



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 03:06 PM EDT

PDB ID : 9N79 / pdb_00009n79
EMDB ID : EMD-49089
Title : SSU processome maturation and disassembly, State M
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

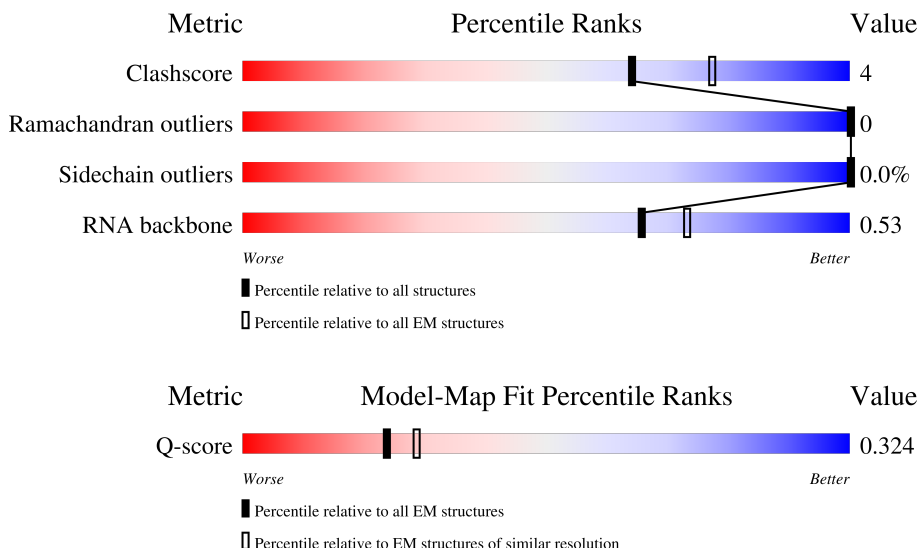
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 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.



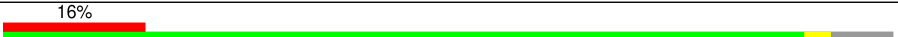
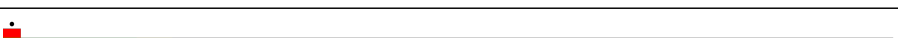
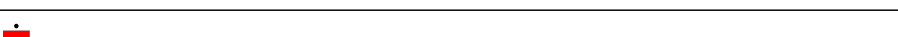
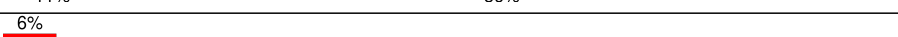
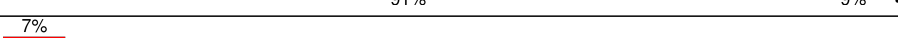
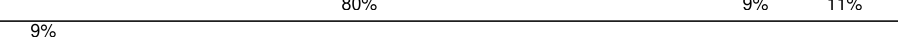
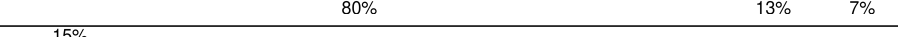
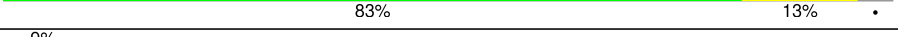
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	L1	1803	
2	L2	334	
3	L3	146	

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Mol	Chain	Length	Quality of chain
4	L4	261	
5	L5	225	
6	L6	236	
7	L7	190	
8	L8	200	
9	L9	197	
10	LC	143	
11	LD	156	
12	LE	130	
13	LF	135	
14	LG	67	
15	N2	5	
16	NA	593	
17	NB	610	
18	NF	151	
19	NG	137	
20	NL	318	
21	NM	255	
22	NP	144	
23	NQ	82	
24	NS	1267	
25	NW	108	
26	SA	504	
27	SB	511	
28	SC	327	

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Mol	Chain	Length	Quality of chain
28	SD	327	
29	SE	126	
29	SF	126	
30	SG	573	
31	SH	367	
32	SI	1183	
33	SJ	252	
33	SK	252	
34	SL	189	
35	SM	290	
36	SP	2493	
37	SR	145	
38	SS	899	
39	ST	810	
40	SU	552	
41	SW	274	
42	SZ	483	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 106665 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1401	Total	C	N	O	P	0	0
			29868	13354	5304	9809	1401		

- Molecule 2 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	88	Total	C	N	O	P	0	0
			1891	842	338	622	89		

- Molecule 3 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	100	Total	C	N	O	S	0	0
			815	515	152	146	2		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L4	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	197	Total	C	N	O	S	0	0
			1558	975	291	289	3		

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	227	Total	C	N	O	S	0	0
			1831	1148	354	326	3		

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L7	186	Total	C	N	O	0	0
			1492	957	267	268		

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	181	Total	C	N	O	S	0	0
			1437	892	287	256	2		

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L9	181	Total	C	N	O	S	0	0
			1470	930	285	254	1		

- Molecule 10 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	LC	120	Total	C	N	O	0	0
			930	598	165	167		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	138	Total	C	N	O	S	0	0
			1119	718	213	185	3		

- Molecule 12 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LE	129	Total	C	N	O	S	0	0
			1022	650	188	181	3		

- Molecule 13 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	LF	130	Total	C	N	O	0	0
			1046	662	204	180		

- Molecule 14 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	62	Total	C	N	O	S	0	0
			490	302	98	89	1		

- Molecule 15 is a RNA chain called U3snoRNA segment.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N2	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	NA	110	Total	C	N	O	S	0	0
			907	562	154	190	1		

- Molecule 17 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	NB	84	Total	C	N	O		0	0
			687	432	137	118			

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	NF	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	NG	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 20 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	NL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 21 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	NM	211	Total	C	N	O	S	0	0
			1688	1070	306	308	4		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	NP	134	Total	C	N	O	S	0	0
			1040	653	193	192	2		

- Molecule 23 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	NQ	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 24 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NS	893	Total	C	N	O	S	0	0
			4947	3014	974	957	2		

- Molecule 25 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	NW	69	Total	C	N	O	0	0
			556	356	103	97		

- Molecule 26 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	SA	384	Total	C	N	O	1	0
			1924	1154	385	385		

- Molecule 27 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	SB	403	Total	C	N	O	0	0
			2009	1203	403	403		

- Molecule 28 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SC	238	Total	C	N	O	S	0	0
			1850	1171	333	336	10		
28	SD	238	Total	C	N	O		0	0
			1198	722	238	238			

- Molecule 29 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SE	121	Total	C	N	O		0	0
			615	373	121	121			
29	SF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 30 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SG	458	Total	C	N	O	S	0	0
			3663	2326	644	683	10		

- Molecule 31 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SH	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 32 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SI	708	Total	C	N	O	S	0	0
			5748	3692	1018	1011	27		

- Molecule 33 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	SJ	213	Total	C	N	O	0	0
			1074	648	213	213		
33	SK	229	Total	C	N	O	0	0
			1160	702	229	229		

- Molecule 34 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SL	148	Total	C	N	O	S	0	0
			1171	750	209	202	10		

- Molecule 35 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SM	219	Total	C	N	O	S	0	0
			1756	1107	325	318	6		

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SP	945	Total	C	N	O	S	0	0
			7764	5052	1269	1422	21		

- Molecule 37 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SR	134	Total	C	N	O	S	0	0
			1052	668	204	178	2		

- Molecule 38 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
38	SS	153	Total	C	N	O	P	S	0	0
			1186	723	231	221	1	10		

- Molecule 39 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	ST	573	Total	C	N	O	S	0	0
			3316	2025	651	635	5		

- Molecule 40 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	SU	532	Total	C	N	O	0	0
			2703	1639	532	532		

- Molecule 41 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SW	182	Total	C	N	O	S	0	0
			1444	923	262	255	4		

- Molecule 42 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SZ	259	Total	C	N	O		0	0
			1314	796	259	259			

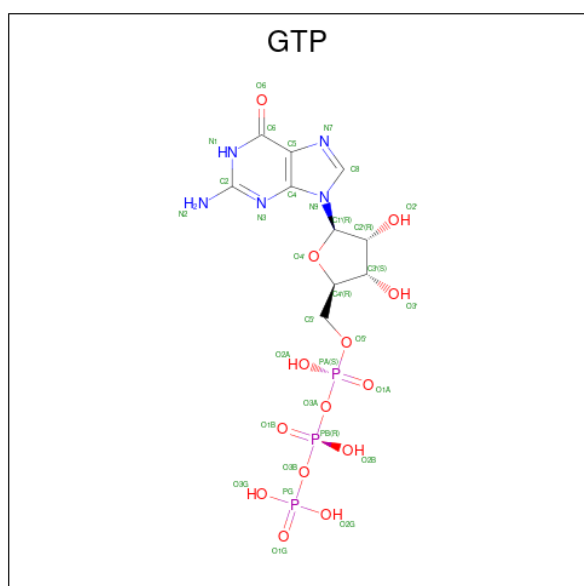
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	L1	46	Total	Mg	0
			46	46	
43	SI	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	NQ	1	Total	Zn	0
			1	1	
44	SL	1	Total	Zn	0
			1	1	

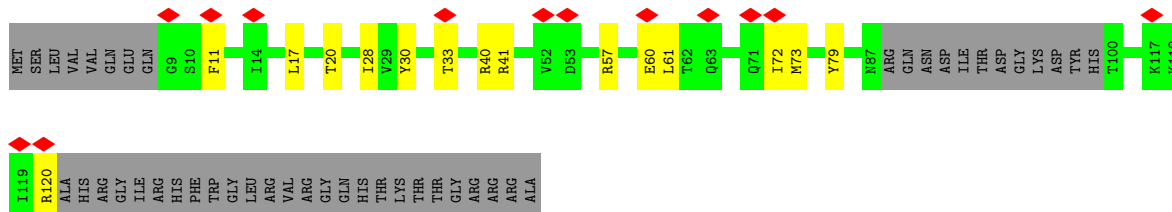
- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	SI	1	32	10	5	14	3	0



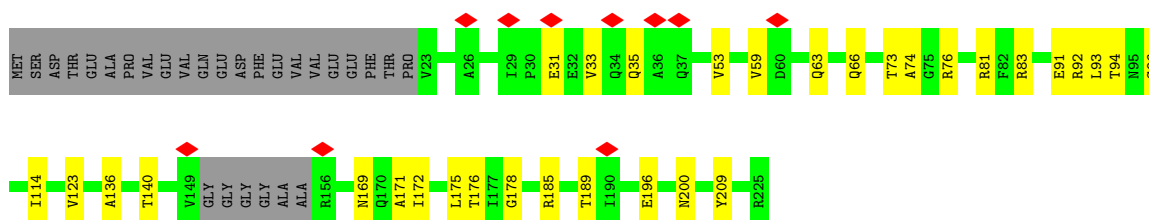
- Molecule 3: 40S ribosomal protein S18-A



