	b	2488	G
10	b	2490	C
10	b	2494	G
10	b	2498	G
10	b	2501	A
10	b	2506	G
10	b	2508	U
10	b	2509	G
10	b	2510	U
10	b	2521	C
10	b	2522	A
10	b	2533	G
10	b	2539	G
10	b	2540	G
10	b	2551	A
10	b	2558	U
10	b	2560	C
10	b	2566	U
10	b	2570	A
10	b	2571	G
10	b	2572	U
10	b	2576	A
10	b	2577	C
10	b	2585	G
10	b	2586	G
10	b	2590	U
10	b	2599	G
10	b	2606	A
10	b	2607	G
10	b	2613	U
10	b	2617	U
10	b	2618	A
10	b	2619	U
10	b	2627	G
10	b	2633	U
10	b	2645	G
10	b	2650	C
10	b	2653	C
10	b	2654	U
10	b	2659	G
10	b	2663	G

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Mol	Chain	Res	Type
10	b	2664	A
10	b	2665	G
10	b	2667	G
10	b	2673	G
10	b	2677	G
10	b	2686	A
10	b	2688	U
10	b	2689	G
10	b	2693	U
10	b	2703	C
10	b	2711	U
10	b	2718	G
10	b	2720	C
10	b	2730	A
10	b	2732	U
10	b	2736	G
10	b	2737	A
10	b	2740	A
10	b	2742	A
10	b	2748	G
10	b	2752	A
10	b	2755	G
10	b	2756	C
10	b	2757	A
10	b	2762	A
10	b	2765	A
10	b	2766	C
10	b	2769	A
10	b	2781	G
10	b	2782	A
10	b	2783	U
10	b	2786	G
10	b	2795	G
10	b	2797	C
10	b	2800	C
10	b	2801	U
10	b	2802	U
10	b	2803	G
10	b	2804	A
10	b	2812	G
10	b	2813	A
10	b	2815	G

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Mol	Chain	Res	Type
10	b	2822	U
10	b	2824	A
10	b	2825	A
10	b	2837	U
10	b	2839	A
10	b	2852	G
10	b	2854	A
10	b	2865	U
10	b	2869	U
10	b	2870	U
10	b	2871	G
10	b	2877	A
10	b	2881	G
10	b	2883	A
10	b	2884	C
10	b	2887	A
10	b	2888	U
10	b	2889	G
10	b	2890	A
10	b	2897	A
10	b	2898	G
10	b	2899	G
10	b	2905	C
29	v	3	G
29	v	5	G
29	v	6	C
29	v	7	A
29	v	8	U
29	v	9	C
29	v	15	A
29	v	16	U
29	v	17	G
29	v	18	G
29	v	20	U
29	v	25	C
29	v	26	C
29	v	27	U
29	v	34	U
29	v	35	C
29	v	36	C
29	v	38	A
29	v	42	G

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Mol	Chain	Res	Type
29	v	45	G
29	v	46	A
29	v	47	U
29	v	48	G
29	v	49	C
29	v	50	G
29	v	52	G
29	v	54	U
29	v	60	C
29	v	62	C
29	v	63	G
29	v	64	C
29	v	65	U
29	v	67	C
29	v	68	C
29	v	70	G
29	v	71	C
29	v	75	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

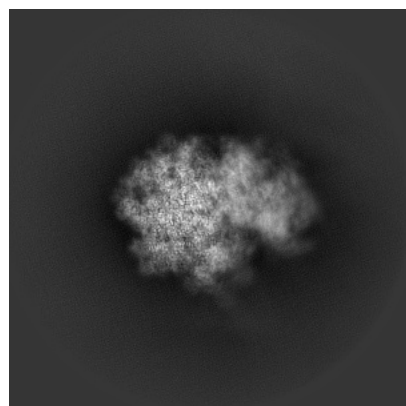
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10891. These allow visual inspection of the internal detail of the map and identification of artifacts.

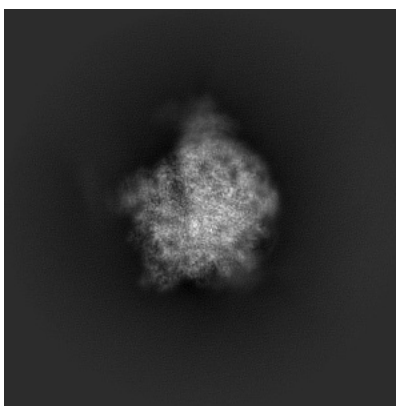
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

