



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:54 AM UTC

PDB ID : 8V84 / pdb_00008v84
EMDB ID : EMD-43021
Title : 60S ribosome biogenesis intermediate (Dbp10 catalytic structure - Overall map)
Authors : Cruz, V.E.; Weirich, C.S.; Peddada, N.; Erzberger, J.P.
Deposited on : 2023-12-04
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:

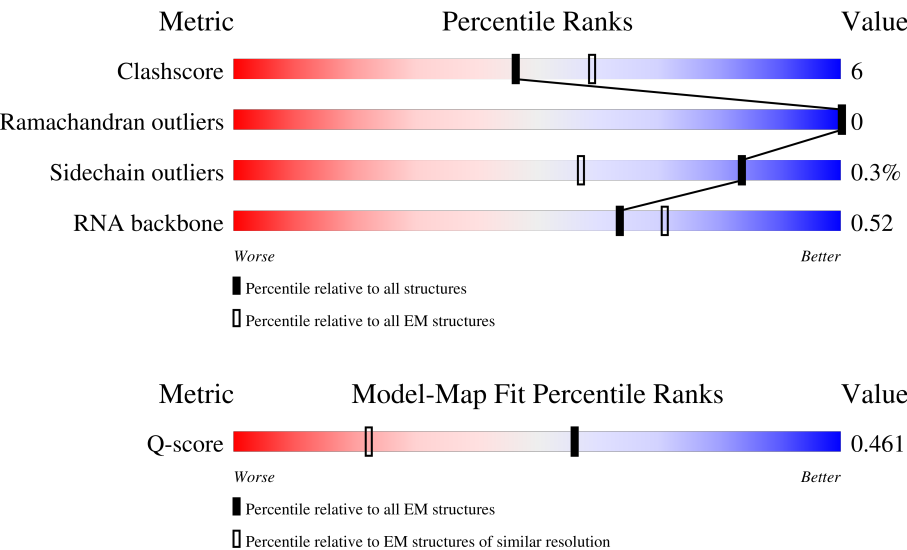
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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	3396	21% 34% 20% 42%
2	2	158	16% 60% 32% 5%
3	3	995	36% 29% 6% 64%

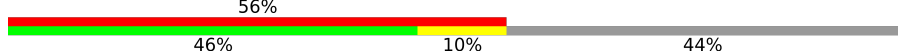
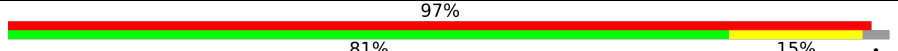
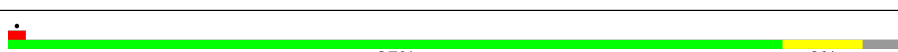
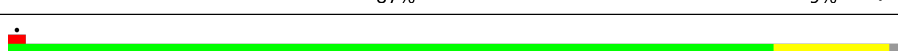
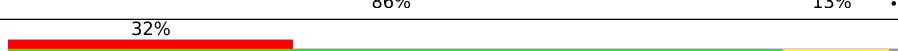
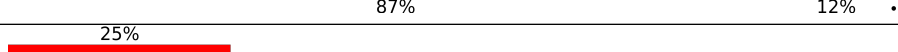
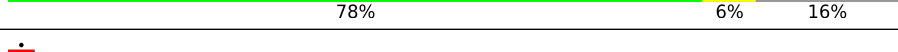
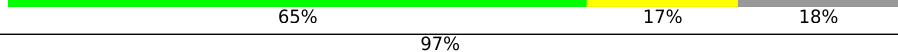
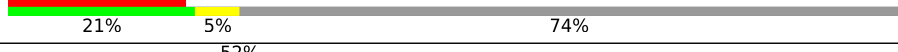
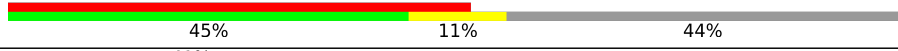
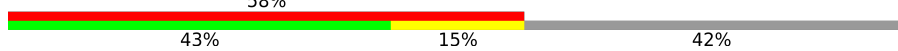
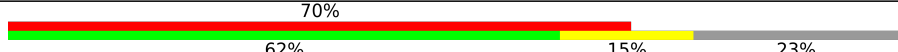
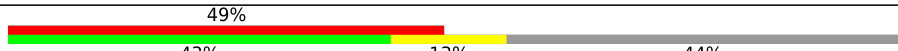
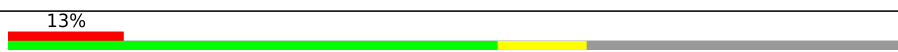
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Mol	Chain	Length	Quality of chain
4	6	232	
5	7	204	
6	8	434	
7	A	291	
8	B	387	
9	C	362	
10	D	505	
11	E	176	
12	F	244	
13	G	256	
14	H	191	
15	I	463	
16	J	427	
17	K	376	
18	L	199	
19	M	138	
20	N	204	
21	O	199	
22	P	184	
23	Q	186	
24	R	306	
25	S	172	
26	T	250	
27	V	137	
28	W	236	

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Mol	Chain	Length	Quality of chain
29	Y	127	
30	Z	453	
31	a	217	
32	b	647	
33	e	130	
34	f	107	
35	h	120	
36	i	100	
37	j	88	
38	l	181	
39	m	807	
40	n	605	
41	o	220	
42	q	618	
43	r	261	
44	t	322	
45	u	199	
46	v	231	
47	w	278	
48	x	295	
49	y	245	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 121244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1970	Total	C	N	O	P	0	0
			42190	18840	7647	13733	1970		

- Molecule 2 is a RNA chain called *Saccharomyces cerevisiae* 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	150	Total	C	N	O	P	0	0
			3189	1426	563	1050	150		

- Molecule 3 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	355	Total	C	N	O	S	0	0
			2884	1842	508	523	11		

- Molecule 4 is a RNA chain called ITS2 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	58	Total	C	N	O	P	0	0
			1227	550	210	409	58		

- Molecule 5 is a protein called 60S ribosomal subunit assembly/export protein LOC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	7	11	Total	C	N	O	0	0
			87	56	15	16		

- Molecule 6 is a protein called Ribosomal RNA-processing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	143	Total	C	N	O	S	0	0
			1203	743	240	216	4		

- Molecule 7 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	255	Total	C	N	O	S	0	0
			2080	1326	372	376	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	331	Total	C	N	O	S	0	0
			2626	1669	484	467	6		

- Molecule 9 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	343	Total	C	N	O	S	0	0
			2611	1643	499	466	3		

- Molecule 10 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	423	Total	C	N	O	S	0	0
			3377	2183	573	609	12		

- Molecule 11 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	151	Total	C	N	O	S	0	0
			1205	780	215	209	1		

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	241	Total	C	N	O	S	0	0
			1936	1246	351	338	1		

- Molecule 13 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	164	Total	C	N	O	S	0	0
			1272	818	217	235	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 15 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	394	Total	C	N	O	S	0	0
			3126	1997	525	593	11		

- Molecule 16 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	151	Total	C	N	O	S	0	0
			1271	793	240	235	3		

- Molecule 17 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	265	Total	C	N	O	S	0	0
			2135	1375	351	405	4		

- Molecule 18 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	110	Total	C	N	O		0	0
			884	552	185	147			

- Molecule 19 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	134	Total	C	N	O	S	0	0
			1041	668	197	174	2		

- Molecule 20 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	177	Total	C	N	O	S	0	0
			1513	948	320	244	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	174	Total	C	N	O	S	0	0
			1386	897	259	229	1		

- Molecule 22 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	137	Total	C	N	O		0	0
			1062	666	198	198			

- Molecule 23 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	144	Total	C	N	O	S	0	0
			1110	704	213	192	1		

- Molecule 24 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	190	Total	C	N	O	S	0	0
			1578	996	297	275	10		

- Molecule 25 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 26 is a protein called Ribosomal RNA-processing protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	79	Total	C	N	O		0	0
			625	390	109	126			

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	122	Total	C	N	O	S	0	0
			903	567	169	160	7		

- Molecule 28 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	125	Total	C	N	O	S	0	0
			984	620	191	173			

- Molecule 30 is a protein called Ribosome biogenesis protein SSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	253	Total	C	N	O	S	0	0
			2020	1280	361	370	9		

- Molecule 31 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	210	Total	C	N	O	S	0	0
			1668	1067	291	301	9		

- Molecule 32 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	423	Total	C	N	O	S	0	0
			3429	2193	586	632	18		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	125	Total	C	N	O	S	0	0
			1010	640	203	166	1		

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 35 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 36 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	84	Total	C	N	O	S	0	0
			665	413	136	114	2		

- Molecule 37 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	72	Total	C	N	O	S	0	0
			571	347	124	95	5		

- Molecule 38 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	176	Total	C	N	O	S	0	0
			1394	896	244	247	7		

- Molecule 39 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	211	Total	C	N	O	S	0	0
			1759	1116	305	333	5		

- Molecule 40 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	337	Total	C	N	O	S	0	0
			2760	1804	462	486	8		

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 42 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	358	Total	C	N	O	S	0	0
			2799	1779	490	518	12		

- Molecule 43 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	200	Total	C	N	O	S	0	0
			1615	1018	306	285	6		

- Molecule 44 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	249	Total	C	N	O	S	0	0
			1973	1258	352	360	3		

- Molecule 45 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	112	Total	C	N	O	S	0	0
			944	594	191	150	9		

- Molecule 46 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	149	Total	C	N	O	S	0	0
			1242	778	242	219	3		

- Molecule 47 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	243	Total	C	N	O	S	0	0
			2058	1334	353	366	5		

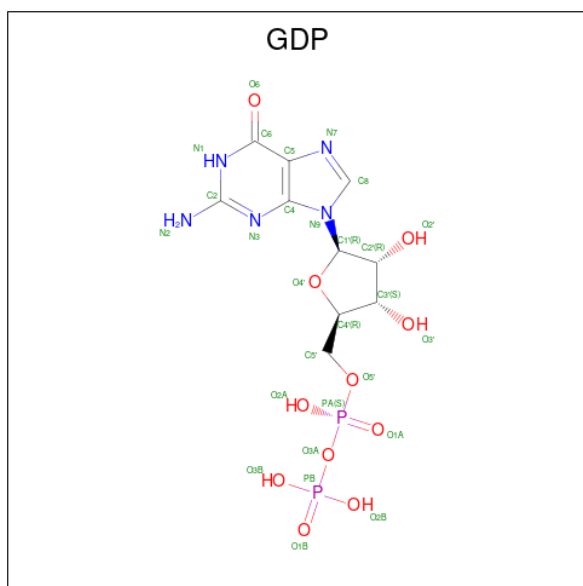
- Molecule 48 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	279	Total	C	N	O	S	0	0
			2362	1500	427	431	4		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 50 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
50	b	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	b	1	Total	Mg	0
			1	1	

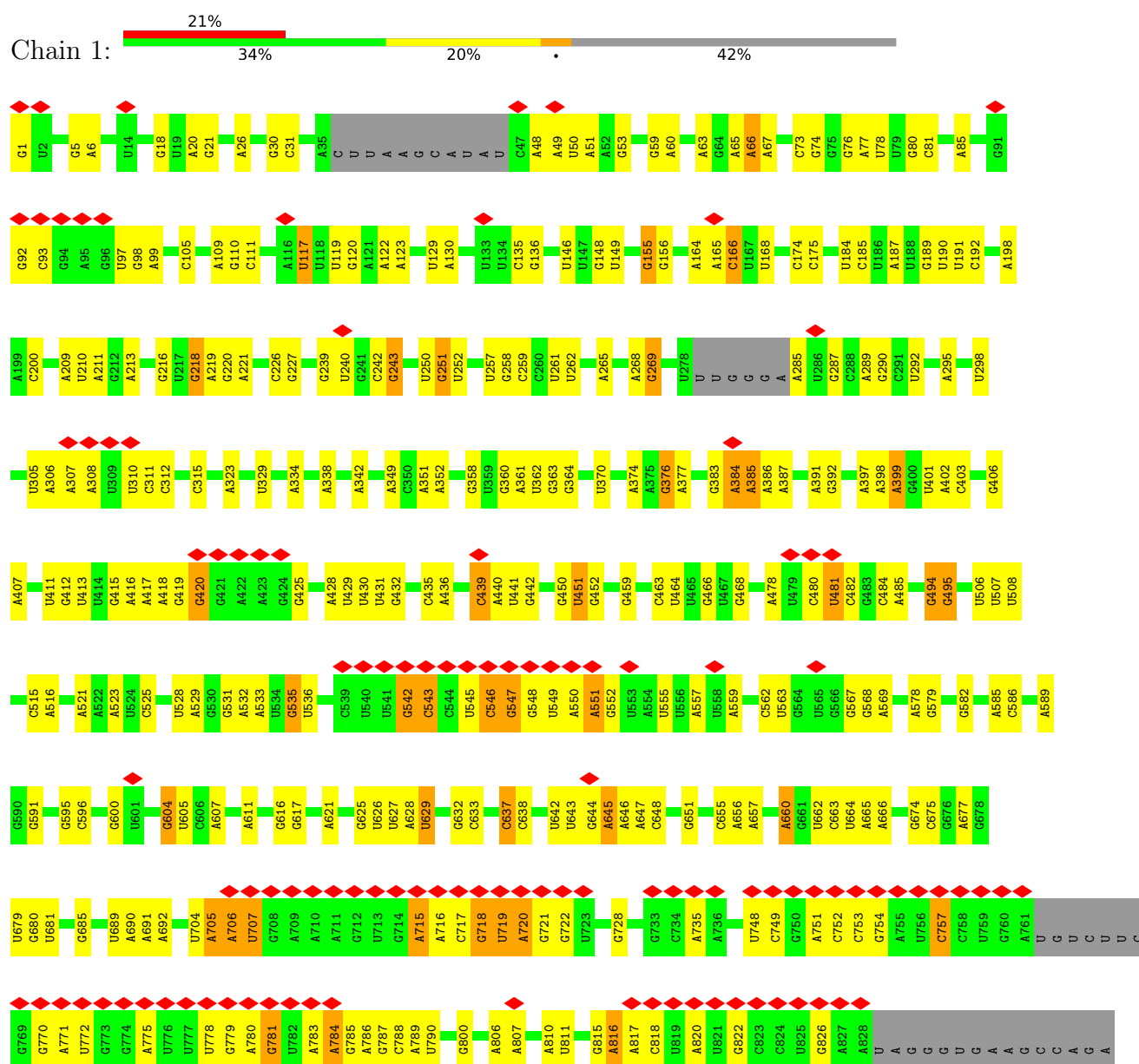
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	j	1	Total	Zn	0
			1	1	
52	u	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

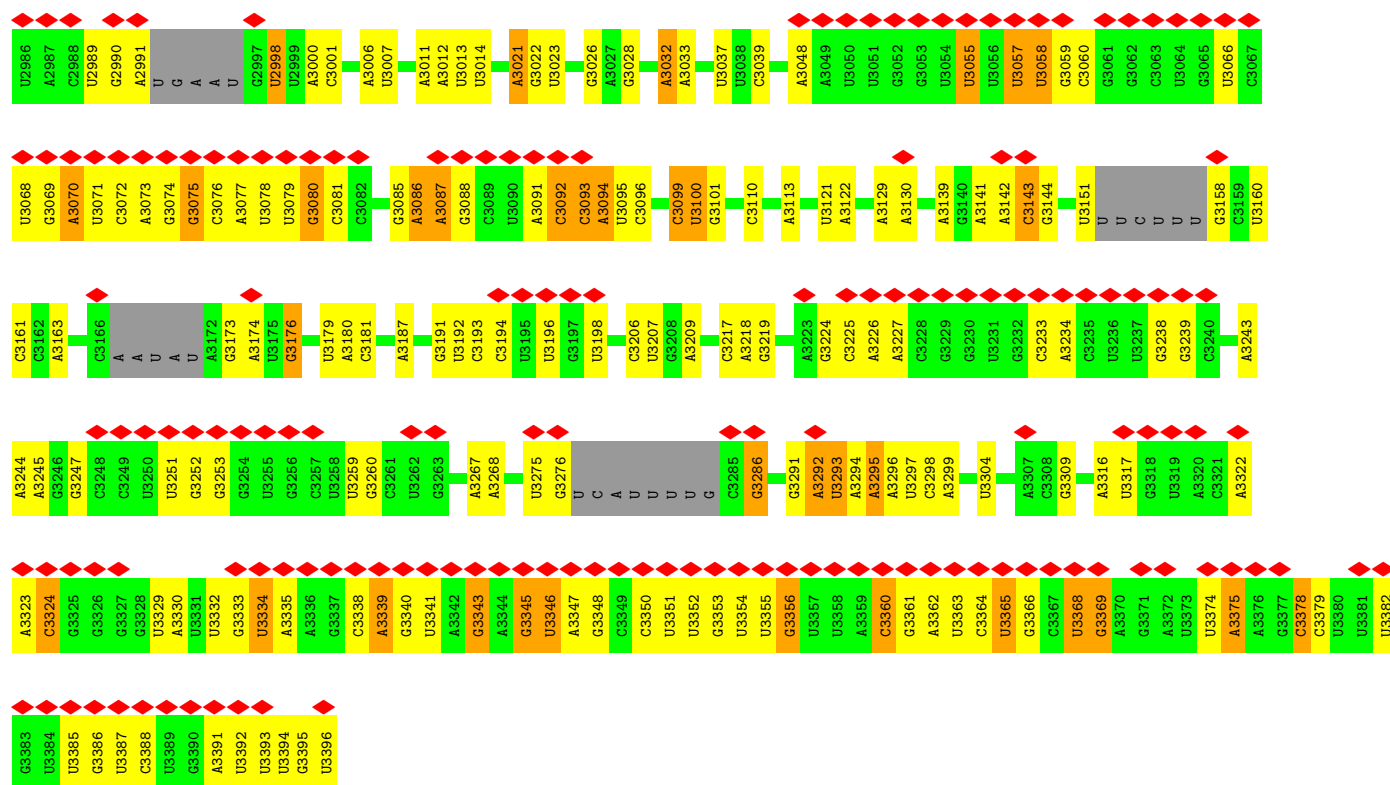
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: *Saccharomyces cerevisiae* 25S ribosomal RNA

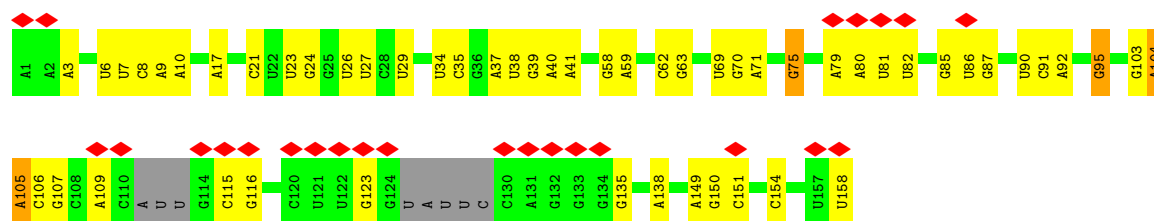




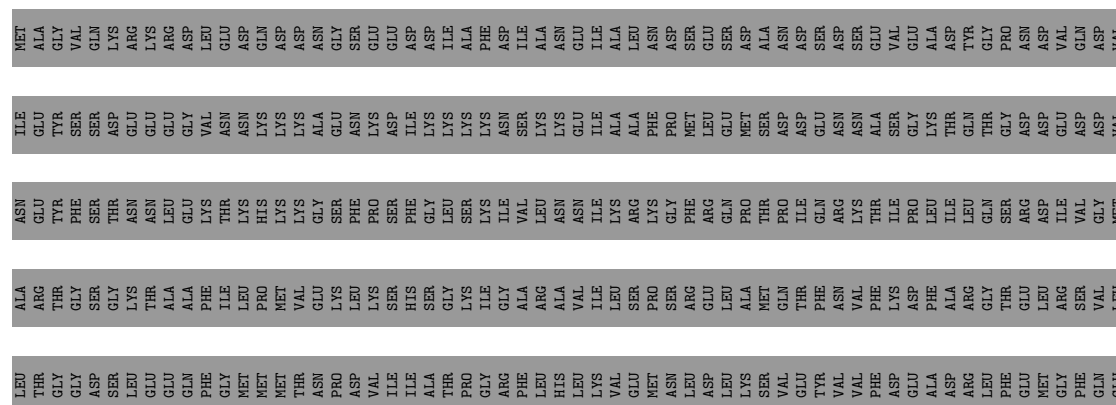


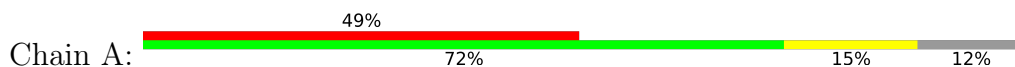


• Molecule 2: *Saccharomyces cerevisiae* 5.8S ribosomal RNA

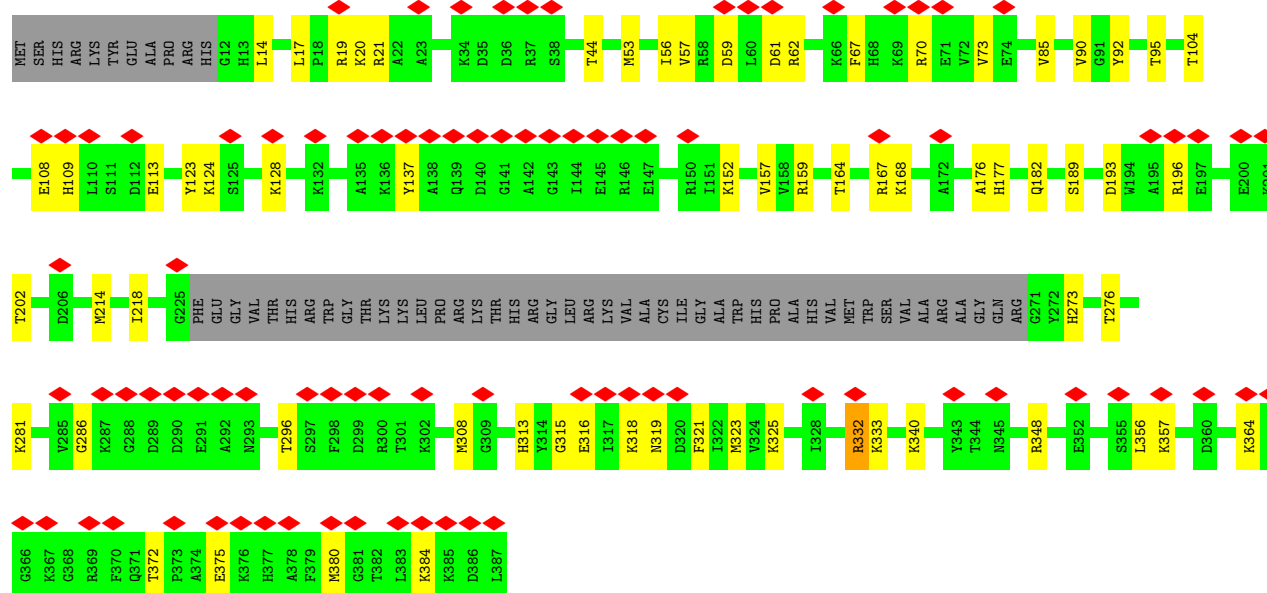


• Molecule 3: ATP-dependent RNA helicase DBP10

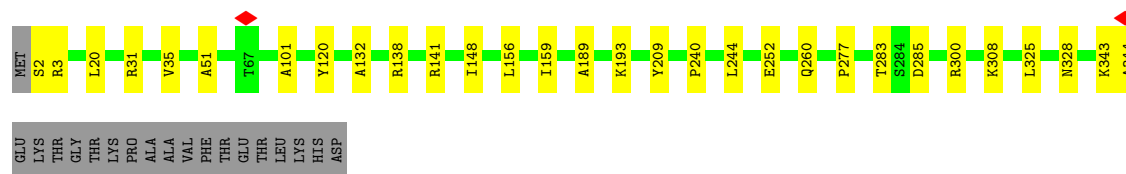




- Molecule 8: Large ribosomal subunit protein uL3

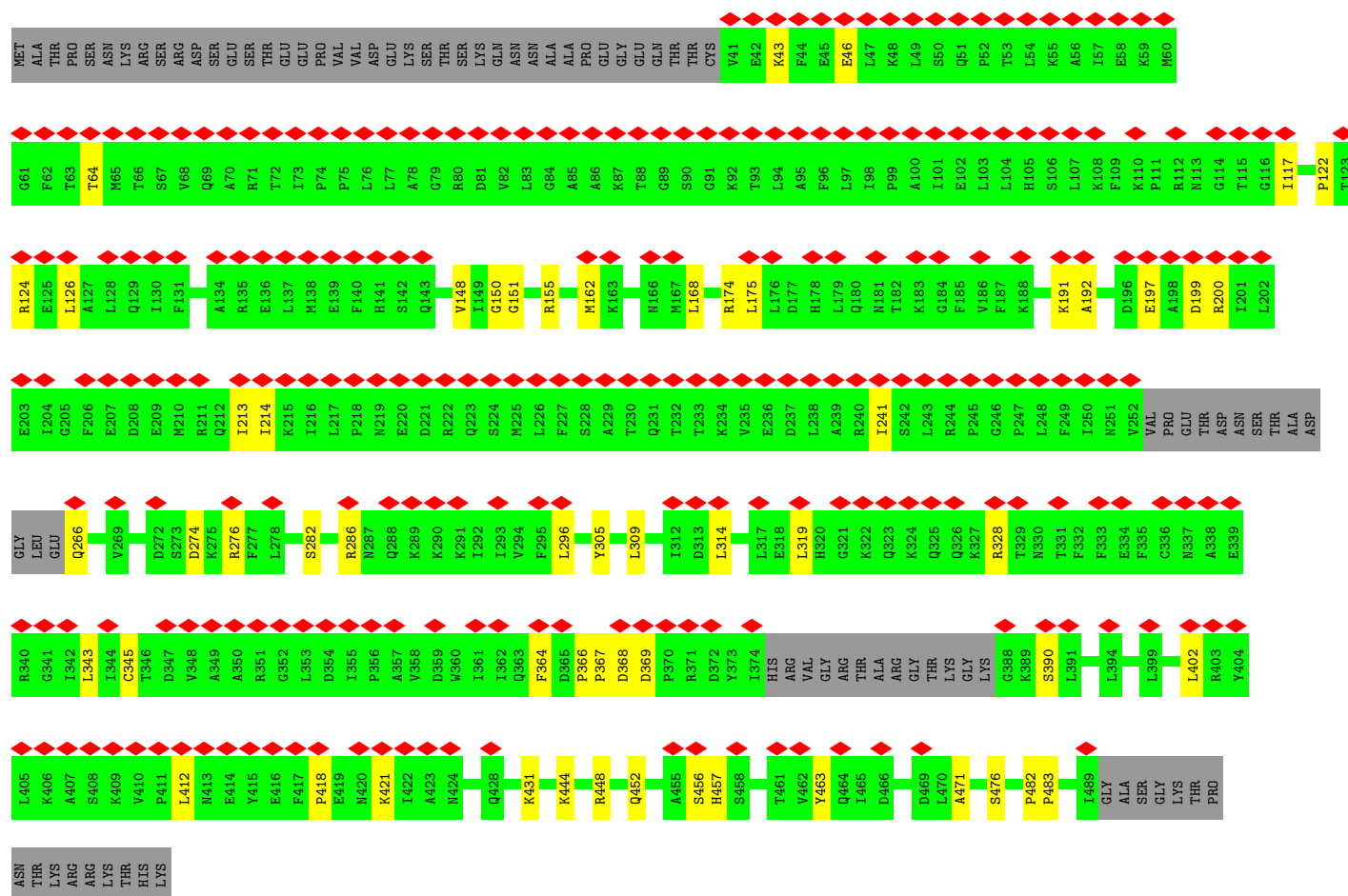


- Molecule 9: 60S ribosomal protein L4-A

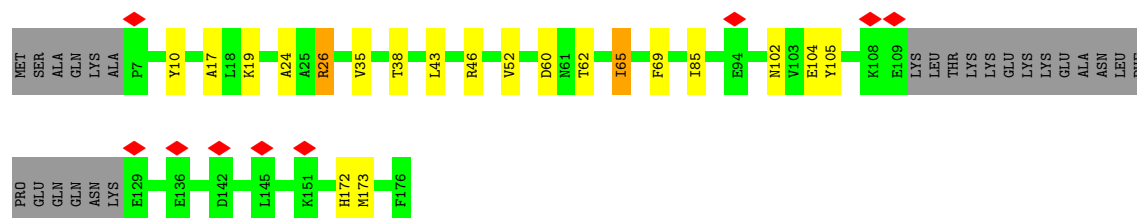
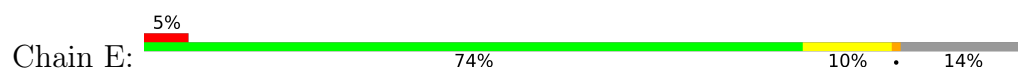


- Molecule 10: ATP-dependent RNA helicase HAS1

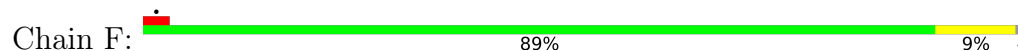




• Molecule 11: 60S ribosomal protein L6-A

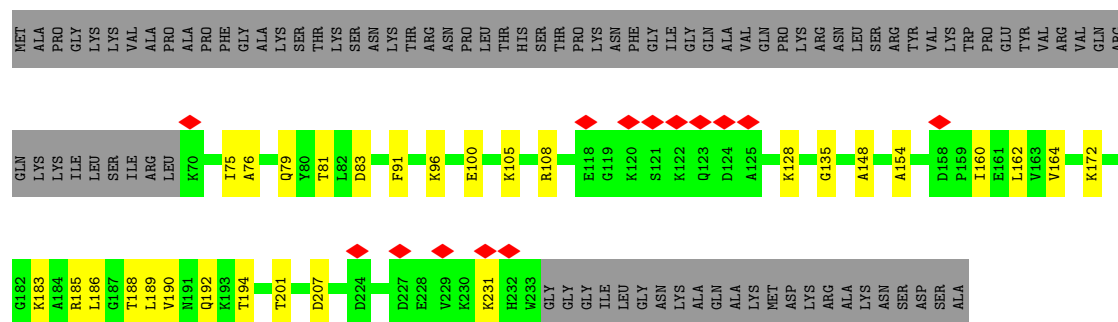


• Molecule 12: 60S ribosomal protein L7-A

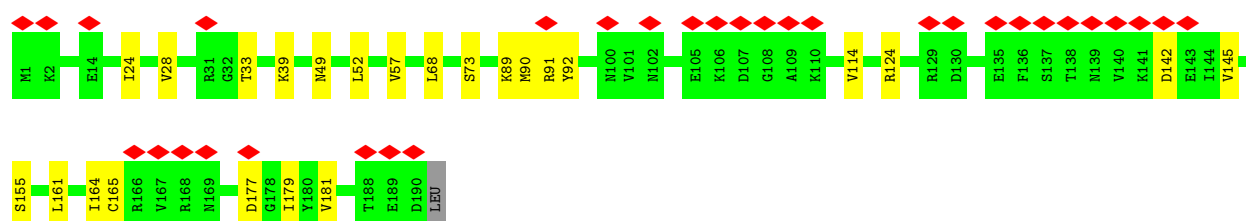
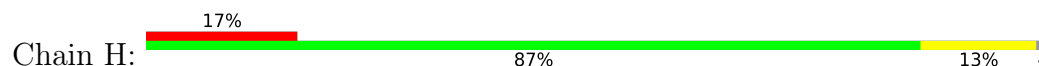