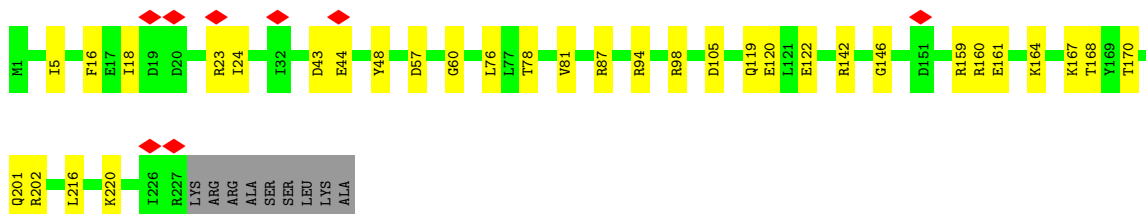
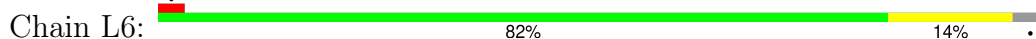
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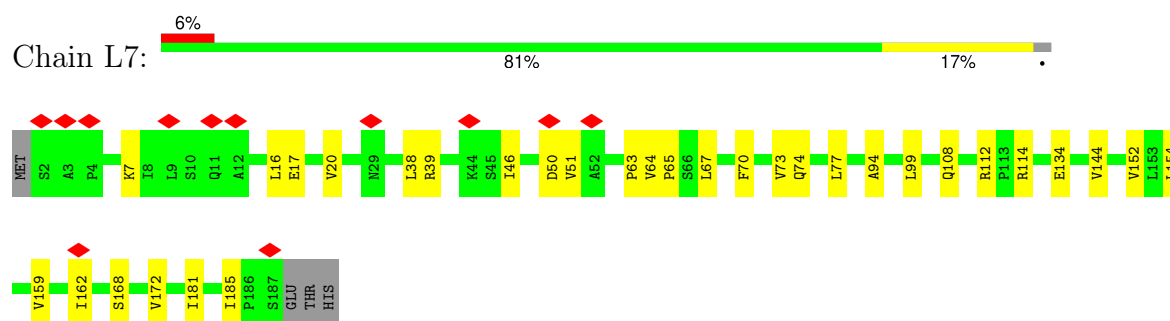
- Molecule 5: 40S ribosomal protein S5



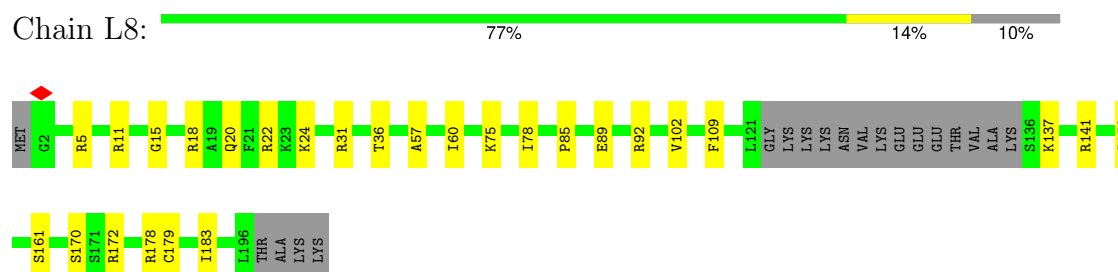
- Molecule 6: 40S ribosomal protein S6-A



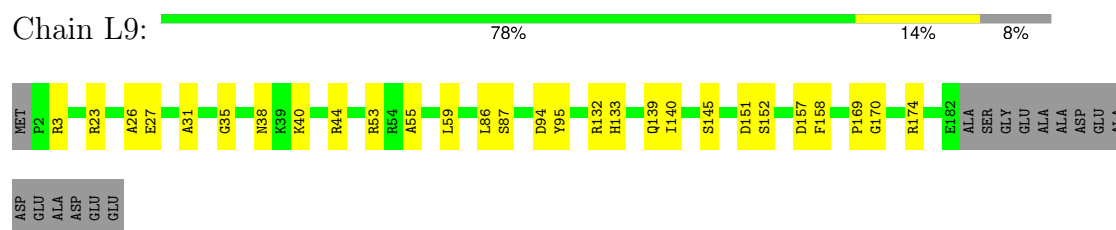
- Molecule 7: 40S ribosomal protein S7-A



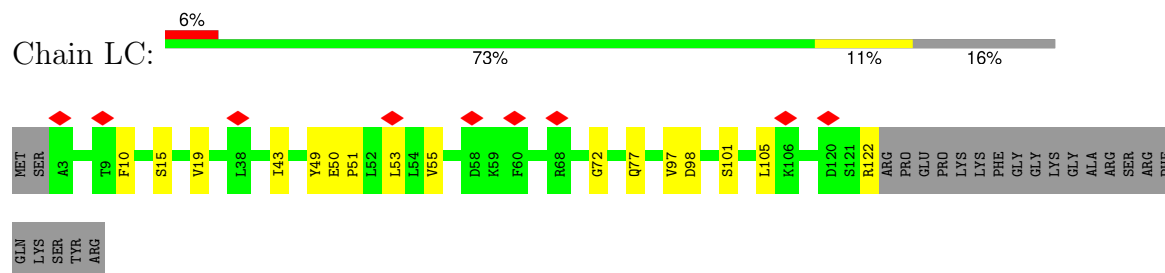
- Molecule 8: 40S ribosomal protein S8-A



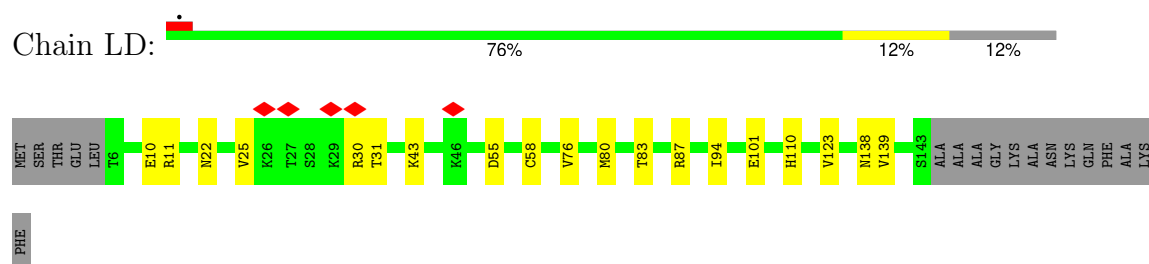
- Molecule 9: 40S ribosomal protein S9-A



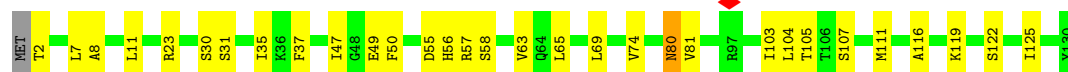
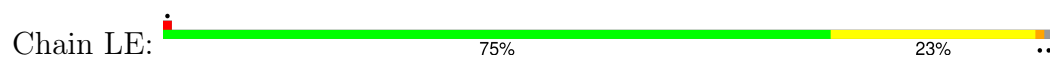
- Molecule 10: 40S ribosomal protein S16-A



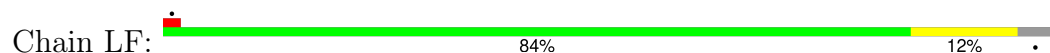
- Molecule 11: 40S ribosomal protein S11-A



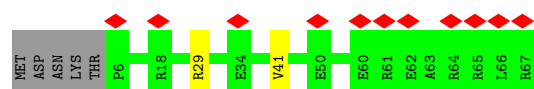
- Molecule 12: 40S ribosomal protein S22-A



- Molecule 13: 40S ribosomal protein S24-A



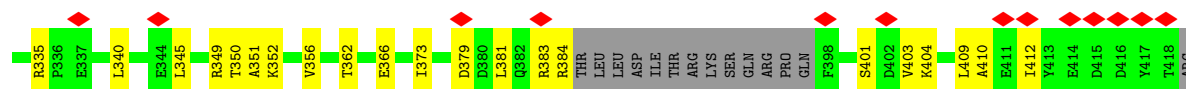
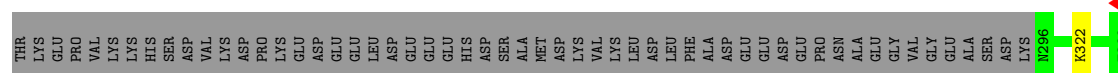
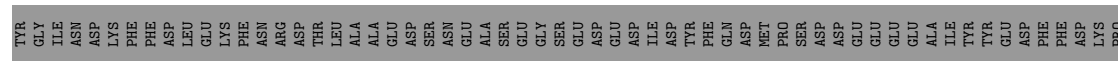
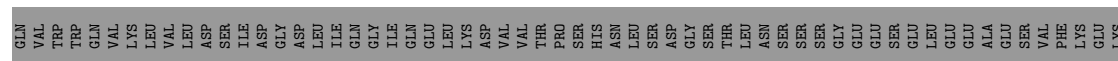
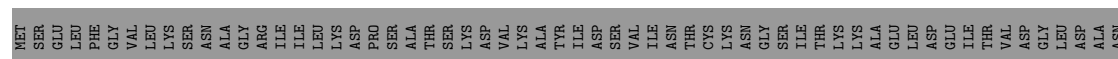
- Molecule 14: 40S ribosomal protein S28-A

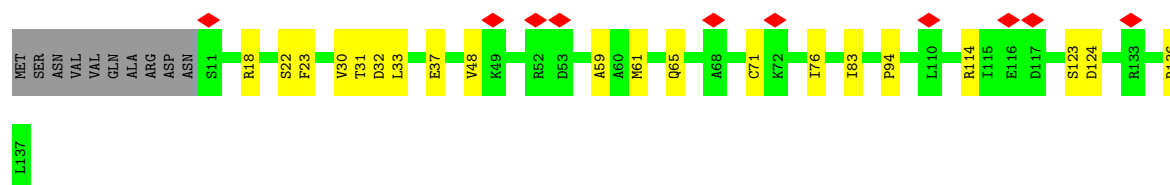


- Molecule 15: U3snoRNA segment

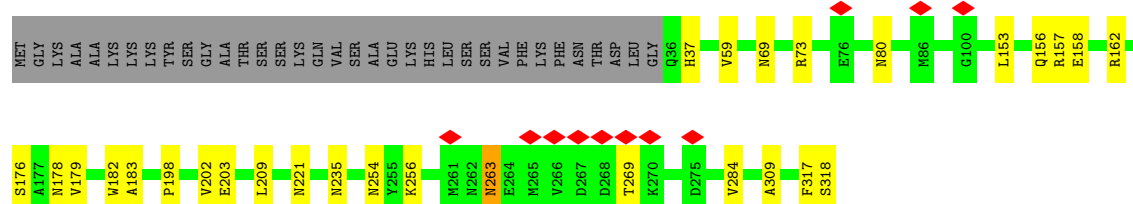
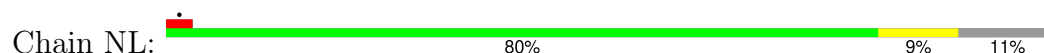