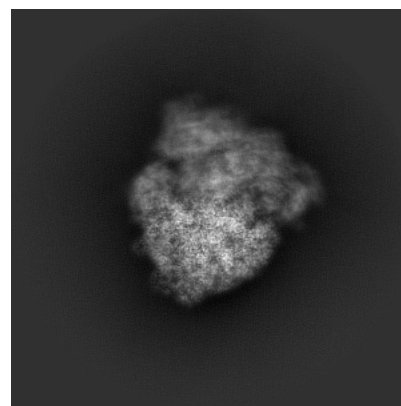
6.1.1 Primary map



X

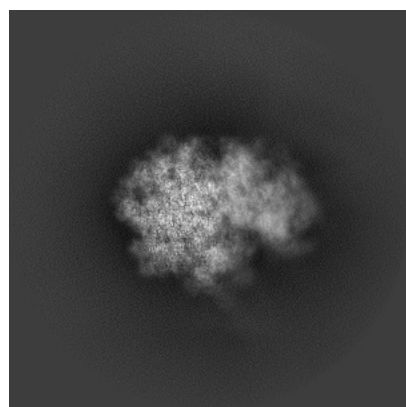


Y

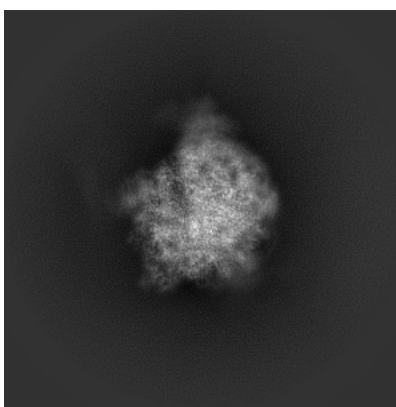


Z

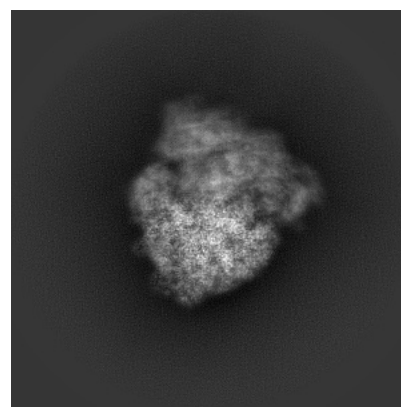
6.1.2 Raw map



X



Y

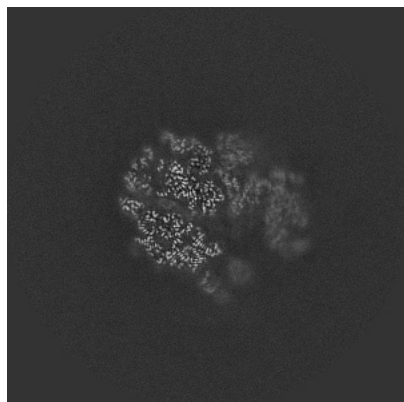


Z

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

6.2 Central slices [i](#)

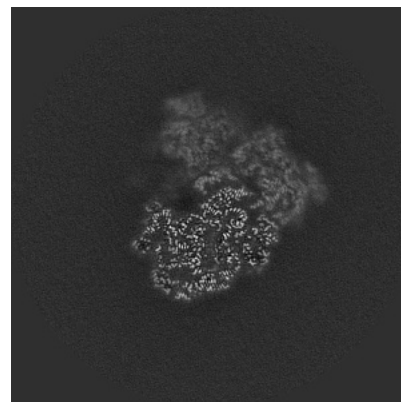
6.2.1 Primary map



X Index: 240

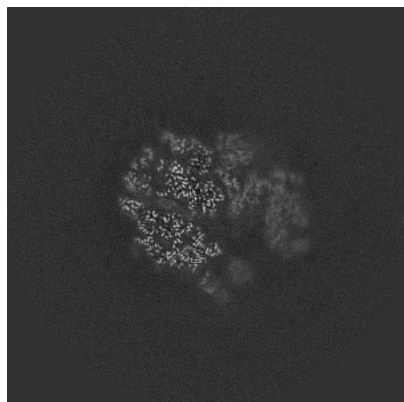


Y Index: 240



Z Index: 240

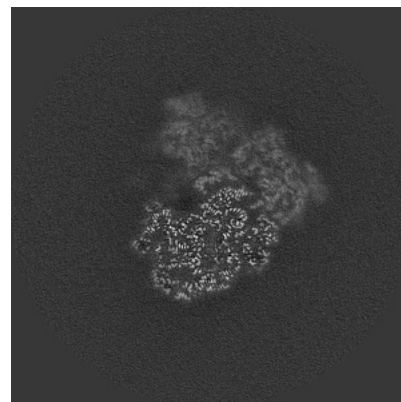
6.2.2 Raw map



X Index: 240



Y Index: 240

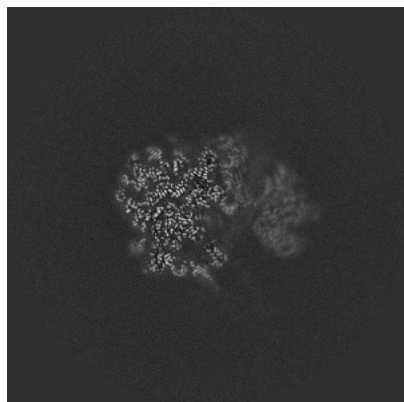


Z Index: 240

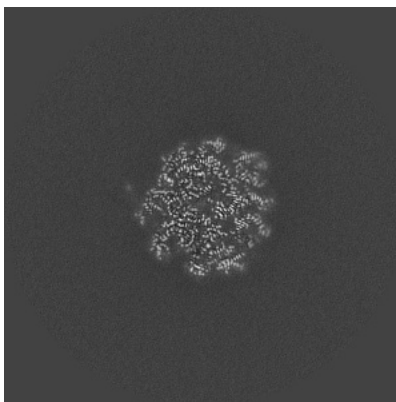
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