• Molecule 13: Large ribosomal subunit protein eL8A

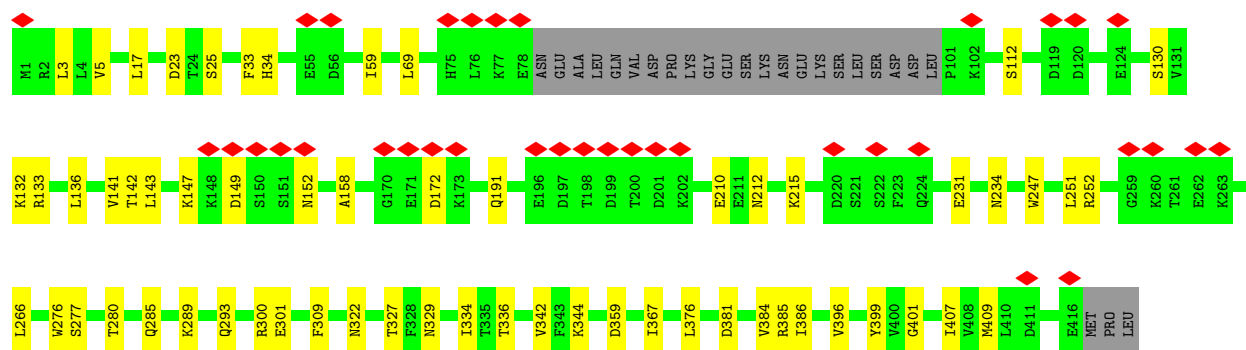




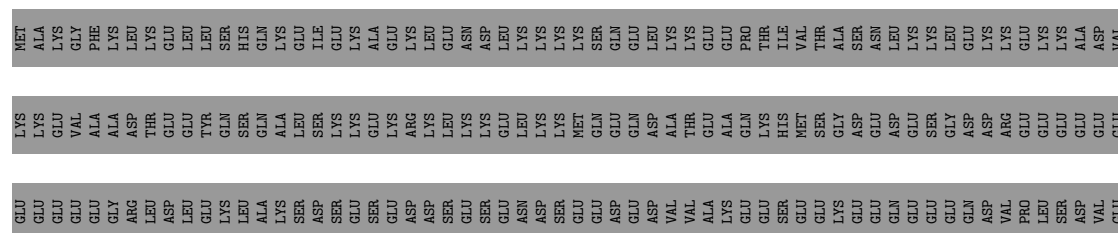
• Molecule 14: Large ribosomal subunit protein uL6A

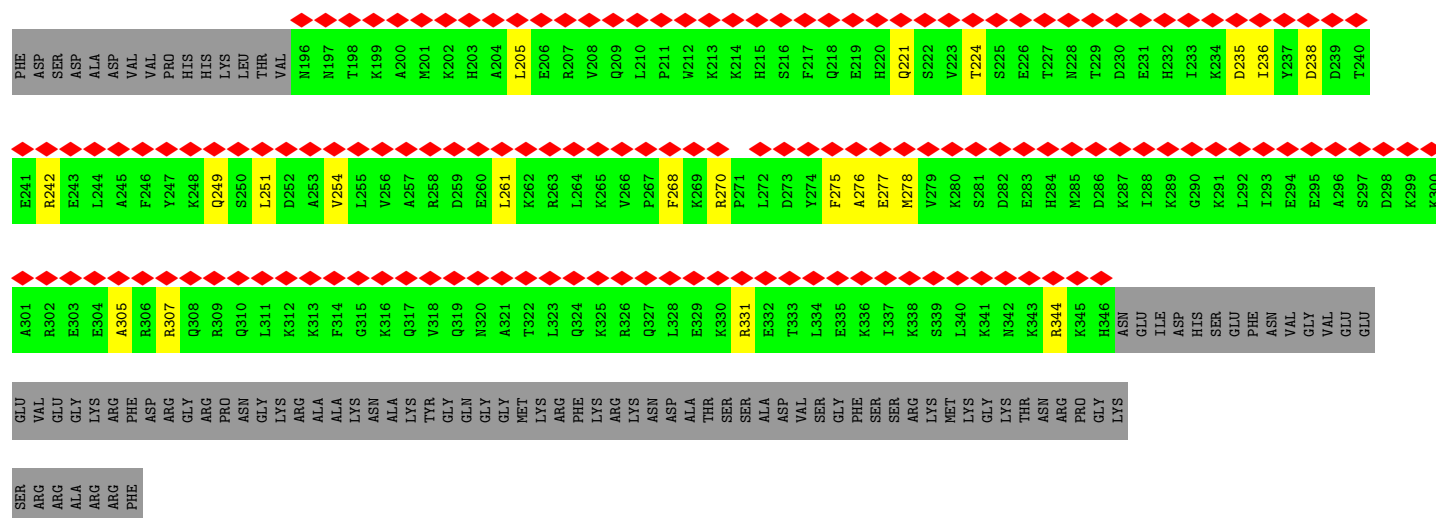


• Molecule 15: Ribosome biogenesis protein NSA1

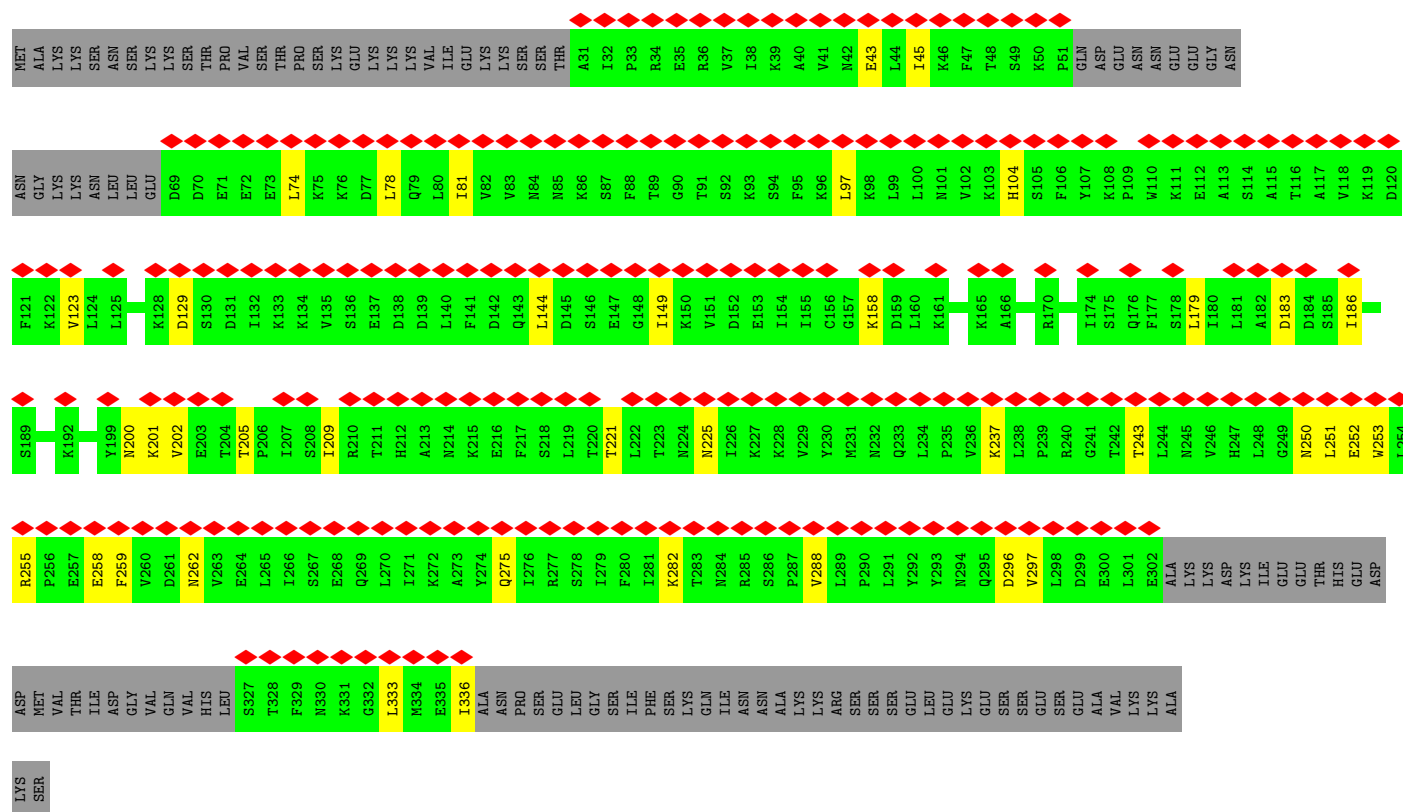


• Molecule 16: rRNA-processing protein EBP2





• Molecule 17: Proteasome-interacting protein CIC1



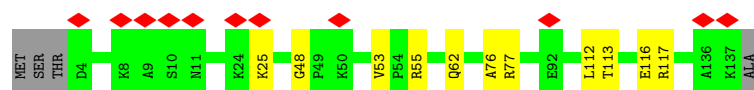
• Molecule 18: 60S ribosomal protein L13-A



ALA
ALA
ALA
THR
PHE
PRO
TLE
GLN
ALA
PRO
ALA
THR
ASP
VAL
GLU
ALA
ARG
VAL
GLN
ASP
ASN
GLY
GLU
SER
ALA
PHE
ARG
THR
LEU
ARG
LEU
ALA
ALA
SER
GLU
LYS
LYS
PHE
ARG
GLY
ILE
ARG
GLU
LYS
ARG
ALA
ALA
GLU
LYS
ALA
ALA
GLU
ALA
GLU
LYS
LYS

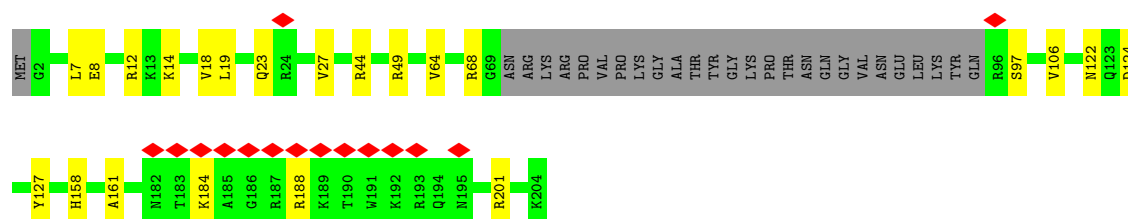
- Molecule 19: 60S ribosomal protein L14-A

Chain M: 



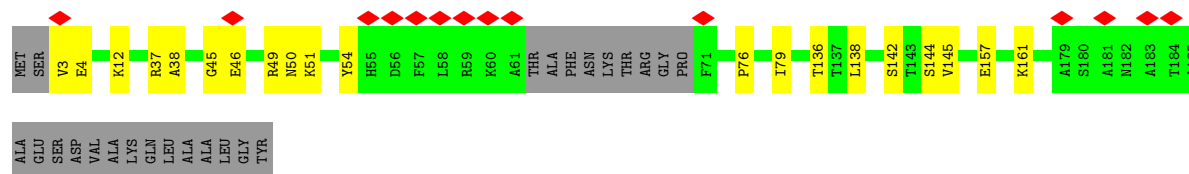
- Molecule 20: Large ribosomal subunit protein eL15A

Chain N: 



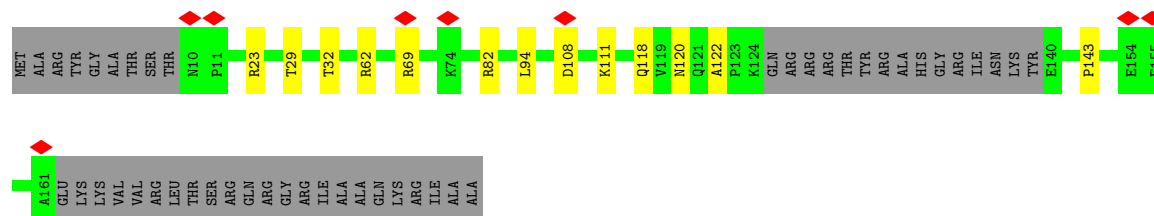
- Molecule 21: Large ribosomal subunit protein uL13A

Chain O: 



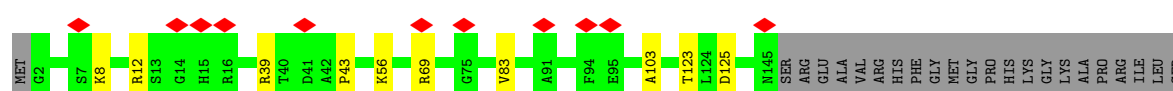
- Molecule 22: 60S ribosomal protein L17-A

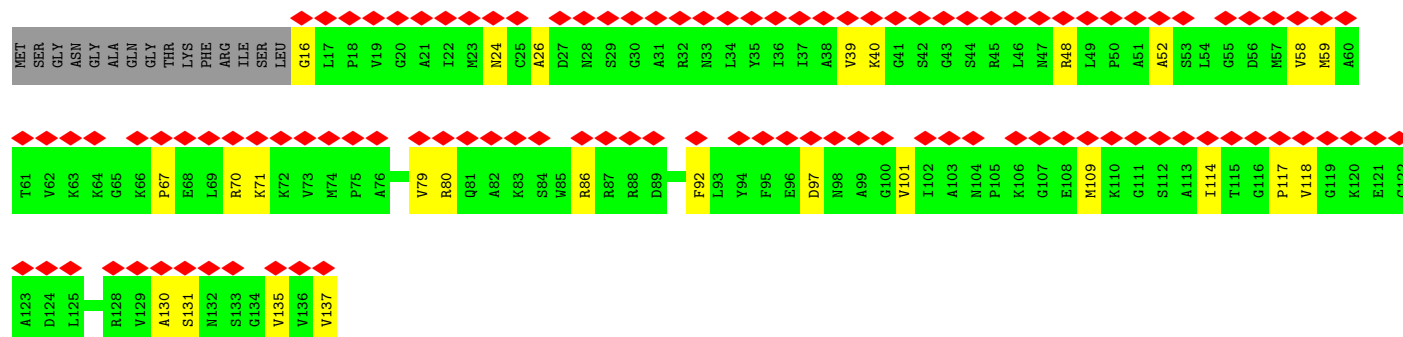
Chain P: 



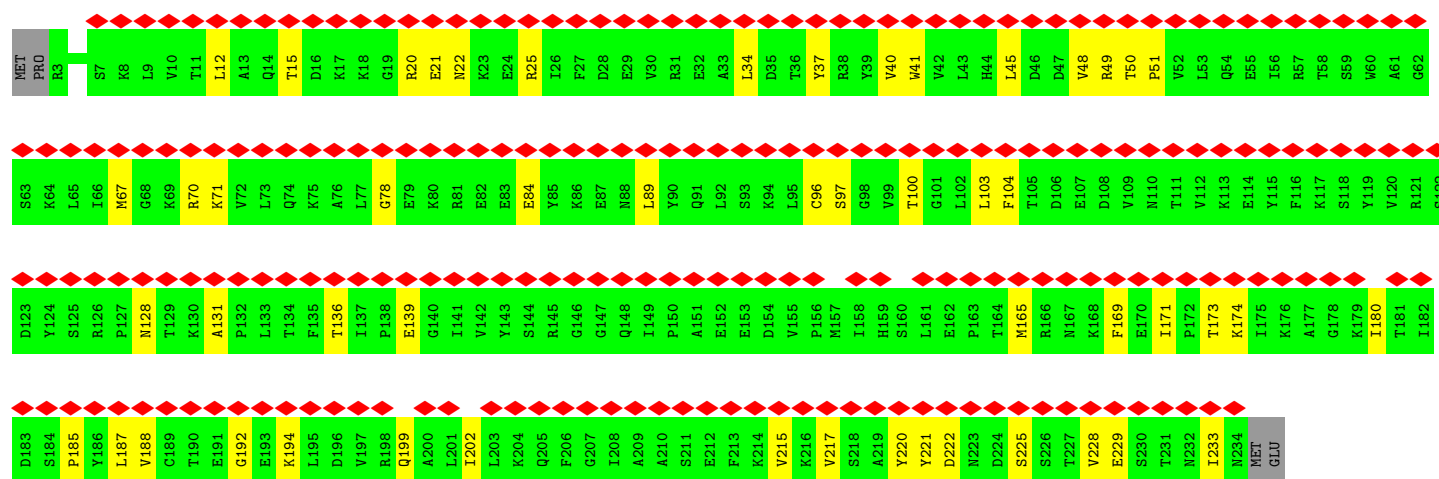
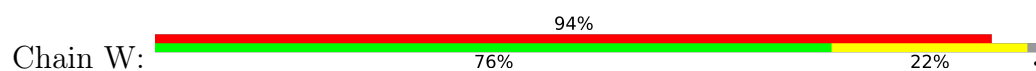
- Molecule 23: 60S ribosomal protein L18-A

Chain Q: 

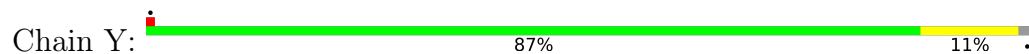




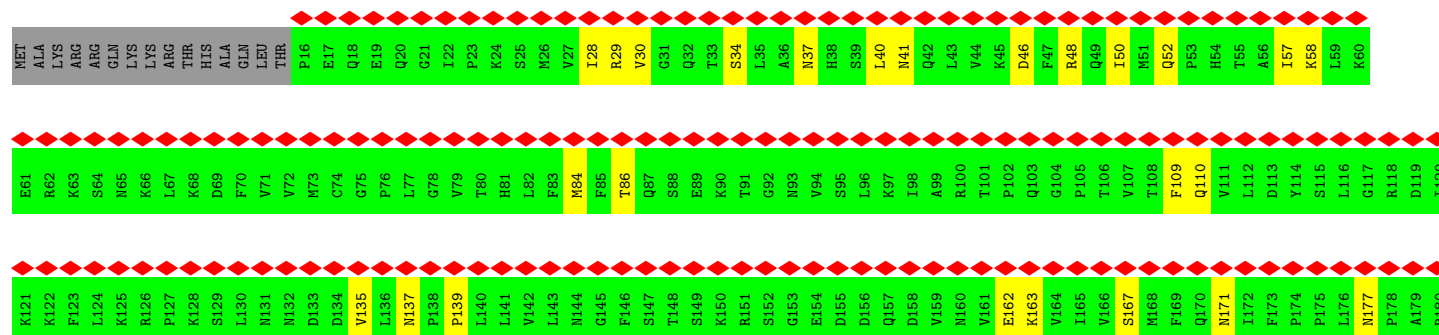
• Molecule 28: Ribosome assembly factor MRT4

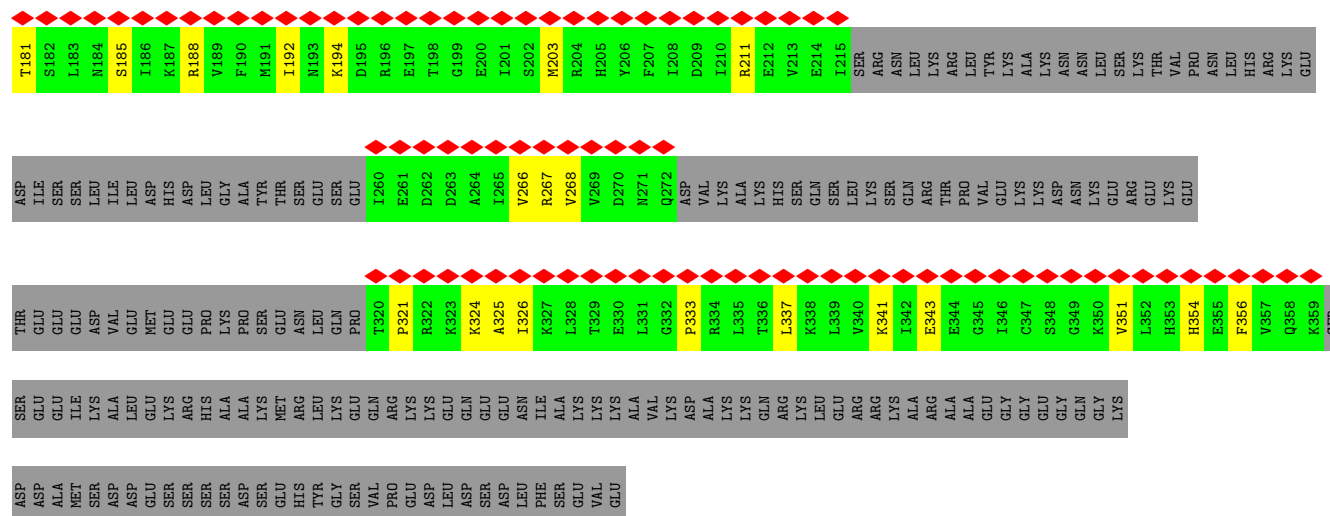


• Molecule 29: 60S ribosomal protein L26-A

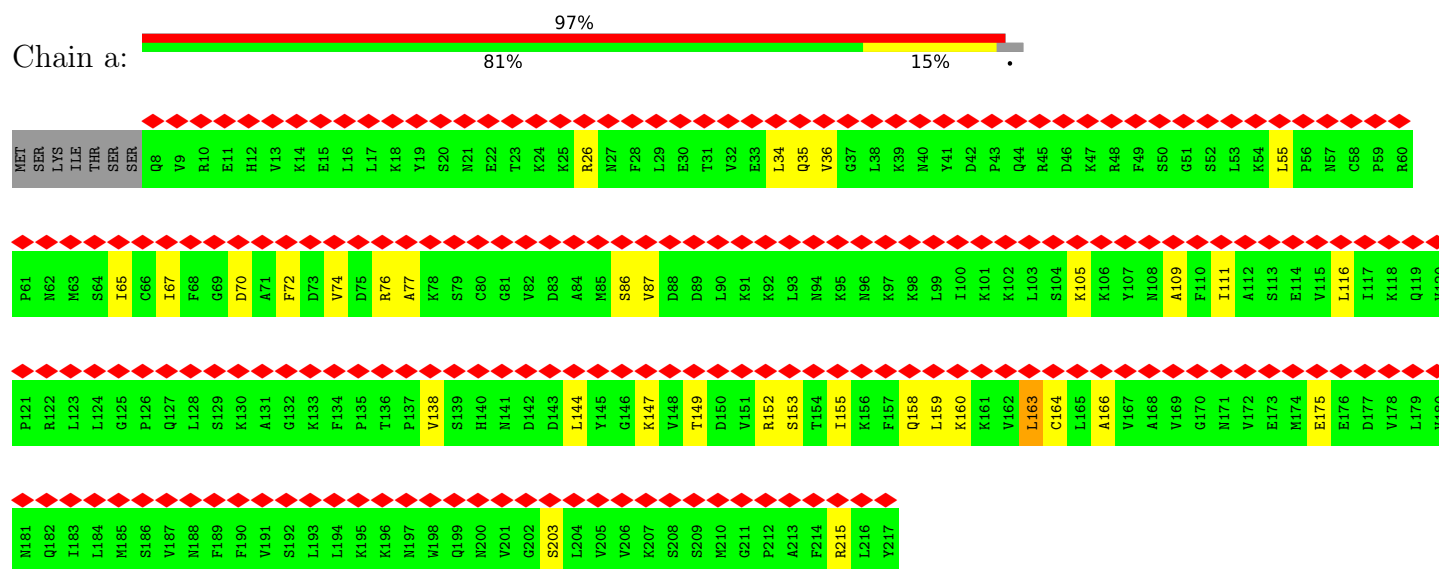


• Molecule 30: Ribosome biogenesis protein SSF1

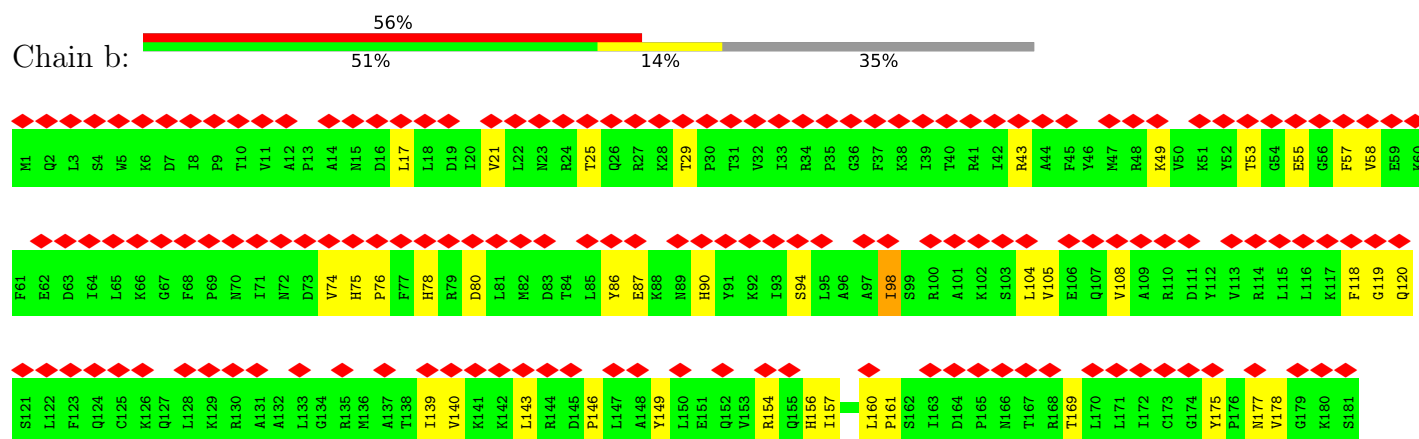


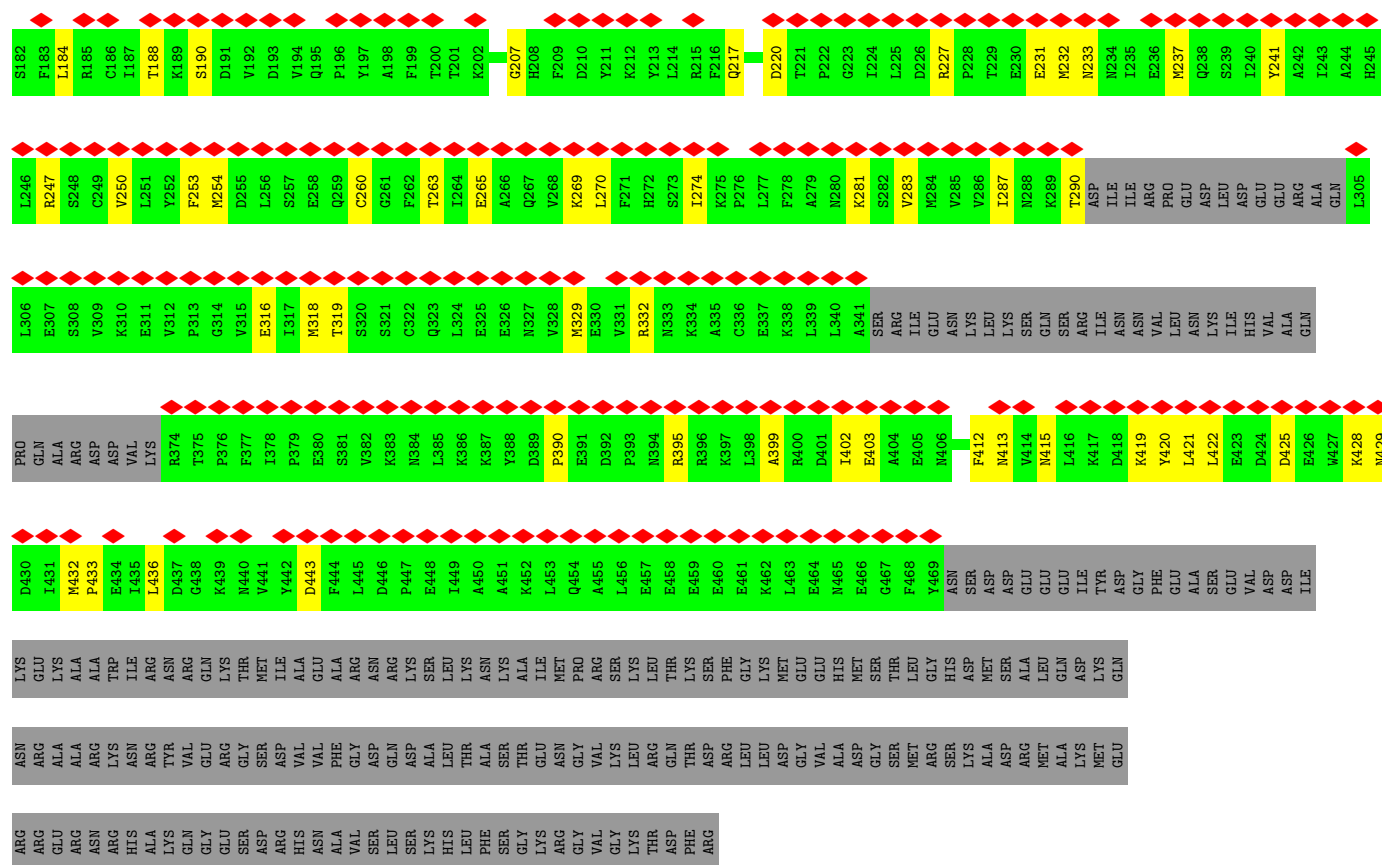


• Molecule 31: Large ribosomal subunit protein uL1A

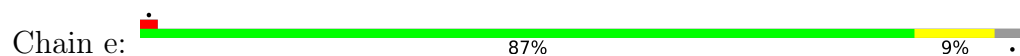


• Molecule 32: Nucleolar GTP-binding protein 1

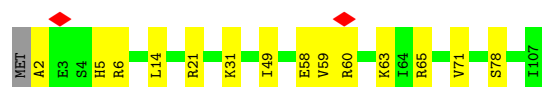
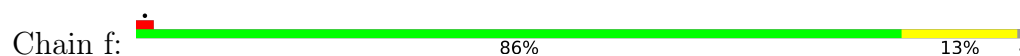




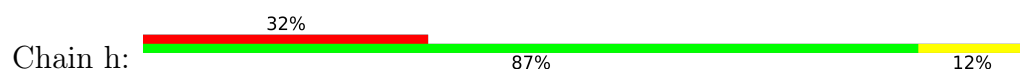
• Molecule 33: 60S ribosomal protein L32