- Molecule 16: U3 small nucleolar RNA-associated protein MPP10

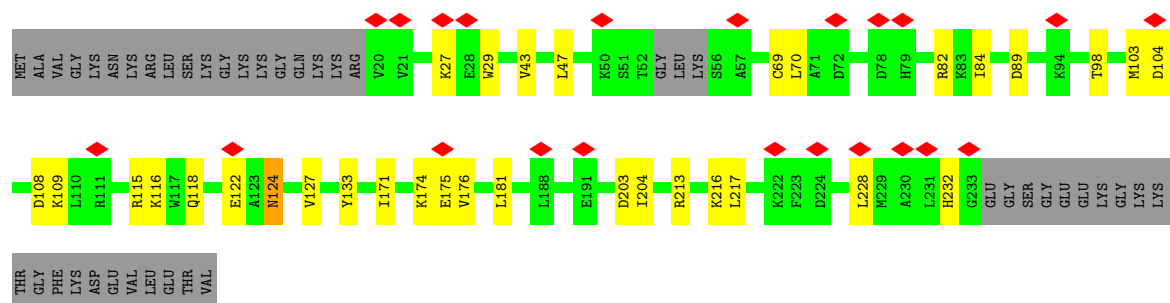
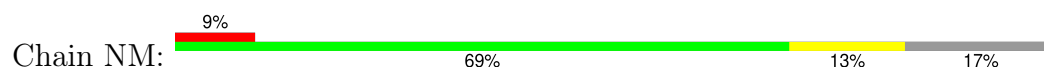




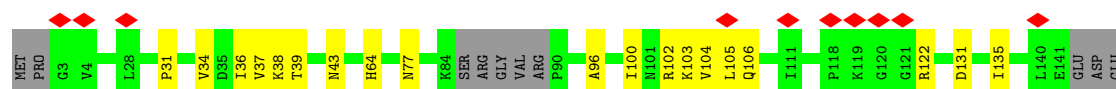
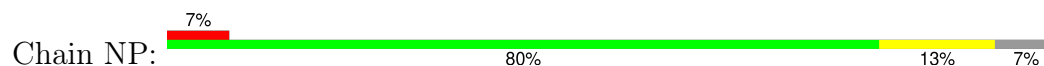
- Molecule 20: Dimethyladenosine transferase



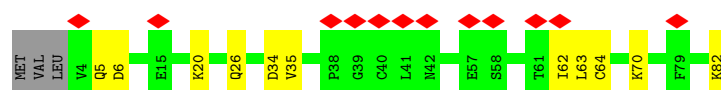
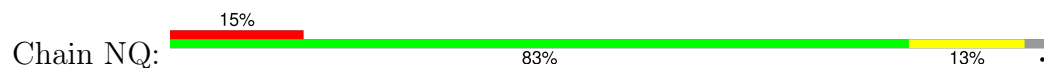
- Molecule 21: Small ribosomal subunit protein eS1A



- Molecule 22: 40S ribosomal protein S19-A

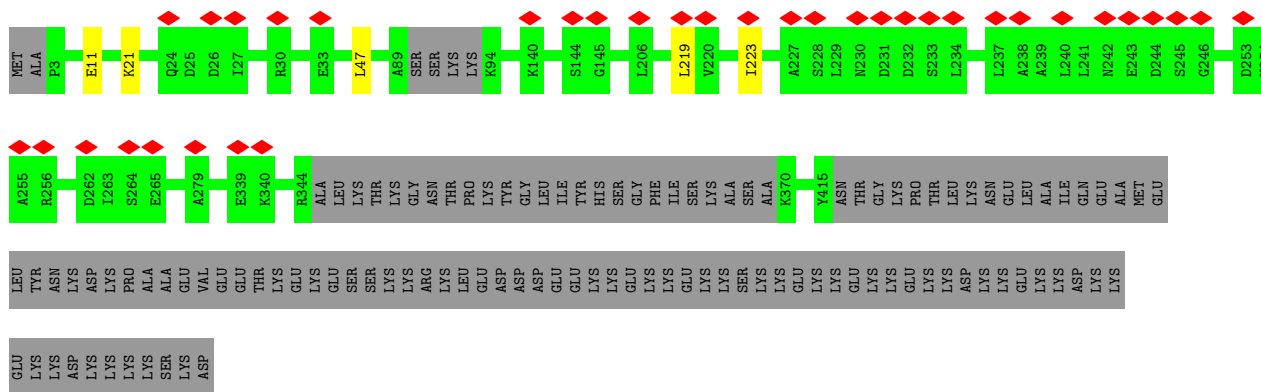


- Molecule 23: 40S ribosomal protein S27-A

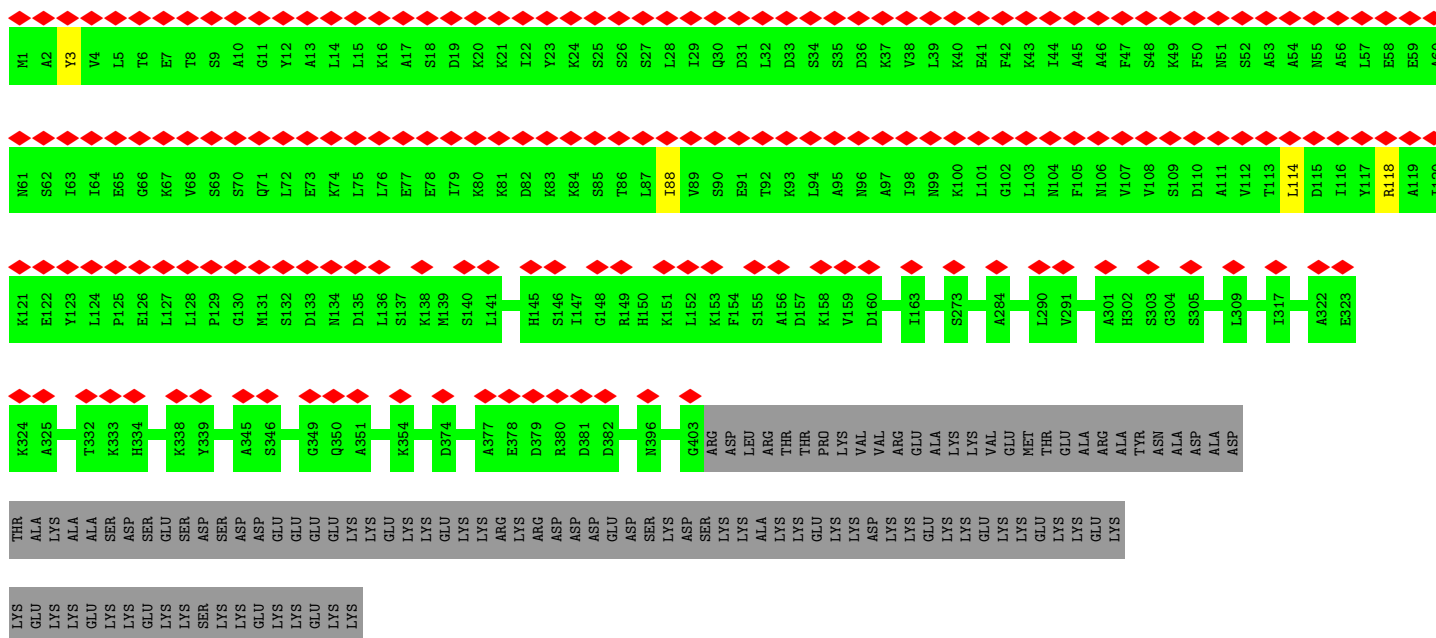
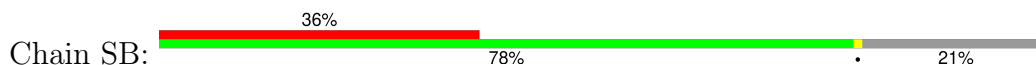