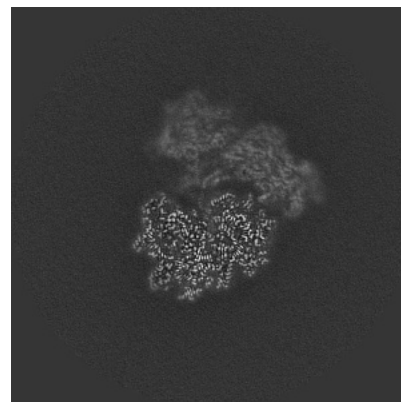
6.3.1 Primary map



X Index: 230

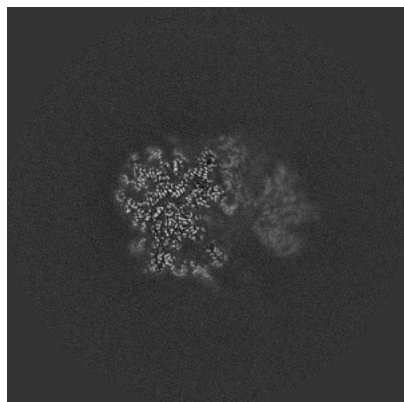


Y Index: 208

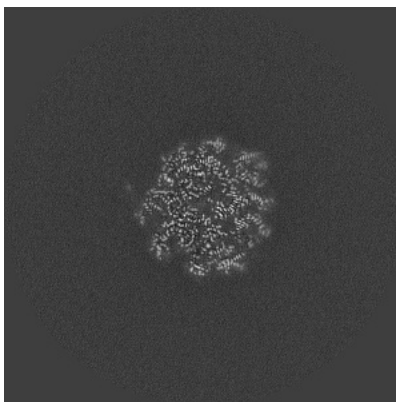


Z Index: 231

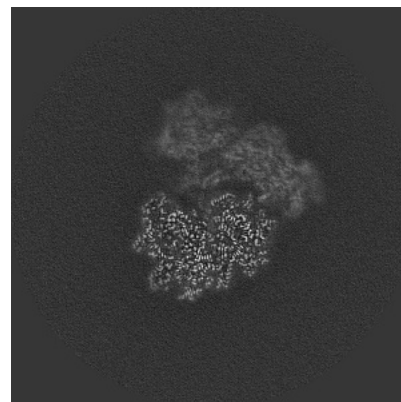
6.3.2 Raw map



X Index: 230



Y Index: 208

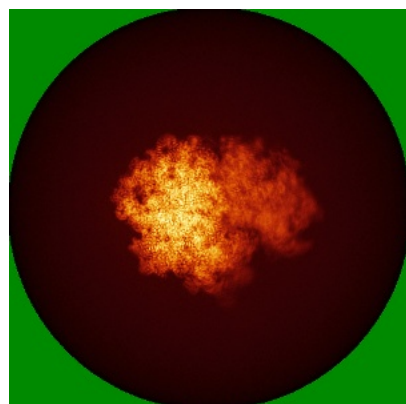


Z Index: 231

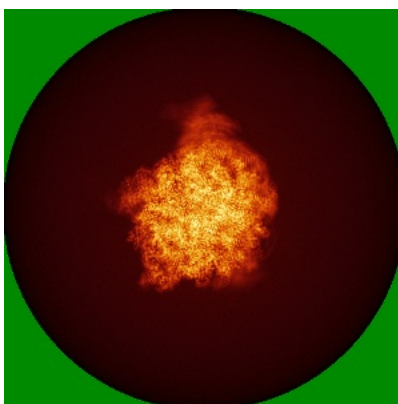
The images above show the largest variance slices of the map in three orthogonal directions.

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

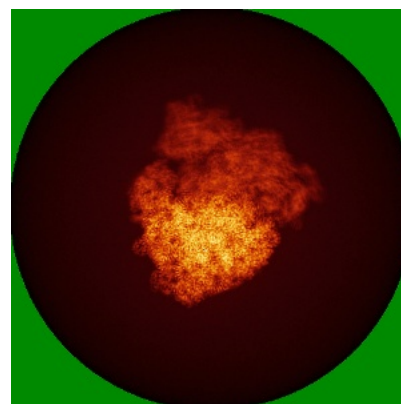
6.4.1 Primary map



X

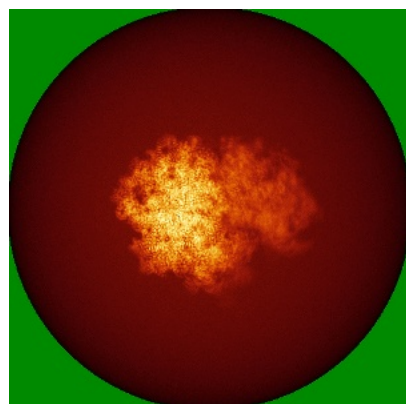


Y

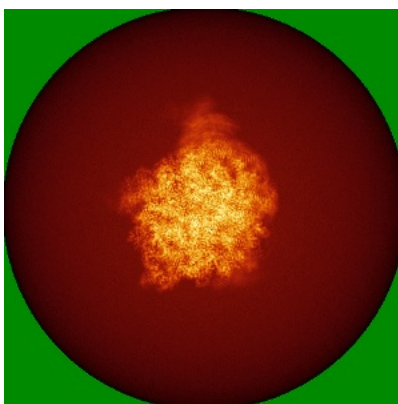


Z

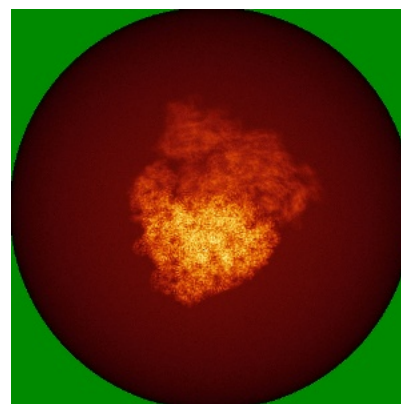
6.4.2 Raw map



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



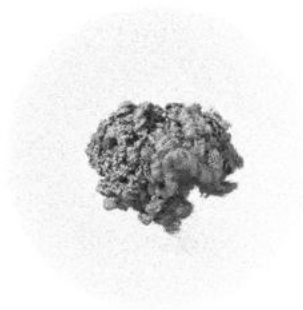
Y



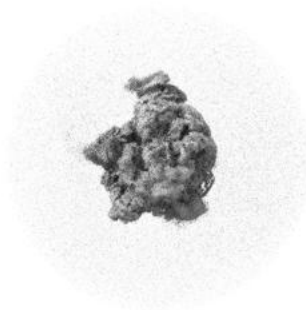
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00741. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

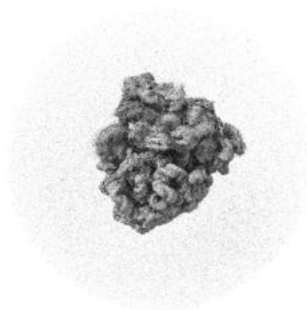
6.5.2 Raw map



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.