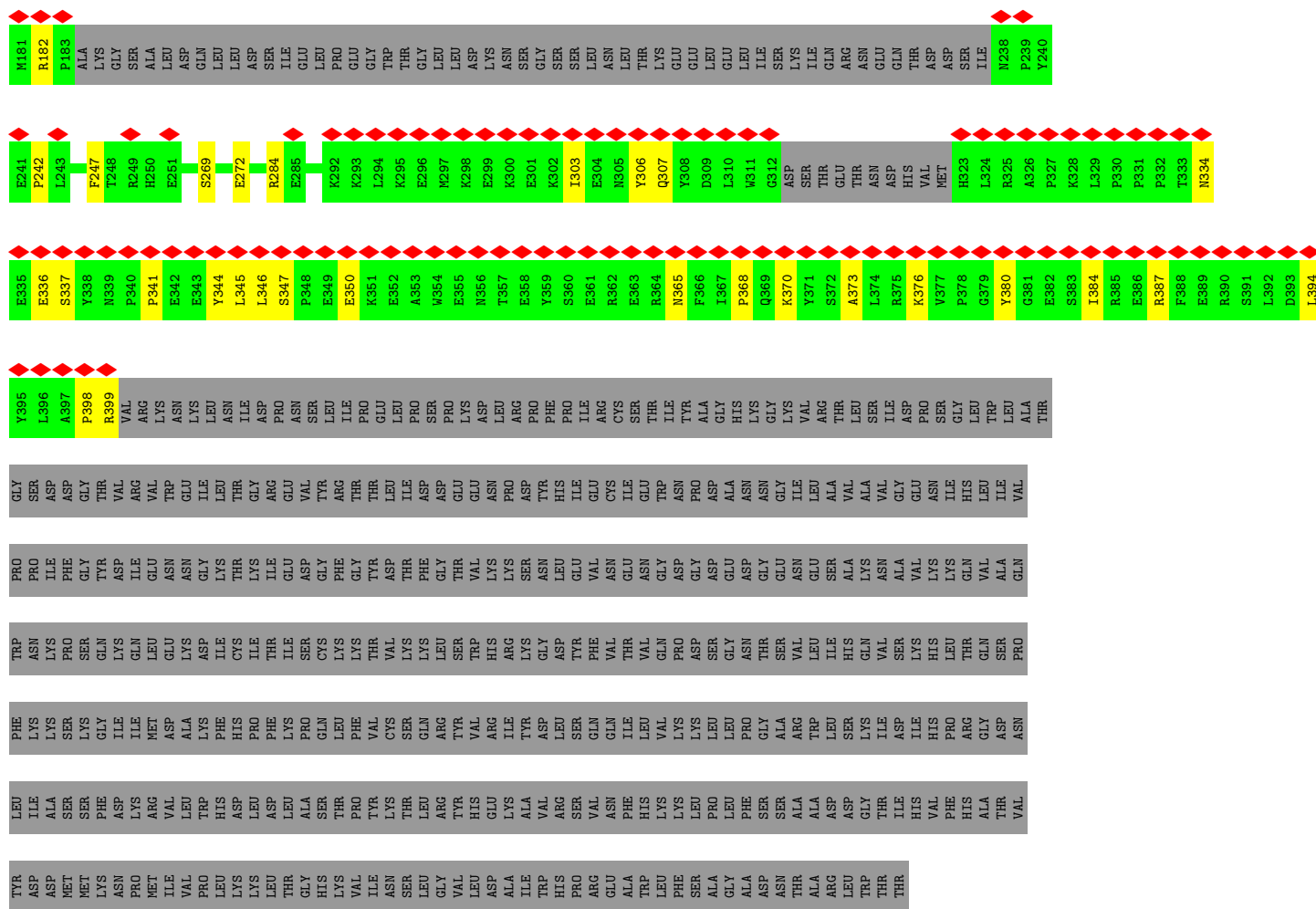


• Molecule 34: 60S ribosomal protein L33-A

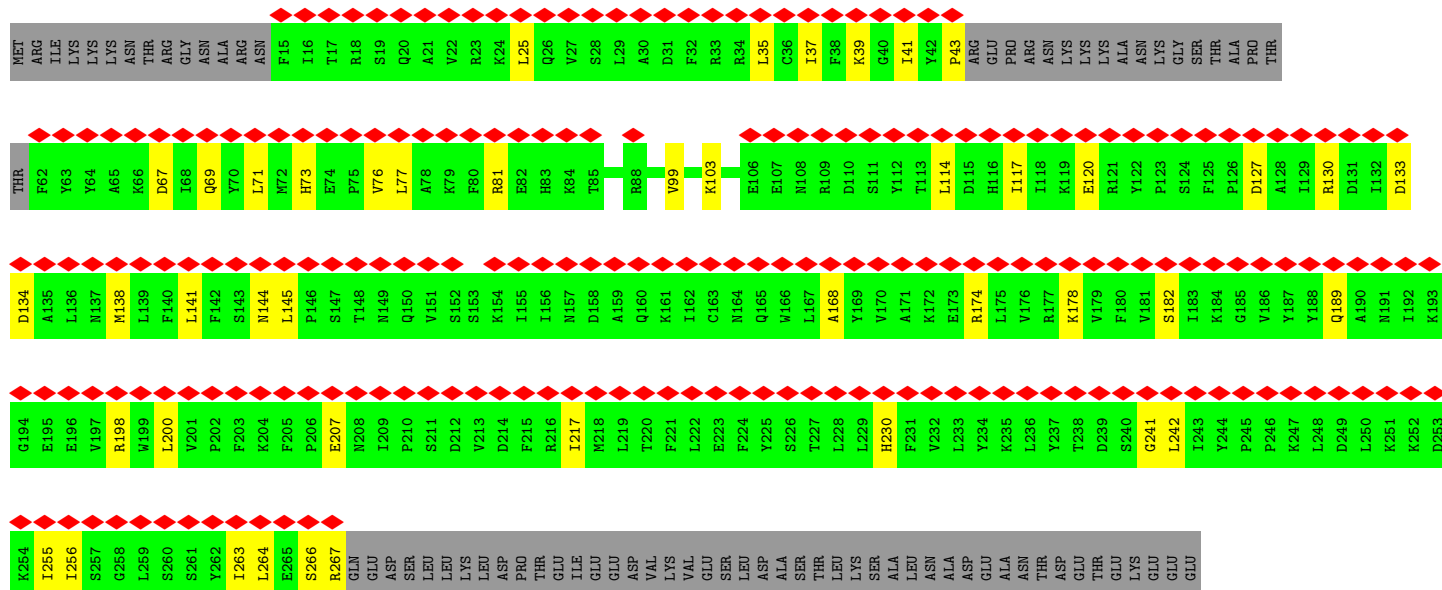
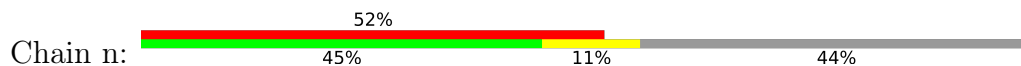


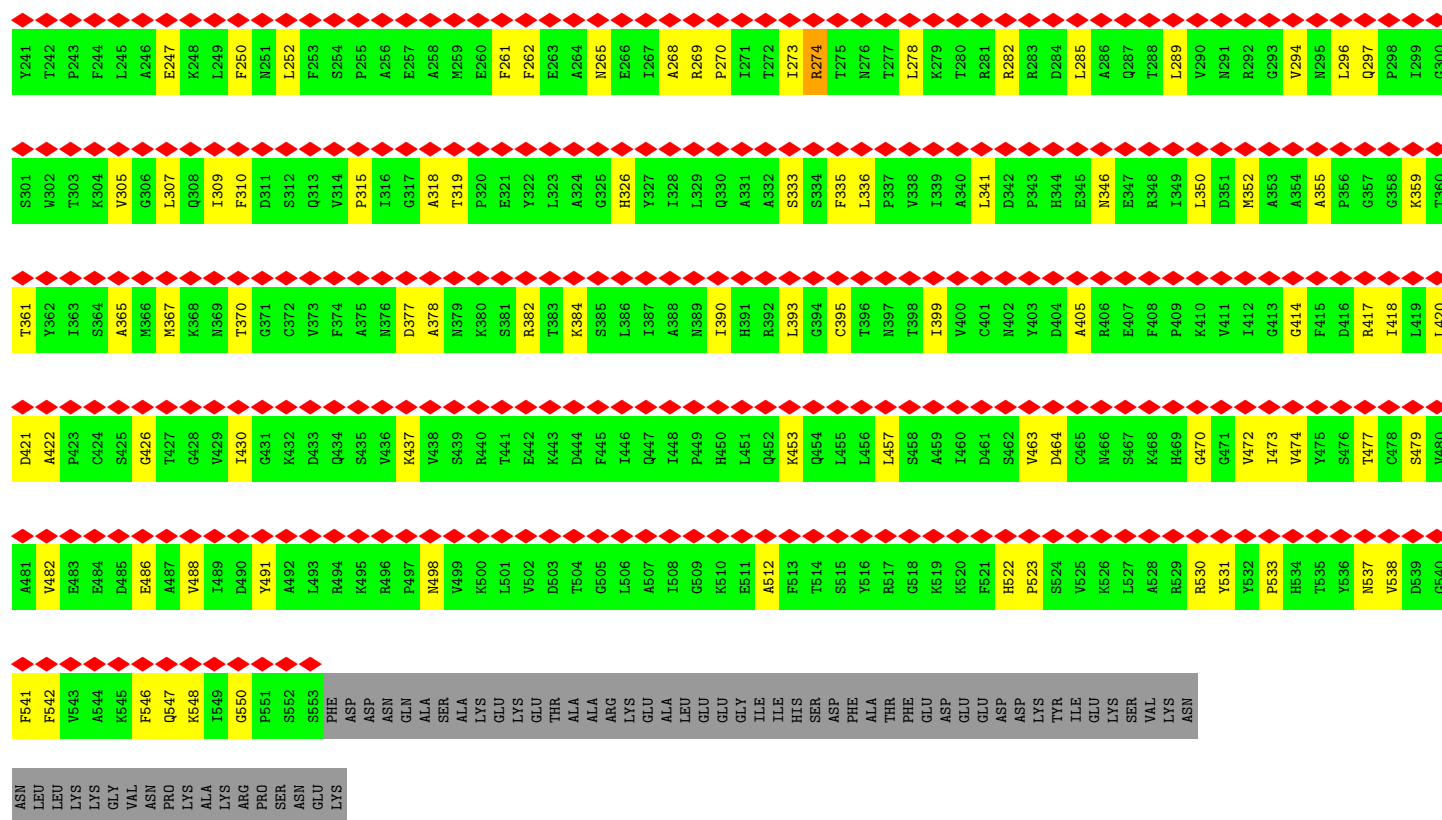
• Molecule 35: 60S ribosomal protein L35-A



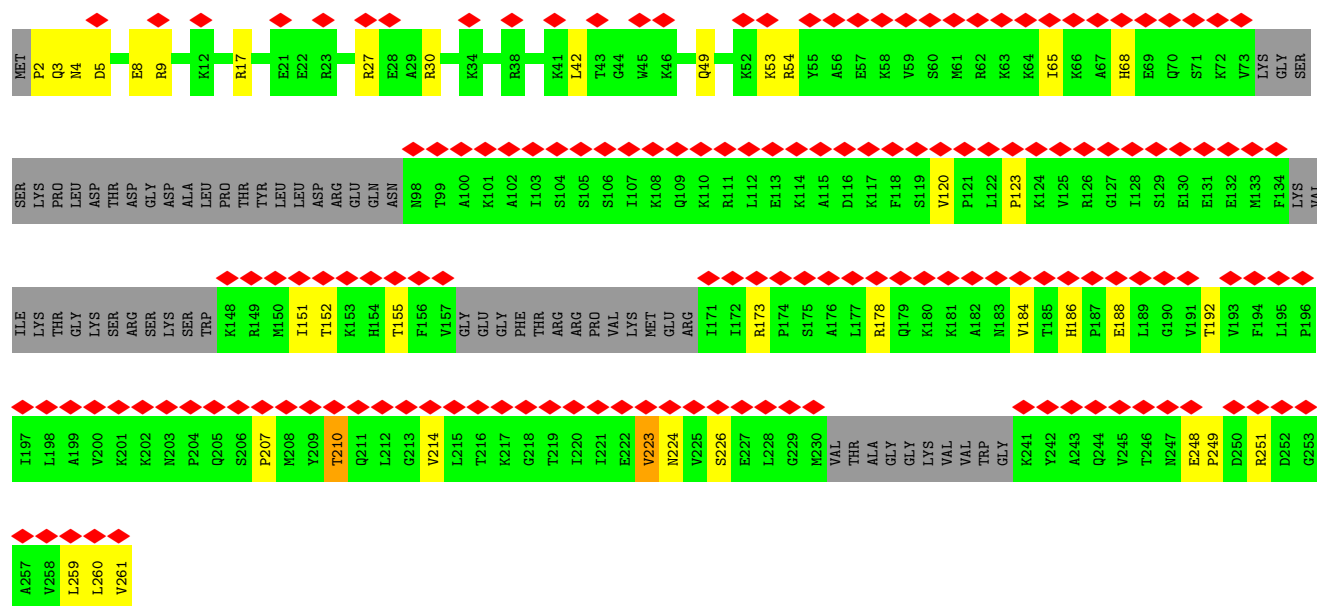


• Molecule 40: Pescadillo homolog



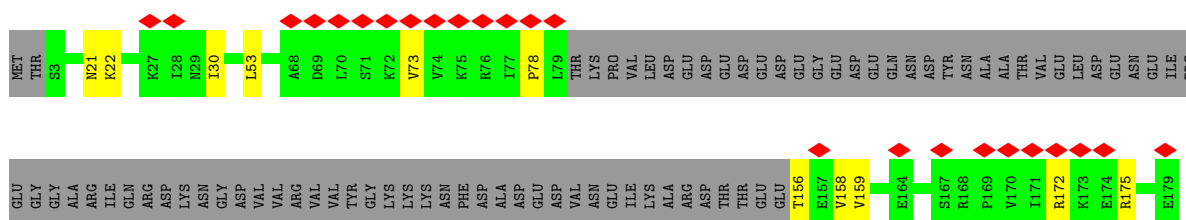


• Molecule 43: Ribosome biogenesis protein NSA2



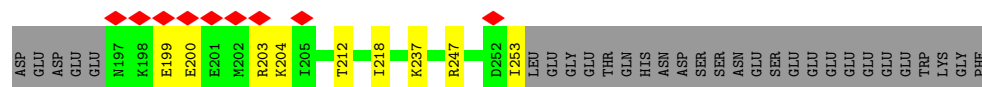
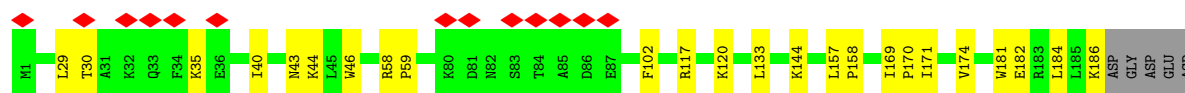
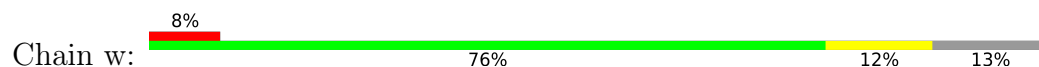
• Molecule 44: Ribosome biogenesis protein RLP7



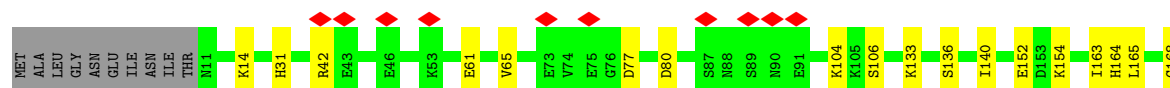
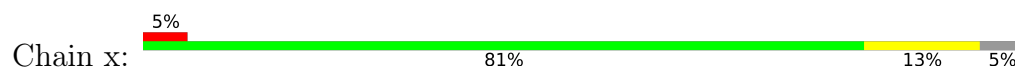




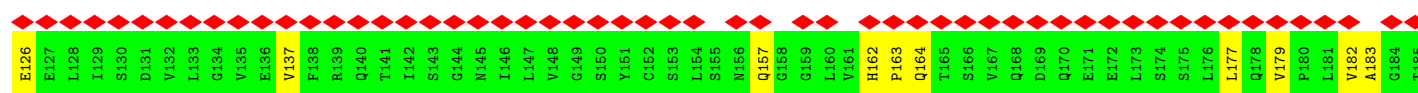
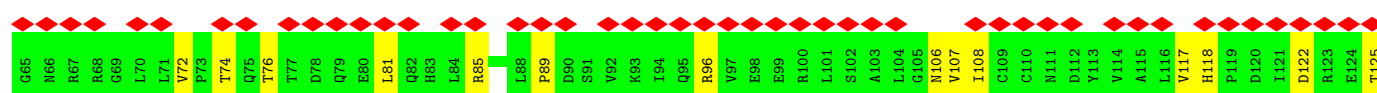
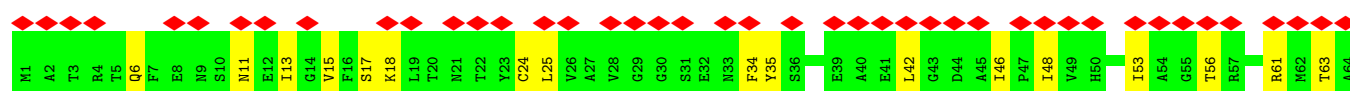
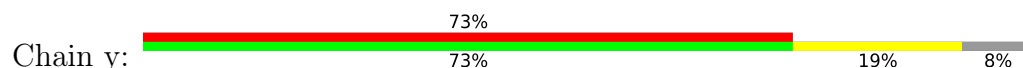
• Molecule 47: Ribosomal RNA-processing protein 1



• Molecule 48: Ribosome production factor 1



• Molecule 49: Eukaryotic translation initiation factor 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	195000	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 ($e^-/\text{\AA}^2$)	39.3	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.16	0/47220	0.25	0/73589
2	2	0.16	0/3562	0.25	0/5542
3	3	0.09	0/2935	0.23	0/3945
4	6	0.10	0/1367	0.24	0/2118
5	7	0.06	0/86	0.15	0/117
6	8	0.10	0/1210	0.21	0/1590
7	A	0.10	0/2126	0.25	0/2868
8	B	0.12	0/2679	0.27	0/3600
9	C	0.17	0/2660	0.30	0/3601
10	D	0.10	0/3441	0.25	0/4642
11	E	0.14	0/1226	0.26	0/1648
12	F	0.17	0/1974	0.30	0/2654
13	G	0.16	0/1294	0.32	0/1751
14	H	0.12	0/1531	0.27	0/2062
15	I	0.14	0/3182	0.30	0/4288
16	J	0.09	0/1289	0.21	0/1715
17	K	0.09	0/2169	0.23	0/2925
18	L	0.18	0/897	0.30	0/1205
19	M	0.14	0/1056	0.26	0/1421
20	N	0.16	0/1544	0.29	0/2065
21	O	0.16	0/1412	0.27	0/1892
22	P	0.14	0/1080	0.28	0/1455
23	Q	0.15	0/1127	0.25	0/1521
24	R	0.17	0/1609	0.29	0/2157
25	S	0.12	0/1468	0.25	0/1973
26	T	0.08	0/626	0.19	0/831
27	V	0.08	0/917	0.22	0/1235
28	W	0.09	0/1902	0.25	0/2564
29	Y	0.16	0/995	0.29	0/1329
30	Z	0.08	0/2051	0.22	0/2758
31	a	0.09	0/1695	0.24	0/2276
32	b	0.10	0/3495	0.26	0/4714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.18	0/1031	0.32	0/1379
34	f	0.17	0/868	0.29	0/1168
35	h	0.13	0/978	0.25	0/1301
36	i	0.13	0/672	0.26	0/894
37	j	0.16	0/583	0.30	0/774
38	l	0.07	0/1425	0.20	0/1922
39	m	0.10	0/1806	0.24	0/2443
40	n	0.09	0/2828	0.22	0/3825
41	o	0.10	0/1129	0.25	0/1502
42	q	0.08	0/2854	0.22	0/3860
43	r	0.09	0/1637	0.22	0/2181
44	t	0.09	0/1999	0.24	0/2690
45	u	0.08	0/964	0.21	0/1283
46	v	0.13	0/1258	0.23	0/1670
47	w	0.15	0/2104	0.28	0/2832
48	x	0.17	0/2408	0.33	0/3230
49	y	0.09	0/1722	0.25	0/2343
All	All	0.14	0/128091	0.26	0/183348

There are no bond length outliers.

There are no bond angle outliers.

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	1	42190	0	21207	456	0
2	2	3189	0	1614	27	0
3	3	2884	0	2970	44	0
4	6	1227	0	622	15	0
5	7	87	0	101	0	0
6	8	1203	0	1291	16	0
7	A	2080	0	2100	33	0
8	B	2626	0	2705	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	2611	0	2724	24	0
10	D	3377	0	3500	35	0
11	E	1205	0	1291	15	0
12	F	1936	0	2032	16	0
13	G	1272	0	1331	23	0
14	H	1510	0	1576	15	0
15	I	3126	0	3178	36	0
16	J	1271	0	1310	19	0
17	K	2135	0	2212	25	0
18	L	884	0	936	11	0
19	M	1041	0	1137	7	0
20	N	1513	0	1564	21	0
21	O	1386	0	1489	18	0
22	P	1062	0	1075	9	0
23	Q	1110	0	1190	10	0
24	R	1578	0	1623	23	0
25	S	1432	0	1470	19	0
26	T	625	0	666	8	0
27	V	903	0	946	18	0
28	W	1870	0	1902	33	0
29	Y	984	0	1075	9	0
30	Z	2020	0	2105	31	0
31	a	1668	0	1753	24	0
32	b	3429	0	3484	68	0
33	e	1010	0	1076	9	0
34	f	850	0	880	9	0
35	h	969	0	1078	9	0
36	i	665	0	721	5	0
37	j	571	0	571	12	0
38	l	1394	0	1426	28	0
39	m	1759	0	1725	32	0
40	n	2760	0	2810	40	0
41	o	1107	0	1159	17	0
42	q	2799	0	2834	61	0
43	r	1615	0	1711	29	0
44	t	1973	0	2083	31	0
45	u	944	0	973	18	0
46	v	1242	0	1317	18	0
47	w	2058	0	2096	22	0
48	x	2362	0	2389	23	0
49	y	1701	0	1697	32	0
50	b	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	b	1	0	0	0	0
52	j	1	0	0	0	0
52	u	1	0	0	0	0
All	All	121244	0	100737	1340	0