- Molecule 24: Probable ATP-dependent RNA helicase DHR1

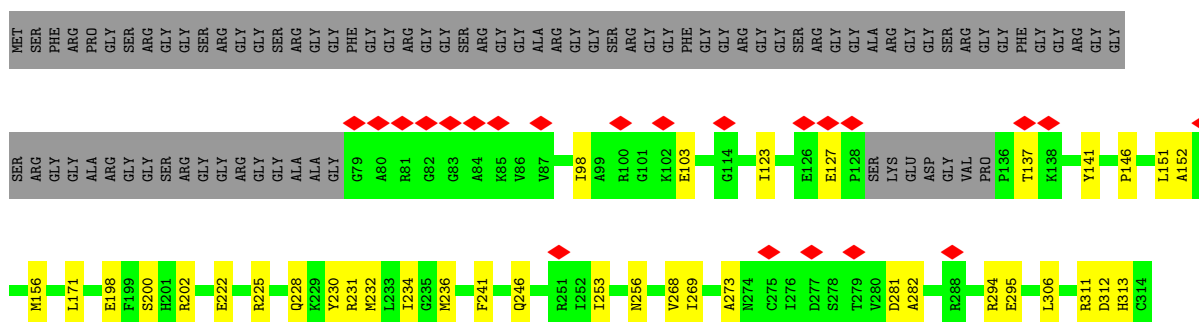


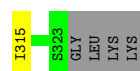


- Molecule 27: Nucleolar protein 58

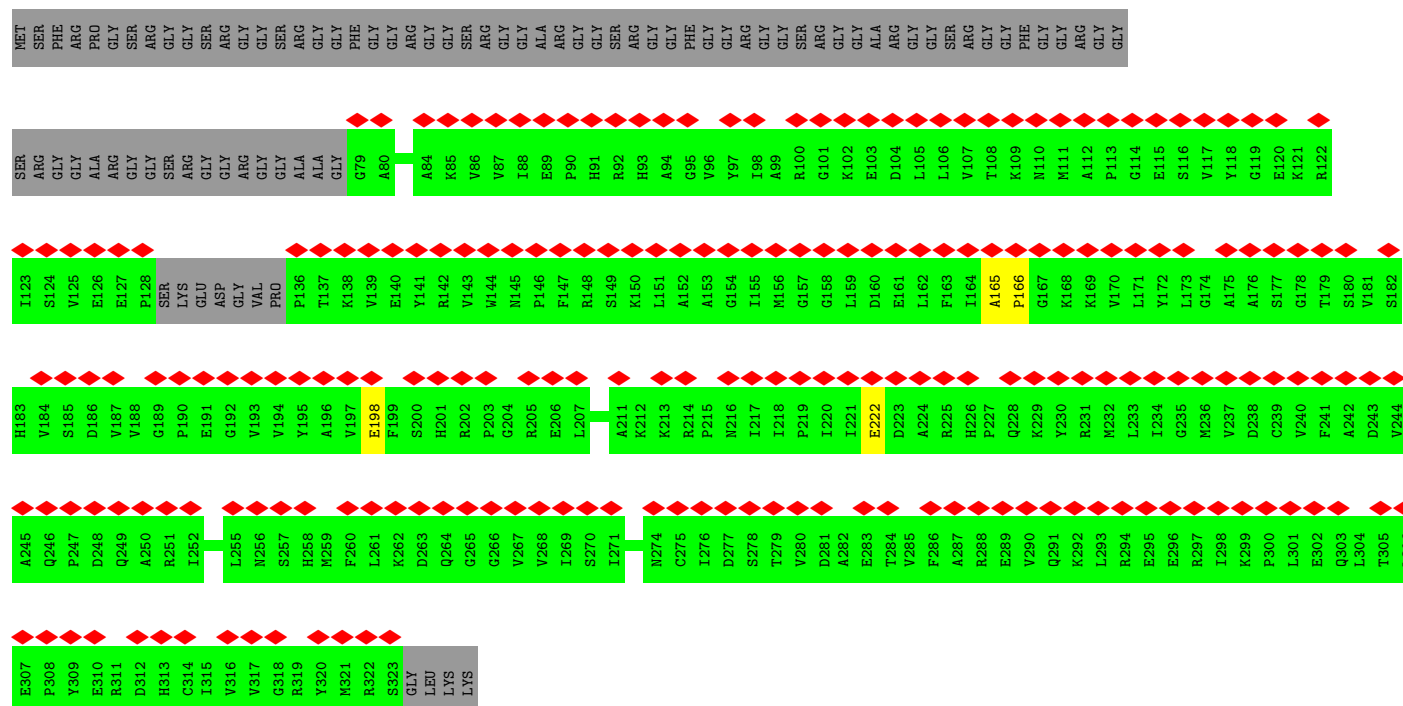
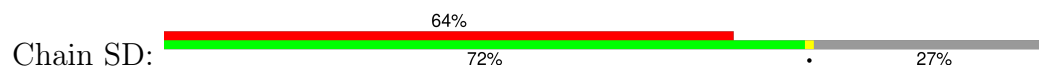


- Molecule 28: rRNA 2'-O-methyltransferase fibrillar

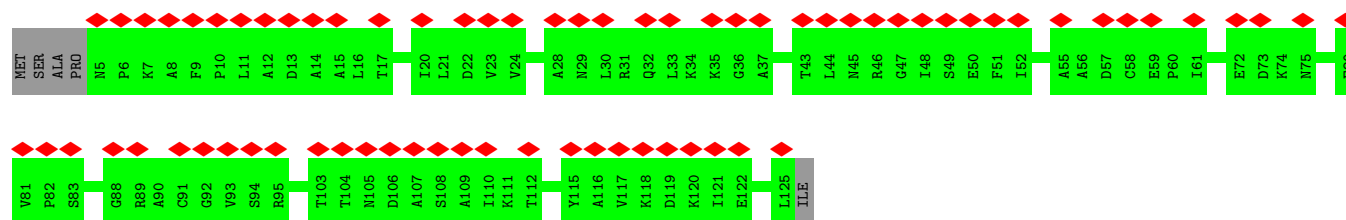




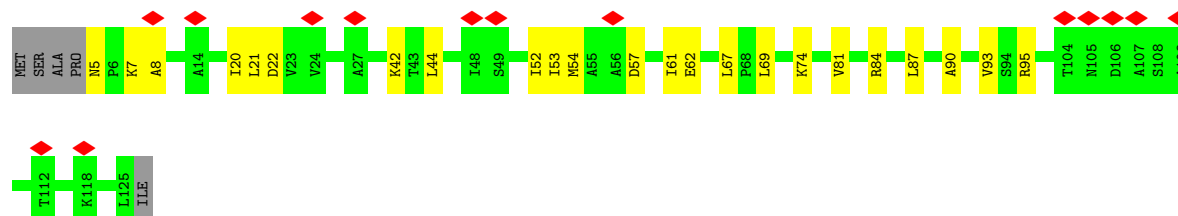
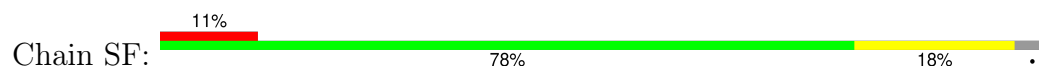
• Molecule 28: rRNA 2'-O-methyltransferase fibrillar



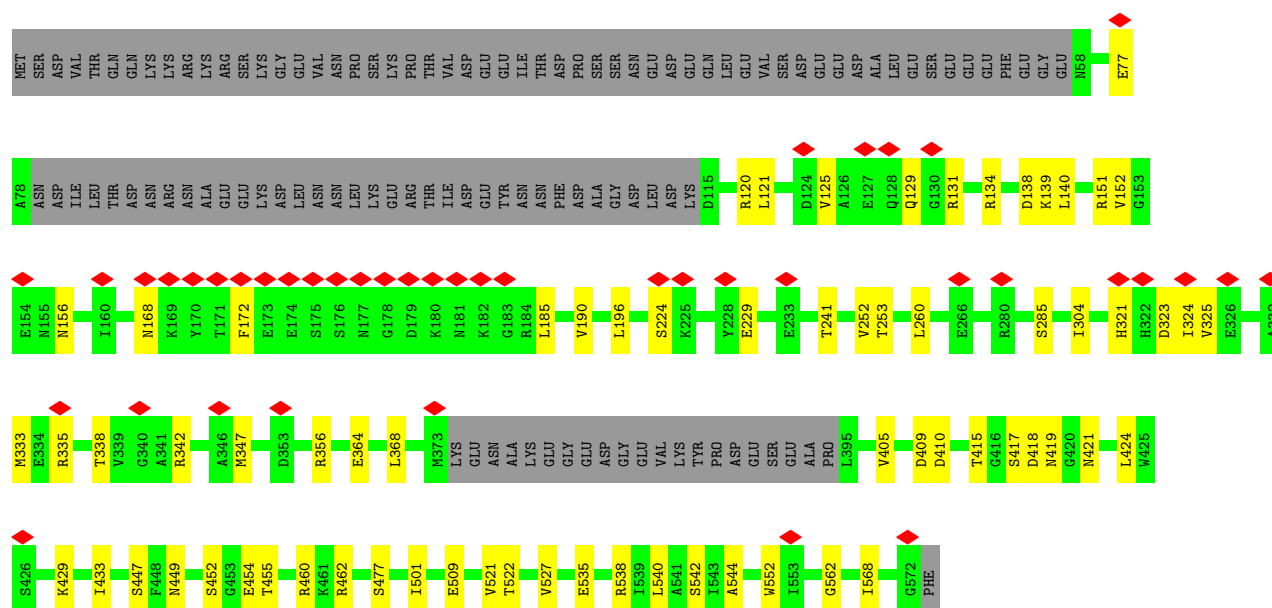
• Molecule 29: 13 kDa ribonucleoprotein-associated protein



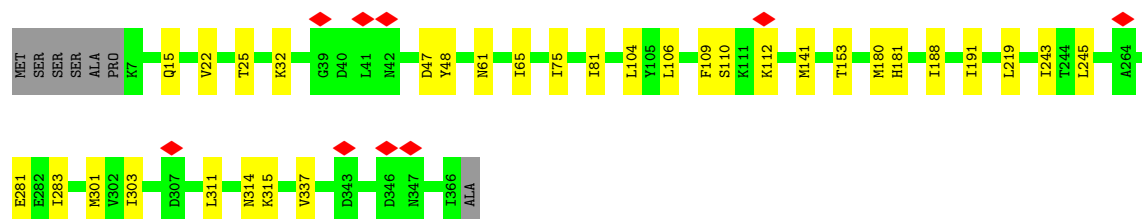
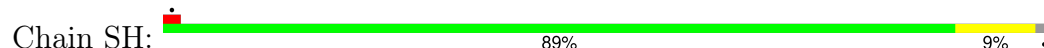
• Molecule 29: 13 kDa ribonucleoprotein-associated protein



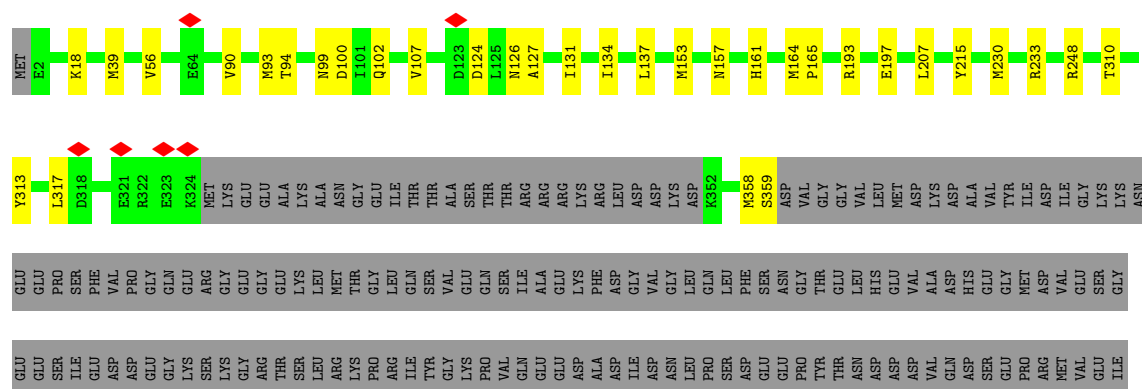
Chain SG:

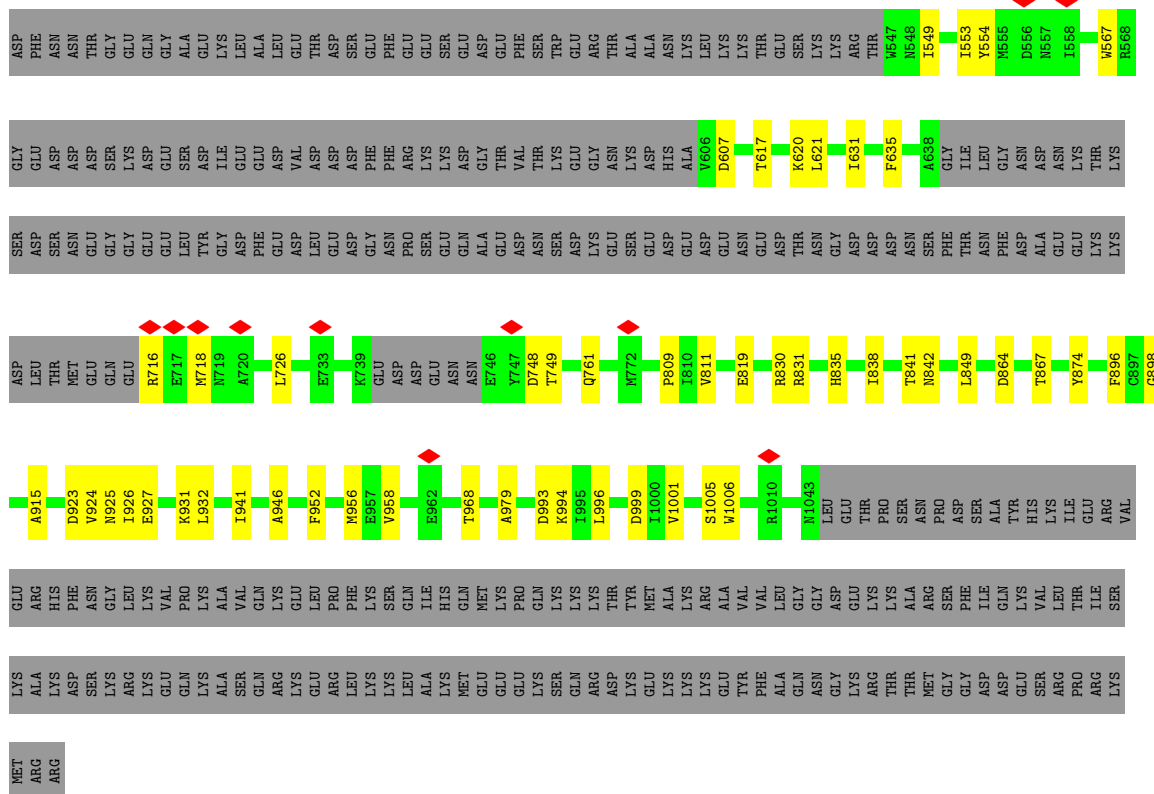


Chain SH:

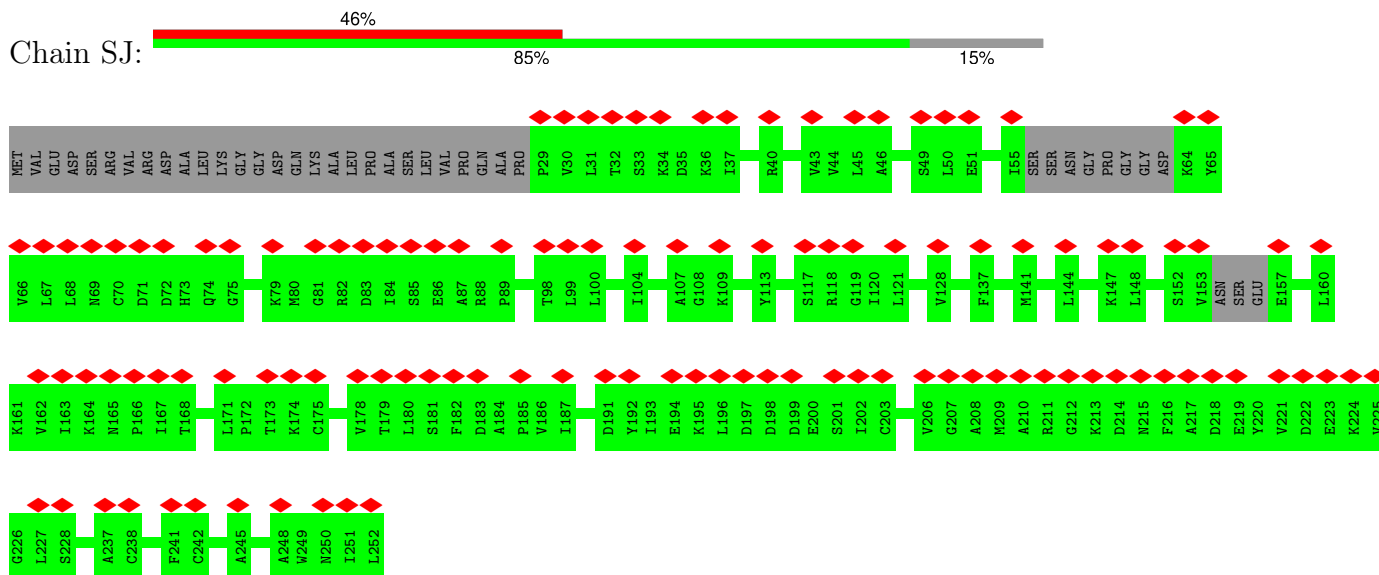


Chain SI:

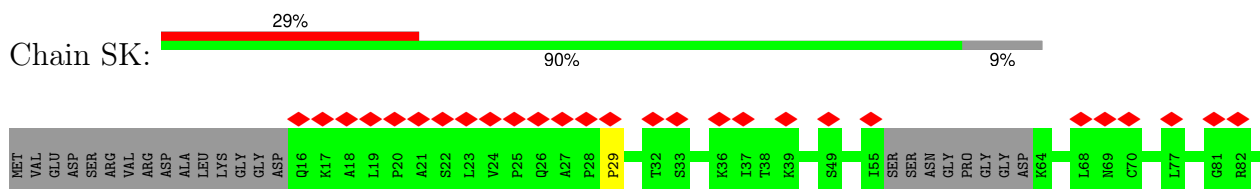


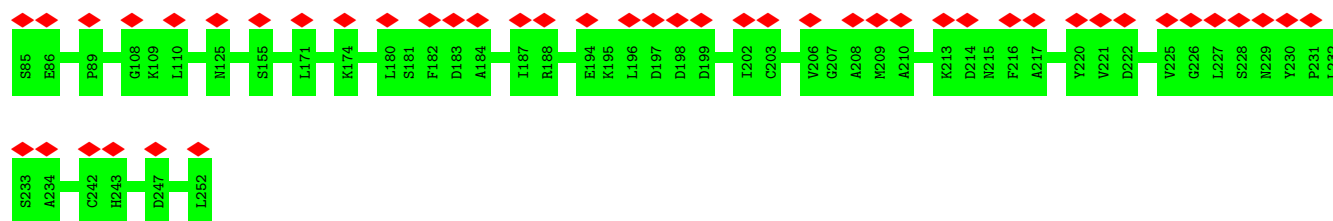


- Molecule 33: Ribosomal RNA small subunit methyltransferase NEP1



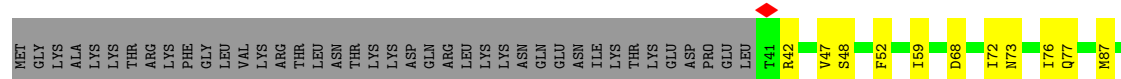
- Molecule 33: Ribosomal RNA small subunit methyltransferase NEP1





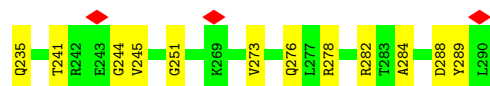
• Molecule 34: rRNA-processing protein FCF1

Chain SL: 63% 15% 22%



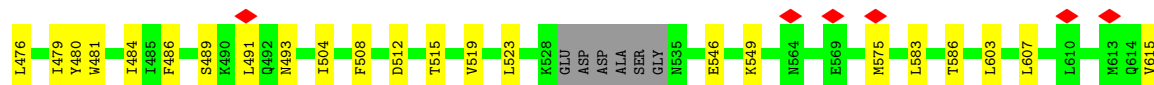
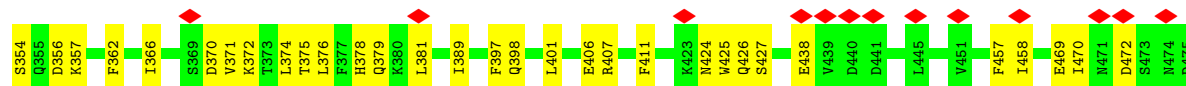
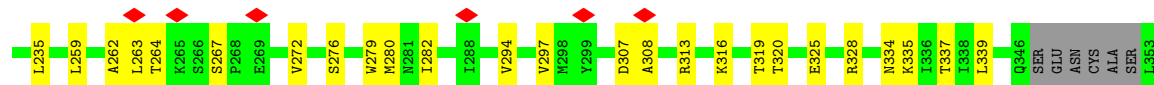
• Molecule 35: U3 small nucleolar ribonucleoprotein protein IMP4

Chain SM: 5% 65% 11% 24%



• Molecule 36: U3 small nucleolar RNA-associated protein 20

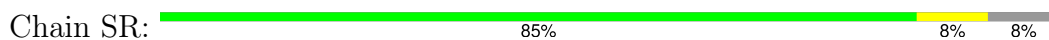
Chain SP: 32% 6% 62%





[illegible]

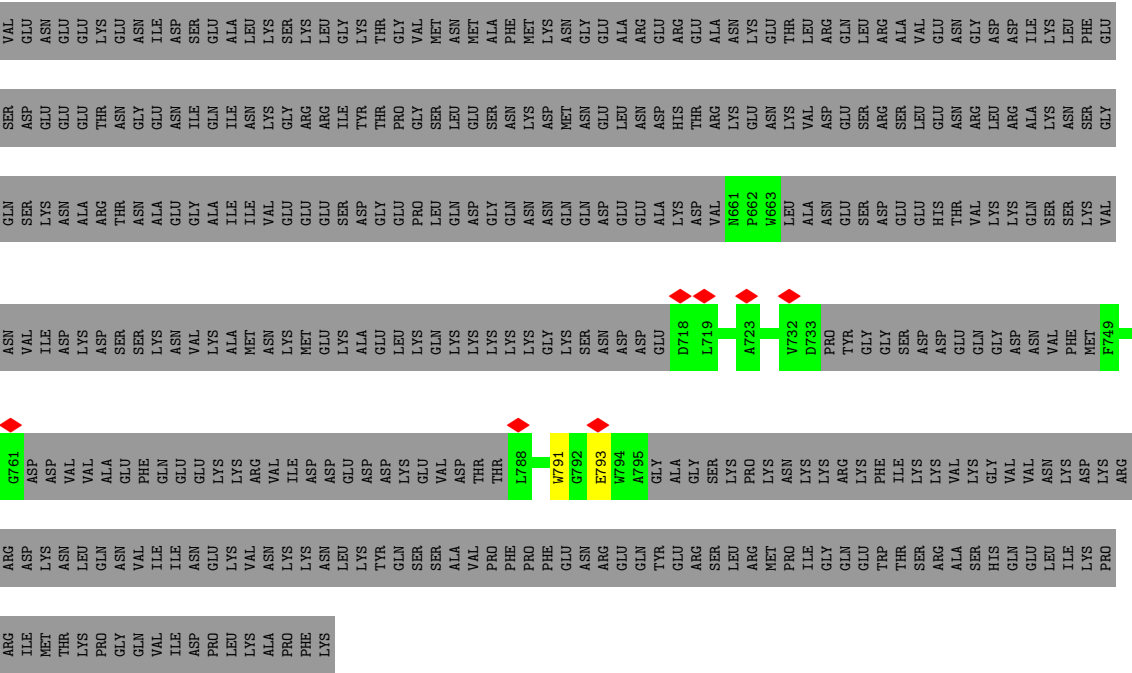
- Molecule 37: 40S ribosomal protein S23-A