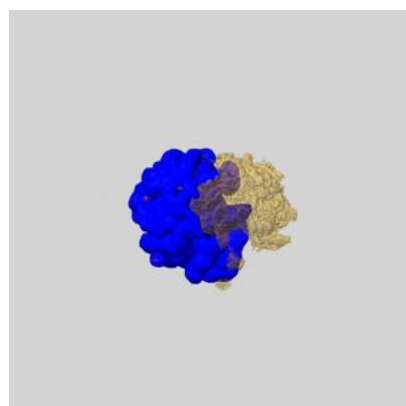
6.6 Mask visualisation [i](#)

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

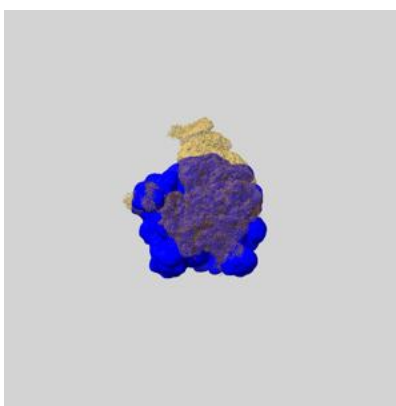
A mask typically either:

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

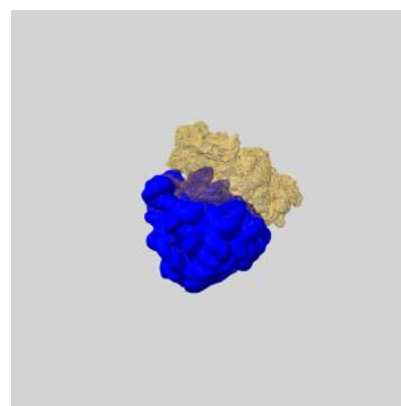
6.6.1 emd_10891_msk_1.map [i](#)