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

All (1340) 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)
24:R:19:ILE:CD1	24:R:29:ARG:HG3	1.87	1.05
24:R:19:ILE:HD11	24:R:29:ARG:CG	1.87	1.04
24:R:19:ILE:HD11	24:R:29:ARG:HG3	1.38	1.02
31:a:67:ILE:HG22	31:a:111:ILE:CG2	1.93	0.98
21:O:38:ALA:O	21:O:138:LEU:HD23	1.64	0.98
1:1:420:G:H1	2:2:3:A:H61	1.12	0.97
21:O:76:PRO:HB3	21:O:138:LEU:HG	1.56	0.87
8:B:332:ARG:HH11	8:B:332:ARG:CG	1.90	0.84
24:R:19:ILE:HD11	24:R:29:ARG:NE	1.95	0.80
25:S:8:GLN:HB2	25:S:64:ILE:HD11	1.62	0.80
38:l:47:VAL:HG11	38:l:66:LEU:HG	1.67	0.77
1:1:728:G:H5'	23:Q:43:PRO:HB2	1.66	0.77
8:B:108:GLU:OE1	8:B:109:HIS:ND1	2.14	0.76
2:2:95:G:OP2	37:j:72:ARG:NH1	2.20	0.75
31:a:67:ILE:HG22	31:a:111:ILE:HG22	1.69	0.75
48:x:164:HIS:HB3	48:x:168:GLY:HA3	1.69	0.75
1:1:1253:U:H5''	1:1:1254:C:H5'	1.69	0.74
21:O:76:PRO:HB3	21:O:138:LEU:CD2	2.17	0.74
1:1:685:G:OP1	18:L:39:ARG:NH2	2.21	0.73
32:b:74:VAL:CG1	32:b:78:HIS:HB2	2.19	0.73
1:1:3151:U:O2'	1:1:3395:G:N2	2.22	0.73
4:6:16:U:H2'	4:6:17:G:H8	1.54	0.73
8:B:59:ASP:HB3	8:B:357:LYS:HE2	1.71	0.73
1:1:3340:G:H1	1:1:3364:C:H42	1.37	0.73
40:n:255:ILE:HG22	40:n:256:ILE:HG12	1.71	0.72
21:O:76:PRO:HB3	21:O:138:LEU:CG	2.19	0.72
26:T:212:VAL:HA	26:T:216:LEU:HB2	1.72	0.72
1:1:2414:G:H1	1:1:2806:U:H3	1.38	0.72
48:x:174:LYS:HE3	48:x:268:LYS:HG3	1.72	0.72
42:q:315:PRO:HG2	42:q:318:ALA:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:332:ARG:HG2	8:B:332:ARG:NH1	2.05	0.71
18:L:42:ARG:NH1	18:L:51:LEU:O	2.24	0.71
32:b:188:THR:HG21	32:b:207:GLY:HA3	1.73	0.71
42:q:463:VAL:HG21	42:q:473:ILE:HG12	1.71	0.71
43:r:49:GLN:HG3	43:r:53:LYS:HE3	1.73	0.71
10:D:319:LEU:HD22	10:D:328:ARG:HG3	1.73	0.70
3:3:652:ILE:HG22	3:3:657:TRP:HB3	1.73	0.70
8:B:313:HIS:HB3	8:B:332:ARG:NH1	2.06	0.70
47:w:182:GLU:OE1	47:w:247:ARG:NH1	2.25	0.70
1:1:3158:G:H22	1:1:3291:G:H1	1.39	0.70
9:C:20:LEU:HD11	9:C:252:GLU:HG3	1.72	0.70
15:I:130:SER:O	48:x:133:LYS:NZ	2.24	0.70
27:V:86:ARG:HH11	27:V:92:PHE:HB3	1.56	0.70
1:1:383:G:O2'	1:1:386:A:N6	2.24	0.70
19:M:55:ARG:NH2	19:M:76:ALA:O	2.24	0.70
4:6:7:C:H5	4:6:21:G:H1	1.39	0.69
1:1:807:A:H61	1:1:934:G:H22	1.38	0.69
12:F:224:ILE:O	25:S:119:ARG:NH2	2.24	0.69
18:L:62:THR:HG22	18:L:64:LYS:H	1.57	0.69
1:1:607:A:OP1	11:E:26:ARG:NH2	2.26	0.69
1:1:2457:G:O2'	1:1:2481:G:N2	2.26	0.69
1:1:959:C:H41	16:J:305:ALA:HB1	1.56	0.69
44:t:197:GLY:HA3	44:t:314:ILE:HB	1.74	0.69
8:B:108:GLU:HG3	8:B:137:TYR:CD1	2.27	0.69
32:b:74:VAL:HG12	32:b:78:HIS:HB2	1.73	0.69
32:b:74:VAL:HG12	32:b:75:HIS:N	2.08	0.69
43:r:4:ASN:O	43:r:9:ARG:NH1	2.26	0.68
1:1:420:G:H1	2:2:3:A:N6	1.87	0.68
8:B:332:ARG:HH11	8:B:332:ARG:HG2	1.57	0.68
42:q:269:ARG:NH1	42:q:538:VAL:O	2.27	0.68
1:1:692:A:OP1	20:N:201:ARG:NH2	2.25	0.68
1:1:1456:A:O2'	22:P:23:ARG:NH2	2.27	0.68
1:1:3158:G:H21	1:1:3291:G:H22	1.41	0.67
31:a:55:LEU:HD11	31:a:155:ILE:HG12	1.77	0.67
7:A:136:VAL:HB	7:A:176:VAL:HG22	1.76	0.67
24:R:19:ILE:HD11	24:R:29:ARG:CD	2.24	0.67
27:V:70:ARG:HG2	27:V:71:LYS:HG3	1.76	0.67
34:f:2:ALA:O	34:f:5:HIS:NE2	2.27	0.66
8:B:108:GLU:HG3	8:B:137:TYR:CG	2.30	0.66
13:G:231:LYS:HA	39:m:242:PRO:HB3	1.76	0.66
10:D:471:ALA:HA	10:D:482:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:51:U:O2'	4:6:54:A:N7	2.30	0.65
7:A:189:ARG:HG2	7:A:218:ARG:HG3	1.78	0.65
34:f:59:VAL:HG12	34:f:60:ARG:HG2	1.79	0.65
11:E:10:TYR:HB3	24:R:113:THR:HG21	1.76	0.65
15:I:215:LYS:HG2	15:I:231:GLU:HG3	1.79	0.65
46:v:188:LEU:HD22	46:v:199:MET:HG2	1.79	0.65
42:q:361:THR:HG21	42:q:393:LEU:HD12	1.79	0.65
17:K:144:LEU:HB3	17:K:149:ILE:HB	1.79	0.65
18:L:105:ASN:HD22	18:L:108:ILE:H	1.43	0.64
1:1:441:U:OP2	24:R:128:ARG:NH1	2.28	0.64
1:1:1231:A:H5''	1:1:1232:C:H5'	1.80	0.64
22:P:122:ALA:HB3	22:P:143:PRO:HB2	1.77	0.64
1:1:675:C:O2'	1:1:679:U:OP1	2.16	0.64
8:B:14:LEU:HD23	8:B:17:LEU:HD12	1.79	0.64
3:3:669:GLU:HB3	3:3:672:LYS:HE3	1.79	0.64
15:I:359:ASP:OD2	15:I:385:ARG:NE	2.31	0.64
1:1:441:U:OP1	24:R:124:ARG:NH1	2.30	0.64
28:W:70:ARG:HE	28:W:97:SER:HA	1.62	0.64
44:t:217:LYS:HB2	44:t:224:PRO:HB3	1.80	0.64
1:1:481:U:H3	1:1:484:C:H41	1.46	0.64
1:1:3379:C:H4'	8:B:315:GLY:HA2	1.79	0.63
17:K:255:ARG:NH2	17:K:258:GLU:OE2	2.32	0.63
15:I:327:THR:HG22	15:I:329:ASN:H	1.63	0.63
1:1:384:A:N7	1:1:385:A:N6	2.46	0.63
1:1:1151:U:H4'	1:1:1152:G:H5''	1.80	0.63
10:D:319:LEU:HG	10:D:343:LEU:HD11	1.79	0.63
32:b:247:ARG:HA	32:b:281:LYS:HE3	1.80	0.63
40:n:368:SER:HB2	40:n:412:VAL:HG12	1.80	0.63
1:1:2468:A:N1	1:1:2477:G:O2'	2.30	0.63
1:1:3329:U:H5''	8:B:308:MET:HE2	1.79	0.63
30:Z:29:ARG:NH1	30:Z:41:ASN:OD1	2.32	0.63
1:1:1222:G:N7	28:W:71:LYS:NZ	2.46	0.63
3:3:557:LEU:H	3:3:560:MET:HE2	1.62	0.63
42:q:417:ARG:HG2	42:q:472:VAL:HB	1.80	0.63
32:b:443:ASP:OD1	45:u:2:ARG:NH1	2.30	0.63
46:v:53:LEU:HD22	46:v:158:VAL:HG21	1.79	0.63
1:1:262:U:OP1	10:D:448:ARG:NH2	2.32	0.62
42:q:377:ASP:OD2	42:q:382:ARG:NH1	2.32	0.62
44:t:67:ALA:HB1	44:t:153:VAL:HG22	1.82	0.62
49:y:53:ILE:HG23	49:y:76:THR:HG22	1.79	0.62
3:3:725:GLU:HA	3:3:728:ARG:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:52:GLN:HB3	30:Z:135:VAL:HG13	1.81	0.62
40:n:25:LEU:O	40:n:81:ARG:NH2	2.32	0.62
44:t:146:ARG:NH1	44:t:147:VAL:O	2.32	0.62
47:w:40:ILE:HG13	47:w:44:LYS:HE3	1.81	0.62
1:1:707:U:O2'	1:1:754:G:N3	2.31	0.62
28:W:45:LEU:HD21	28:W:215:VAL:HG13	1.82	0.62
1:1:1169:A:H4'	12:F:219:LYS:HE2	1.82	0.62
32:b:425:ASP:HA	32:b:428:LYS:HG3	1.82	0.62
15:I:212:ASN:OD1	15:I:215:LYS:NZ	2.31	0.62
49:y:107:VAL:HB	49:y:118:HIS:HB2	1.81	0.62
1:1:251:G:O6	46:v:175:ARG:NH2	2.25	0.62
4:6:25:G:N2	17:K:200:ASN:OD1	2.33	0.62
40:n:127:ASP:OD1	40:n:130:ARG:NH2	2.33	0.62
1:1:2961:G:H21	1:1:2971:A:H62	1.47	0.61
47:w:171:ILE:HG23	47:w:237:LYS:HE2	1.82	0.61
49:y:18:LYS:NZ	49:y:63:THR:O	2.33	0.61
1:1:3297:U:O4	8:B:124:LYS:NZ	2.33	0.61
38:l:23:ASN:HB3	38:l:92:HIS:HB3	1.81	0.61
8:B:67:PHE:HA	8:B:70:ARG:HD2	1.83	0.61
30:Z:137:ASN:ND2	30:Z:185:SER:O	2.32	0.61
1:1:216:G:OP1	29:Y:16:ARG:NH1	2.33	0.61
1:1:2442:G:N2	1:1:2505:U:O2	2.34	0.61
1:1:3057:U:H3'	1:1:3058:U:H4'	1.83	0.61
1:1:269:G:H5''	20:N:14:LYS:HE3	1.83	0.61
1:1:3343:G:H3'	1:1:3361:G:H21	1.66	0.61
8:B:164:THR:HG22	8:B:177:HIS:H	1.64	0.61
25:S:155:ARG:HD3	25:S:172:TYR:CD1	2.35	0.61
1:1:3385:U:H2'	1:1:3386:G:H8	1.66	0.61
1:1:1:G:N2	1:1:1:G:OP2	2.31	0.61
1:1:591:G:O2'	11:E:17:ALA:O	2.18	0.61
32:b:43:ARG:NH1	32:b:119:GLY:O	2.34	0.61
32:b:433:PRO:HG3	45:u:90:LEU:HD11	1.83	0.61
1:1:633:C:O2'	34:f:21:ARG:O	2.16	0.60
27:V:24:ASN:ND2	27:V:97:ASP:OD2	2.34	0.60
44:t:208:ILE:HD12	44:t:251:ILE:HG12	1.82	0.60
8:B:57:VAL:HG22	8:B:73:VAL:HG22	1.82	0.60
9:C:283:THR:HG22	9:C:285:ASP:H	1.66	0.60
13:G:100:GLU:OE1	13:G:108:ARG:NH1	2.34	0.60
1:1:2968:G:H2'	1:1:2969:A:C8	2.37	0.60
1:1:3037:U:H5''	8:B:348:ARG:HD2	1.84	0.60
2:2:69:U:H2'	2:2:70:G:O4'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:71:A:OP2	29:Y:51:ARG:NH1	2.34	0.60
24:R:19:ILE:HD12	24:R:29:ARG:HG3	1.83	0.60
1:1:1236:G:N2	1:1:1244:A:OP1	2.35	0.60
1:1:3233:C:H2'	1:1:3234:A:C8	2.36	0.60
7:A:56:LEU:HD22	7:A:58:HIS:HE1	1.66	0.59
13:G:183:LYS:HG2	13:G:194:THR:HB	1.84	0.59
19:M:48:GLY:HA3	19:M:53:VAL:HB	1.84	0.59
49:y:74:THR:O	49:y:96:ARG:NH2	2.33	0.59
1:1:250:U:H4'	1:1:251:G:H5'	1.84	0.59
1:1:2353:G:OP2	22:P:82:ARG:NH2	2.35	0.59
1:1:3369:G:N1	8:B:380:MET:O	2.33	0.59
24:R:19:ILE:CD1	24:R:29:ARG:CG	2.61	0.59
42:q:341:LEU:HB2	42:q:474:VAL:HG21	1.83	0.59
42:q:414:GLY:HA2	42:q:464:ASP:HB2	1.83	0.59
25:S:71:LYS:O	25:S:73:LYS:NZ	2.33	0.59
1:1:155:G:H1	10:D:155:ARG:HH22	1.49	0.59
3:3:363:ASP:O	3:3:367:ASN:ND2	2.32	0.59
10:D:296:LEU:HD21	10:D:305:TYR:HD2	1.67	0.59
1:1:2968:G:H2'	1:1:2969:A:H8	1.67	0.59
40:n:242:LEU:HA	40:n:266:SER:HA	1.85	0.59
1:1:3234:A:H61	1:1:3253:G:H1	1.49	0.59
16:J:236:ILE:O	16:J:242:ARG:NH2	2.34	0.59
42:q:273:ILE:HD13	42:q:309:ILE:HD11	1.84	0.59
1:1:364:G:OP2	37:j:52:LYS:NZ	2.26	0.59
1:1:822:G:O6	1:1:903:U:O2	2.20	0.59
1:1:3293:U:HO2'	1:1:3294:A:H8	1.51	0.59
3:3:682:ARG:NH1	32:b:237:MET:SD	2.76	0.59
29:Y:118:LEU:HD11	29:Y:122:LYS:HE2	1.84	0.59
1:1:543:C:H2'	1:1:548:G:H22	1.67	0.58
1:1:2369:G:H2'	1:1:2370:G:H8	1.67	0.58
1:1:292:U:OP2	20:N:68:ARG:NH2	2.36	0.58
3:3:690:GLU:OE2	3:3:707:ARG:NH1	2.36	0.58
17:K:129:ASP:HB3	17:K:158:LYS:HE3	1.85	0.58
28:W:136:THR:HG22	28:W:187:LEU:HG	1.85	0.58
1:1:3055:U:O3'	1:1:3087:A:N6	2.36	0.58
32:b:420:TYR:HB3	32:b:422:LEU:HG	1.86	0.58
8:B:44:THR:HA	8:B:340:LYS:HE2	1.85	0.58
17:K:333:LEU:HD22	44:t:165:LEU:HD12	1.85	0.58
32:b:422:LEU:HD12	32:b:428:LYS:HA	1.83	0.58
45:u:66:ASP:OD1	45:u:67:SER:N	2.37	0.58
48:x:80:ASP:OD2	48:x:212:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:545:LEU:HD21	3:3:652:ILE:HD12	1.85	0.58
7:A:284:LEU:HD21	47:w:43:ASN:HB3	1.84	0.58
8:B:372:THR:OG1	8:B:375:GLU:OE1	2.21	0.58
40:n:168:ALA:HB1	40:n:264:LEU:HD11	1.84	0.58
1:1:2442:G:N1	1:1:2505:U:N3	2.43	0.58
3:3:498:ILE:HG21	3:3:522:ARG:HD3	1.86	0.58
27:V:80:ARG:HD3	27:V:117:PRO:HG2	1.86	0.58
39:m:337:SER:HA	40:n:182:SER:HA	1.85	0.58
44:t:87:LYS:HB3	44:t:89:GLU:HG2	1.85	0.58
1:1:3066:U:O2	1:1:3075:G:O6	2.22	0.58
7:A:113:TYR:HB2	7:A:224:ILE:HD11	1.84	0.58
8:B:332:ARG:HH11	8:B:332:ARG:HG3	1.69	0.58
47:w:133:LEU:HB3	47:w:184:LEU:HD11	1.86	0.58
11:E:102:ASN:ND2	11:E:104:GLU:OE1	2.36	0.57
15:I:234:ASN:O	15:I:289:LYS:NZ	2.37	0.57
49:y:74:THR:HA	49:y:96:ARG:HE	1.69	0.57
1:1:1299:U:O2'	43:r:42:LEU:O	2.20	0.57
31:a:203:SER:OG	31:a:215:ARG:NH1	2.36	0.57
1:1:412:G:OP1	22:P:62:ARG:NH1	2.36	0.57
1:1:1348:U:OP1	23:Q:39:ARG:NH1	2.37	0.57
8:B:168:LYS:O	8:B:319:ASN:ND2	2.37	0.57
17:K:43:GLU:OE2	41:o:217:GLU:N	2.37	0.57
40:n:69:GLN:O	40:n:73:HIS:ND1	2.28	0.57
31:a:159:LEU:HD11	31:a:163:LEU:HA	1.87	0.57
1:1:648:C:N3	6:8:390:ARG:NH2	2.52	0.57
40:n:35:LEU:HB3	40:n:71:LEU:HD11	1.86	0.57
47:w:182:GLU:HG2	47:w:186:LYS:HE3	1.86	0.57
1:1:73:C:O2'	18:L:105:ASN:OD1	2.22	0.57
1:1:1138:U:H2'	1:1:1139:G:H8	1.68	0.57
3:3:371:ILE:HG12	3:3:375:ILE:HD12	1.85	0.57
9:C:31:ARG:HG3	9:C:120:TYR:HE1	1.68	0.57
15:I:334:ILE:HG12	15:I:344:LYS:HG2	1.86	0.57
39:m:387:ARG:HG3	40:n:141:LEU:HD22	1.86	0.57
42:q:296:LEU:HD13	42:q:307:LEU:HD13	1.85	0.57
1:1:1199:C:H2'	1:1:1200:A:H8	1.70	0.57
13:G:75:ILE:HD11	20:N:18:VAL:HG13	1.87	0.57
32:b:188:THR:HG23	32:b:190:SER:H	1.69	0.57
40:n:428:GLN:HB2	40:n:447:TYR:HB3	1.87	0.57
25:S:109:ASP:OD2	25:S:113:ARG:NH1	2.37	0.57
25:S:152:LEU:HD12	25:S:172:TYR:HE2	1.70	0.57
1:1:706:A:N3	1:1:715:A:N6	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:123:THR:OG1	23:Q:125:ASP:OD1	2.22	0.57
2:2:154:C:H5'	13:G:181:LYS:HD3	1.86	0.56
26:T:191:GLN:NE2	30:Z:326:ILE:O	2.38	0.56
37:j:60:GLY:HA2	37:j:64:MET:HE2	1.87	0.56
40:n:433:PHE:O	40:n:437:ASN:ND2	2.34	0.56
1:1:2450:G:N1	1:1:2497:U:N3	2.53	0.56
13:G:96:LYS:NZ	13:G:207:ASP:OD1	2.35	0.56
17:K:104:HIS:HB2	17:K:262:ASN:HD21	1.69	0.56
20:N:64:VAL:HG21	20:N:106:VAL:CG2	2.34	0.56
30:Z:354:HIS:HE1	30:Z:356:PHE:HB2	1.71	0.56
31:a:35:GLN:HG3	31:a:166:ALA:HB2	1.86	0.56
44:t:137:GLY:O	44:t:181:LYS:NZ	2.35	0.56
1:1:3158:G:N2	1:1:3291:G:H22	2.04	0.56
28:W:78:GLY:HA3	28:W:84:GLU:HA	1.86	0.56
48:x:205:ARG:HD2	48:x:208:GLN:HE21	1.70	0.56
2:2:40:A:H2'	2:2:41:A:C8	2.41	0.56
7:A:135:PRO:O	16:J:221:GLN:NE2	2.38	0.56
47:w:218:ILE:HD12	47:w:253:ILE:HG21	1.87	0.56
1:1:2473:C:O2	1:1:2474:G:N2	2.38	0.56
1:1:2961:G:H2'	1:1:2962:U:C6	2.41	0.56
1:1:3268:A:OP1	11:E:46:ARG:NH2	2.38	0.56
31:a:67:ILE:HG22	31:a:111:ILE:HG21	1.83	0.56
44:t:279:GLY:O	44:t:288:LYS:NZ	2.32	0.56
1:1:655:C:H2'	1:1:656:A:H8	1.71	0.56
1:1:679:U:OP2	7:A:270:ARG:NH2	2.36	0.56
6:8:330:LYS:HG3	6:8:340:ILE:HD11	1.87	0.56
17:K:275:GLN:HB3	17:K:297:VAL:HG11	1.86	0.56
21:O:54:TYR:HD2	21:O:145:VAL:HG11	1.70	0.56
30:Z:48:ARG:HD3	30:Z:57:ILE:HA	1.87	0.56
39:m:134:ARG:HD3	39:m:136:ILE:HD11	1.88	0.56
1:1:905:U:H2'	1:1:906:A:H8	1.71	0.56
13:G:172:LYS:NZ	39:m:247:PHE:O	2.34	0.56
32:b:403:GLU:HG3	32:b:412:PHE:HB3	1.87	0.56
48:x:176:SER:HB3	48:x:264:THR:HB	1.87	0.56
3:3:707:ARG:HA	32:b:90:HIS:HE1	1.71	0.56
9:C:35:VAL:HG21	9:C:244:LEU:HD21	1.88	0.56
34:f:58:GLU:HG2	34:f:63:LYS:HG3	1.88	0.56
1:1:596:C:OP1	12:F:33:ARG:NH1	2.39	0.55
1:1:1307:G:H4'	1:1:1308:A:H5'	1.87	0.55
7:A:128:ASN:ND2	16:J:278:MET:SD	2.79	0.55
15:I:336:THR:HG22	15:I:342:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:51:LYS:HZ3	21:O:144:SER:HB2	1.70	0.55
1:1:269:G:OP2	20:N:44:ARG:NH1	2.33	0.55
1:1:779:G:O2'	1:1:781:G:O4'	2.24	0.55
1:1:1278:A:O2'	28:W:15:THR:O	2.21	0.55
34:f:49:ILE:HD11	34:f:71:VAL:HG22	1.87	0.55
1:1:251:G:N2	46:v:181:GLU:OE1	2.39	0.55
32:b:74:VAL:CG1	32:b:75:HIS:N	2.69	0.55
38:l:53:LYS:O	38:l:56:THR:OG1	2.24	0.55
39:m:341:PRO:HG2	39:m:344:TYR:HD2	1.71	0.55
1:1:2467:G:H21	1:1:2488:A:H62	1.54	0.55
25:S:10:ILE:HG12	25:S:26:ARG:HG3	1.87	0.55
30:Z:57:ILE:HG13	30:Z:58:LYS:HG3	1.88	0.55
31:a:65:ILE:HG12	31:a:109:ALA:HB3	1.87	0.55
32:b:415:ASN:HD21	32:b:429:ASN:HD21	1.53	0.55
37:j:21:ARG:NH1	37:j:41:ALA:O	2.32	0.55
1:1:1188:U:OP1	1:1:1210:U:O2'	2.23	0.55
33:e:89:THR:HG22	33:e:117:ILE:HG12	1.88	0.55
38:l:40:GLN:NE2	38:l:63:LEU:O	2.39	0.55
42:q:498:ASN:HB3	42:q:550:GLY:H	1.72	0.55
1:1:3295:A:H2'	1:1:3296:A:C8	2.42	0.55
11:E:35:VAL:O	11:E:38:THR:OG1	2.24	0.55
48:x:163:ILE:HG12	48:x:170:THR:HG23	1.89	0.55
1:1:754:G:H1	1:1:779:G:H1'	1.70	0.55
11:E:43:LEU:HD11	11:E:85:ILE:HG13	1.88	0.55
31:a:138:VAL:HG13	31:a:147:LYS:HG3	1.88	0.55
32:b:74:VAL:HG11	32:b:78:HIS:CB	2.35	0.55
1:1:662:U:H2'	1:1:663:C:C6	2.42	0.55
27:V:80:ARG:NH1	27:V:117:PRO:O	2.33	0.55
29:Y:54:ASP:HB2	29:Y:70:ILE:HD13	1.89	0.55
1:1:3057:U:OP1	1:1:3058:U:O2'	2.25	0.55
6:8:385:GLU:OE1	6:8:388:ARG:NH1	2.39	0.55
10:D:274:ASP:HA	10:D:476:SER:HB3	1.89	0.55
6:8:314:LYS:O	6:8:319:GLN:NE2	2.41	0.54
15:I:17:LEU:HD13	15:I:34:HIS:HB3	1.87	0.54
32:b:74:VAL:HG11	32:b:78:HIS:HB2	1.89	0.54
1:1:3039:C:OP1	8:B:62:ARG:NH1	2.36	0.54
8:B:56:ILE:HG21	8:B:356:LEU:HD22	1.89	0.54
10:D:43:LYS:HB2	10:D:46:GLU:HG3	1.90	0.54
12:F:82:LYS:HE2	12:F:191:VAL:HB	1.89	0.54
3:3:679:LEU:HD13	32:b:237:MET:HE1	1.88	0.54
30:Z:267:ARG:HB3	30:Z:321:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:343:GLU:HG2	30:Z:351:VAL:HG22	1.88	0.54
38:l:2:ARG:HE	38:l:39:LEU:HD23	1.72	0.54
1:1:361:A:O3'	37:j:45:ARG:NH2	2.41	0.54
1:1:987:U:H3	1:1:1097:G:H1	1.55	0.54
1:1:2462:A:H2'	1:1:2463:G:C8	2.43	0.54
1:1:2966:G:N2	38:l:166:GLN:O	2.40	0.54
2:2:29:U:H5''	18:L:27:ASP:HB3	1.89	0.54
1:1:2420:C:O2'	1:1:2421:U:OP1	2.25	0.54
30:Z:48:ARG:HB3	30:Z:57:ILE:HG22	1.88	0.54
44:t:84:LYS:HB3	44:t:90:THR:HG21	1.88	0.54
4:6:230:A:OP2	44:t:292:ARG:NH2	2.41	0.54
7:A:99:LEU:HB3	7:A:112:PHE:HB2	1.90	0.54
15:I:266:LEU:O	15:I:285:GLN:NE2	2.39	0.54
28:W:22:ASN:OD1	28:W:25:ARG:NH2	2.40	0.54
41:o:149:GLN:HG2	41:o:164:VAL:HG12	1.89	0.54
1:1:3099:C:O2'	1:1:3100:U:O5'	2.25	0.54
26:T:181:GLU:O	26:T:184:THR:OG1	2.26	0.54
26:T:219:ILE:HD11	48:x:42:ARG:HD3	1.89	0.54
39:m:152:GLU:OE2	39:m:154:GLN:NE2	2.40	0.54
39:m:365:ASN:O	39:m:380:TYR:OH	2.25	0.54
1:1:664:U:H2'	1:1:665:A:H8	1.72	0.54
1:1:2366:C:H2'	1:1:2367:A:H8	1.73	0.54
1:1:1197:A:H5'	1:1:1198:C:H4'	1.88	0.54
13:G:154:ALA:HB2	13:G:186:LEU:HD12	1.88	0.54
18:L:107:GLU:OE2	36:i:18:THR:OG1	2.26	0.54
31:a:67:ILE:HD11	31:a:77:ALA:HB2	1.90	0.54
31:a:87:VAL:HB	31:a:116:LEU:HD21	1.89	0.54
1:1:358:G:N2	1:1:361:A:OP2	2.34	0.54
9:C:325:LEU:O	12:F:41:ARG:NH2	2.36	0.54
19:M:55:ARG:HD3	25:S:70:THR:HB	1.89	0.54
1:1:3060:C:O2	1:1:3332:U:O2'	2.25	0.53
31:a:67:ILE:CD1	31:a:77:ALA:HB2	2.38	0.53
1:1:1257:C:H42	1:1:1261:G:H22	1.54	0.53
10:D:124:ARG:CZ	10:D:456:SER:HB2	2.38	0.53
16:J:277:GLU:HB2	39:m:158:GLY:HA3	1.90	0.53
44:t:150:PRO:HB2	44:t:153:VAL:HG21	1.90	0.53
1:1:2891:U:H2'	1:1:2892:A:H8	1.73	0.53
44:t:211:ARG:NE	44:t:322:ASN:OD1	2.41	0.53
1:1:644:G:H2'	1:1:645:A:H5'	1.91	0.53
21:O:76:PRO:CB	21:O:138:LEU:CD2	2.87	0.53
28:W:96:CYS:HB3	28:W:100:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:99:VAL:HG12	40:n:103:LYS:HE2	1.91	0.53
1:1:1230:G:H5''	28:W:49:ARG:HD2	1.90	0.53
15:I:384:VAL:HG13	15:I:407:ILE:HD13	1.89	0.53
26:T:195:VAL:HG11	30:Z:266:VAL:HG11	1.89	0.53
32:b:421:LEU:O	45:u:80:ARG:NH1	2.42	0.53
41:o:95:VAL:HG12	41:o:164:VAL:HG22	1.89	0.53
42:q:269:ARG:HH12	42:q:533:PRO:HB3	1.72	0.53
1:1:198:A:N3	1:1:218:G:O2'	2.41	0.53
1:1:305:U:H2'	1:1:306:A:C8	2.43	0.53
1:1:546:C:OP1	1:1:547:G:N2	2.41	0.53
1:1:1256:G:H2'	1:1:1257:C:C6	2.44	0.53
2:2:9:A:H2'	2:2:10:A:C8	2.44	0.53
8:B:113:GLU:HG3	8:B:167:ARG:HH21	1.74	0.53
32:b:157:ILE:HG13	32:b:160:LEU:HD12	1.89	0.53
1:1:385:A:OP2	48:x:31:HIS:NE2	2.42	0.53
1:1:664:U:H2'	1:1:665:A:C8	2.44	0.53
3:3:653:ILE:HA	3:3:657:TRP:CD1	2.44	0.53
8:B:316:GLU:OE2	8:B:318:LYS:NZ	2.38	0.53
14:H:57:VAL:HG23	14:H:68:LEU:HD13	1.90	0.53
1:1:515:C:H5'	9:C:343:LYS:HE3	1.92	0.53
1:1:604:G:H2'	1:1:605:U:C6	2.43	0.53
13:G:185:ARG:O	13:G:188:THR:OG1	2.27	0.53
17:K:202:VAL:HG22	17:K:237:LYS:HE2	1.91	0.53
1:1:3394:U:H2'	1:1:3395:G:C8	2.44	0.52
21:O:46:GLU:HG3	21:O:49:ARG:H	1.73	0.52
40:n:189:GLN:HB2	40:n:198:ARG:HG2	1.91	0.52
42:q:265:ASN:OD1	42:q:269:ARG:NH2	2.42	0.52
15:I:276:TRP:HB3	15:I:300:ARG:HD2	1.90	0.52
24:R:109:LYS:O	24:R:113:THR:HG23	2.09	0.52
38:l:58:VAL:HG11	38:l:63:LEU:HD13	1.91	0.52
1:1:164:A:O2'	1:1:166:C:O4'	2.27	0.52
1:1:806:A:H61	1:1:935:U:H3'	1.74	0.52
1:1:1290:A:H2'	1:1:1291:A:C8	2.45	0.52
1:1:3158:G:N2	1:1:3291:G:H1	2.05	0.52
3:3:353:GLU:HG2	3:3:589:TYR:HB2	1.91	0.52
1:1:435:C:H2'	1:1:436:A:C8	2.44	0.52
1:1:3023:U:H5	1:1:3032:A:N7	2.07	0.52
39:m:373:ALA:HB3	39:m:376:LYS:HG3	1.90	0.52
1:1:1129:A:OP1	43:r:251:ARG:NH2	2.43	0.52
14:H:90:MET:HG2	14:H:181:VAL:HA	1.92	0.52
42:q:200:THR:O	42:q:204:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:359:LYS:NZ	42:q:421:ASP:OD2	2.42	0.52
45:u:66:ASP:OD1	45:u:103:ARG:NH1	2.42	0.52
10:D:148:VAL:HG23	10:D:168:LEU:HD11	1.91	0.52
1:1:770:G:H4'	1:1:771:A:H5'	1.92	0.52
1:1:1203:A:H4'	1:1:1204:A:C8	2.44	0.52
1:1:3163:A:N1	1:1:3286:G:O6	2.42	0.52
8:B:56:ILE:HD13	8:B:356:LEU:HD13	1.92	0.52
12:F:89:ILE:HD11	12:F:229:PHE:HB3	1.90	0.52
1:1:2428:U:H2'	1:1:2429:G:C8	2.45	0.52
40:n:409:HIS:HD2	40:n:427:ILE:HD11	1.74	0.52
1:1:435:C:H2'	1:1:436:A:H8	1.75	0.52
1:1:1107:C:H2'	1:1:1108:U:C6	2.44	0.52
7:A:192:GLU:HB2	7:A:215:ILE:HD11	1.91	0.52
12:F:189:ILE:HG23	12:F:190:THR:HG23	1.91	0.52
15:I:5:VAL:HG21	15:I:384:VAL:HG21	1.90	0.52
49:y:24:CYS:HB3	49:y:48:ILE:HG12	1.92	0.52
49:y:42:LEU:HD13	49:y:46:ILE:HD11	1.91	0.52
1:1:428:A:H2'	1:1:429:U:C6	2.45	0.52
8:B:90:VAL:HG13	8:B:104:THR:HG22	1.90	0.52
30:Z:354:HIS:CE1	30:Z:356:PHE:HB2	2.45	0.52
39:m:336:GLU:HG2	40:n:182:SER:HB2	1.91	0.52
1:1:3233:C:H2'	1:1:3234:A:H8	1.74	0.51
7:A:38:SER:HB2	7:A:68:LYS:HG2	1.93	0.51
44:t:142:LEU:HD11	44:t:179:LEU:HD22	1.92	0.51
1:1:981:U:O2'	1:1:1105:A:O2'	2.28	0.51
1:1:3338:C:H2'	1:1:3339:A:C8	2.45	0.51
3:3:790:LEU:O	42:q:537:ASN:ND2	2.43	0.51
45:u:33:ARG:HE	45:u:35:LYS:HD3	1.75	0.51
1:1:542:G:O6	1:1:549:U:O2	2.27	0.51
1:1:655:C:H2'	1:1:656:A:C8	2.45	0.51
1:1:2495:C:H2'	1:1:2496:C:C6	2.45	0.51
1:1:3080:G:H2'	1:1:3081:C:C6	2.46	0.51
38:l:51:VAL:HG13	42:q:399:ILE:HD11	1.91	0.51
43:r:173:ARG:O	43:r:178:ARG:NH2	2.43	0.51
1:1:1888:U:H2'	1:1:1889:G:C8	2.46	0.51
1:1:2990:G:O3'	8:B:21:ARG:NH2	2.44	0.51
4:6:20:U:H2'	4:6:21:G:C8	2.45	0.51
8:B:152:LYS:HG3	8:B:189:SER:HA	1.92	0.51
9:C:31:ARG:HG3	9:C:120:TYR:CE1	2.45	0.51
10:D:266:GLN:N	10:D:390:SER:O	2.43	0.51
30:Z:109:PHE:HB3	30:Z:337:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:289:A:H2'	1:1:290:G:H8	1.76	0.51
1:1:656:A:H2'	1:1:657:A:C8	2.45	0.51
1:1:3309:G:O2'	22:P:69:ARG:NH2	2.44	0.51
15:I:147:LYS:HE2	15:I:149:ASP:HB3	1.93	0.51
28:W:45:LEU:HB3	28:W:48:VAL:HG21	1.93	0.51
1:1:531:G:H2'	1:1:532:A:C8	2.46	0.51
1:1:644:G:O6	6:8:398:ARG:NH2	2.40	0.51
1:1:1455:U:H2'	1:1:1456:A:H8	1.74	0.51
1:1:257:U:H2'	1:1:258:G:H8	1.75	0.51
1:1:665:A:H2'	1:1:666:A:C8	2.46	0.51
1:1:2450:G:N1	1:1:2497:U:C2	2.78	0.51
4:6:16:U:H2'	4:6:17:G:C8	2.40	0.51
13:G:81:THR:HG21	13:G:181:LYS:HG3	1.93	0.51
25:S:80:ARG:HG3	25:S:124:LEU:HD11	1.91	0.51
1:1:1885:U:O2'	1:1:1886:A:H5''	2.10	0.51
1:1:3163:A:H2	1:1:3286:G:H1	1.55	0.51
10:D:444:LYS:HE2	10:D:483:PRO:HB3	1.93	0.51
28:W:173:THR:HG23	28:W:180:ILE:HG23	1.93	0.51
42:q:282:ARG:HD3	42:q:305:VAL:HA	1.92	0.51
49:y:85:ARG:NH2	49:y:89:PRO:O	2.43	0.51
1:1:1221:A:N7	28:W:20:ARG:NH2	2.59	0.50
1:1:2414:G:OP1	38:l:72:LYS:NZ	2.42	0.50
1:1:2855:U:H2'	1:1:2856:G:C8	2.46	0.50
3:3:557:LEU:HD21	3:3:652:ILE:HG23	1.93	0.50
3:3:697:ASP:OD1	3:3:697:ASP:N	2.41	0.50
7:A:47:HIS:HB3	7:A:119:THR:HG21	1.92	0.50
20:N:27:VAL:HG21	20:N:124:ASP:OD1	2.11	0.50
40:n:41:ILE:HD12	40:n:67:ASP:HB3	1.93	0.50
42:q:512:ALA:HB2	42:q:530:ARG:HB2	1.92	0.50
13:G:162:LEU:HD23	20:N:7:LEU:HD11	1.93	0.50
39:m:128:TYR:CE2	39:m:134:ARG:HB3	2.46	0.50
43:r:155:THR:HG22	43:r:214:VAL:HA	1.93	0.50
49:y:42:LEU:HD12	49:y:48:ILE:HD11	1.93	0.50
1:1:439:C:C4	33:e:128:LEU:HD11	2.47	0.50
1:1:1307:G:N7	1:1:2369:G:H1'	2.27	0.50
2:2:75:G:OP2	29:Y:74:TYR:OH	2.26	0.50
3:3:352:LEU:HD12	3:3:524:ALA:HB3	1.94	0.50
3:3:540:GLU:HA	3:3:543:TYR:HD2	1.76	0.50
42:q:252:LEU:HD13	42:q:482:VAL:HG21	1.92	0.50