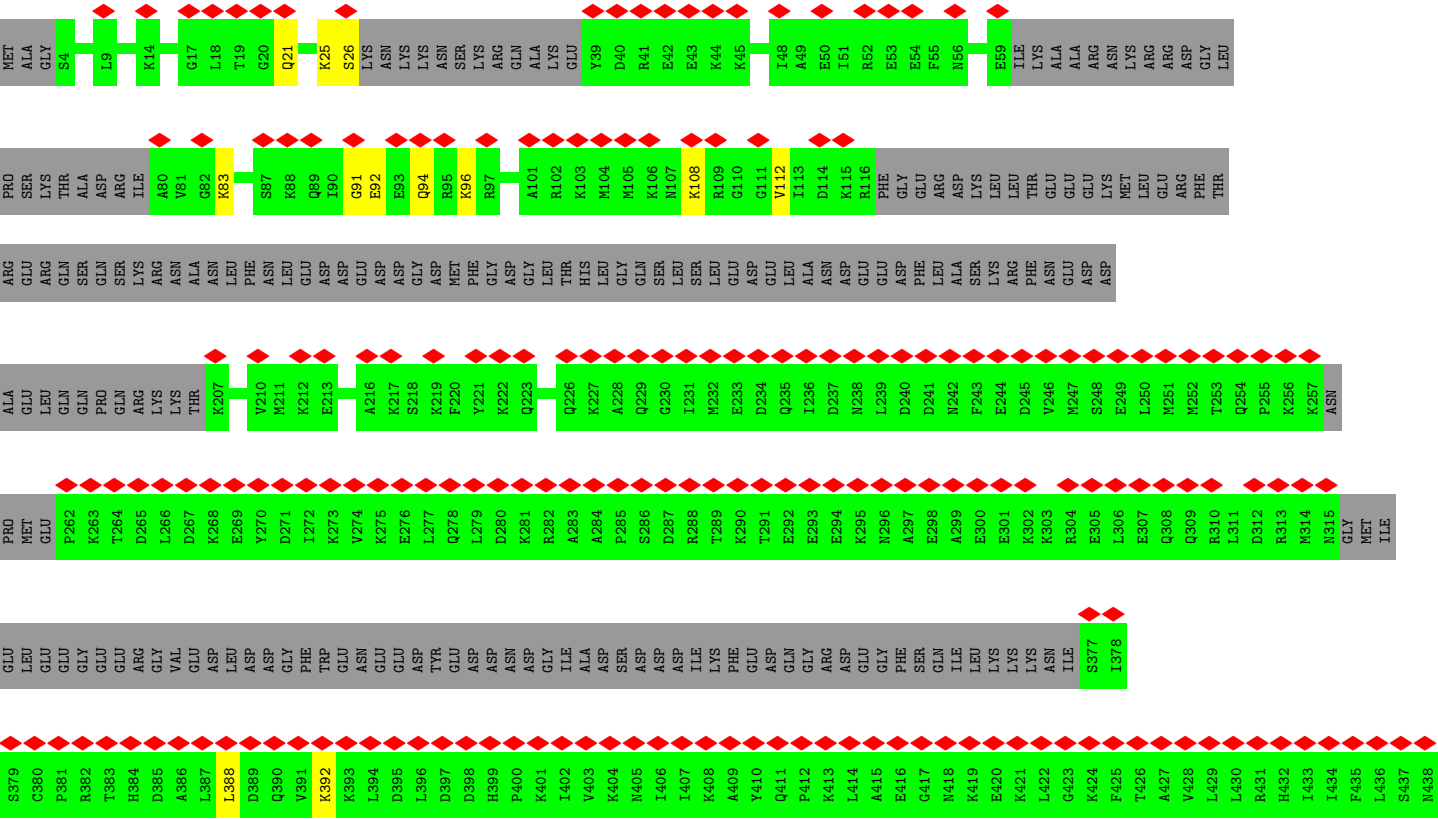
- Molecule 38: U3 small nucleolar RNA-associated protein 14

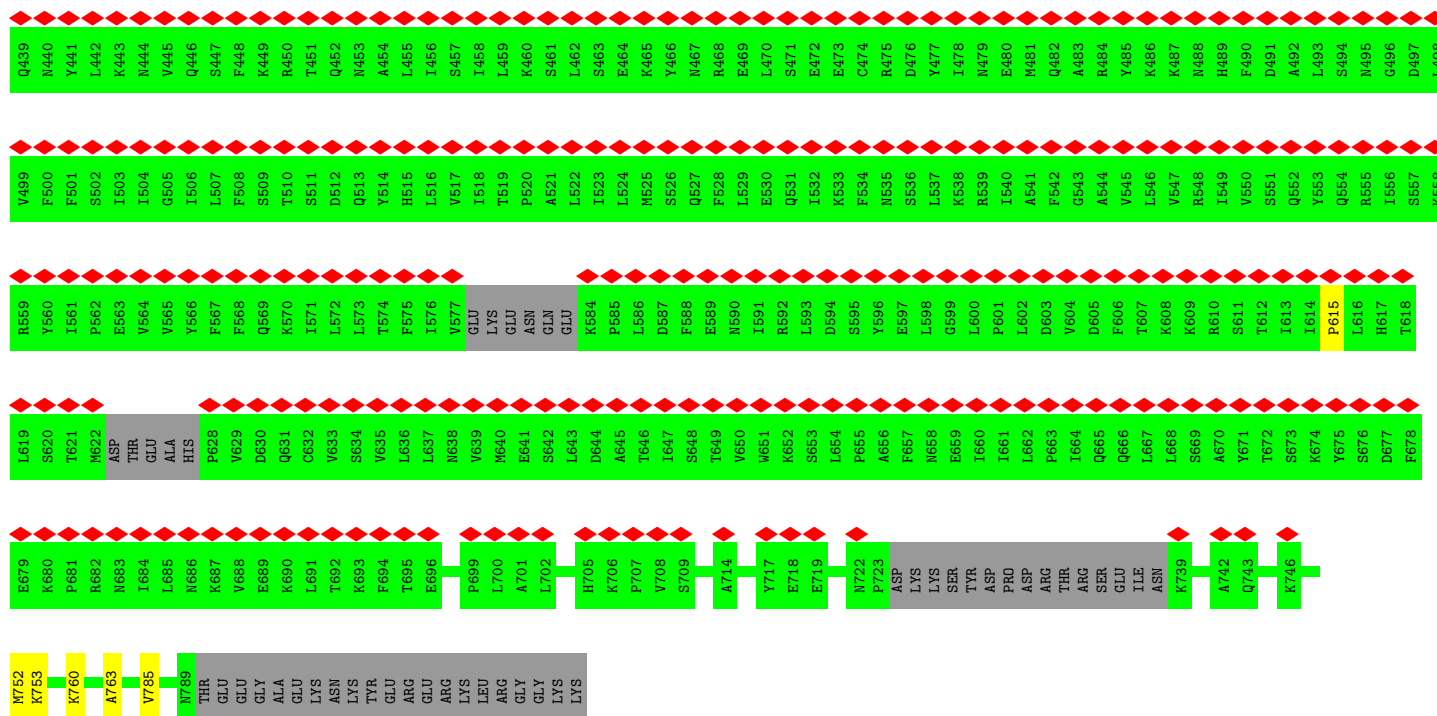


GLU	ILE	LYS	GLU	ILE	MET
GLU	VAL	LEU	GLU	ASP	ALA
LEU	GLN	SER	ASP	GLU	LYS
SER	ASN	LEU	PRO	GLN	LYS
THR	ARG	THR	PHE	ASP	LYS
ALA	ARG	ASP	GLU	LEU	SER
LYS	ARG	MET	GLU	MET	LYS
MET	ALA	MET	ILE	PRO	SER
THR	HIS	ASN	SER	LEU	ARG
P370	LEU	VAL	GLU	SER	SER
+	ILE	ASP	ASP	GLN	LYS
L382	PHE	ASP	GLU	VAL	SER
L386	PRO	ARG	GLU	TRP	SER
M387	LEU	GLN	ASP	GLU	ARG
F388	ASN	VAL	ILE	MET	ARG
R389	LYS	VAL	GLU	ASP	VAL
+	ASN	ILE	LEU	GLU	LEU
K393	PRO	GLU	ASN	LYS	ASP
+	THR	ASN	THR	THR	ALA
L397	GLU	ALA	ILE	ALA	LEU
K403	HIS	ASN	THR	GLN	GLN
+	ASN	LEU	SER	SER	LEU
K411	HIS	LEU	LYS	ASN	LEU
E412	ALA	LYS	LEU	GLY	ALA
L413	PHE	GLY	ILE	ASN	GLU
+	ARG	THR	THR	ASP	ARG
S423	THR	TYR	SER	ASP	GLY
+	GLN	GLU	SER	ALA	GLU
S424	ASP	VAL	LYS	ILE	PHE
D425	VAL	VAL	ALA	PRO	ASP
E426	VAL	PRO	PRO	GLN	ASN
+	PRO	LEU	LYS	LEU	ASN
R439	GLN	PRO	ARG	LYS	SER
M440	THR	GLN	LEU	LEU	ASP
+	GLU	ARG	ASP	PHE	ASN
R466	LEU	ILE	GLN	GLN	ASP
+	GLN	GLN	THR	THR	LYS
R474	GLU	GLN	GLY	ASP	ARG
+	LYS	ARG	SER	ILE	HIS
K482	VAL	HIS	GLY	SER	ASP
MET	ASN	ASP	GLU	GLU	ALA
LEU	GLN	ARG	ALA	SER	LYS
ASP	VAL	LYS	ASN	GLY	ARG
ARG	LEU	ALA	GLU	SER	ARG
ASN	GLN	LYS	TYR	ASN	GLY
SER	GLU	TYR	VAL	SER	GLY
ASP	SER	GLU	LEU	ASP	THR
ASP	ASN	ILE	PRO	GLU	VAL
GLU	LEU	SER	PHE	GLN	VAL
GLU	ALA	GLN	ALA	GLU	LEU
ASP	ASN	ARG	ASN	SER	LEU
GLY	PRO	GLU	ALA	SER	LYS
ARG	GLU	VAL	ALA	GLU	ARG
VAL	LYS	SER	ALA	SER	GLY
GLN	ASP	LYS	GLY	ASP	LYS
THR	SER	TRP	ALA	THR	GLY
LEU	LYS	ASN	SER	GLY	THR
SER	PHE	ASP	GLY	GLU	THR