X



Y

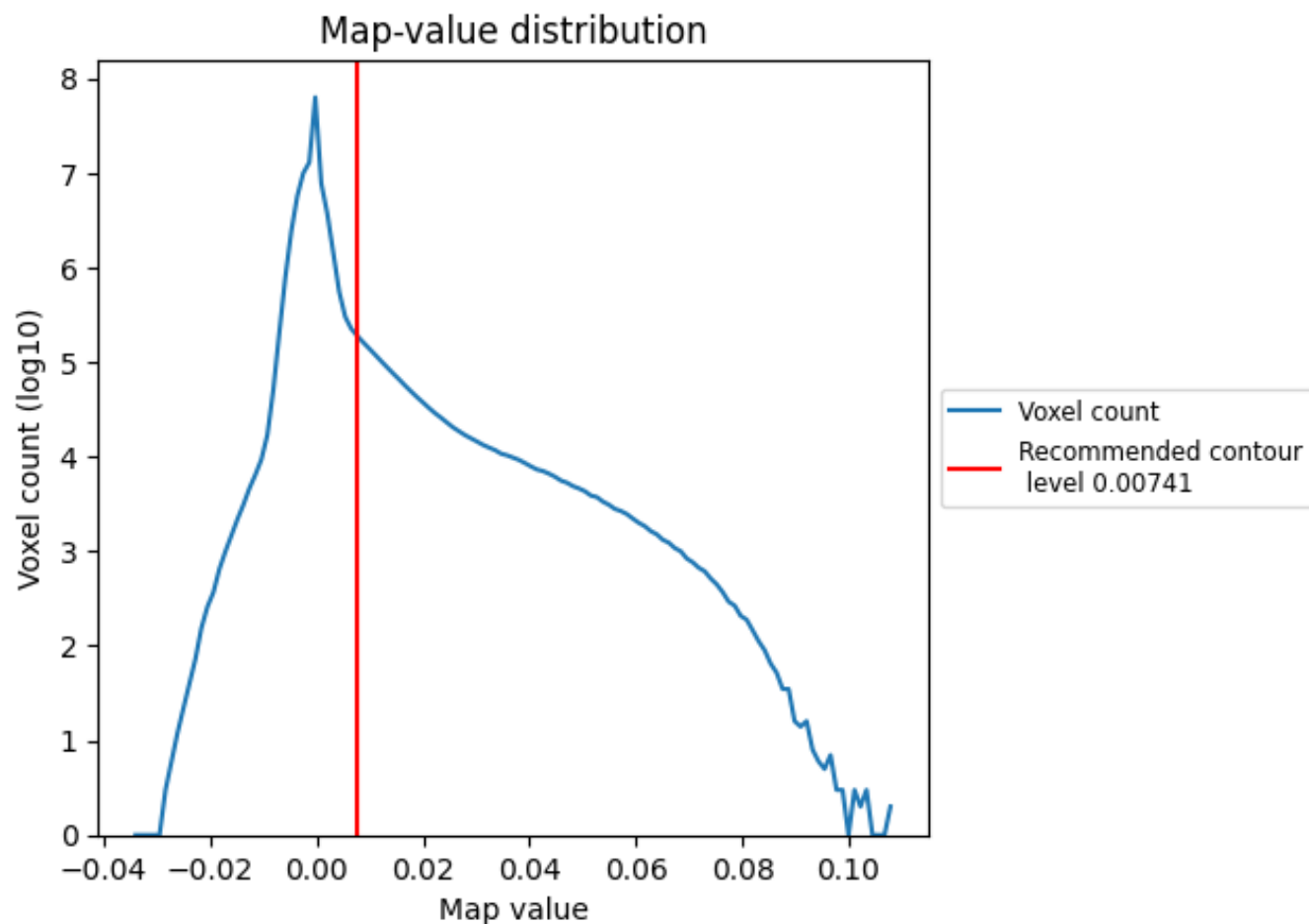


Z

7 Map analysis [i](#)

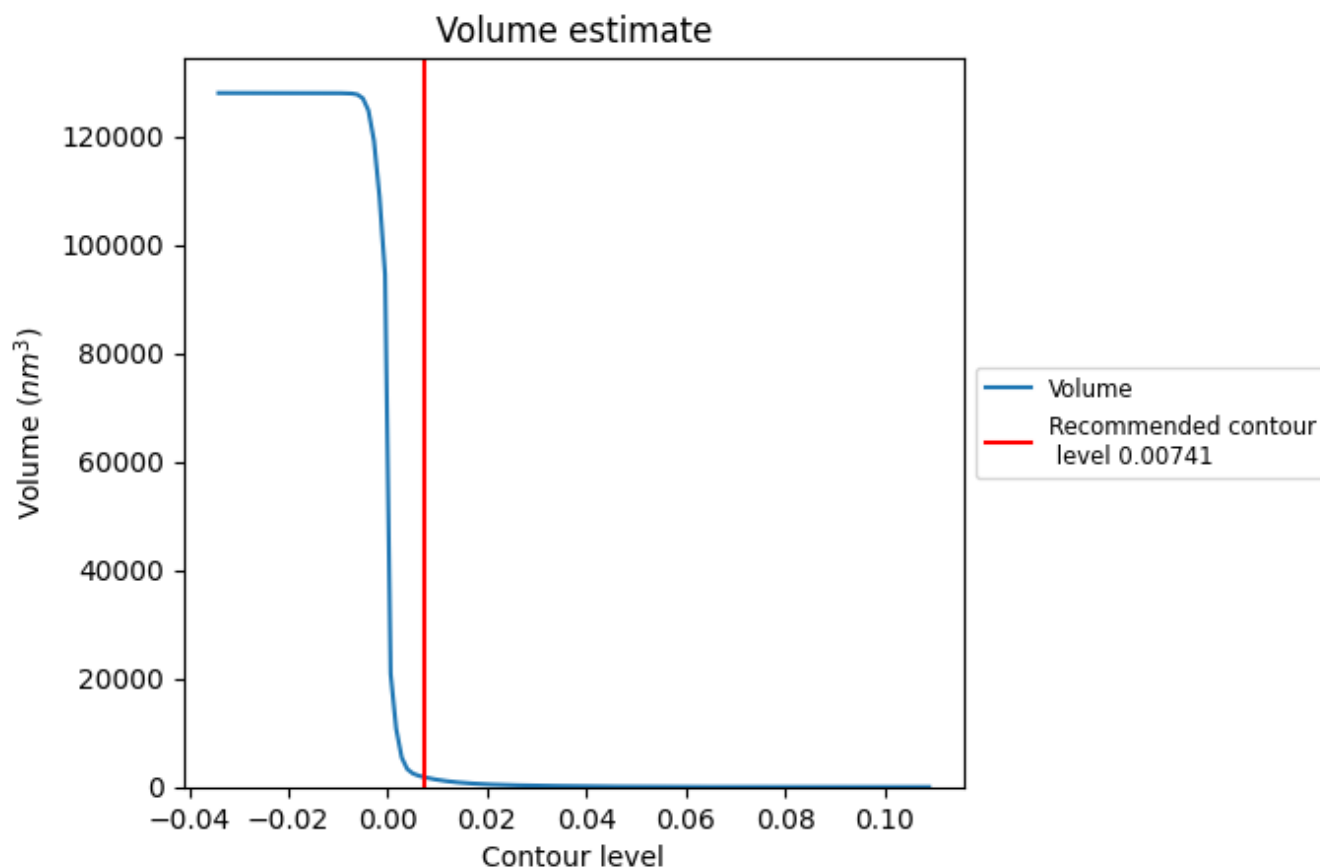
This section contains the results of statistical analysis of the map.

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.