1:1:30:G:H5''	20:N:188:ARG:NH2	2.27	0.50
1:1:748:U:H2'	1:1:749:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1138:U:H2'	1:1:1139:G:C8	2.45	0.50
1:1:1277:C:O2'	1:1:1278:A:O5'	2.30	0.50
36:i:45:ARG:HD3	36:i:93:ILE:HD11	1.93	0.50
1:1:5:G:H2'	1:1:6:A:H8	1.77	0.50
1:1:156:G:H22	18:L:91:ARG:HH12	1.60	0.50
35:h:12:LYS:NZ	35:h:20:GLN:OE1	2.43	0.50
48:x:189:ARG:O	48:x:245:ARG:NH2	2.44	0.50
1:1:411:U:H2'	1:1:412:G:H8	1.77	0.50
1:1:585:A:H2'	1:1:586:C:C6	2.46	0.50
1:1:757:C:N3	1:1:775:A:N6	2.53	0.50
1:1:1399:A:H2	2:2:8:C:HO2'	1.60	0.50
1:1:2357:A:H2'	1:1:2358:A:C8	2.46	0.50
8:B:61:ASP:CG	32:b:413:ASN:HD21	2.20	0.50
27:V:130:ALA:O	49:y:106:ASN:ND2	2.36	0.50
47:w:181:TRP:HZ3	47:w:212:THR:HB	1.75	0.50
1:1:787:G:H2'	1:1:788:C:C6	2.47	0.50
1:1:3000:A:H2'	1:1:3001:C:C6	2.47	0.50
21:O:157:GLU:HG3	21:O:161:LYS:HE3	1.94	0.50
23:Q:83:VAL:O	23:Q:103:ALA:HA	2.12	0.50
32:b:120:GLN:HG2	43:r:152:THR:HG21	1.93	0.50
41:o:121:ARG:HD3	41:o:176:LEU:HB2	1.93	0.50
42:q:289:LEU:HB3	42:q:294:VAL:HB	1.94	0.50
49:y:162:HIS:HD2	49:y:164:GLN:HB2	1.75	0.50
1:1:439:C:H42	24:R:134:TYR:HE1	1.59	0.50
1:1:642:U:H2'	1:1:643:U:O4'	2.12	0.50
1:1:1280:C:H2'	1:1:1281:G:H8	1.75	0.50
1:1:2891:U:H2'	1:1:2892:A:C8	2.47	0.50
32:b:161:PRO:HB3	43:r:3:GLN:HG2	1.94	0.50
49:y:15:VAL:HA	49:y:61:ARG:HG2	1.94	0.50
4:6:227:C:N4	44:t:153:VAL:O	2.46	0.49
28:W:165:MET:HG3	28:W:169:PHE:HD2	1.77	0.49
32:b:86:TYR:O	32:b:149:TYR:OH	2.29	0.49
1:1:3252:G:H2'	1:1:3253:G:C8	2.47	0.49
24:R:86:TYR:HE1	24:R:113:THR:HG22	1.76	0.49
38:l:93:ALA:HB2	38:l:132:ILE:HD12	1.93	0.49
42:q:232:LEU:HD13	42:q:247:GLU:HG2	1.94	0.49
1:1:1126:G:OP1	16:J:331:ARG:NH1	2.45	0.49
17:K:123:VAL:HA	17:K:179:LEU:O	2.12	0.49
1:1:3193:C:H2'	1:1:3194:C:C6	2.47	0.49
3:3:557:LEU:HB3	3:3:559:PRO:HD2	1.95	0.49
7:A:179:PHE:HD1	7:A:188:VAL:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:158:HIS:HB3	20:N:161:ALA:HB3	1.95	0.49
24:R:111:ARG:HG3	33:e:87:MET:HE3	1.93	0.49
1:1:397:A:H5'	1:1:399:A:OP1	2.12	0.49
1:1:494:G:O2'	1:1:495:G:H8	1.95	0.49
1:1:1206:G:H4'	43:r:54:ARG:HB3	1.94	0.49
1:1:3057:U:H5''	1:1:3086:A:N1	2.27	0.49
4:6:43:A:H2'	4:6:44:G:H8	1.77	0.49
8:B:113:GLU:HB3	8:B:176:ALA:HB2	1.94	0.49
39:m:306:TYR:O	40:n:230:HIS:NE2	2.34	0.49
41:o:149:GLN:HG3	41:o:166:VAL:HG23	1.93	0.49
42:q:350:LEU:HB3	42:q:418:ILE:HG12	1.94	0.49
48:x:106:SER:OG	48:x:152:GLU:OE2	2.29	0.49
1:1:2597:U:H3'	1:1:2598:G:H8	1.78	0.49
1:1:3139:A:H4'	8:B:20:LYS:HD3	1.94	0.49
35:h:85:THR:HG22	35:h:87:ALA:H	1.76	0.49
49:y:177:LEU:HB3	49:y:179:VAL:HG22	1.93	0.49
1:1:909:G:H3'	1:1:910:G:C8	2.48	0.49
1:1:1132:C:H2'	1:1:1133:A:H8	1.76	0.49
1:1:2830:G:H2'	1:1:2831:G:C8	2.48	0.49
4:6:45:U:O2'	17:K:243:THR:O	2.30	0.49
10:D:309:LEU:HD22	10:D:314:LEU:HD23	1.94	0.49
10:D:402:LEU:HD22	10:D:412:LEU:HD13	1.94	0.49
42:q:346:ASN:H	42:q:370:THR:HG23	1.76	0.49
1:1:567:G:H2'	1:1:568:G:C8	2.47	0.49
1:1:1104:G:H2'	1:1:1105:A:H8	1.78	0.49
1:1:3096:C:H5''	8:B:325:LYS:NZ	2.27	0.49
7:A:260:ALA:HA	7:A:263:ARG:HE	1.78	0.49
8:B:193:ASP:OD1	8:B:196:ARG:NH2	2.46	0.49
8:B:214:MET:HE2	8:B:281:LYS:HE2	1.95	0.49
12:F:96:PRO:HB2	12:F:99:PRO:HD2	1.94	0.49
32:b:87:GLU:HG2	32:b:90:HIS:HD2	1.78	0.49
43:r:248:GLU:HG3	43:r:251:ARG:HH21	1.78	0.49
1:1:660:A:N1	1:1:941:G:O2'	2.44	0.49
1:1:2603:G:H2'	1:1:2604:U:C6	2.47	0.49
1:1:3330:A:N6	1:1:3374:U:O2	2.45	0.49
32:b:104:LEU:HB3	32:b:139:ILE:HD13	1.95	0.49
44:t:146:ARG:HA	44:t:194:VAL:HG12	1.94	0.49
49:y:53:ILE:O	49:y:56:THR:OG1	2.31	0.49
1:1:953:G:H1	1:1:1142:G:H2'	1.78	0.49
1:1:2892:A:H2'	1:1:2893:C:C6	2.48	0.49
1:1:3340:G:N2	1:1:3365:U:O2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:21:C:OP1	9:C:193:LYS:NZ	2.36	0.49
4:6:48:A:H4'	17:K:74:LEU:HD21	1.94	0.49
14:H:28:VAL:HG13	14:H:33:THR:HG22	1.95	0.49
1:1:53:G:OP2	37:j:48:ASN:ND2	2.43	0.48
1:1:431:U:OP1	34:f:65:ARG:NH1	2.43	0.48
1:1:1454:A:H3'	1:1:1455:U:H5''	1.94	0.48
7:A:280:ALA:HB2	46:v:78:PRO:HG3	1.94	0.48
8:B:53:MET:O	8:B:364:LYS:NZ	2.44	0.48
8:B:108:GLU:CD	8:B:109:HIS:HD1	2.15	0.48
14:H:177:ASP:O	43:r:17:ARG:NH1	2.46	0.48
27:V:86:ARG:NH1	27:V:92:PHE:HB3	2.28	0.48
30:Z:268:VAL:HB	30:Z:324:LYS:HD2	1.94	0.48
44:t:186:LEU:O	44:t:190:ILE:HG12	2.12	0.48
1:1:2463:G:N2	31:a:164:CYS:SG	2.86	0.48
27:V:39:VAL:HG12	27:V:58:VAL:HG12	1.95	0.48
27:V:79:VAL:HG13	27:V:118:VAL:HG13	1.95	0.48
32:b:329:MET:HA	32:b:332:ARG:HG2	1.94	0.48
32:b:390:PRO:O	32:b:395:ARG:NH1	2.47	0.48
1:1:2428:U:H2'	1:1:2429:G:H8	1.77	0.48
3:3:597:SER:N	3:3:659:ALA:O	2.44	0.48
7:A:130:LEU:HD22	16:J:276:ALA:HB3	1.96	0.48
8:B:108:GLU:CD	8:B:108:GLU:O	2.56	0.48
25:S:155:ARG:CZ	25:S:172:TYR:HD1	2.26	0.48
1:1:92:G:H5'	1:1:93:C:H5''	1.95	0.48
1:1:411:U:H2'	1:1:412:G:C8	2.49	0.48
1:1:3393:U:H2'	1:1:3394:U:C6	2.49	0.48
41:o:184:LEU:HD23	41:o:184:LEU:H	1.77	0.48
1:1:2442:G:O6	1:1:2505:U:O4	2.30	0.48
9:C:120:TYR:CE2	9:C:277:PRO:HB3	2.49	0.48
33:e:101:SER:HA	33:e:125:ARG:HH11	1.78	0.48
45:u:1:MET:HE3	45:u:15:PRO:HG2	1.96	0.48
1:1:168:U:H5''	46:v:172:ARG:HH12	1.79	0.48
1:1:2465:G:O6	1:1:2491:A:N6	2.47	0.48
1:1:2855:U:H2'	1:1:2856:G:H8	1.79	0.48
1:1:3294:A:OP1	8:B:128:LYS:NZ	2.43	0.48
9:C:120:TYR:CE2	9:C:277:PRO:CB	2.96	0.48
9:C:138:ARG:HH21	9:C:240:PRO:HB2	1.78	0.48
17:K:97:LEU:HD11	17:K:205:THR:HB	1.94	0.48
28:W:139:GLU:HB3	28:W:185:PRO:HD3	1.96	0.48
44:t:78:VAL:HG22	44:t:305:ALA:HA	1.94	0.48
49:y:72:VAL:HB	49:y:76:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:y:126:GLU:HG3	49:y:137:VAL:HG11	1.95	0.48
1:1:117:U:O2'	1:1:119:U:OP2	2.27	0.48
1:1:525:C:OP2	19:M:77:ARG:NH2	2.41	0.48
1:1:2449:A:H2'	1:1:2450:G:C8	2.49	0.48
1:1:2450:G:C2	1:1:2497:U:C2	3.02	0.48
1:1:2900:A:C8	43:r:2:PRO:HD3	2.49	0.48
15:I:147:LYS:HD3	15:I:152:ASN:HB2	1.96	0.48
28:W:37:TYR:HB2	28:W:104:PHE:HB3	1.96	0.48
44:t:100:ILE:HD13	44:t:309:VAL:HB	1.95	0.48
49:y:13:ILE:HG23	49:y:34:PHE:HZ	1.79	0.48
49:y:17:SER:HB3	49:y:34:PHE:HE2	1.77	0.48
1:1:406:G:OP1	1:1:1415:U:O2'	2.27	0.48
1:1:464:U:H5''	24:R:75:LYS:HD2	1.96	0.48
1:1:651:G:O2'	1:1:1435:A:OP1	2.32	0.48
1:1:1385:C:OP1	9:C:141:ARG:NH1	2.35	0.48
1:1:2347:U:OP2	6:8:360:LYS:NZ	2.31	0.48
30:Z:211:ARG:O	30:Z:325:ALA:N	2.39	0.48
33:e:126:LEU:O	48:x:154:LYS:NZ	2.42	0.48
40:n:76:VAL:HG21	40:n:117:ILE:HD11	1.95	0.48
48:x:193:HIS:HB3	48:x:223:ASP:HB2	1.95	0.48
21:O:142:SER:HA	21:O:145:VAL:HG22	1.96	0.48
1:1:50:U:H2'	1:1:51:A:H8	1.79	0.47
1:1:2423:U:O2	1:1:2607:G:O6	2.32	0.47
1:1:3345:G:H2'	1:1:3346:U:H4'	1.96	0.47
3:3:543:TYR:OH	3:3:639:THR:O	2.26	0.47
13:G:81:THR:HG22	13:G:179:ILE:HG22	1.95	0.47
28:W:34:LEU:HD21	28:W:89:LEU:HD21	1.96	0.47
42:q:457:LEU:HD11	42:q:491:TYR:HE1	1.79	0.47
40:n:114:LEU:HD22	40:n:117:ILE:HD12	1.95	0.47
1:1:704:U:H3'	1:1:705:A:H5''	1.96	0.47
1:1:3093:C:OP2	27:V:48:ARG:NH1	2.47	0.47
1:1:3267:A:H2'	11:E:69:PHE:CZ	2.50	0.47
8:B:159:ARG:HG2	8:B:182:GLN:HA	1.96	0.47
14:H:49:ASN:HD21	14:H:52:LEU:HD12	1.80	0.47
35:h:70:TYR:CD1	35:h:73:LYS:HD2	2.49	0.47
1:1:987:U:H2'	1:1:988:U:C6	2.49	0.47
14:H:89:LYS:HG2	14:H:145:VAL:HG22	1.95	0.47
40:n:411:ILE:HG12	40:n:427:ILE:HB	1.95	0.47
42:q:470:GLY:HA3	42:q:547:GLN:HE22	1.79	0.47
1:1:2383:C:H2'	1:1:2384:A:C8	2.50	0.47
10:D:117:ILE:HG23	10:D:192:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:60:ASP:OD1	11:E:62:THR:OG1	2.29	0.47
25:S:152:LEU:HD12	25:S:172:TYR:CE2	2.48	0.47
49:y:157:GLN:NE2	49:y:201:ASP:O	2.48	0.47
1:1:2366:C:H2'	1:1:2367:A:C8	2.49	0.47
1:1:3323:A:H2'	1:1:3324:C:C6	2.50	0.47
3:3:653:ILE:HA	3:3:657:TRP:HD1	1.78	0.47
1:1:377:A:H1'	1:1:392:G:N2	2.29	0.47
1:1:528:U:H2'	1:1:529:A:C8	2.50	0.47
1:1:595:G:H2'	1:1:596:C:C6	2.49	0.47
1:1:952:A:H4'	1:1:968:G:N2	2.30	0.47
1:1:1342:C:OP1	23:Q:12:ARG:NH1	2.48	0.47
1:1:2357:A:H2'	1:1:2358:A:H8	1.80	0.47
1:1:3080:G:H2'	1:1:3081:C:H6	1.78	0.47
1:1:3294:A:H2'	1:1:3295:A:O4'	2.15	0.47
3:3:469:HIS:HD2	27:V:67:PRO:HG2	1.79	0.47
4:6:33:U:O3'	4:6:34:A:H8	1.98	0.47
12:F:98:LYS:HB3	12:F:99:PRO:HD3	1.95	0.47
27:V:118:VAL:O	27:V:137:VAL:N	2.42	0.47
42:q:355:ALA:O	42:q:382:ARG:NH2	2.48	0.47
44:t:101:LEU:HD11	44:t:130:ARG:HB3	1.95	0.47
44:t:302:SER:HB2	44:t:307:ALA:HB2	1.95	0.47
49:y:108:ILE:HD12	49:y:117:VAL:HG12	1.97	0.47
1:1:129:U:H2'	1:1:130:A:C8	2.50	0.47
1:1:184:U:H2'	1:1:185:C:C6	2.49	0.47
1:1:285:A:O2'	1:1:287:G:N7	2.41	0.47
1:1:3113:A:OP1	14:H:73:SER:OG	2.33	0.47
10:D:418:PRO:HB2	10:D:421:LYS:HB2	1.95	0.47
17:K:78:LEU:HD23	17:K:259:PHE:CZ	2.50	0.47
39:m:334:ASN:OD1	40:n:458:SER:OG	2.32	0.47
1:1:20:A:H2'	1:1:21:G:C8	2.50	0.47
1:1:1240:A:H2'	1:1:1241:U:C6	2.50	0.47
1:1:1464:G:H2'	1:1:1465:A:C8	2.50	0.47
6:8:367:GLU:OE1	6:8:370:ARG:NH1	2.35	0.47
15:I:277:SER:HB2	15:I:301:GLU:O	2.15	0.47
42:q:289:LEU:HD12	42:q:296:LEU:HD11	1.95	0.47
1:1:905:U:H2'	1:1:906:A:C8	2.49	0.47
1:1:1142:G:H5''	1:1:1143:A:OP2	2.15	0.47
38:l:135:ALA:HB3	38:l:139:VAL:HB	1.97	0.47
44:t:77:ARG:NH2	44:t:303:ASN:OD1	2.48	0.47
1:1:2369:G:H2'	1:1:2370:G:C8	2.49	0.46
3:3:710:LEU:HD12	32:b:90:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:143:PHE:HA	7:A:149:TYR:HB3	1.97	0.46
25:S:12:ARG:HB3	25:S:24:LEU:HD23	1.97	0.46
48:x:272:ARG:O	48:x:276:GLU:HB2	2.15	0.46
1:1:627:U:H2'	1:1:628:A:C8	2.51	0.46
1:1:784:A:H8	23:Q:69:ARG:HD2	1.80	0.46
1:1:1202:A:H5'	1:1:1203:A:H5''	1.95	0.46
1:1:1893:A:N6	1:1:2342:U:H3	2.14	0.46
1:1:2429:G:H2'	1:1:2430:A:C8	2.50	0.46
1:1:3343:G:N2	1:1:3362:A:OP1	2.45	0.46
10:D:319:LEU:HB2	10:D:345:CYS:HB3	1.97	0.46
10:D:366:PRO:HB3	10:D:463:TYR:CE1	2.50	0.46
24:R:86:TYR:CE1	24:R:113:THR:HG22	2.50	0.46
39:m:387:ARG:HB3	40:n:138:MET:HE1	1.97	0.46
1:1:305:U:O4	7:A:92:ARG:NH2	2.46	0.46
1:1:637:C:H2'	1:1:638:C:C6	2.49	0.46
1:1:3291:G:H4'	1:1:3292:A:C8	2.51	0.46
8:B:296:THR:OG1	8:B:357:LYS:O	2.28	0.46
15:I:191:GLN:NE2	15:I:322:ASN:OD1	2.40	0.46
21:O:76:PRO:CA	21:O:138:LEU:HD21	2.45	0.46
27:V:117:PRO:HA	27:V:135:VAL:HG13	1.97	0.46
28:W:220:TYR:CE2	28:W:229:GLU:HB2	2.51	0.46
43:r:151:ILE:HD11	43:r:173:ARG:HG2	1.97	0.46
49:y:163:PRO:HA	49:y:183:ALA:HB1	1.98	0.46
1:1:258:G:H2'	1:1:259:C:C6	2.51	0.46
7:A:176:VAL:HG23	7:A:193:ILE:HD11	1.97	0.46
8:B:123:TYR:CZ	8:B:124:LYS:HG3	2.51	0.46
20:N:64:VAL:CG2	20:N:106:VAL:CG2	2.94	0.46
28:W:131:ALA:O	28:W:192:GLY:N	2.40	0.46
38:l:122:SER:HB2	38:l:125:ILE:HD11	1.97	0.46
1:1:209:A:O2'	1:1:211:A:OP2	2.29	0.46
1:1:507:U:H2'	1:1:508:U:C6	2.51	0.46
1:1:3075:G:N3	1:1:3075:G:H2'	2.31	0.46
15:I:376:LEU:HD21	15:I:409:MET:HE3	1.97	0.46
17:K:45:ILE:HG13	17:K:251:LEU:HD21	1.98	0.46
17:K:183:ASP:HB3	17:K:186:ILE:HG22	1.97	0.46
21:O:3:VAL:HG13	21:O:4:GLU:HG3	1.98	0.46
30:Z:28:ILE:HG13	30:Z:84:MET:HG2	1.98	0.46
35:h:70:TYR:HD1	35:h:73:LYS:HD2	1.81	0.46
37:j:39:TYR:CD1	37:j:40:PRO:HA	2.50	0.46
46:v:196:TYR:HA	46:v:199:MET:HE3	1.96	0.46
46:v:214:ASP:OD1	46:v:218:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:97:U:H2'	1:1:98:G:O4'	2.15	0.46
1:1:1132:C:H2'	1:1:1133:A:C8	2.50	0.46
1:1:3385:U:H2'	1:1:3386:G:C8	2.47	0.46
10:D:162:MET:HE3	36:i:24:PRO:HD2	1.97	0.46
15:I:399:TYR:CZ	15:I:401:GLY:HA2	2.51	0.46
17:K:201:LYS:O	17:K:205:THR:OG1	2.30	0.46
21:O:50:ASN:OD1	21:O:136:THR:OG1	2.22	0.46
31:a:76:ARG:HB3	31:a:144:LEU:HD22	1.96	0.46
39:m:168:MET:O	39:m:182:ARG:NH2	2.48	0.46
1:1:5:G:H2'	1:1:6:A:C8	2.50	0.46
1:1:3353:G:O2'	1:1:3356:G:OP2	2.33	0.46
1:1:3394:U:H2'	1:1:3395:G:H8	1.81	0.46
7:A:139:PHE:HB2	16:J:224:THR:HG22	1.98	0.46
9:C:156:LEU:HD12	9:C:159:ILE:HD12	1.97	0.46
22:P:118:GLN:NE2	22:P:120:ASN:OD1	2.42	0.46
32:b:178:VAL:HG11	32:b:253:PHE:HB3	1.97	0.46
41:o:98:LEU:HD23	41:o:162:LEU:HD22	1.97	0.46
49:y:182:VAL:HG22	49:y:221:ILE:HG12	1.97	0.46
1:1:3091:A:O2'	1:1:3092:C:H4'	2.16	0.46
1:1:3332:U:H2'	1:1:3333:G:O4'	2.16	0.46
1:1:3353:G:O2'	1:1:3356:G:H5''	2.16	0.46
7:A:151:LEU:HA	16:J:205:LEU:HD13	1.98	0.46
7:A:170:LYS:HZ1	16:J:277:GLU:HB3	1.80	0.46
24:R:114:LYS:HB3	33:e:87:MET:HE1	1.97	0.46
29:Y:71:SER:N	29:Y:81:GLN:O	2.47	0.46
48:x:77:ASP:OD1	48:x:77:ASP:N	2.49	0.46
1:1:431:U:H2'	1:1:432:G:C8	2.51	0.46
1:1:789:A:H2'	1:1:790:U:C6	2.51	0.46
1:1:3110:C:O3'	14:H:155:SER:OG	2.30	0.46
7:A:44:ARG:NH2	7:A:117:LEU:O	2.38	0.46
21:O:12:LYS:HD2	21:O:37:ARG:NH2	2.30	0.46
39:m:269:SER:HB3	39:m:272:GLU:HB2	1.97	0.46
1:1:1307:G:H2'	1:1:2369:G:H4'	1.97	0.46
1:1:2440:G:H2'	1:1:2441:A:C8	2.51	0.46
1:1:2481:G:H2'	1:1:2482:U:C6	2.51	0.46
1:1:2816:G:H2'	1:1:2817:A:C8	2.52	0.46
1:1:3360:C:H2'	1:1:3361:G:H8	1.81	0.46
30:Z:167:SER:O	30:Z:171:ASN:ND2	2.34	0.46
32:b:118:PHE:O	32:b:120:GLN:NE2	2.49	0.46
32:b:227:ARG:HH12	32:b:233:ASN:HD21	1.64	0.46
38:l:108:LEU:HD21	38:l:141:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:80:G:H2'	1:1:81:C:H6	1.81	0.45
1:1:753:C:H2'	1:1:754:G:C8	2.51	0.45
3:3:357:LEU:HD12	3:3:371:ILE:HD11	1.98	0.45
7:A:36:ILE:HG23	7:A:88:PHE:HD1	1.81	0.45
27:V:101:VAL:HB	27:V:109:MET:HE1	1.98	0.45
1:1:374:A:N3	1:1:376:G:H5''	2.31	0.45
2:2:103:G:OP2	2:2:105:A:O2'	2.28	0.45
21:O:76:PRO:O	21:O:138:LEU:HD21	2.17	0.45
39:m:345:LEU:HD21	39:m:370:LYS:HB2	1.98	0.45
42:q:377:ASP:OD1	42:q:378:ALA:N	2.50	0.45
44:t:234:ILE:HA	44:t:237:GLU:HG2	1.97	0.45
47:w:169:ILE:HB	47:w:170:PRO:HD3	1.97	0.45
1:1:258:G:H2'	1:1:259:C:H6	1.81	0.45
15:I:381:ASP:OD2	15:I:385:ARG:NH1	2.37	0.45
21:O:79:ILE:HD12	21:O:138:LEU:HD11	1.98	0.45
1:1:784:A:C8	23:Q:69:ARG:HD2	2.51	0.45
1:1:822:G:O6	1:1:903:U:C2	2.69	0.45
1:1:1362:G:H2'	1:1:1363:A:C8	2.52	0.45
1:1:3006:A:H2'	1:1:3007:U:O4'	2.16	0.45
1:1:3091:A:H2'	1:1:3094:A:N7	2.31	0.45
14:H:92:TYR:CZ	14:H:142:ASP:HA	2.52	0.45
22:P:29:THR:HA	22:P:32:THR:HG22	1.99	0.45
25:S:155:ARG:CZ	25:S:172:TYR:CD1	2.99	0.45
40:n:174:ARG:NH2	40:n:357:ALA:O	2.36	0.45
45:u:33:ARG:HH21	45:u:35:LYS:HD3	1.82	0.45
1:1:451:U:H2'	1:1:452:G:C8	2.52	0.45
1:1:1353:U:H1'	24:R:39:THR:HG21	1.98	0.45
1:1:2440:G:H2'	1:1:2441:A:H8	1.81	0.45
1:1:2595:A:H5''	1:1:2596:U:H5	1.81	0.45
28:W:12:LEU:O	43:r:68:HIS:NE2	2.50	0.45
28:W:128:ASN:HA	28:W:194:LYS:HG3	1.99	0.45
33:e:79:VAL:HG13	33:e:111:ARG:HG2	1.98	0.45
38:l:17:ALA:HA	38:l:21:GLY:H	1.82	0.45
43:r:184:VAL:HG21	43:r:223:VAL:HG21	1.97	0.45
1:1:901:G:H2'	1:1:902:G:C8	2.51	0.45
1:1:1404:G:N2	1:1:1407:A:OP2	2.36	0.45
1:1:2441:A:H2'	1:1:2442:G:C8	2.52	0.45
1:1:2470:C:H5''	31:a:26:ARG:HD2	1.99	0.45
2:2:149:A:H2'	2:2:150:G:C8	2.51	0.45
24:R:68:GLU:HG3	47:w:117:ARG:NH1	2.32	0.45
28:W:217:VAL:HB	28:W:233:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:270:LEU:O	32:b:274:ILE:HG13	2.16	0.45
38:l:95:TYR:HD1	38:l:125:ILE:HG12	1.81	0.45
1:1:2441:A:H2'	1:1:2442:G:H8	1.82	0.45
6:8:315:ASP:OD1	6:8:316:GLU:N	2.47	0.45
20:N:124:ASP:N	20:N:127:TYR:O	2.43	0.45
27:V:40:LYS:HD2	27:V:59:MET:HE2	1.98	0.45
41:o:93:ILE:HG23	41:o:164:VAL:HG13	1.98	0.45
1:1:1390:A:N6	1:1:1418:A:O2'	2.49	0.45
1:1:1891:A:H2'	1:1:1892:G:C8	2.52	0.45
1:1:2809:C:H2'	1:1:2810:C:C6	2.52	0.45
1:1:2819:A:H2'	1:1:2820:A:C8	2.52	0.45
1:1:3000:A:H2'	1:1:3001:C:H6	1.82	0.45
2:2:6:U:H2'	2:2:7:U:C6	2.52	0.45
3:3:444:HIS:NE2	3:3:631:GLU:HB2	2.32	0.45
3:3:594:VAL:HG12	3:3:661:ASN:HD21	1.81	0.45
3:3:689:PHE:HB3	3:3:699:MET:HG2	1.99	0.45
25:S:90:MET:HE1	25:S:114:HIS:NE2	2.31	0.45
41:o:101:GLY:HA3	44:t:62:VAL:HG13	1.99	0.45
1:1:239:G:H2'	1:1:240:U:C6	2.52	0.45
1:1:2498:U:H2'	1:1:2499:U:C6	2.52	0.45
10:D:276:ARG:HB3	10:D:364:PHE:CZ	2.52	0.45
32:b:184:LEU:O	32:b:188:THR:HG22	2.17	0.45
32:b:316:GLU:HB3	32:b:318:MET:HE2	1.99	0.45
35:h:66:VAL:HG12	35:h:80:LEU:HD11	1.99	0.45
37:j:75:LYS:HE2	37:j:75:LYS:HB3	1.80	0.45
42:q:453:LYS:HA	42:q:488:VAL:HG13	1.99	0.45
45:u:22:VAL:HG22	45:u:28:GLU:HG2	1.99	0.45
45:u:45:ASN:HB3	45:u:48:LYS:HG3	1.99	0.45
48:x:140:ILE:HD11	48:x:165:LEU:HB3	1.99	0.45
1:1:226:C:H2'	1:1:227:G:O4'	2.17	0.45
1:1:628:A:H2'	1:1:629:U:O4'	2.16	0.45
1:1:679:U:H2'	1:1:680:G:C8	2.52	0.45
3:3:693:ARG:HB2	3:3:696:ASP:OD1	2.18	0.45
11:E:10:TYR:H	24:R:86:TYR:HH	1.60	0.45
1:1:689:U:O4	9:C:209:TYR:OH	2.23	0.44
1:1:1151:U:H5'	1:1:1307:G:H21	1.82	0.44
1:1:2486:A:OP1	31:a:105:LYS:NZ	2.50	0.44
3:3:504:VAL:HG23	3:3:523:THR:HB	1.98	0.44
13:G:148:ALA:HA	13:G:201:THR:HG22	1.98	0.44
1:1:63:A:N3	1:1:78:U:O2'	2.46	0.44
1:1:665:A:H2'	1:1:666:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1405:U:OP2	33:e:59:SER:OG	2.29	0.44
1:1:2608:G:H2'	1:1:2609:A:H8	1.82	0.44
1:1:3072:C:H2'	1:1:3073:A:O4'	2.18	0.44
1:1:3296:A:H2'	1:1:3297:U:C6	2.52	0.44
27:V:16:GLY:N	27:V:52:ALA:O	2.51	0.44
32:b:75:HIS:CG	32:b:76:PRO:HD2	2.52	0.44
32:b:432:MET:HE3	45:u:81:TYR:HD1	1.81	0.44
41:o:94:TYR:CZ	41:o:96:SER:HB3	2.52	0.44
44:t:98:ASP:HB3	44:t:184:TYR:CZ	2.52	0.44
47:w:46:TRP:CE2	47:w:102:PHE:HB2	2.52	0.44
1:1:431:U:H2'	1:1:432:G:H8	1.83	0.44
1:1:789:A:H2'	1:1:790:U:H6	1.81	0.44
15:I:386:ILE:HB	15:I:396:VAL:HB	1.98	0.44
25:S:135:VAL:O	25:S:141:LYS:HE3	2.18	0.44
30:Z:30:VAL:HB	30:Z:86:THR:HG22	1.99	0.44
30:Z:177:ASN:O	30:Z:181:THR:OG1	2.29	0.44
39:m:347:SER:HB3	39:m:350:GLU:HG2	2.00	0.44
44:t:276:GLU:OE2	44:t:291:GLN:NE2	2.50	0.44
1:1:965:A:H2'	1:1:966:U:C6	2.53	0.44
1:1:3021:A:H2	1:1:3033:A:H62	1.65	0.44
3:3:469:HIS:CD2	3:3:473:ARG:HH21	2.35	0.44
7:A:116:ASN:HB2	7:A:220:VAL:HG23	1.98	0.44
15:I:142:THR:HB	15:I:158:ALA:HB3	1.99	0.44
15:I:280:THR:HG22	15:I:293:GLN:HG3	1.98	0.44
30:Z:139:PRO:HD3	30:Z:188:ARG:HH21	1.83	0.44
38:l:47:VAL:HG12	38:l:67:GLY:HA3	1.99	0.44
42:q:278:LEU:HG	42:q:365:ALA:HA	2.00	0.44
42:q:422:ALA:HB3	42:q:477:THR:HG22	1.98	0.44
1:1:120:G:C5	13:G:128:LYS:HB3	2.51	0.44
1:1:551:A:H2'	1:1:552:G:H8	1.81	0.44
1:1:800:G:H22	9:C:101:ALA:HA	1.82	0.44
1:1:1176:C:H2'	1:1:1177:G:N2	2.32	0.44
1:1:2420:C:H2'	1:1:2421:U:C6	2.53	0.44
1:1:2475:G:H2'	1:1:2476:C:C6	2.52	0.44
1:1:2962:U:H2'	1:1:2963:C:C6	2.53	0.44
1:1:3375:A:OP2	1:1:3378:C:N4	2.51	0.44
9:C:260:GLN:HE21	46:v:73:VAL:HG22	1.82	0.44
10:D:122:PRO:HD2	10:D:126:LEU:HD23	1.98	0.44
11:E:102:ASN:H	11:E:105:TYR:HB3	1.82	0.44
20:N:8:GLU:O	20:N:12:ARG:HG2	2.18	0.44
21:O:45:GLY:HA2	21:O:49:ARG:HH21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:364:VAL:HG22	40:n:386:ASN:HB3	2.00	0.44
46:v:156:THR:HB	46:v:159:VAL:HB	1.99	0.44
47:w:200:GLU:HG3	47:w:204:LYS:HE3	2.00	0.44
1:1:257:U:H2'	1:1:258:G:C8	2.52	0.44
1:1:626:U:O2'	1:1:1399:A:O2'	2.35	0.44
3:3:467:ASP:O	3:3:471:ARG:HG3	2.18	0.44
8:B:17:LEU:HD23	8:B:19:ARG:HG3	2.00	0.44
32:b:169:THR:HG23	32:b:217:GLN:HG3	2.00	0.44
43:r:207:PRO:O	43:r:210:THR:HG22	2.18	0.44
1:1:1420:C:C5	9:C:189:ALA:HB2	2.53	0.44
4:6:57:U:H3	41:o:173:ILE:HG22	1.82	0.44
32:b:436:LEU:HD22	45:u:90:LEU:HD22	2.00	0.44
40:n:133:ASP:OD1	40:n:134:ASP:N	2.50	0.44
41:o:97:ARG:HD2	41:o:163:GLN:HG2	2.00	0.44
45:u:50:LYS:HA	45:u:55:PHE:CD2	2.53	0.44
47:w:30:THR:HA	47:w:35:LYS:HE3	1.98	0.44
49:y:18:LYS:HB3	49:y:25:LEU:HB2	2.00	0.44
1:1:815:G:N3	1:1:816:A:H1'	2.33	0.44
1:1:1101:G:OP2	12:F:196:LYS:NZ	2.50	0.44
3:3:792:HIS:CE1	42:q:270:PRO:HD3	2.53	0.44
6:8:309:ASN:HA	6:8:312:GLU:HG2	2.00	0.44
32:b:21:VAL:HG21	32:b:57:PHE:CE1	2.53	0.44
32:b:29:THR:OG1	32:b:49:LYS:NZ	2.51	0.44
32:b:263:THR:HG22	32:b:265:GLU:H	1.83	0.44
39:m:398:PRO:HG3	40:n:43:PRO:HG2	1.99	0.44
48:x:61:GLU:OE2	48:x:235:GLN:NE2	2.51	0.44
1:1:947:G:H2'	1:1:948:C:C6	2.53	0.44
1:1:2461:A:N3	1:1:2461:A:H2'	2.33	0.44
6:8:269:ILE:HG12	6:8:275:ARG:HG2	2.00	0.44
30:Z:46:ASP:HB3	30:Z:333:PRO:HD3	2.00	0.44
1:1:184:U:H2'	1:1:185:C:H6	1.82	0.43
1:1:616:G:H2'	1:1:617:G:C8	2.53	0.43
1:1:2491:A:H2'	1:1:2492:C:C6	2.53	0.43
1:1:3070:A:H5''	1:1:3072:C:H41	1.82	0.43
4:6:19:U:H2'	4:6:20:U:C6	2.53	0.43
4:6:20:U:H2'	4:6:21:G:H8	1.83	0.43
20:N:14:LYS:HA	20:N:19:LEU:HD22	2.00	0.43
32:b:227:ARG:NH2	32:b:231:GLU:O	2.51	0.43
38:l:50:HIS:CE1	38:l:51:VAL:HG23	2.53	0.43
40:n:77:LEU:HD21	40:n:81:ARG:HH21	1.83	0.43
40:n:144:ASN:ND2	40:n:207:GLU:OE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:5:ASP:HB2	43:r:8:GLU:HB2	1.99	0.43
47:w:117:ARG:HB3	47:w:120:LYS:HE2	2.00	0.43
1:1:242:C:O2'	1:1:243:G:H8	2.01	0.43
1:1:718:G:O2'	1:1:719:U:H3'	2.17	0.43
1:1:1137:C:H2'	1:1:1138:U:C6	2.53	0.43
1:1:3026:G:O2'	43:r:2:PRO:HG2	2.18	0.43
8:B:313:HIS:O	8:B:333:LYS:HE3	2.18	0.43
15:I:17:LEU:O	15:I:33:PHE:N	2.51	0.43
31:a:70:ASP:HB2	31:a:72:PHE:CE1	2.53	0.43
32:b:250:VAL:HB	32:b:283:VAL:HG22	1.99	0.43
42:q:418:ILE:HD12	42:q:463:VAL:HG23	2.00	0.43
1:1:3238:G:H2'	1:1:3239:G:O4'	2.18	0.43
8:B:332:ARG:O	8:B:333:LYS:HB2	2.18	0.43
10:D:151:GLY:O	10:D:452:GLN:NE2	2.51	0.43
15:I:251:LEU:O	15:I:252:ARG:NH1	2.43	0.43
17:K:336:ILE:HD13	44:t:186:LEU:HD13	2.00	0.43
19:M:25:LYS:HE3	19:M:62:GLN:HG2	2.00	0.43
20:N:64:VAL:HG21	20:N:106:VAL:HG23	2.00	0.43
42:q:463:VAL:O	42:q:548:LYS:NZ	2.46	0.43
1:1:1191:U:H4'	1:1:1192:C:H5''	1.99	0.43
1:1:1259:A:N6	28:W:67:MET:SD	2.91	0.43
1:1:1890:U:H2'	1:1:1891:A:C8	2.54	0.43
1:1:2426:U:H3	1:1:2603:G:H22	1.65	0.43
8:B:92:TYR:HB2	8:B:157:VAL:HB	1.99	0.43
13:G:91:PHE:HD1	13:G:189:LEU:HD21	1.83	0.43
16:J:261:LEU:HD12	16:J:268:PHE:HD2	1.83	0.43
21:O:54:TYR:CD2	21:O:145:VAL:HG11	2.52	0.43
28:W:41:TRP:HB2	28:W:103:LEU:HB3	2.00	0.43
28:W:188:VAL:O	28:W:199:GLN:NE2	2.51	0.43
28:W:222:ASP:HB3	28:W:225:SER:HB3	2.01	0.43
39:m:284:ARG:HH22	46:v:180:ARG:HH22	1.66	0.43
44:t:99:PHE:O	44:t:184:TYR:OH	2.36	0.43