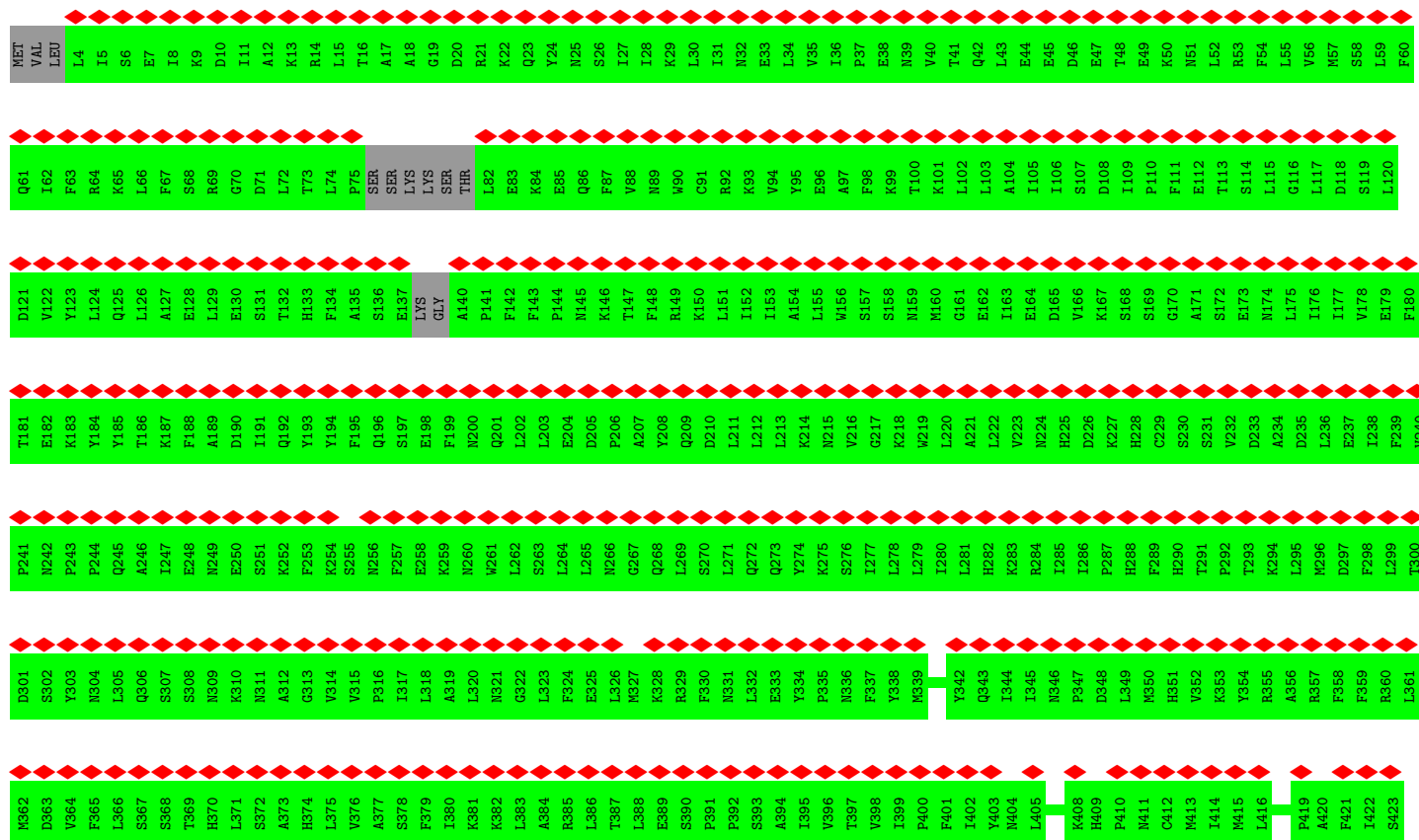


● Molecule 39: Nucleolar complex protein 14





● Molecule 40: Nucleolar complex protein 4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.203	Depositor
Minimum map value	-0.289	Depositor
Average map value	0.094	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7G, SEP, GTP, 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	L1	0.14	0/33399	0.27	0/52011
2	L2	0.10	0/2078	0.23	0/3226
3	L3	0.14	0/825	0.34	0/1109
4	L4	0.15	0/2097	0.35	0/2823
5	L5	0.18	0/1575	0.42	0/2127
6	L6	0.15	0/1855	0.34	0/2478
7	L7	0.18	0/1517	0.41	0/2044
8	L8	0.15	0/1462	0.35	0/1955
9	L9	0.16	0/1495	0.36	0/2003
10	LC	0.14	0/945	0.35	0/1274
11	LD	0.16	0/1145	0.32	0/1543
12	LE	0.17	0/1039	0.41	0/1395
13	LF	0.16	0/1060	0.35	0/1412
14	LG	0.12	0/492	0.31	0/659
15	N2	0.09	0/109	0.24	0/166
16	NA	0.18	0/916	0.43	0/1228
17	NB	0.17	0/694	0.39	0/912
18	NF	0.15	0/1215	0.31	0/1638
19	NG	0.17	0/952	0.35	0/1279
20	NL	0.17	0/2305	0.36	0/3116
21	NM	0.15	0/1713	0.36	0/2305
22	NP	0.18	0/1056	0.41	0/1416
23	NQ	0.19	0/605	0.35	0/817
24	NS	0.15	0/4994	0.38	0/6900
25	NW	0.17	0/564	0.41	0/758
26	SA	0.14	0/1931	0.30	0/2693
27	SB	0.13	0/2015	0.31	0/2813
28	SC	0.16	0/1885	0.39	0/2543
28	SD	0.12	0/1210	0.31	0/1689
29	SE	0.13	0/621	0.32	0/871
29	SF	0.15	0/928	0.34	0/1262
30	SG	0.13	0/3735	0.33	0/5028