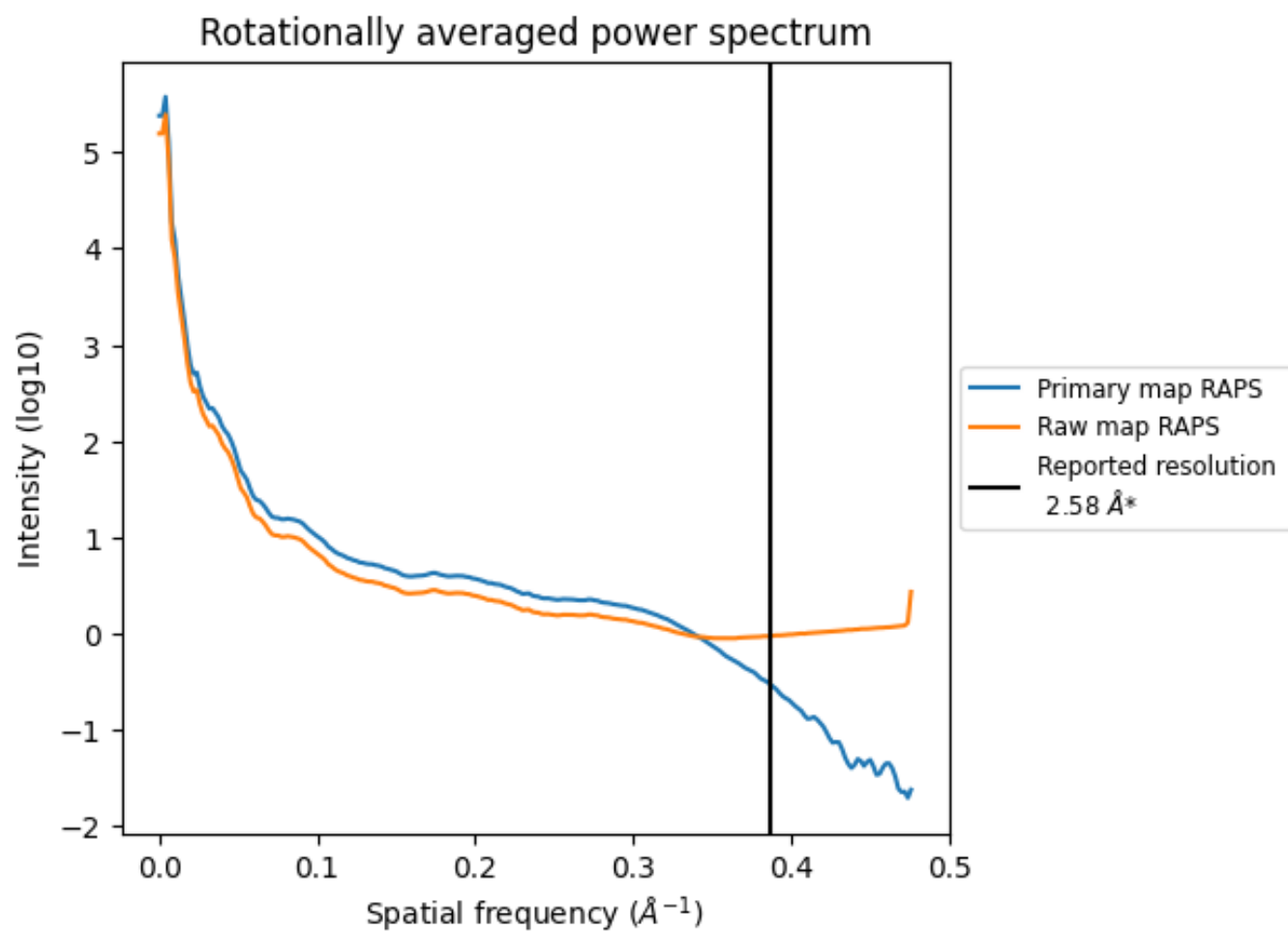
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1796 nm^3 ; this corresponds to an approximate mass of 1623 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 ⓘ