1:1:952:A:H2'	1:1:953:G:O4'	2.17	0.43
1:1:1108:U:H2'	1:1:1109:U:H6	1.84	0.43
2:2:40:A:H2'	2:2:41:A:H8	1.82	0.43
32:b:287:ILE:HD11	32:b:319:THR:HG22	1.99	0.43
38:l:100:LYS:O	38:l:104:GLU:HG3	2.18	0.43
47:w:170:PRO:O	47:w:174:VAL:HG13	2.19	0.43
1:1:148:G:O6	13:G:135:GLY:HA3	2.18	0.43
1:1:149:U:OP1	20:N:49:ARG:NH2	2.46	0.43
1:1:415:G:H2'	1:1:416:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1151:U:OP1	1:1:1307:G:N2	2.52	0.43
1:1:1281:G:C2	1:1:1282:G:C8	3.07	0.43
1:1:3343:G:H21	1:1:3361:G:H3'	1.84	0.43
2:2:107:G:H4'	2:2:138:A:H5'	1.99	0.43
3:3:470:ALA:O	3:3:473:ARG:HG2	2.19	0.43
8:B:218:ILE:HG13	8:B:276:THR:HG23	2.01	0.43
8:B:286:GLY:HA3	8:B:321:PHE:CZ	2.53	0.43
10:D:200:ARG:NH2	10:D:368:ASP:O	2.51	0.43
12:F:126:LEU:O	12:F:130:ILE:HG12	2.18	0.43
16:J:275:PHE:HB2	39:m:164:ALA:HB1	2.01	0.43
30:Z:110:GLN:O	30:Z:337:LEU:HA	2.19	0.43
40:n:351:LYS:HG2	40:n:352:TYR:H	1.83	0.43
42:q:352:MET:SD	42:q:420:LEU:HB2	2.59	0.43
1:1:3243:A:H4'	8:B:95:THR:HG22	2.00	0.43
2:2:58:G:O6	37:j:63:ARG:NH1	2.51	0.43
7:A:32:ARG:NH1	39:m:143:VAL:O	2.52	0.43
13:G:190:VAL:HG12	13:G:192:GLN:HG2	2.00	0.43
32:b:55:GLU:HA	32:b:58:VAL:HG22	1.99	0.43
42:q:352:MET:HE3	42:q:405:ALA:HB1	2.00	0.43
1:1:562:C:H2'	1:1:563:U:C6	2.54	0.43
1:1:1169:A:H2'	1:1:1170:A:C8	2.54	0.43
1:1:2434:U:H5''	1:1:2435:G:H8	1.83	0.43
6:8:267:ASN:O	6:8:269:ILE:HG13	2.19	0.43
10:D:282:SER:O	10:D:286:ARG:HG3	2.19	0.43
15:I:210:GLU:HB2	15:I:247:TRP:CE2	2.54	0.43
20:N:184:LYS:HE3	20:N:184:LYS:HB2	1.82	0.43
30:Z:50:ILE:HD11	30:Z:333:PRO:HD2	2.01	0.43
42:q:367:MET:O	42:q:370:THR:HG22	2.18	0.43
1:1:67:A:O2'	1:1:315:C:O2	2.36	0.43
1:1:2476:C:H2'	1:1:2477:G:H8	1.83	0.43
10:D:191:LYS:HA	10:D:191:LYS:HD3	1.86	0.43
15:I:132:LYS:HD3	15:I:136:LEU:HD21	2.00	0.43
15:I:141:VAL:N	15:I:158:ALA:O	2.43	0.43
31:a:74:VAL:HG21	31:a:86:SER:HB2	2.00	0.43
34:f:31:LYS:NZ	34:f:78:SER:O	2.51	0.43
35:h:44:ILE:HA	35:h:47:VAL:HG12	2.01	0.43
42:q:231:LEU:HD23	42:q:250:PHE:CZ	2.54	0.43
1:1:2388:U:H3	1:1:2991:A:H2	1.67	0.43
3:3:634:TYR:OH	3:3:638:ARG:NH1	2.52	0.43
11:E:24:ALA:HB3	11:E:26:ARG:HH21	1.84	0.43
22:P:94:LEU:HD23	22:P:94:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:170:HIS:CE1	39:m:179:ARG:HH21	2.37	0.43
39:m:394:LEU:O	39:m:399:ARG:NH2	2.38	0.43
40:n:37:ILE:HD11	40:n:217:ILE:HG23	1.99	0.43
40:n:355:PRO:O	40:n:359:LEU:HG	2.19	0.43
42:q:285:LEU:HD12	42:q:326:HIS:HB3	2.01	0.43
49:y:122:ASP:O	49:y:125:THR:OG1	2.35	0.43
1:1:155:G:H4'	1:1:156:G:H2'	2.00	0.42
2:2:37:A:OP2	35:h:86:ARG:HD2	2.19	0.42
3:3:517:VAL:HA	3:3:520:VAL:HG12	2.00	0.42
10:D:367:PRO:O	10:D:457:HIS:NE2	2.41	0.42
13:G:83:ASP:OD1	13:G:83:ASP:N	2.46	0.42
15:I:336:THR:HG23	15:I:367:ILE:HD13	2.01	0.42
16:J:344:ARG:NH2	43:r:260:LEU:O	2.52	0.42
17:K:81:ILE:HG23	17:K:243:THR:HG23	2.00	0.42
26:T:202:LEU:HD22	30:Z:268:VAL:HG13	2.01	0.42
28:W:221:TYR:HB2	28:W:228:VAL:HG12	2.00	0.42
40:n:178:LYS:HB2	40:n:189:GLN:HB3	2.01	0.42
41:o:92:ILE:HG12	41:o:138:GLU:HG3	2.01	0.42
42:q:390:ILE:HG23	42:q:395:CYS:HB2	2.00	0.42
1:1:1303:A:OP2	1:1:2826:U:N3	2.31	0.42
1:1:3234:A:N6	1:1:3253:G:H1	2.14	0.42
3:3:490:ASP:CG	3:3:519:ARG:HH21	2.27	0.42
8:B:56:ILE:HD11	8:B:323:MET:SD	2.60	0.42
16:J:235:ASP:HB2	16:J:238:ASP:HB2	2.01	0.42
22:P:108:ASP:HB3	22:P:111:LYS:HE2	2.01	0.42
29:Y:55:GLU:HB2	29:Y:108:LYS:HB3	2.01	0.42
31:a:67:ILE:HD11	31:a:77:ALA:CB	2.48	0.42
39:m:387:ARG:HH21	40:n:200:LEU:HD23	1.84	0.42
40:n:374:ASP:OD1	40:n:374:ASP:N	2.49	0.42
40:n:380:ILE:HG22	40:n:381:LEU:HD12	2.02	0.42
48:x:136:SER:O	48:x:140:ILE:HG12	2.19	0.42
49:y:206:THR:OG1	49:y:207:GLY:N	2.52	0.42
1:1:342:A:OP2	2:2:21:C:N4	2.52	0.42
1:1:362:U:O4	37:j:24:ARG:NH2	2.52	0.42
1:1:412:G:H2'	1:1:413:U:C6	2.54	0.42
1:1:506:U:H2'	1:1:507:U:O4'	2.19	0.42
1:1:591:G:H1'	11:E:19:LYS:HG3	2.01	0.42
1:1:3160:U:H2'	1:1:3161:C:C6	2.54	0.42
9:C:2:SER:OG	9:C:3:ARG:N	2.52	0.42
18:L:44:ALA:HA	46:v:30:ILE:HD13	2.00	0.42
28:W:45:LEU:HB3	28:W:48:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:34:LEU:HG	31:a:36:VAL:HG13	2.01	0.42
32:b:74:VAL:CG1	32:b:75:HIS:H	2.31	0.42
42:q:235:ILE:HD13	42:q:262:PHE:HE2	1.84	0.42
42:q:430:ILE:HD13	42:q:437:LYS:HB3	2.01	0.42
43:r:259:LEU:HB3	43:r:261:VAL:HG13	2.00	0.42
1:1:289:A:H5'	20:N:97:SER:HB3	2.01	0.42
1:1:1123:U:H2'	1:1:1124:U:C6	2.55	0.42
12:F:236:ILE:HD12	12:F:236:ILE:HA	1.88	0.42
15:I:309:PHE:CD1	15:I:334:ILE:HG13	2.54	0.42
29:Y:39:LEU:HD22	29:Y:43:TYR:HE2	1.85	0.42
30:Z:34:SER:HA	30:Z:40:LEU:HD12	2.01	0.42
31:a:175:GLU:OE1	31:a:175:GLU:N	2.53	0.42
32:b:25:THR:HG21	32:b:53:THR:HA	2.01	0.42
32:b:419:LYS:NZ	49:y:35:TYR:OH	2.46	0.42
42:q:204:MET:HG2	42:q:234:ASP:HB3	2.01	0.42
45:u:10:SER:HB2	45:u:53:LYS:HB2	2.02	0.42
1:1:973:A:H2'	1:1:974:G:C8	2.55	0.42
2:2:26:U:O2'	9:C:51:ALA:O	2.37	0.42
18:L:93:ILE:HD12	18:L:93:ILE:HA	1.85	0.42
28:W:50:THR:N	28:W:51:PRO:HD2	2.35	0.42
42:q:310:PHE:C	43:r:123:PRO:HG3	2.43	0.42
42:q:473:ILE:HB	42:q:546:PHE:HB2	2.00	0.42
1:1:786:A:H4'	1:1:787:G:H5'	2.01	0.42
7:A:88:PHE:HB3	7:A:100:TRP:HB2	2.01	0.42
17:K:221:THR:O	17:K:225:ASN:ND2	2.34	0.42
32:b:57:PHE:CE1	32:b:140:VAL:HG21	2.54	0.42
32:b:80:ASP:HB3	32:b:241:TYR:CD2	2.54	0.42
42:q:274:ARG:HB2	42:q:335:PHE:CZ	2.55	0.42
44:t:132:LYS:HE3	44:t:308:PRO:HG3	2.01	0.42
46:v:197:LYS:HE3	46:v:197:LYS:HB2	1.82	0.42
1:1:123:A:OP1	13:G:105:LYS:NZ	2.49	0.42
1:1:2989:U:H2'	1:1:2990:G:H8	1.84	0.42
14:H:124:ARG:HD3	14:H:164:ILE:HG13	2.02	0.42
15:I:59:ILE:HG22	15:I:143:LEU:HD21	2.02	0.42
18:L:103:ASN:O	36:i:22:PRO:HB3	2.20	0.42
29:Y:83:ASP:OD1	29:Y:83:ASP:N	2.52	0.42
38:l:168:ASP:N	38:l:168:ASP:OD1	2.52	0.42
1:1:1286:A:H8	1:1:1287:A:H1'	1.83	0.42
1:1:3073:A:H2'	1:1:3074:G:C8	2.54	0.42
3:3:789:PHE:CZ	42:q:537:ASN:HB2	2.54	0.42
8:B:19:ARG:HB3	8:B:273:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:132:ALA:HB2	9:C:148:ILE:HG21	2.01	0.42
10:D:175:LEU:HD23	10:D:213:ILE:HD13	2.01	0.42
11:E:52:VAL:CG1	11:E:65:ILE:HB	2.50	0.42
14:H:90:MET:HE1	14:H:161:LEU:HB3	2.02	0.42
14:H:91:ARG:NH2	28:W:174:LYS:HG2	2.35	0.42
32:b:98:ILE:HG12	32:b:143:LEU:HD21	2.02	0.42
38:l:2:ARG:NE	38:l:39:LEU:HD23	2.34	0.42
1:1:645:A:H8	1:1:2373:A:C6	2.38	0.42
1:1:1139:G:H2'	1:1:1140:G:H8	1.85	0.42
1:1:3192:U:H2'	1:1:3193:C:C6	2.55	0.42
7:A:170:LYS:HD3	39:m:156:THR:HB	2.01	0.42
10:D:274:ASP:OD1	10:D:274:ASP:N	2.49	0.42
14:H:92:TYR:HB3	14:H:179:ILE:HG12	2.02	0.42
15:I:23:ASP:OD1	15:I:25:SER:OG	2.35	0.42
16:J:251:LEU:HA	16:J:254:VAL:HG12	2.02	0.42
23:Q:8:LYS:HE3	23:Q:8:LYS:HB3	1.92	0.42
25:S:112:ALA:O	25:S:115:ARG:NH1	2.53	0.42
46:v:208:TYR:O	46:v:210:GLN:N	2.53	0.42
1:1:85:A:N1	1:1:99:A:H5''	2.35	0.42
1:1:966:U:H2'	1:1:967:A:H8	1.84	0.42
1:1:3013:U:H2'	1:1:3014:U:C6	2.55	0.42
1:1:3225:C:H2'	1:1:3226:A:H8	1.85	0.42
1:1:3297:U:H2'	1:1:3298:C:H6	1.85	0.42
3:3:676:LEU:O	3:3:680:GLN:HG2	2.19	0.42
6:8:393:ASN:ND2	6:8:402:GLU:O	2.53	0.42
12:F:176:TYR:CZ	12:F:197:GLN:HG2	2.55	0.42
24:R:181:ASN:ND2	48:x:246:TYR:OH	2.44	0.42
28:W:21:GLU:OE1	28:W:21:GLU:N	2.50	0.42
32:b:94:SER:HB3	32:b:146:PRO:HB3	2.01	0.42
32:b:160:LEU:HD23	32:b:160:LEU:HA	1.94	0.42
32:b:254:MET:HB2	32:b:287:ILE:HG22	2.02	0.42
42:q:297:GLN:HB3	42:q:310:PHE:HE2	1.84	0.42
43:r:186:HIS:HE1	43:r:188:GLU:HB3	1.84	0.42
1:1:349:A:C4	2:2:24:G:H1'	2.55	0.41
1:1:752:C:H2'	1:1:753:C:C6	2.54	0.41
1:1:2413:A:H2'	1:1:2414:G:H8	1.85	0.41
3:3:682:ARG:HD2	32:b:232:MET:O	2.19	0.41
7:A:62:GLU:OE1	36:i:74:LYS:NZ	2.50	0.41
7:A:180:SER:OG	16:J:249:GLN:OE1	2.25	0.41
16:J:307:ARG:HA	16:J:307:ARG:HD2	1.76	0.41
20:N:49:ARG:NH1	20:N:49:ARG:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:303:ILE:O	39:m:307:GLN:NE2	2.53	0.41
39:m:346:LEU:HD22	39:m:368:PRO:HD2	2.01	0.41
42:q:426:GLY:H	42:q:479:SER:HB2	1.85	0.41
43:r:224:ASN:ND2	43:r:226:SER:OG	2.47	0.41
47:w:58:ARG:HB3	47:w:59:PRO:HD2	2.02	0.41
1:1:351:A:N1	48:x:14:LYS:HD3	2.35	0.41
1:1:535:G:N2	1:1:536:U:O4	2.27	0.41
1:1:2507:C:H2'	1:1:2508:U:C5	2.55	0.41
1:1:3298:C:C2	1:1:3299:A:C8	3.08	0.41
1:1:3391:A:H2'	1:1:3392:U:C6	2.55	0.41
2:2:26:U:H2'	2:2:27:U:C6	2.55	0.41
3:3:688:VAL:HG21	32:b:156:HIS:NE2	2.35	0.41
6:8:397:LYS:HG2	6:8:398:ARG:H	1.84	0.41
7:A:176:VAL:HG21	16:J:254:VAL:HB	2.02	0.41
8:B:59:ASP:OD1	8:B:59:ASP:N	2.51	0.41
30:Z:52:GLN:O	30:Z:188:ARG:NH2	2.52	0.41
32:b:177:ASN:HB3	32:b:260:CYS:SG	2.61	0.41
32:b:290:THR:HG21	32:b:319:THR:HB	2.02	0.41
1:1:417:A:H2'	1:1:418:A:C8	2.54	0.41
1:1:485:A:H5''	24:R:127:LEU:HD11	2.02	0.41
1:1:674:G:O6	23:Q:56:LYS:NZ	2.53	0.41
1:1:705:A:OP1	1:1:705:A:H8	2.03	0.41
1:1:1458:U:H2'	1:1:1459:C:C6	2.55	0.41
1:1:1883:A:H2'	1:1:1884:A:O4'	2.20	0.41
2:2:95:G:O2'	37:j:81:GLY:O	2.28	0.41
12:F:214:TRP:CD2	12:F:219:LYS:HD3	2.55	0.41
20:N:23:GLN:HG3	20:N:122:ASN:OD1	2.21	0.41
25:S:155:ARG:NH1	25:S:172:TYR:CE1	2.88	0.41
32:b:154:ARG:HA	32:b:157:ILE:HG22	2.01	0.41
34:f:14:LEU:HD11	34:f:31:LYS:HB2	2.02	0.41
41:o:197:LYS:HA	41:o:200:MET:HG2	2.01	0.41
41:o:197:LYS:HG2	41:o:200:MET:HE2	2.02	0.41
42:q:453:LYS:HG2	42:q:488:VAL:HA	2.02	0.41
46:v:207:ILE:HG13	46:v:208:TYR:H	1.86	0.41
1:1:31:C:H5	20:N:188:ARG:HH12	1.68	0.41
1:1:1202:A:C5'	1:1:1203:A:H5''	2.50	0.41
1:1:3073:A:H2'	1:1:3074:G:H8	1.83	0.41
1:1:3091:A:O2'	1:1:3093:C:H2'	2.21	0.41
1:1:3176:G:OP2	34:f:6:ARG:HB2	2.20	0.41
1:1:3334:U:H4'	1:1:3335:A:H5'	2.01	0.41
1:1:3387:U:H2'	1:1:3388:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:332:MET:HE1	30:Z:163:LYS:HD3	2.01	0.41
13:G:186:LEU:HD23	13:G:186:LEU:HA	1.93	0.41
15:I:172:ASP:OD1	15:I:172:ASP:N	2.54	0.41
19:M:112:LEU:HD22	19:M:116:GLU:HB3	2.03	0.41
26:T:202:LEU:O	26:T:205:GLN:HG2	2.21	0.41
31:a:149:THR:HA	31:a:152:ARG:HG2	2.01	0.41
38:l:152:GLU:O	38:l:156:MET:HG3	2.20	0.41
45:u:57:LYS:HE3	45:u:64:ALA:HA	2.02	0.41
47:w:199:GLU:H	47:w:199:GLU:CD	2.28	0.41
48:x:104:LYS:HB2	48:x:152:GLU:OE2	2.20	0.41
1:1:419:G:H2'	1:1:420:G:C8	2.56	0.41
1:1:1293:U:H2'	1:1:1294:A:H8	1.84	0.41
1:1:2606:G:O5'	38:l:60:ARG:NH1	2.48	0.41
1:1:3094:A:H2'	1:1:3095:U:C6	2.55	0.41
6:8:329:GLN:O	6:8:333:LEU:HG	2.21	0.41
12:F:86:VAL:O	12:F:114:GLY:HA2	2.19	0.41
25:S:138:GLN:HA	25:S:141:LYS:HB2	2.02	0.41
27:V:131:SER:HA	49:y:61:ARG:HD3	2.02	0.41
30:Z:162:GLU:OE2	30:Z:194:LYS:NZ	2.53	0.41
38:l:108:LEU:HD22	38:l:169:ILE:HG12	2.02	0.41
40:n:365:PHE:CD2	40:n:409:HIS:HB2	2.56	0.41
42:q:205:ILE:HG22	42:q:209:LYS:HE3	2.03	0.41
49:y:11:ASN:HB3	49:y:207:GLY:HA3	2.01	0.41
1:1:450:G:H2'	1:1:451:U:C6	2.56	0.41
1:1:956:U:H2'	1:1:957:C:O4'	2.20	0.41
1:1:1199:C:H2'	1:1:1200:A:C8	2.53	0.41
2:2:91:C:H2'	2:2:92:A:C8	2.55	0.41
7:A:43:TYR:N	7:A:46:ARG:HH21	2.19	0.41
7:A:130:LEU:HD11	16:J:270:ARG:HD2	2.03	0.41
9:C:300:ARG:O	23:Q:39:ARG:NH2	2.40	0.41
10:D:43:LYS:HG2	10:D:64:THR:HG22	2.03	0.41
42:q:522:HIS:CG	42:q:523:PRO:HD2	2.55	0.41
43:r:186:HIS:CE1	43:r:188:GLU:HB3	2.55	0.41
47:w:29:LEU:HD23	47:w:29:LEU:HA	1.94	0.41
1:1:704:U:C3'	1:1:705:A:H5''	2.51	0.41
1:1:3055:U:N3	1:1:3086:A:N7	2.69	0.41
13:G:108:ARG:NH2	39:m:272:GLU:OE2	2.54	0.41
14:H:24:ILE:HD11	14:H:39:LYS:HE3	2.01	0.41
30:Z:52:GLN:NE2	30:Z:57:ILE:HD13	2.35	0.41
31:a:55:LEU:HB2	31:a:153:SER:HB3	2.02	0.41
35:h:35:LYS:HA	35:h:41:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:241:GLY:O	40:n:267:ARG:N	2.54	0.41
42:q:269:ARG:HH22	42:q:533:PRO:HB3	1.86	0.41
44:t:99:PHE:HB3	44:t:308:PRO:HB3	2.02	0.41
45:u:76:ASN:HB3	49:y:96:ARG:HB3	2.02	0.41
45:u:82:ASN:HB3	45:u:85:LEU:HB3	2.02	0.41
1:1:417:A:H2'	1:1:418:A:H8	1.85	0.41
1:1:429:U:H2'	1:1:430:U:H6	1.86	0.41
1:1:516:A:H5''	9:C:344:ALA:HB2	2.03	0.41
1:1:1105:A:H2'	1:1:1106:G:C8	2.55	0.41
1:1:1105:A:H2'	1:1:1106:G:H8	1.86	0.41
1:1:1240:A:O2'	1:1:1241:U:OP1	2.32	0.41
1:1:1373:A:H2'	1:1:1374:G:C8	2.56	0.41
1:1:3322:A:H2'	1:1:3323:A:C8	2.56	0.41
3:3:679:LEU:O	3:3:682:ARG:HG3	2.21	0.41
13:G:160:ILE:O	13:G:164:VAL:HG13	2.21	0.41
14:H:114:VAL:HG11	14:H:165:CYS:SG	2.61	0.41
15:I:3:LEU:HD21	15:I:386:ILE:HD11	2.02	0.41
17:K:252:GLU:OE1	17:K:252:GLU:N	2.53	0.41
17:K:296:ASP:OD1	17:K:296:ASP:N	2.54	0.41
33:e:32:TRP:CZ2	33:e:53:PRO:HD2	2.56	0.41
41:o:113:GLN:HE22	44:t:56:VAL:H	1.68	0.41
47:w:144:LYS:HE3	47:w:144:LYS:HB3	1.84	0.41
1:1:334:A:O2'	46:v:22:LYS:HE2	2.20	0.41
1:1:360:G:H2'	1:1:361:A:C8	2.55	0.41
1:1:720:A:OP1	1:1:784:A:N6	2.51	0.41
1:1:810:A:H2'	1:1:811:U:C6	2.56	0.41
1:1:1184:A:H2'	1:1:1185:C:C6	2.56	0.41
1:1:1317:A:O2'	1:1:1318:A:H3'	2.21	0.41
1:1:2970:C:O2'	1:1:2972:G:N7	2.32	0.41
1:1:3343:G:H2'	1:1:3361:G:N3	2.36	0.41
1:1:3368:U:OP2	8:B:384:LYS:HD3	2.20	0.41
2:2:39:G:H1'	2:2:104:A:N6	2.36	0.41
8:B:85:VAL:HG22	8:B:202:THR:HG22	2.03	0.41
17:K:250:ASN:HB3	17:K:253:TRP:CD1	2.56	0.41
17:K:282:LYS:HB3	17:K:288:VAL:HG12	2.03	0.41
19:M:113:THR:O	19:M:117:ARG:HG3	2.21	0.41
26:T:207:LYS:HB3	26:T:236:LYS:NZ	2.36	0.41
28:W:171:ILE:HD11	28:W:202:ILE:HD13	2.03	0.41
30:Z:341:LYS:HB3	30:Z:354:HIS:CD2	2.55	0.41
32:b:17:LEU:O	32:b:21:VAL:HG22	2.21	0.41
32:b:105:VAL:HA	32:b:108:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:184:LEU:HD22	32:b:220:ASP:HB3	2.01	0.41
32:b:399:ALA:HA	32:b:402:ILE:HG12	2.02	0.41
45:u:78:PRO:HG3	49:y:81:LEU:HG	2.02	0.41
1:1:174:C:H2'	1:1:175:C:C6	2.56	0.41
1:1:363:G:OP2	37:j:56:ARG:NH2	2.40	0.41
1:1:2412:G:C2	1:1:2810:C:N3	2.89	0.41
1:1:2486:A:H1'	1:1:2487:U:C6	2.56	0.41
10:D:150:GLY:HA2	10:D:174:ARG:NH1	2.36	0.41
10:D:197:GLU:HB3	10:D:200:ARG:HB3	2.03	0.41
10:D:199:ASP:OD1	10:D:199:ASP:N	2.54	0.41
10:D:200:ARG:NH1	10:D:369:ASP:OD1	2.54	0.41
11:E:172:HIS:CD2	11:E:173:MET:HG2	2.56	0.41
13:G:76:ALA:O	13:G:79:GLN:HG2	2.21	0.41
38:l:52:ALA:O	38:l:56:THR:HG23	2.21	0.41
38:l:153:SER:HB3	38:l:162:VAL:HG22	2.03	0.41
41:o:96:SER:OG	41:o:163:GLN:HB2	2.21	0.41
42:q:352:MET:HE2	42:q:420:LEU:HD13	2.03	0.41
42:q:477:THR:OG1	42:q:542:PHE:HB3	2.21	0.41
48:x:242:ARG:NH1	48:x:262:GLN:HB2	2.35	0.41
1:1:644:G:C2'	1:1:645:A:H5'	2.51	0.40
1:1:1146:C:H4'	1:1:1331:U:C4	2.56	0.40
1:1:2481:G:H2'	1:1:2482:U:H6	1.85	0.40
1:1:3191:G:H2'	1:1:3192:U:C6	2.56	0.40
1:1:3251:U:H2'	1:1:3252:G:C8	2.56	0.40
10:D:431:LYS:HE3	10:D:431:LYS:HB2	1.81	0.40
24:R:54:LYS:HB2	24:R:63:TYR:CE1	2.56	0.40
32:b:265:GLU:HG2	32:b:269:LYS:HE3	2.02	0.40
38:l:15:LYS:HG2	38:l:79:PHE:HD2	1.86	0.40
39:m:384:ILE:HG21	40:n:145:LEU:HD21	2.02	0.40
42:q:384:LYS:HD3	42:q:384:LYS:HA	1.90	0.40
49:y:107:VAL:HG23	49:y:108:ILE:HG12	2.03	0.40
1:1:168:U:H5''	46:v:172:ARG:NH1	2.36	0.40
1:1:778:U:H2'	1:1:779:G:O4'	2.21	0.40
1:1:1121:U:H2'	1:1:1122:U:C6	2.55	0.40
1:1:1276:U:H2'	1:1:1277:C:C6	2.56	0.40
1:1:2607:G:C2	1:1:2608:G:C8	3.09	0.40
1:1:3048:A:C8	1:1:3091:A:N6	2.89	0.40
9:C:308:LYS:HE2	9:C:308:LYS:HB3	1.93	0.40
9:C:328:ASN:OD1	12:F:48:ASN:ND2	2.55	0.40
10:D:214:ILE:HG21	10:D:241:ILE:HG22	2.03	0.40
17:K:209:ILE:HB	17:K:225:ASN:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:155:ARG:CD	25:S:172:TYR:CD1	3.03	0.40
27:V:26:ALA:HB1	27:V:114:ILE:HG23	2.03	0.40
30:Z:192:ILE:HG12	30:Z:203:MET:HG2	2.02	0.40
38:l:20:ILE:O	38:l:94:LYS:HB2	2.21	0.40
47:w:200:GLU:HA	47:w:203:ARG:HG2	2.04	0.40
1:1:66:A:N6	1:1:76:G:H1'	2.36	0.40
1:1:261:U:H2'	1:1:262:U:C6	2.56	0.40
1:1:1364:C:H2'	1:1:1365:G:C8	2.56	0.40
1:1:1870:C:H2'	1:1:1871:U:C6	2.56	0.40
1:1:2998:U:OP1	1:1:3143:C:N4	2.54	0.40
6:8:307:LYS:O	6:8:311:MET:HG3	2.21	0.40
15:I:69:LEU:HB3	15:I:112:SER:HB3	2.04	0.40
28:W:40:VAL:O	28:W:220:TYR:HA	2.21	0.40
35:h:23:ASP:O	35:h:26:LYS:HG2	2.21	0.40
42:q:261:PHE:CE1	42:q:533:PRO:HG2	2.56	0.40
42:q:268:ALA:HB3	43:r:120:VAL:HG22	2.03	0.40
42:q:333:SER:HB2	42:q:541:PHE:HB2	2.03	0.40
43:r:27:ARG:HG2	43:r:30:ARG:NH2	2.36	0.40
46:v:198:LYS:HE3	46:v:198:LYS:HB2	1.87	0.40
47:w:157:LEU:HA	47:w:157:LEU:HD12	1.85	0.40
47:w:157:LEU:HB3	47:w:158:PRO:HD3	2.04	0.40
1:1:1139:G:H2'	1:1:1140:G:C8	2.57	0.40
1:1:1290:A:H2'	1:1:1291:A:H8	1.86	0.40
1:1:1455:U:H4'	1:1:1455:U:OP1	2.21	0.40
1:1:2856:G:H21	43:r:192:THR:HG21	1.86	0.40
1:1:3340:G:H1	1:1:3364:C:N4	2.13	0.40
28:W:12:LEU:HD21	43:r:65:ILE:HD13	2.03	0.40
32:b:237:MET:HA	32:b:237:MET:HE2	2.02	0.40
39:m:160:ILE:H	39:m:160:ILE:HG13	1.59	0.40
40:n:39:LYS:NZ	40:n:120:GLU:OE1	2.54	0.40
43:r:249:PRO:HB3	43:r:255:VAL:HG22	2.03	0.40
49:y:6:GLN:HG3	49:y:208:LEU:HB2	2.03	0.40
1:1:407:A:C2	2:2:17:A:H1'	2.57	0.40
1:1:632:G:H2'	1:1:633:C:C6	2.55	0.40
3:3:686:GLU:HG3	3:3:691:PHE:HD2	1.86	0.40
15:I:133:ARG:HD2	48:x:274:ILE:O	2.22	0.40
31:a:158:GLN:HG2	31:a:160:LYS:HE2	2.04	0.40
38:l:38:ARG:HE	38:l:52:ALA:HB1	1.86	0.40
42:q:336:LEU:HD13	42:q:531:TYR:CE1	2.56	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	
3	3	347/995 (35%)	338 (97%)	9 (3%)	0	100	100
5	7	9/204 (4%)	9 (100%)	0	0	100	100
6	8	139/434 (32%)	135 (97%)	4 (3%)	0	100	100
7	A	251/291 (86%)	244 (97%)	7 (3%)	0	100	100
8	B	327/387 (84%)	319 (98%)	8 (2%)	0	100	100
9	C	341/362 (94%)	334 (98%)	7 (2%)	0	100	100
10	D	417/505 (83%)	408 (98%)	9 (2%)	0	100	100
11	E	147/176 (84%)	144 (98%)	3 (2%)	0	100	100
12	F	239/244 (98%)	236 (99%)	3 (1%)	0	100	100
13	G	162/256 (63%)	156 (96%)	6 (4%)	0	100	100
14	H	188/191 (98%)	183 (97%)	5 (3%)	0	100	100
15	I	390/463 (84%)	382 (98%)	8 (2%)	0	100	100
16	J	149/427 (35%)	147 (99%)	2 (1%)	0	100	100
17	K	259/376 (69%)	255 (98%)	4 (2%)	0	100	100
18	L	108/199 (54%)	107 (99%)	1 (1%)	0	100	100
19	M	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
20	N	173/204 (85%)	171 (99%)	2 (1%)	0	100	100
21	O	170/199 (85%)	169 (99%)	1 (1%)	0	100	100
22	P	133/184 (72%)	126 (95%)	7 (5%)	0	100	100
23	Q	142/186 (76%)	141 (99%)	1 (1%)	0	100	100
24	R	188/306 (61%)	186 (99%)	2 (1%)	0	100	100
25	S	168/172 (98%)	164 (98%)	4 (2%)	0	100	100
26	T	77/250 (31%)	77 (100%)	0	0	100	100
27	V	120/137 (88%)	120 (100%)	0	0	100	100
28	W	230/236 (98%)	226 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Y	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
30	Z	247/453 (54%)	245 (99%)	2 (1%)	0	100	100
31	a	208/217 (96%)	198 (95%)	10 (5%)	0	100	100
32	b	417/647 (64%)	406 (97%)	11 (3%)	0	100	100
33	e	123/130 (95%)	123 (100%)	0	0	100	100
34	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
35	h	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
36	i	82/100 (82%)	78 (95%)	4 (5%)	0	100	100
37	j	70/88 (80%)	67 (96%)	3 (4%)	0	100	100
38	l	174/181 (96%)	171 (98%)	3 (2%)	0	100	100
39	m	205/807 (25%)	196 (96%)	9 (4%)	0	100	100
40	n	329/605 (54%)	321 (98%)	8 (2%)	0	100	100
41	o	131/220 (60%)	131 (100%)	0	0	100	100
42	q	356/618 (58%)	347 (98%)	9 (2%)	0	100	100
43	r	190/261 (73%)	184 (97%)	6 (3%)	0	100	100
44	t	245/322 (76%)	241 (98%)	4 (2%)	0	100	100
45	u	110/199 (55%)	110 (100%)	0	0	100	100
46	v	145/231 (63%)	143 (99%)	2 (1%)	0	100	100
47	w	239/278 (86%)	233 (98%)	6 (2%)	0	100	100
48	x	275/295 (93%)	264 (96%)	11 (4%)	0	100	100
49	y	223/245 (91%)	216 (97%)	7 (3%)	0	100	100
All	All	9119/13773 (66%)	8919 (98%)	200 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	316/870 (36%)	316 (100%)	0	100	100
5	7	11/181 (6%)	11 (100%)	0	100	100
6	8	128/388 (33%)	128 (100%)	0	100	100
7	A	232/263 (88%)	232 (100%)	0	100	100
8	B	278/323 (86%)	277 (100%)	1 (0%)	84	93
9	C	273/289 (94%)	273 (100%)	0	100	100
10	D	371/440 (84%)	371 (100%)	0	100	100
11	E	131/153 (86%)	129 (98%)	2 (2%)	57	81
12	F	204/205 (100%)	204 (100%)	0	100	100
13	G	133/208 (64%)	133 (100%)	0	100	100
14	H	170/171 (99%)	170 (100%)	0	100	100
15	I	352/410 (86%)	352 (100%)	0	100	100
16	J	139/383 (36%)	139 (100%)	0	100	100
17	K	245/346 (71%)	245 (100%)	0	100	100
18	L	89/159 (56%)	89 (100%)	0	100	100
19	M	106/109 (97%)	106 (100%)	0	100	100
20	N	153/176 (87%)	153 (100%)	0	100	100
21	O	144/162 (89%)	144 (100%)	0	100	100
22	P	109/146 (75%)	109 (100%)	0	100	100
23	Q	118/151 (78%)	118 (100%)	0	100	100
24	R	171/274 (62%)	171 (100%)	0	100	100
25	S	155/156 (99%)	155 (100%)	0	100	100
26	T	69/219 (32%)	69 (100%)	0	100	100
27	V	94/105 (90%)	94 (100%)	0	100	100
28	W	209/213 (98%)	209 (100%)	0	100	100
29	Y	108/110 (98%)	108 (100%)	0	100	100
30	Z	234/413 (57%)	233 (100%)	1 (0%)	84	93
31	a	191/198 (96%)	190 (100%)	1 (0%)	81	92
32	b	380/573 (66%)	378 (100%)	2 (0%)	81	92
33	e	108/111 (97%)	108 (100%)	0	100	100
34	f	90/91 (99%)	90 (100%)	0	100	100
35	h	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	i	70/82 (85%)	70 (100%)	0	100	100
37	j	59/71 (83%)	59 (100%)	0	100	100
38	l	151/156 (97%)	150 (99%)	1 (1%)	76	90
39	m	193/723 (27%)	192 (100%)	1 (0%)	81	92
40	n	305/548 (56%)	302 (99%)	3 (1%)	68	86
41	o	118/199 (59%)	116 (98%)	2 (2%)	53	79
42	q	304/535 (57%)	301 (99%)	3 (1%)	68	86
43	r	178/229 (78%)	176 (99%)	2 (1%)	65	85
44	t	220/287 (77%)	220 (100%)	0	100	100
45	u	98/180 (54%)	97 (99%)	1 (1%)	68	86
46	v	134/205 (65%)	133 (99%)	1 (1%)	76	90
47	w	225/257 (88%)	225 (100%)	0	100	100
48	x	263/276 (95%)	260 (99%)	3 (1%)	65	85
49	y	193/211 (92%)	193 (100%)	0	100	100
All	All	8126/12060 (67%)	8102 (100%)	24 (0%)	84	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	B	332	ARG
11	E	26	ARG
11	E	65	ILE
30	Z	37	ASN
31	a	163	LEU
32	b	98	ILE
32	b	175	TYR
38	l	24	ILE
39	m	160	ILE
40	n	263	ILE
40	n	363	PHE
40	n	371	VAL
41	o	102	PHE
41	o	185	VAL
42	q	274	ARG
42	q	319	THR
42	q	486	GLU
43	r	210	THR

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Mol	Chain	Res	Type
43	r	223	VAL
45	u	109	LYS
46	v	21	ASN
48	x	65	VAL
48	x	213	LEU
48	x	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	351	ASN
3	3	469	HIS
3	3	503	ASN
3	3	506	ASN
3	3	680	GLN
3	3	792	HIS
7	A	159	ASN
7	A	246	ASN
8	B	163	HIS
8	B	182	GLN
9	C	18	ASN
9	C	48	GLN
9	C	196	ASN
9	C	213	ASN
9	C	260	GLN
10	D	105	HIS
10	D	288	GLN
10	D	310	ASN
10	D	452	GLN
11	E	61	ASN
12	F	81	HIS
12	F	244	ASN
13	G	232	HIS
14	H	96	HIS
14	H	169	ASN
15	I	269	GLN
15	I	286	HIS
15	I	293	GLN
16	J	215	HIS
16	J	221	GLN
17	K	262	ASN
17	K	295	GLN

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Mol	Chain	Res	Type
18	L	99	HIS
18	L	129	ASN
19	M	41	GLN
20	N	139	HIS
21	O	55	HIS
22	P	45	GLN
22	P	50	GLN
23	Q	9	GLN
25	S	74	ASN
28	W	199	GLN
29	Y	110	HIS
31	a	21	ASN
32	b	70	ASN
32	b	90	HIS
32	b	233	ASN
32	b	327	ASN
32	b	429	ASN
33	e	13	HIS
33	e	20	HIS
33	e	49	ASN
33	e	104	ASN
34	f	88	ASN
35	h	59	ASN
35	h	99	GLN
39	m	170	HIS
39	m	307	GLN
39	m	365	ASN
40	n	150	GLN
40	n	386	ASN
40	n	410	GLN
40	n	428	GLN
41	o	103	HIS
41	o	160	HIS
42	q	537	ASN
43	r	179	GLN
44	t	233	ASN
44	t	242	HIS
46	v	21	ASN
46	v	25	GLN
46	v	33	ASN
46	v	210	GLN
48	x	208	GLN

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Mol	Chain	Res	Type
48	x	244	HIS
49	y	156	ASN
49	y	170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1950/3396 (57%)	392 (20%)	6 (0%)
2	2	147/158 (93%)	27 (18%)	0
4	6	54/232 (23%)	18 (33%)	0
All	All	2151/3786 (56%)	437 (20%)	6 (0%)

All (437) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	18	G
1	1	26	A
1	1	48	A
1	1	49	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	74	G
1	1	77	A
1	1	105	C
1	1	109	A
1	1	110	G
1	1	111	C
1	1	117	U
1	1	122	A
1	1	135	C
1	1	136	G
1	1	146	U
1	1	155	G
1	1	165	A
1	1	166	C
1	1	187	A
1	1	189	G
1	1	190	U
1	1	191	U

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Mol	Chain	Res	Type
1	1	192	C
1	1	200	C
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	221	A
1	1	243	G
1	1	251	G
1	1	252	U
1	1	265	A
1	1	268	A
1	1	269	G
1	1	295	A
1	1	298	U
1	1	307	A
1	1	308	A
1	1	310	U
1	1	311	C
1	1	312	C
1	1	323	A
1	1	329	U
1	1	338	A
1	1	352	A
1	1	370	U
1	1	376	G
1	1	384	A
1	1	385	A
1	1	387	A
1	1	391	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	420	G
1	1	425	G
1	1	439	C
1	1	440	A
1	1	442	G
1	1	451	U

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Mol	Chain	Res	Type
1	1	459	G
1	1	463	C
1	1	466	G
1	1	468	G
1	1	478	A
1	1	480	C
1	1	481	U
1	1	482	C
1	1	494	G
1	1	495	G
1	1	521	A
1	1	523	A
1	1	533	A
1	1	535	G
1	1	542	G
1	1	543	C
1	1	545	U
1	1	546	C
1	1	547	G
1	1	550	A
1	1	551	A
1	1	555	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	582	G
1	1	589	A
1	1	600	G
1	1	604	G
1	1	611	A
1	1	621	A
1	1	625	G
1	1	629	U
1	1	637	C
1	1	645	A
1	1	646	A
1	1	647	A
1	1	660	A
1	1	677	A
1	1	681	U

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Mol	Chain	Res	Type
1	1	690	A
1	1	691	A
1	1	705	A
1	1	706	A
1	1	707	U
1	1	715	A
1	1	716	A
1	1	717	C
1	1	718	G
1	1	719	U
1	1	720	A
1	1	721	G
1	1	722	G
1	1	735	A
1	1	751	A
1	1	757	C
1	1	772	U
1	1	780	A
1	1	781	G
1	1	783	A
1	1	784	A
1	1	785	G
1	1	816	A
1	1	817	A
1	1	818	C
1	1	820	A
1	1	826	G
1	1	908	G
1	1	909	G
1	1	910	G
1	1	936	A
1	1	944	C
1	1	957	C
1	1	958	C
1	1	959	C
1	1	960	U
1	1	962	A
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	985	U

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Mol	Chain	Res	Type
1	1	1103	A
1	1	1111	U
1	1	1116	G
1	1	1117	G
1	1	1125	U
1	1	1127	G
1	1	1128	U
1	1	1131	G
1	1	1132	C
1	1	1143	A
1	1	1145	G
1	1	1159	A
1	1	1160	C
1	1	1177	G
1	1	1178	G
1	1	1180	A
1	1	1181	U
1	1	1191	U
1	1	1197	A
1	1	1198	C
1	1	1202	A
1	1	1203	A
1	1	1204	A
1	1	1221	A
1	1	1222	G
1	1	1235	U
1	1	1239	C
1	1	1241	U
1	1	1245	A
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1271	A
1	1	1272	C
1	1	1278	A
1	1	1286	A
1	1	1287	A
1	1	1301	A
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U

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Mol	Chain	Res	Type
1	1	1308	A
1	1	1309	U
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1386	A
1	1	1387	G
1	1	1391	C
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1450	G
1	1	1452	A
1	1	1455	U
1	1	1464	G
1	1	1864	A
1	1	1866	C
1	1	1867	A
1	1	1868	G
1	1	1872	C
1	1	1873	U
1	1	1874	A
1	1	1875	G
1	1	1880	U
1	1	1881	A
1	1	1885	U
1	1	1886	A
1	1	1887	A
1	1	2347	U
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2385	G

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Mol	Chain	Res	Type
1	1	2387	A
1	1	2388	U
1	1	2393	G
1	1	2398	A
1	1	2402	A
1	1	2419	A
1	1	2420	C
1	1	2421	U
1	1	2433	U
1	1	2434	U
1	1	2435	G
1	1	2436	U
1	1	2438	A
1	1	2440	G
1	1	2445	A
1	1	2447	A
1	1	2451	G
1	1	2452	G
1	1	2453	U
1	1	2461	A
1	1	2468	A
1	1	2469	G
1	1	2473	C
1	1	2474	G
1	1	2475	G
1	1	2487	U
1	1	2491	A
1	1	2497	U
1	1	2501	U
1	1	2507	C
1	1	2596	U
1	1	2600	C
1	1	2602	G
1	1	2603	G
1	1	2606	G
1	1	2611	U
1	1	2809	C
1	1	2817	A
1	1	2819	A
1	1	2820	A
1	1	2821	C
1	1	2822	U

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Mol	Chain	Res	Type
1	1	2823	G
1	1	2824	G
1	1	2828	G
1	1	2838	A
1	1	2841	G
1	1	2844	C
1	1	2845	A
1	1	2847	A
1	1	2848	G
1	1	2866	U
1	1	2867	C
1	1	2868	U
1	1	2898	G
1	1	2899	C
1	1	2961	G
1	1	2964	G
1	1	2967	A
1	1	2968	G
1	1	2970	C
1	1	2971	A
1	1	2998	U
1	1	3011	A
1	1	3012	A
1	1	3021	A
1	1	3022	G
1	1	3028	G
1	1	3032	A
1	1	3055	U
1	1	3057	U
1	1	3058	U
1	1	3059	G
1	1	3068	U
1	1	3069	G
1	1	3070	A
1	1	3071	U
1	1	3075	G
1	1	3076	C
1	1	3077	A
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3085	G

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Mol	Chain	Res	Type
1	1	3086	A
1	1	3087	A
1	1	3088	G
1	1	3092	C
1	1	3093	C
1	1	3094	A
1	1	3099	C
1	1	3100	U
1	1	3101	G
1	1	3122	A
1	1	3129	A
1	1	3130	A
1	1	3141	A
1	1	3142	A
1	1	3143	C
1	1	3144	G
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3198	U
1	1	3206	C
1	1	3207	U
1	1	3209	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3224	G
1	1	3227	A
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3259	U
1	1	3260	G
1	1	3275	U
1	1	3276	G
1	1	3286	G
1	1	3292	A

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Mol	Chain	Res	Type
1	1	3293	U
1	1	3295	A
1	1	3304	U
1	1	3316	A
1	1	3317	U
1	1	3324	C
1	1	3334	U
1	1	3339	A
1	1	3341	U
1	1	3343	G
1	1	3345	G
1	1	3346	U
1	1	3347	A
1	1	3348	G
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3354	U
1	1	3355	U
1	1	3356	G
1	1	3360	C
1	1	3363	U
1	1	3365	U
1	1	3366	G
1	1	3368	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
1	1	3396	U
2	2	23	U
2	2	34	U
2	2	35	C
2	2	38	U
2	2	59	A
2	2	62	C
2	2	63	G
2	2	75	G
2	2	79	A
2	2	80	A
2	2	81	U
2	2	82	U

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Mol	Chain	Res	Type
2	2	85	G
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	104	A
2	2	105	A
2	2	106	C
2	2	109	A
2	2	115	C
2	2	116	G
2	2	123	G
2	2	135	G
2	2	151	C
2	2	158	U
4	6	4	U
4	6	5	C
4	6	6	U
4	6	7	C
4	6	24	A
4	6	33	U
4	6	43	A
4	6	47	A
4	6	48	A
4	6	49	C
4	6	52	G
4	6	54	A
4	6	56	U
4	6	58	G
4	6	59	C
4	6	228	U
4	6	229	U
4	6	231	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	720	A
1	1	1240	A
1	1	1301	A
1	1	1886	A
1	1	2420	C

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Mol	Chain	Res	Type
1	1	3121	U

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
50	GDP	b	801	51	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)

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
50	GDP	b	801	51	-	5/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	b	801	GDP	C5-C4	3.11	1.47	1.38
50	b	801	GDP	C6-N1	-2.44	1.34	1.38
50	b	801	GDP	C5-N7	-2.06	1.34	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	b	801	GDP	C5-C4-N3	-6.04	118.77	128.39
50	b	801	GDP	C2-N3-C4	5.03	120.97	112.30
50	b	801	GDP	N9-C4-N3	4.43	134.82	125.95
50	b	801	GDP	C6-C5-N7	3.34	136.37	130.29
50	b	801	GDP	C4-C5-N7	-2.58	106.58	110.67
50	b	801	GDP	O6-C6-C5	-2.11	120.96	126.53

There are no chirality outliers.

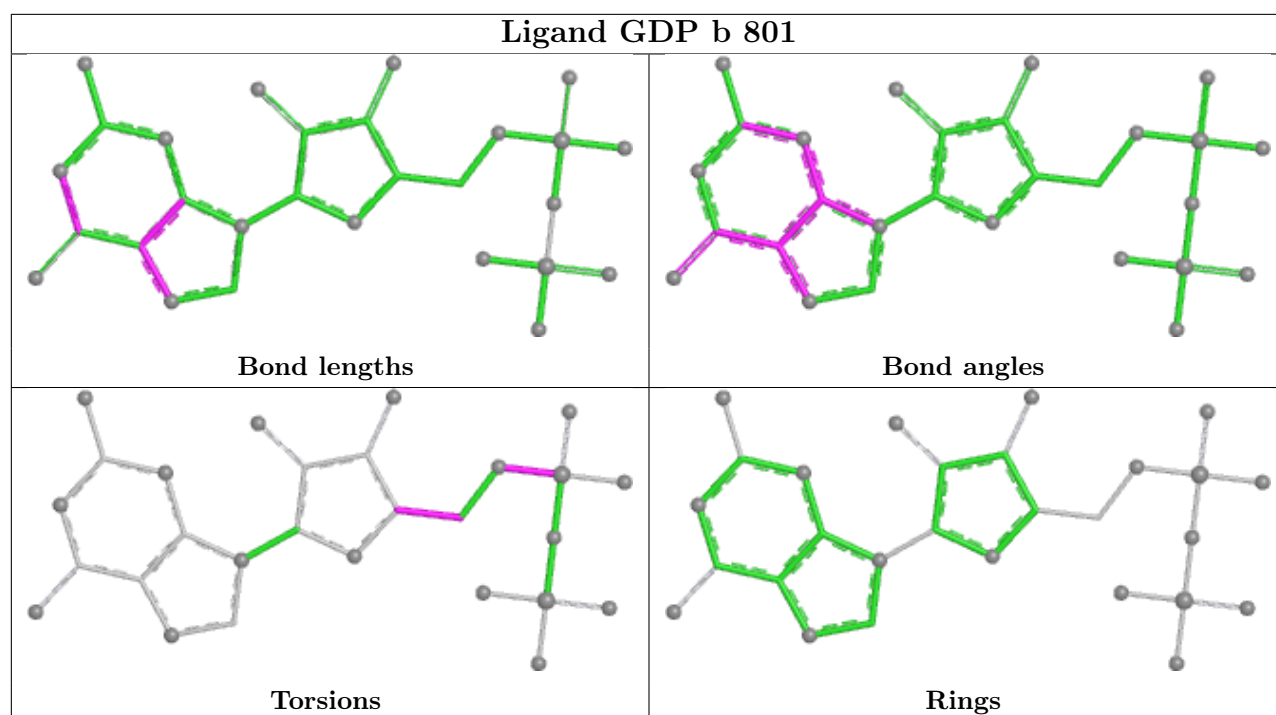
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	b	801	GDP	C5'-O5'-PA-O3A
50	b	801	GDP	C5'-O5'-PA-O2A
50	b	801	GDP	O4'-C4'-C5'-O5'
50	b	801	GDP	C3'-C4'-C5'-O5'
50	b	801	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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



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.

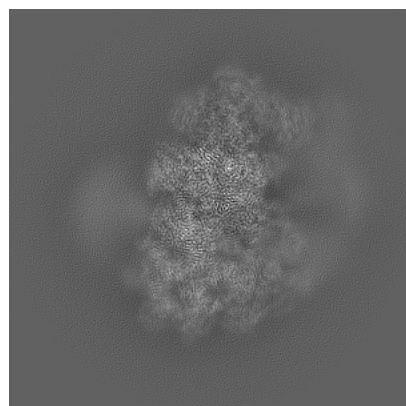
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43021. These allow visual inspection of the internal detail of the map and identification of artifacts.

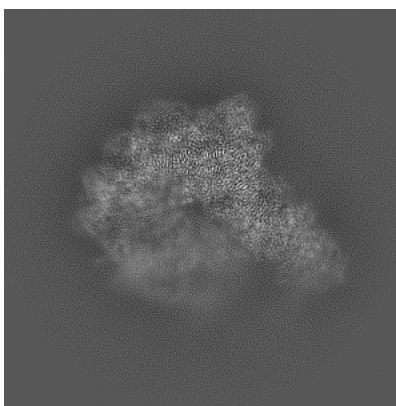
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

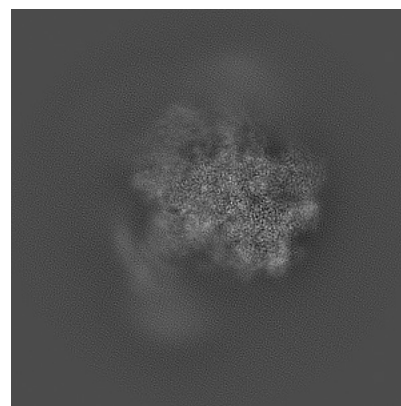
6.1.1 Primary map



X

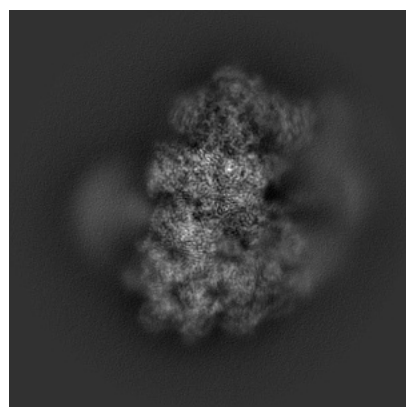


Y

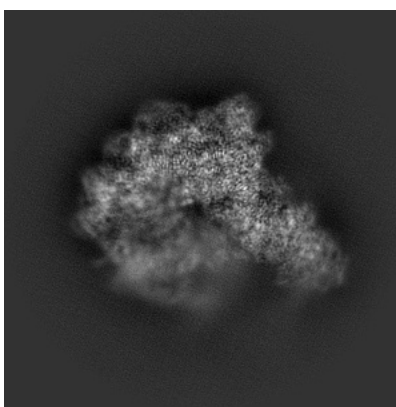


Z

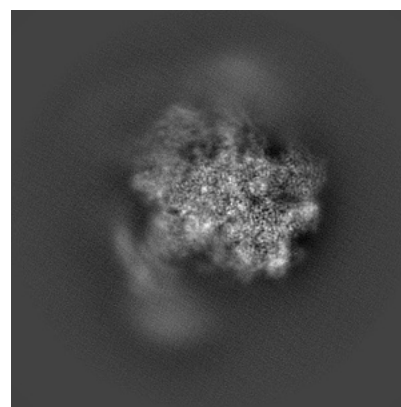
6.1.2 Raw map



X



Y

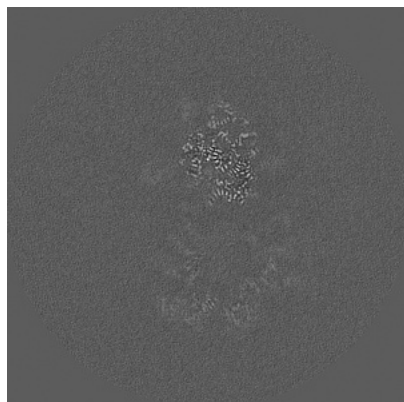


Z

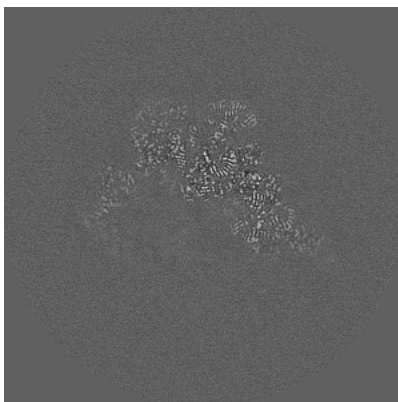
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

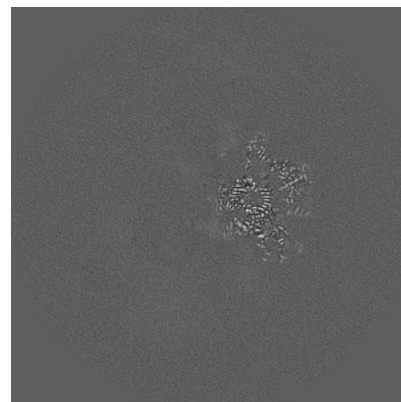
6.2.1 Primary map



X Index: 200

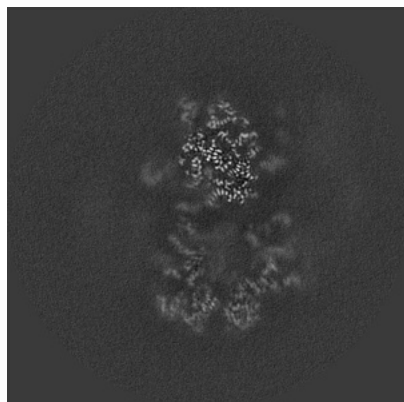


Y Index: 200

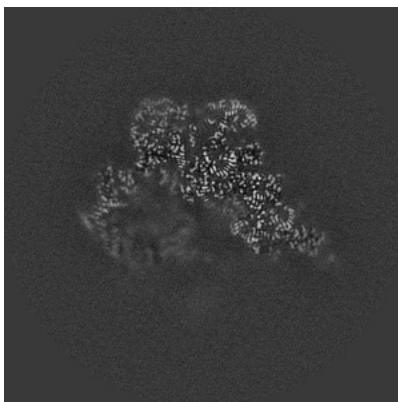


Z Index: 200

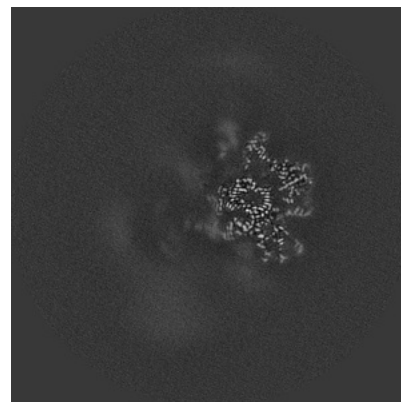
6.2.2 Raw map



X Index: 200



Y Index: 200

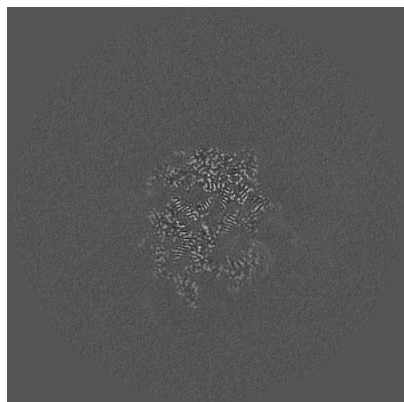


Z Index: 200

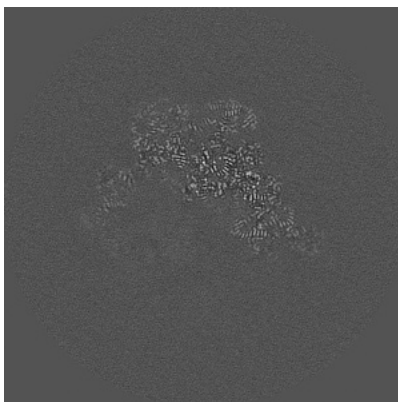
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

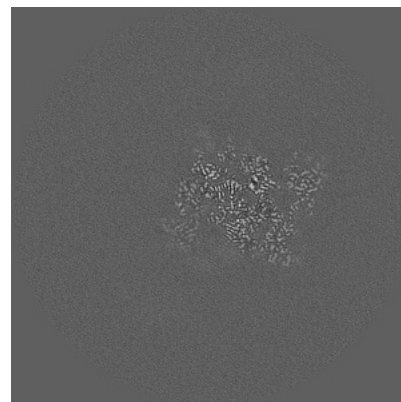
6.3.1 Primary map



X Index: 249

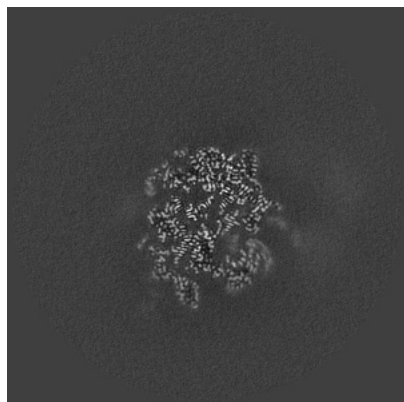


Y Index: 199

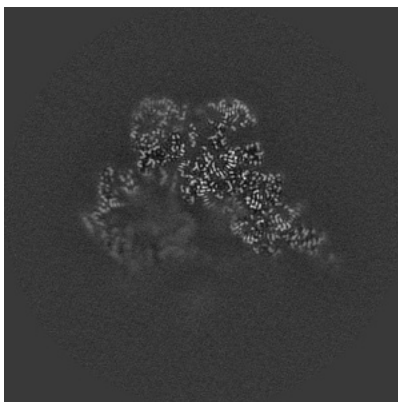


Z Index: 240

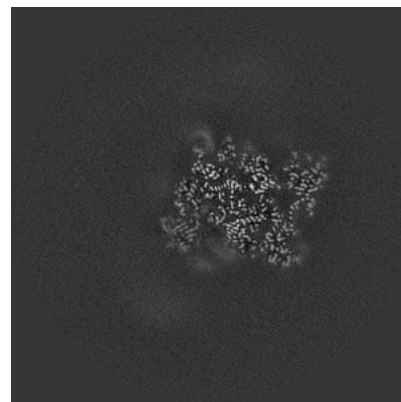
6.3.2 Raw map



X Index: 250



Y Index: 201

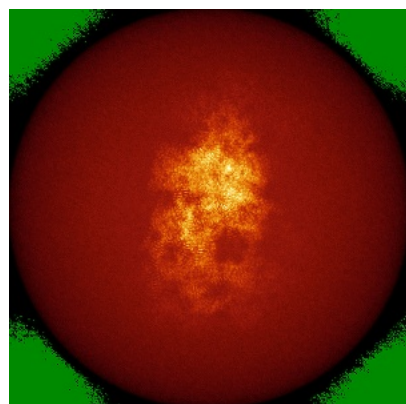


Z Index: 240

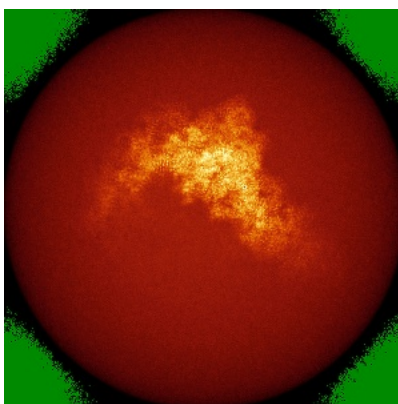
The images above show the largest variance slices of the map in three orthogonal directions.