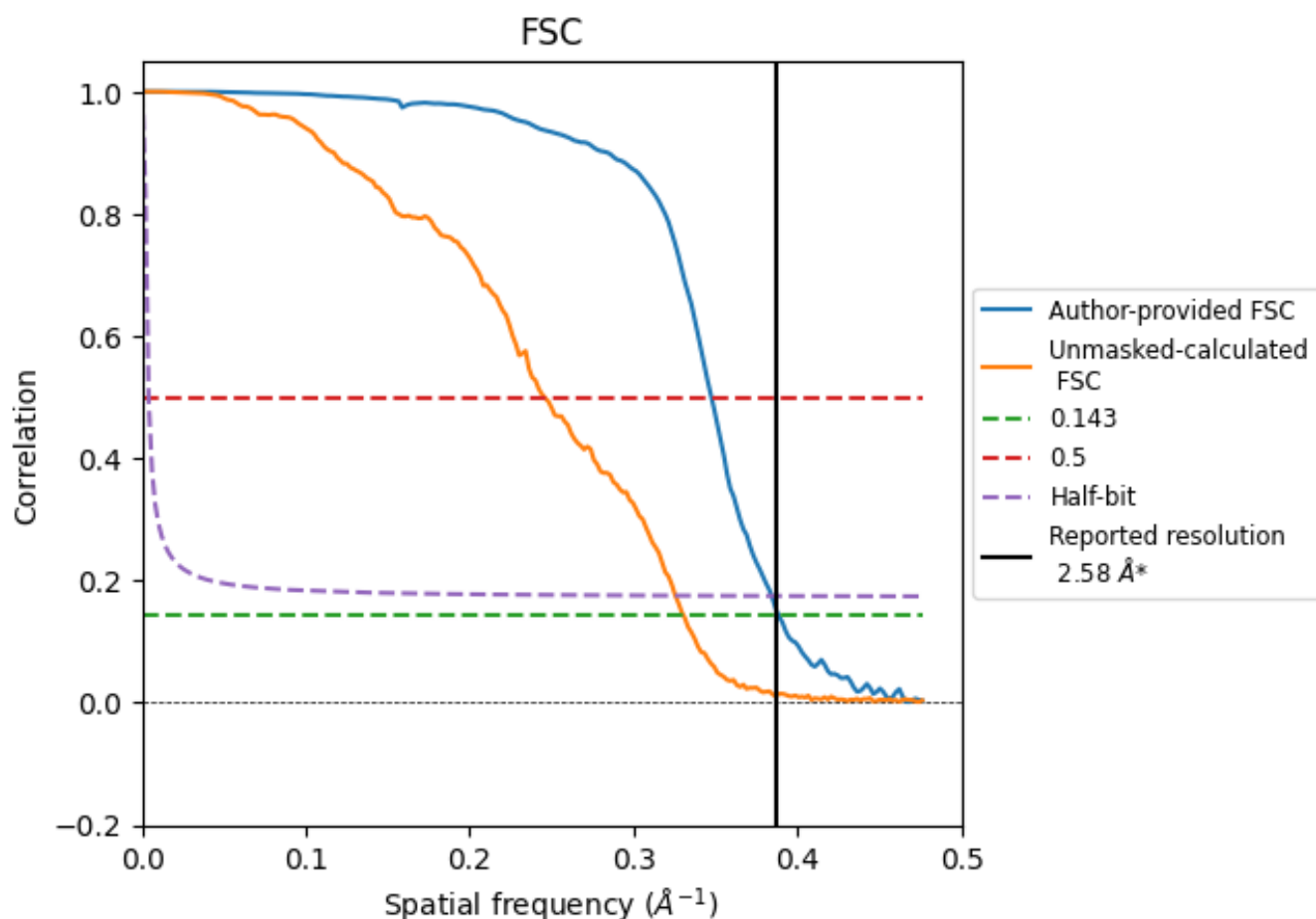


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

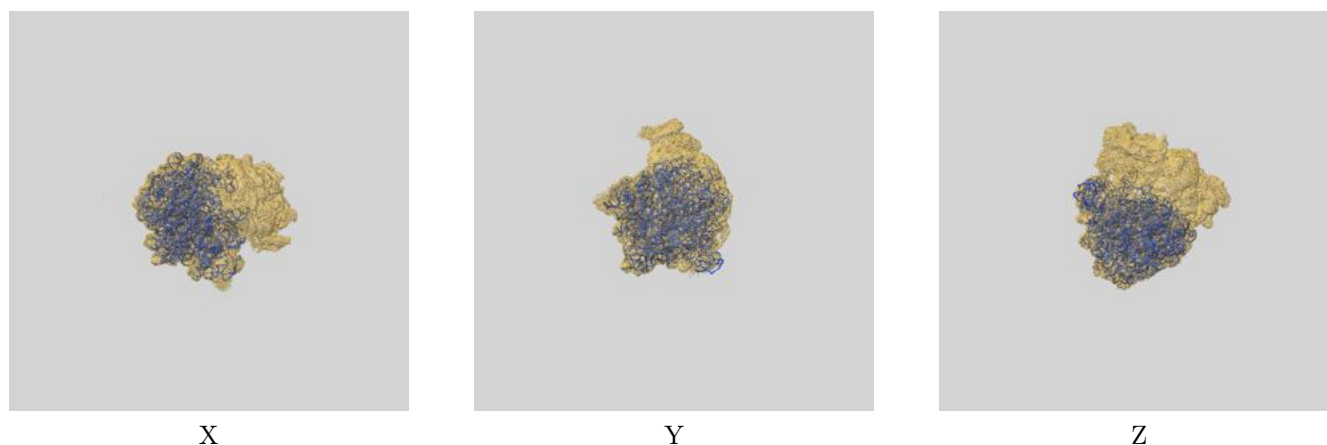
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.88	2.60
Unmasked-calculated*	3.03	4.07	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.58 by more than 10 %

9 Map-model fit [i](#)

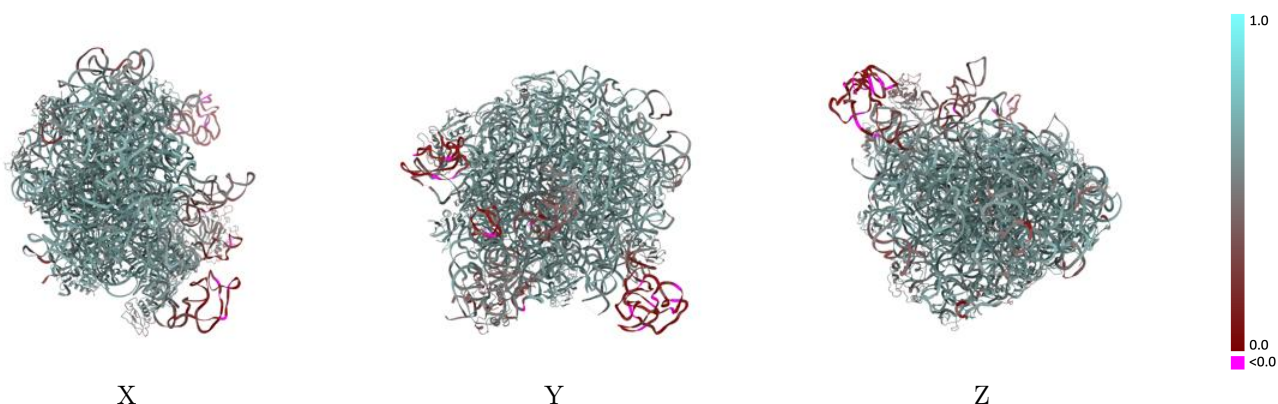
This section contains information regarding the fit between EMDB map EMD-10891 and PDB model 6YS3. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



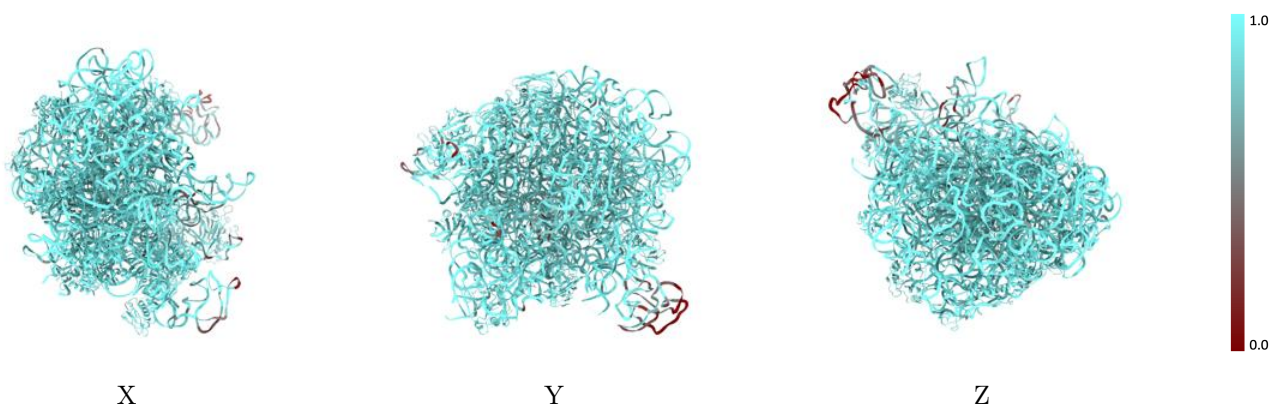
The images above show the 3D surface view of the map at the recommended contour level 0.00741 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