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

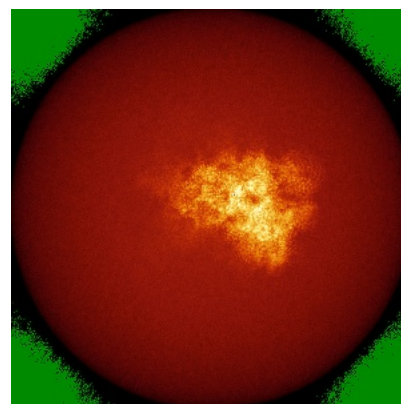
6.4.1 Primary map



X

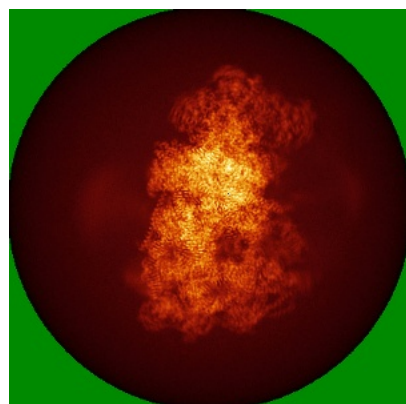


Y

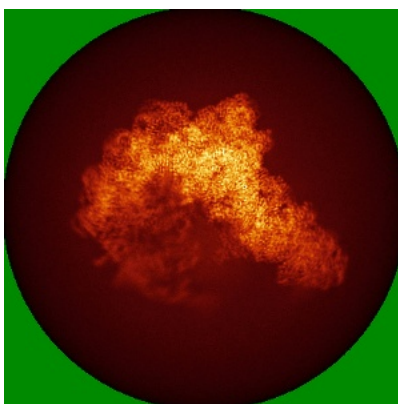


Z

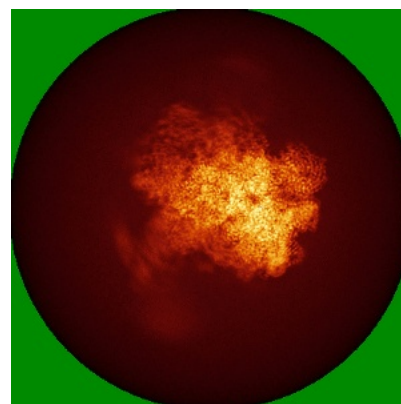
6.4.2 Raw map



X



Y

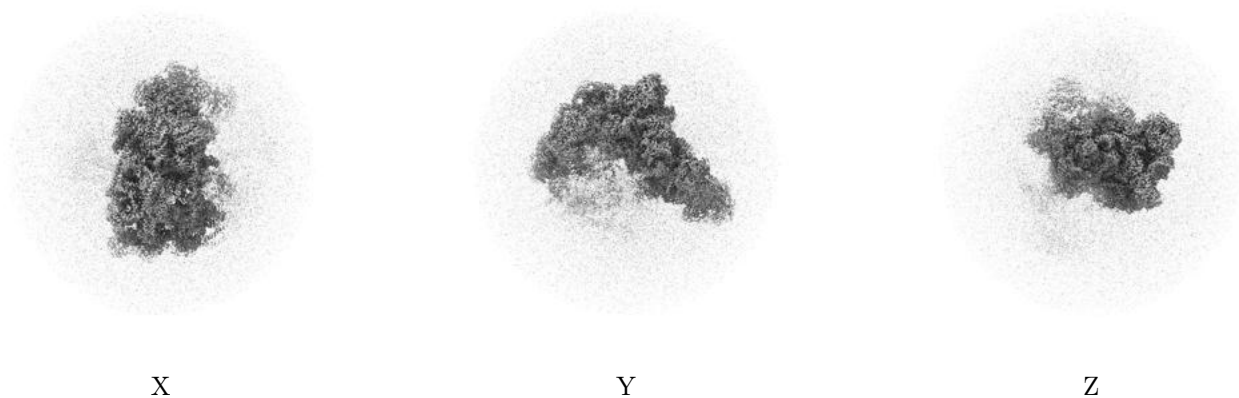


Z

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

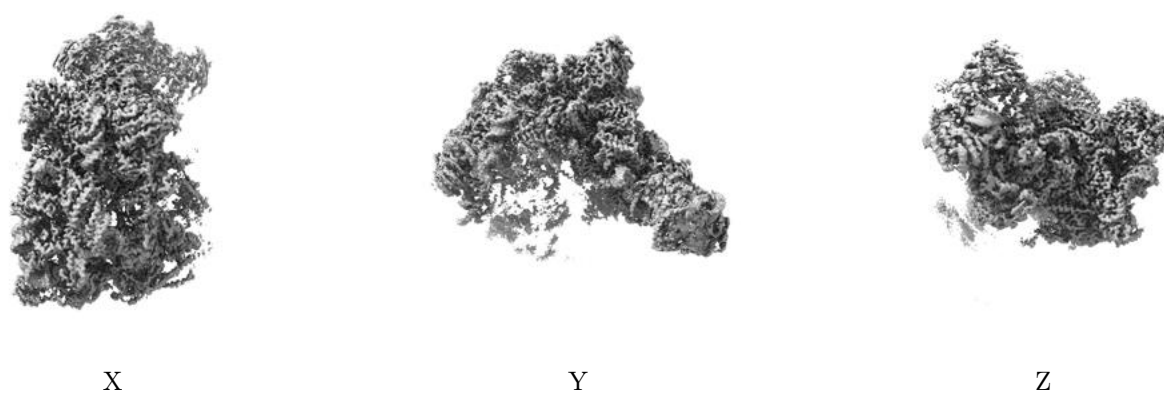
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

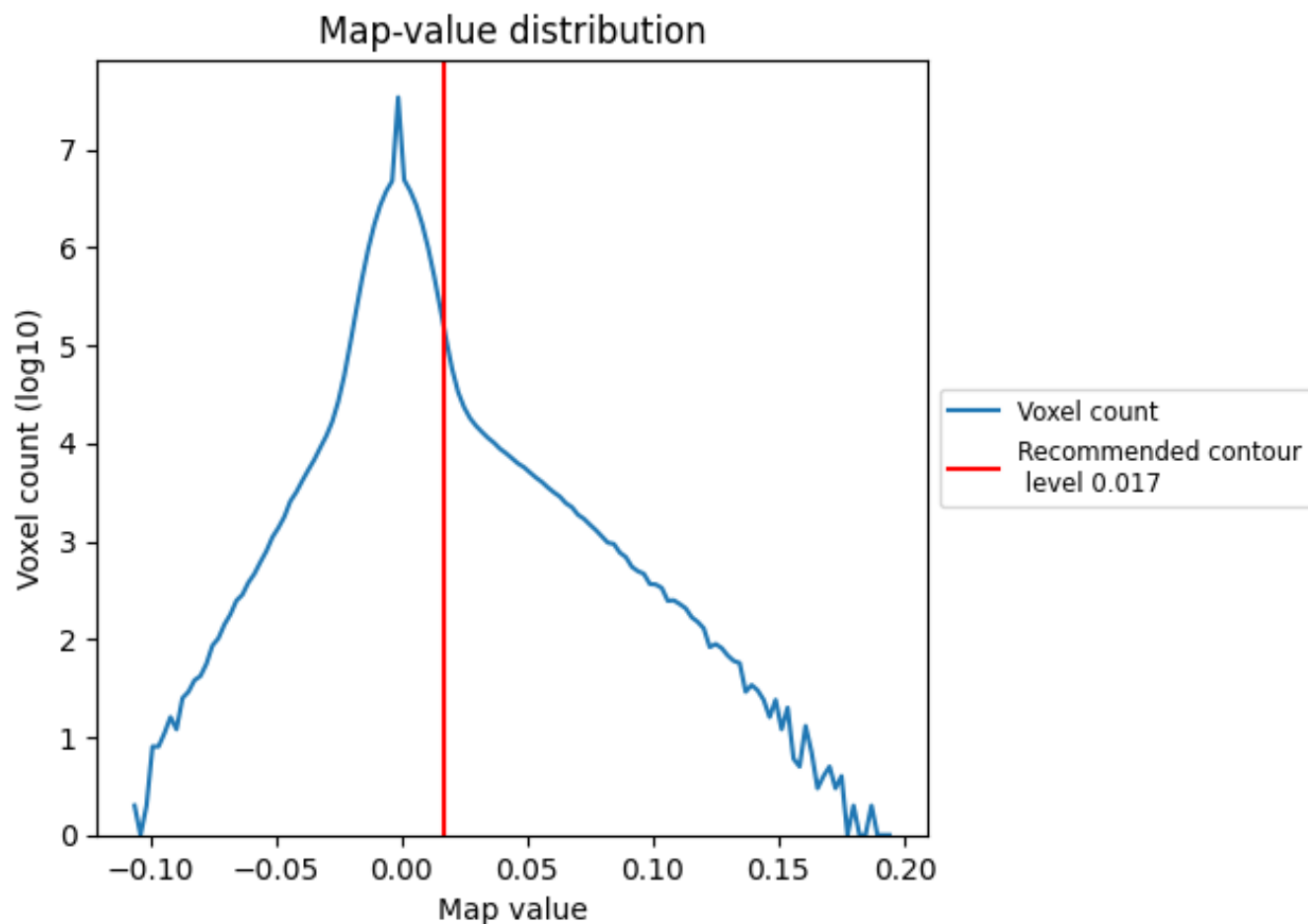
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

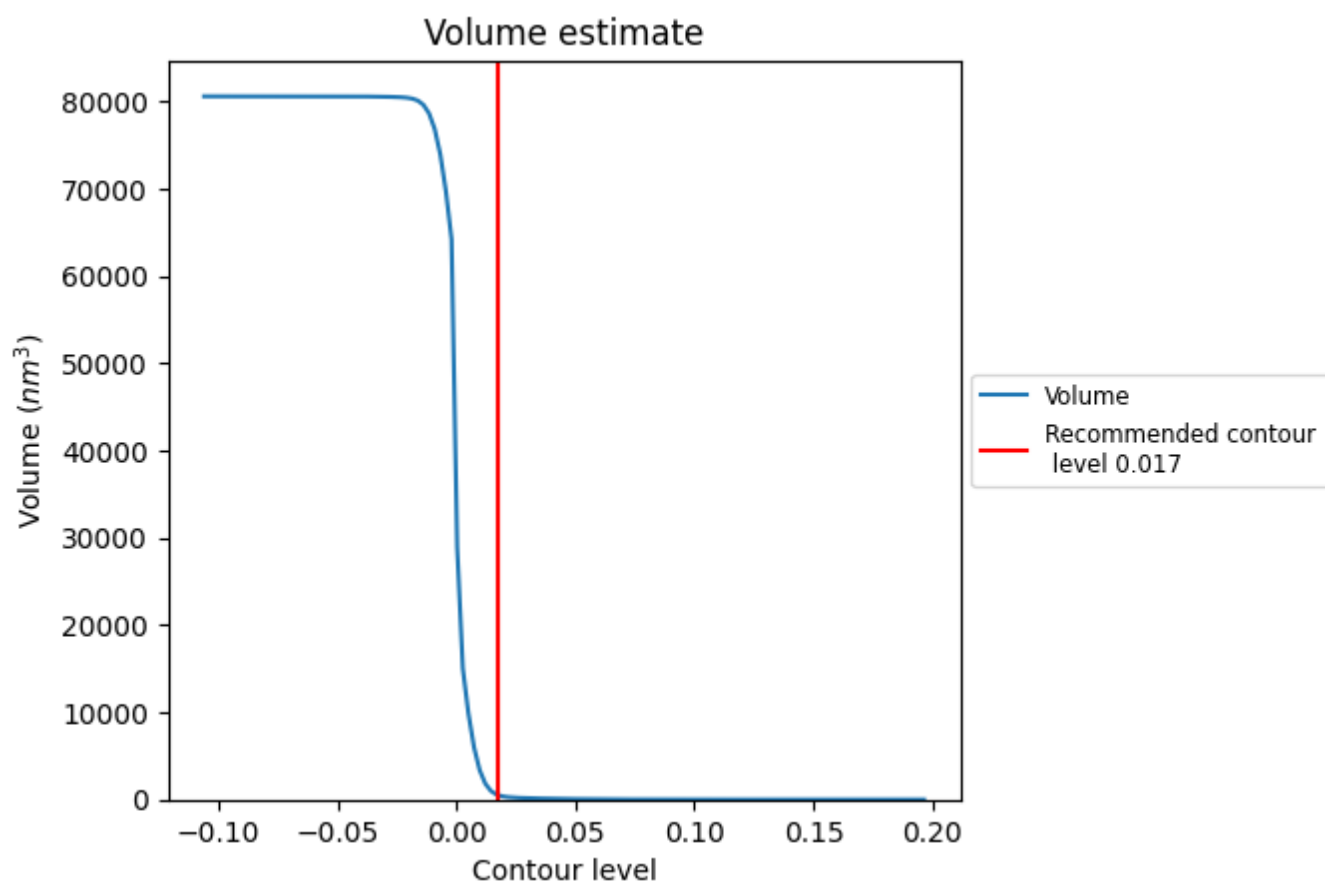
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

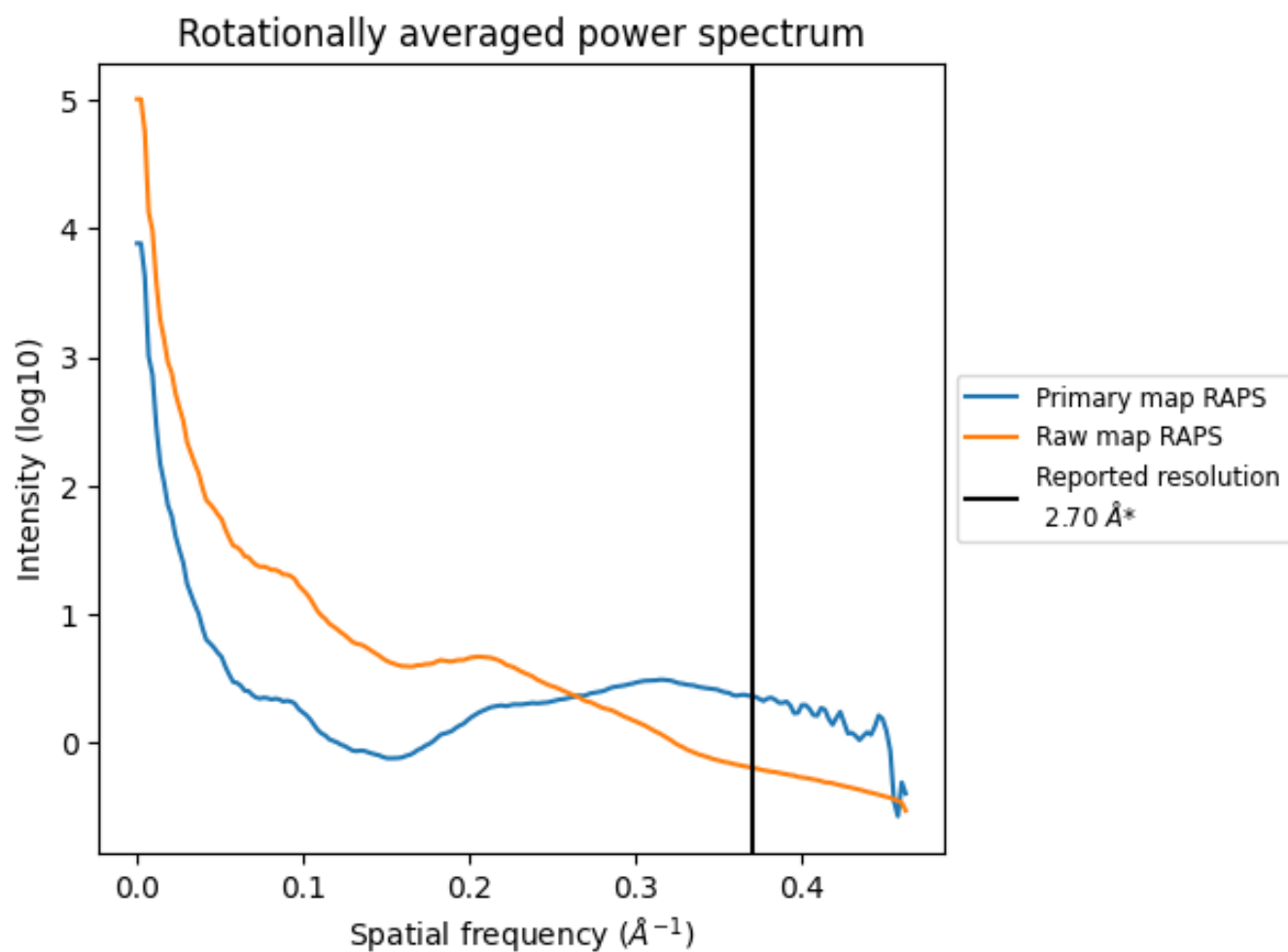
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm^3 ; this corresponds to an approximate mass of 500 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 ⓘ

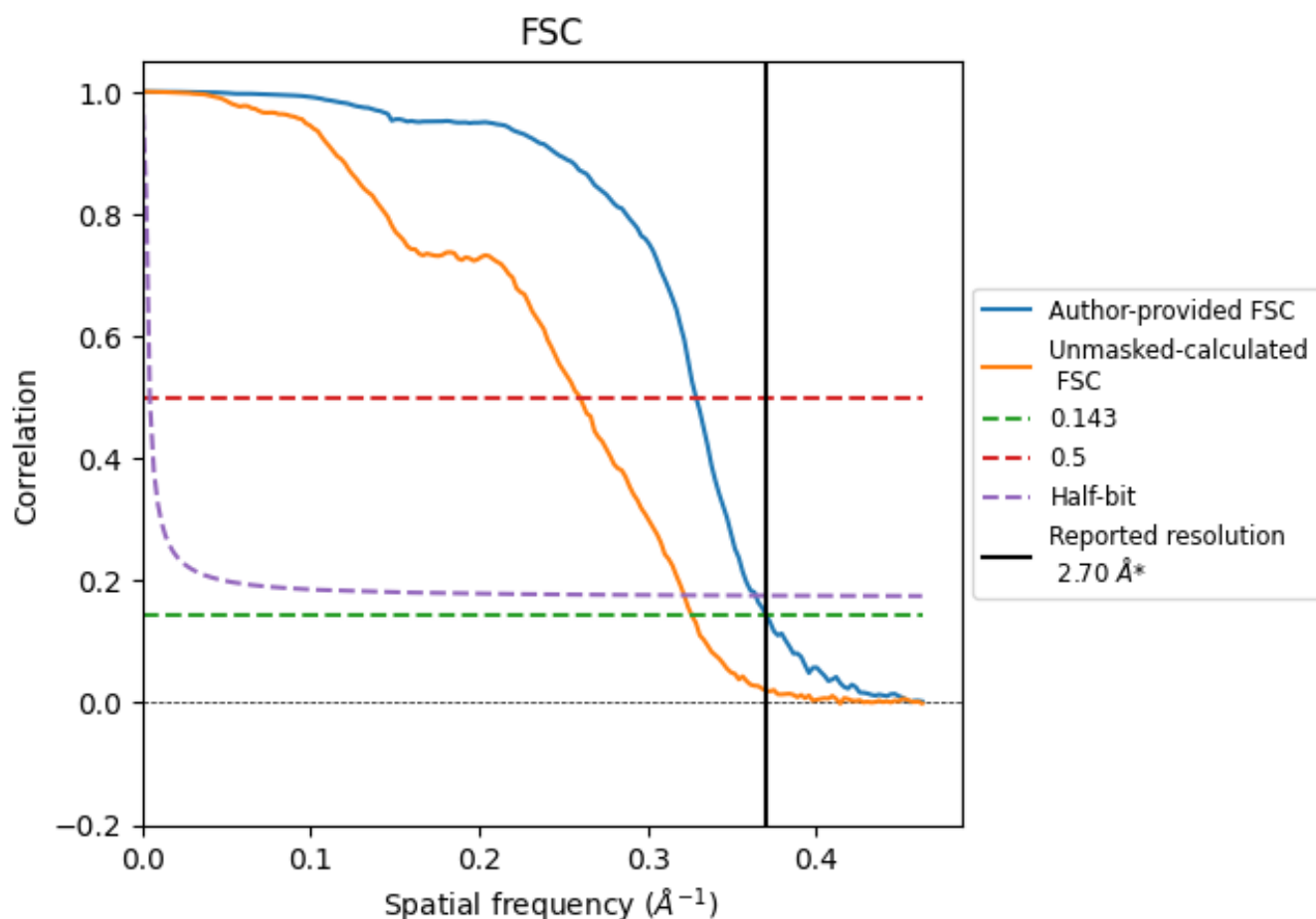


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 [i](#)

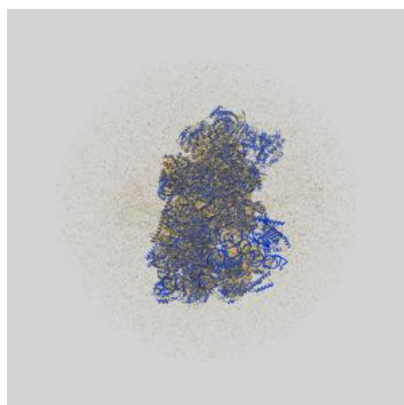
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.04	2.75
Unmasked-calculated*	3.07	3.85	3.11

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

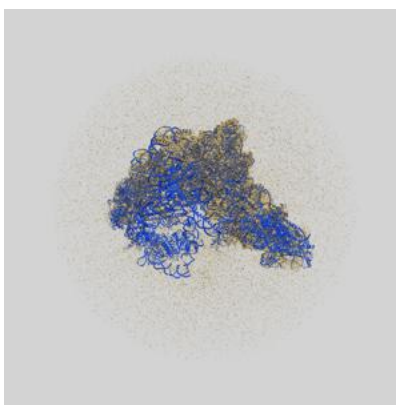
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43021 and PDB model 8V84. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

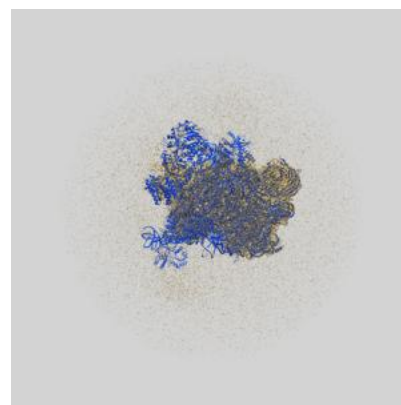
9.1 Map-model overlay [i](#)



X



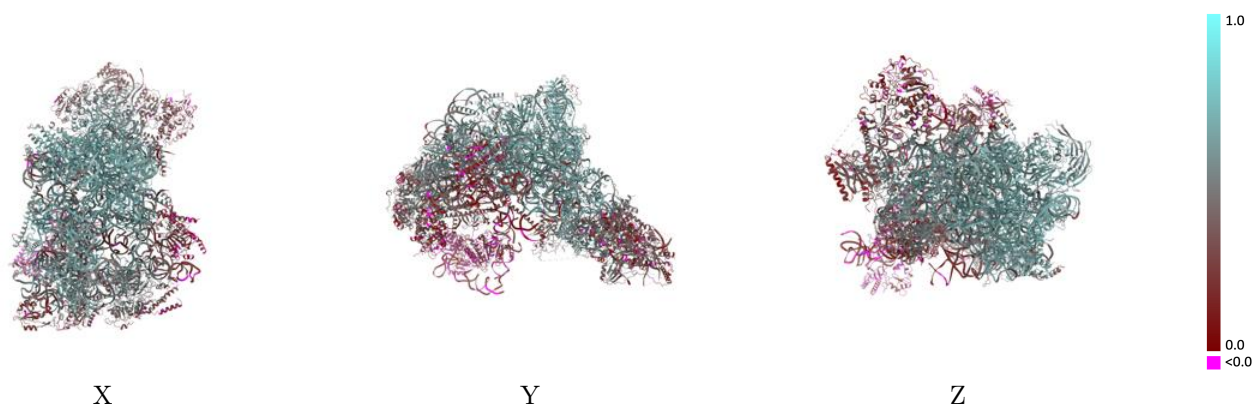
Y



Z

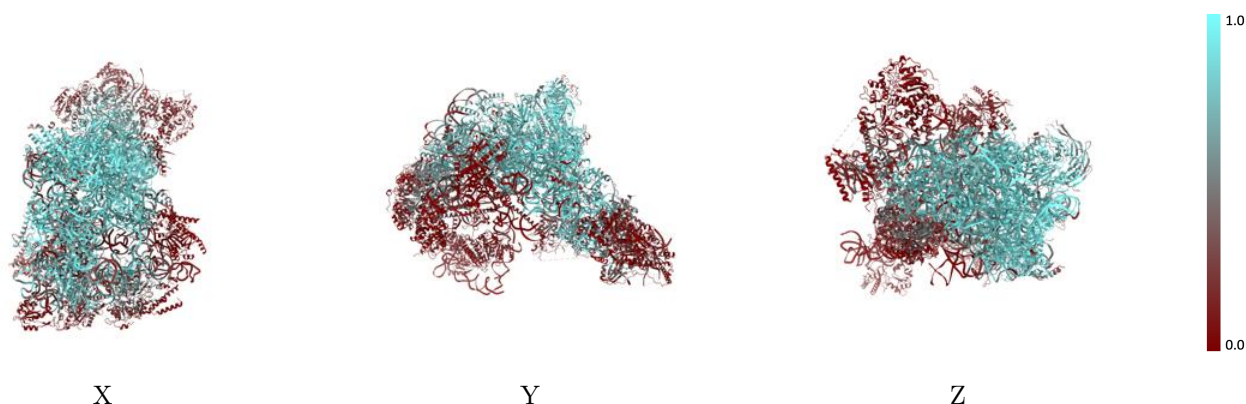
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



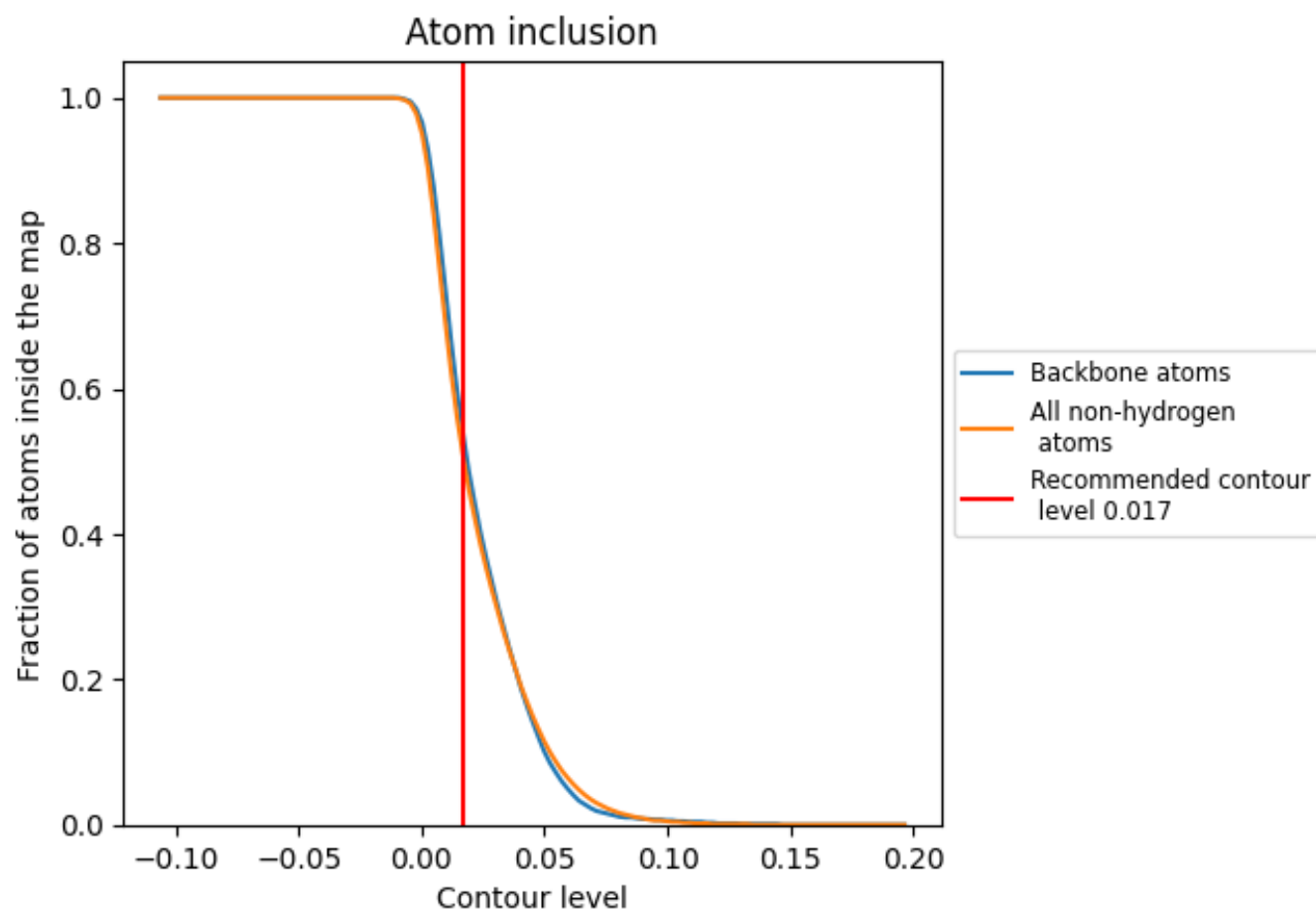
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 50% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.4610
1	0.5930	0.4840
2	0.7680	0.5770
3	0.0400	0.2020
6	0.3750	0.4080
7	0.0000	0.0610
8	0.2940	0.3920
A	0.3730	0.4550
B	0.5990	0.5370
C	0.9320	0.6810
D	0.3600	0.4430
E	0.7860	0.6140
F	0.8360	0.6280
G	0.7510	0.5860
H	0.6300	0.5610
I	0.7720	0.6080
J	0.0810	0.2700
K	0.1850	0.3550
L	0.8800	0.6470
M	0.7550	0.6090
N	0.8160	0.6170
O	0.8030	0.6240
P	0.8090	0.6270
Q	0.8520	0.6520
R	0.8490	0.6450
S	0.5760	0.5380
T	0.0150	0.1610
V	0.1960	0.3830
W	0.0970	0.3140
Y	0.8800	0.6540
Z	0.0200	0.1950
a	0.0010	0.0370
b	0.1890	0.3620
e	0.9100	0.6770
f	0.9030	0.6760



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Chain	Atom inclusion	Q-score
h	 0.5580	 0.5340
i	 0.5990	 0.5490
j	 0.8830	 0.6590
l	 0.0070	 0.1190
m	 0.2230	 0.3350
n	 0.0780	 0.2610
o	 0.2790	 0.3640
q	 0.0080	 0.1190
r	 0.2010	 0.3570
t	 0.1400	 0.3230
u	 0.2160	 0.3700
v	 0.6360	 0.5550
w	 0.7720	 0.5970
x	 0.8100	 0.6170
y	 0.2390	 0.4130