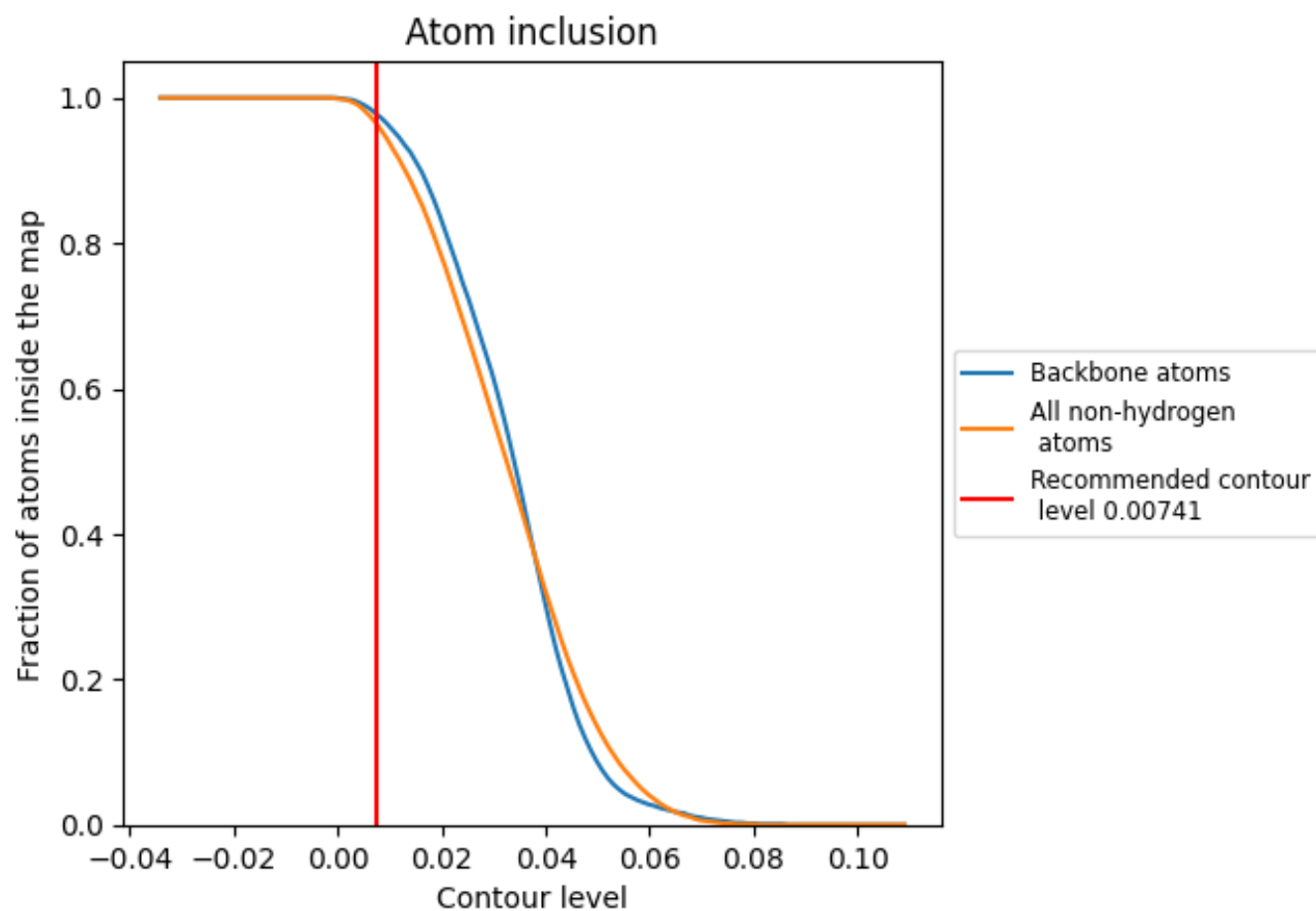
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00741).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00741) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.5680
0	 0.9680	 0.5890
1	 0.9250	 0.5280
2	 0.9630	 0.5880
3	 0.9830	 0.6010
4	 0.9280	 0.5590
6	 0.9800	 0.6240
7	 0.9800	 0.6330
8	 0.9690	 0.5930
a	 0.9870	 0.5370
b	 0.9750	 0.5750
c	 0.9720	 0.6040
d	 0.9630	 0.6020
e	 0.9400	 0.5640
f	 0.8810	 0.3830
g	 0.9220	 0.4980
h	 0.8870	 0.4860
j	 0.9660	 0.6040
k	 0.9560	 0.5900
l	 0.9610	 0.5910
m	 0.9660	 0.6000
n	 0.9860	 0.6090
o	 0.9470	 0.4960
p	 0.9410	 0.5770
q	 0.9770	 0.6140
r	 0.9560	 0.5860
s	 0.9610	 0.6020
t	 0.9430	 0.5570
u	 0.9450	 0.5310
v	 0.7420	 0.3480
w	 0.9420	 0.5670
y	 0.9730	 0.6070
z	 0.7430	 0.3460