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SH	0.14	0/2832	0.32	0/3825
32	SI	0.14	0/5879	0.33	0/7920
33	SJ	0.13	0/1080	0.33	0/1508
33	SK	0.17	0/1170	0.42	1/1639 (0.1%)
34	SL	0.18	0/1193	0.40	0/1611
35	SM	0.15	0/1792	0.34	0/2425
36	SP	0.14	0/7933	0.33	2/10729 (0.0%)
37	SR	0.13	0/1069	0.32	0/1427
38	SS	0.15	0/1184	0.40	0/1567
39	ST	0.12	0/3338	0.30	0/4580
40	SU	0.11	0/2726	0.30	0/3825
41	SW	0.17	0/1470	0.38	0/1980
42	SZ	0.12	0/1326	0.32	0/1859
All	All	0.14	0/111424	0.32	3/158388 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	SK	29	PRO	CA-N-CD	-9.49	98.71	112.00
36	SP	2	ALA	CA-C-N	7.26	130.73	120.28
36	SP	2	ALA	C-N-CA	7.26	130.73	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	L1	29868	0	15038	173	0
2	L2	1891	0	955	12	0
3	L3	815	0	850	13	0
4	L4	2056	0	2140	21	0
5	L5	1558	0	1629	25	0
6	L6	1831	0	1931	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L7	1492	0	1581	20	0
8	L8	1437	0	1458	22	0
9	L9	1470	0	1554	20	0
10	LC	930	0	983	12	0
11	LD	1119	0	1186	13	0
12	LE	1022	0	1060	22	0
13	LF	1046	0	1114	11	0
14	LG	490	0	529	1	0
15	N2	100	0	51	0	0
16	NA	907	0	893	23	0
17	NB	687	0	747	15	0
18	NF	1192	0	1255	9	0
19	NG	941	0	979	14	0
20	NL	2262	0	2330	18	0
21	NM	1688	0	1756	26	0
22	NP	1040	0	1057	15	0
23	NQ	595	0	613	9	0
24	NS	4947	0	3060	26	0
25	NW	556	0	596	11	0
26	SA	1924	0	946	3	0
27	SB	2009	0	1010	2	0
28	SC	1850	0	1889	27	0
28	SD	1198	0	625	2	0
29	SE	615	0	331	0	0
29	SF	916	0	964	19	0
30	SG	3663	0	3684	48	0
31	SH	2781	0	2878	26	0
32	SI	5748	0	5873	72	0
33	SJ	1074	0	514	0	0
33	SK	1160	0	570	0	0
34	SL	1171	0	1229	23	0
35	SM	1756	0	1765	23	0
36	SP	7764	0	7883	98	0
37	SR	1052	0	1120	12	0
38	SS	1186	0	1134	14	0
39	ST	3316	0	2190	21	0
40	SU	2703	0	1302	1	0
41	SW	1444	0	1526	22	0
42	SZ	1314	0	649	2	0
43	L1	46	0	0	0	0
43	SI	1	0	0	0	0
44	NQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	SL	1	0	0	0	0
45	SI	32	0	12	0	0
All	All	106665	0	83439	773	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (773) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:976:G:H1	1:L1:1023:A:HO2'	1.15	0.91
1:L1:904:G:N2	1:L1:1000:C:O2	2.06	0.89
5:L5:63:GLN:NE2	5:L5:66:GLN:OE1	2.06	0.88
13:LF:36:SER:OG	13:LF:39:GLU:OE1	1.93	0.87
1:L1:191:C:N3	8:L8:137:LYS:NZ	2.24	0.86
1:L1:1034:C:HO2'	12:LE:2:THR:N	1.75	0.85
35:SM:235:GLN:NE2	35:SM:251:GLY:O	2.11	0.84
1:L1:127:G:N7	6:L6:202:ARG:NH2	2.25	0.84
32:SI:864:ASP:OD2	32:SI:867:THR:OG1	1.96	0.84
29:SF:52:ILE:HG21	29:SF:67:LEU:HD23	1.60	0.83
7:L7:67:LEU:HD22	7:L7:94:ALA:HB2	1.61	0.81
41:SW:202:ILE:HG23	41:SW:226:LEU:HD21	1.62	0.81
1:L1:622:A:O2'	1:L1:1032:G:OP2	1.98	0.80
32:SI:932:LEU:O	32:SI:1005:SER:OG	1.98	0.80
29:SF:7:LYS:NZ	29:SF:62:GLU:OE2	2.14	0.80
20:NL:162:ARG:O	20:NL:176:SER:OG	2.00	0.79
11:LD:80:MET:SD	11:LD:83:THR:OG1	2.39	0.79
5:L5:196:GLU:OE2	5:L5:200:ASN:ND2	2.15	0.79
32:SI:56:VAL:HG22	37:SR:52:ILE:HD12	1.65	0.79
13:LF:86:GLU:OE2	13:LF:90:ARG:NE	2.15	0.79
3:L3:28:ILE:HD13	3:L3:61:LEU:HD11	1.65	0.79
9:L9:139:GLN:NE2	9:L9:140:ILE:O	2.17	0.78
5:L5:73:THR:OG1	5:L5:91:GLU:OE2	2.00	0.78
30:SG:522:THR:OG1	30:SG:542:SER:OG	2.02	0.78
36:SP:149:GLU:OE2	36:SP:153:ASN:ND2	2.18	0.77
1:L1:904:G:N1	1:L1:1000:C:N3	2.33	0.77
1:L1:780:A:OP1	30:SG:335:ARG:NH2	2.18	0.77
11:LD:101:GLU:OE1	37:SR:12:ALA:N	2.18	0.76
28:SC:294:ARG:NH1	34:SL:131:SER:OG	2.18	0.76
20:NL:254:ASN:ND2	20:NL:317:PHE:O	2.19	0.76
6:L6:161:GLU:OE1	6:L6:168:THR:OG1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:NF:140:LYS:NZ	18:NF:142:GLU:OE2	2.18	0.75
20:NL:256:LYS:NZ	20:NL:269:THR:O	2.19	0.75
18:NF:101:HIS:NE2	18:NF:108:ASP:OD2	2.18	0.75
35:SM:241:THR:OG1	35:SM:244:GLY:O	2.01	0.75
1:L1:358:U:O2'	1:L1:360:A:OP1	2.05	0.74
36:SP:264:THR:O	36:SP:313:ARG:NH1	2.19	0.74
1:L1:1779:U:OP2	1:L1:1781:A:N6	2.21	0.74
1:L1:578:U:OP2	32:SI:874:TYR:OH	2.04	0.73
1:L1:1080:U:O2'	1:L1:1082:C:OP1	2.03	0.73
41:SW:154:LYS:NZ	41:SW:177:LEU:O	2.22	0.73
1:L1:330:G:OP2	8:L8:172:ARG:NH1	2.22	0.73
12:LE:81:VAL:O	12:LE:122:SER:OG	2.05	0.73
1:L1:1050:G:OP1	23:NQ:70:LYS:NZ	2.14	0.73
1:L1:869:A:OP1	18:NF:94:LYS:NZ	2.20	0.72
11:LD:101:GLU:OE1	37:SR:13:ARG:N	2.21	0.72
1:L1:706:A:N6	1:L1:732:G:O2'	2.23	0.72
6:L6:98:ARG:NH1	6:L6:105:ASP:OD1	2.22	0.72
19:NG:37:GLU:OE1	21:NM:27:LYS:NZ	2.22	0.72
19:NG:31:THR:OG1	19:NG:37:GLU:O	2.06	0.71
1:L1:742:U:O2'	1:L1:743:U:OP1	2.08	0.71
35:SM:123:VAL:HG12	35:SM:125:PRO:HD2	1.71	0.71
36:SP:438:GLU:OE2	36:SP:749:LYS:NZ	2.22	0.71
31:SH:301:MET:HE1	31:SH:311:LEU:HB2	1.73	0.70
25:NW:92:ILE:HD11	25:NW:102:THR:HG23	1.73	0.70
1:L1:392:G:OP2	8:L8:24:LYS:NZ	2.20	0.70
30:SG:333:MET:SD	30:SG:335:ARG:NH1	2.65	0.70
1:L1:810:G:N2	7:L7:108:GLN:OE1	2.24	0.70
1:L1:1471:A:OP1	5:L5:185:ARG:NH1	2.24	0.70
2:L2:0:M7G:O2'	24:NS:96:ARG:NH2	2.25	0.70
1:L1:1540:G:OP2	3:L3:40:ARG:NH2	2.24	0.70
1:L1:447:U:O2'	4:L4:27:TYR:O	2.10	0.70
21:NM:127:VAL:HG13	21:NM:176:VAL:HG11	1.74	0.70
41:SW:169:ASP:OD2	41:SW:170:ASP:N	2.25	0.70
16:NA:352:LYS:NZ	35:SM:284:ALA:O	2.25	0.69
7:L7:99:LEU:O	7:L7:112:ARG:NH2	2.26	0.69
29:SF:57:ASP:O	29:SF:84:ARG:NH1	2.25	0.69
2:L2:253:G:OP2	29:SF:95:ARG:NH2	2.26	0.69
35:SM:276:GLN:O	35:SM:278:ARG:NH1	2.26	0.69
1:L1:72:A:N7	6:L6:167:LYS:NZ	2.40	0.69
9:L9:38:ASN:OD1	9:L9:40:LYS:N	2.25	0.69
1:L1:1584:G:O4'	5:L5:76:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:99:C:OP2	1:L1:378:A:O2'	2.06	0.69
20:NL:156:GLN:NE2	20:NL:158:GLU:OE2	2.25	0.69
1:L1:779:U:O4	13:LF:10:ARG:NH1	2.25	0.69
5:L5:31:GLU:OE2	5:L5:35:GLN:NE2	2.25	0.68
28:SC:311:ARG:O	28:SC:313:HIS:ND1	2.21	0.68
31:SH:104:LEU:HD12	31:SH:141:MET:SD	2.33	0.68
1:L1:1482:C:O2'	10:LC:72:GLY:O	2.12	0.68
1:L1:93:A:O4'	4:L4:3:ARG:NH1	2.25	0.68
3:L3:120:ARG:NH2	39:ST:94:GLN:OE1	2.26	0.68
22:NP:38:LYS:O	22:NP:39:THR:OG1	2.12	0.68
11:LD:30:ARG:NH1	11:LD:31:THR:OG1	2.27	0.68
34:SL:73:ASN:ND2	38:SS:440:MET:O	2.27	0.67
41:SW:204:ARG:NH1	41:SW:250:LEU:O	2.28	0.67
9:L9:53:ARG:NH2	34:SL:91:LEU:O	2.27	0.67
8:L8:89:GLU:OE1	8:L8:92:ARG:NH2	2.28	0.66
1:L1:1778:G:OP2	20:NL:162:ARG:NH2	2.28	0.66
36:SP:424:ASN:OD1	36:SP:427:SER:OG	2.13	0.66
28:SC:202:ARG:NH1	29:SF:69:LEU:O	2.29	0.66
3:L3:17:LEU:O	3:L3:20:THR:OG1	2.08	0.66
19:NG:61:MET:O	19:NG:65:GLN:NE2	2.28	0.66
1:L1:576:G:O3'	16:NA:322:LYS:NZ	2.28	0.66
1:L1:886:U:OP2	21:NM:216:LYS:NZ	2.28	0.66
12:LE:55:ASP:OD2	12:LE:57:ARG:NH1	2.28	0.66
28:SC:151:LEU:HD11	28:SC:241:PHE:CE2	2.29	0.66
23:NQ:5:GLN:NE2	23:NQ:6:ASP:O	2.29	0.66
36:SP:354:SER:OG	36:SP:356:ASP:OD2	2.13	0.66
1:L1:110:U:OP1	1:L1:753:A:O2'	2.13	0.66
1:L1:1616:G:O5'	5:L5:81:ARG:NH1	2.29	0.66
5:L5:74:ALA:O	10:LC:122:ARG:NH2	2.29	0.66
16:NA:373:ILE:HD12	35:SM:245:VAL:HG11	1.78	0.66
1:L1:1480:G:OP1	22:NP:64:HIS:NE2	2.28	0.65
19:NG:114:ARG:NH1	21:NM:69:CYS:SG	2.69	0.65
37:SR:27:ASN:OD1	37:SR:28:ASN:N	2.29	0.65
29:SF:53:ILE:HD11	29:SF:81:VAL:HG13	1.77	0.65
1:L1:539:G:OP2	1:L1:539:G:N2	2.19	0.65
36:SP:489:SER:OG	36:SP:493:ASN:ND2	2.29	0.65
9:L9:94:ASP:OD2	9:L9:95:TYR:N	2.30	0.65
1:L1:1179:G:OP1	39:ST:91:GLY:N	2.30	0.65
12:LE:111:MET:HE1	12:LE:119:LYS:HD3	1.79	0.65
1:L1:1606:C:OP1	35:SM:123:VAL:HG13	1.98	0.64
1:L1:1802:A:OP1	21:NM:115:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SI:617:THR:OG1	32:SI:620:LYS:NZ	2.21	0.64
6:L6:48:TYR:OH	6:L6:119:GLN:O	2.05	0.64
1:L1:1581:C:OP1	35:SM:116:ARG:NH2	2.32	0.63
2:L2:15:U:OP1	38:SS:466:ARG:NH2	2.32	0.63
1:L1:460:A:O2'	4:L4:27:TYR:OH	2.15	0.63
7:L7:38:LEU:HD22	7:L7:77:LEU:HD21	1.81	0.63
28:SC:230:TYR:OH	28:SC:256:ASN:OD1	2.16	0.63
20:NL:157:ARG:NH2	20:NL:203:GLU:OE1	2.31	0.63
1:L1:1085:G:N2	1:L1:1088:A:OP2	2.25	0.62
1:L1:1555:A:O2'	1:L1:1556:A:O5'	2.17	0.62
30:SG:347:MET:HE3	30:SG:356:ARG:NH2	2.14	0.62
4:L4:21:ASP:OD2	4:L4:24:SER:N	2.32	0.62
34:SL:87:MET:O	34:SL:91:LEU:N	2.33	0.62
41:SW:131:ASN:O	41:SW:135:LYS:N	2.30	0.62
21:NM:70:LEU:HD12	21:NM:82:ARG:HB2	1.80	0.62
36:SP:603:LEU:HD23	36:SP:607:LEU:HD23	1.82	0.62
1:L1:1082:C:O2'	1:L1:1083:G:OP1	2.17	0.62
12:LE:30:SER:OG	12:LE:58:SER:O	2.18	0.62
32:SI:124:ASP:OD1	32:SI:126:ASN:N	2.31	0.62
36:SP:491:LEU:HD12	36:SP:491:LEU:O	2.00	0.62
1:L1:1534:G:OP1	3:L3:57:ARG:NH1	2.32	0.62
17:NB:580:ARG:NH1	34:SL:47:VAL:O	2.33	0.62
2:L2:17:G:O2'	38:SS:474:ARG:NH2	2.32	0.62
22:NP:77:ASN:OD1	22:NP:96:ALA:N	2.33	0.62
1:L1:1499:G:OP1	22:NP:122:ARG:NH1	2.33	0.61
1:L1:195:G:N7	8:L8:141:ARG:NH2	2.47	0.61
1:L1:1796:C:N4	41:SW:226:LEU:HD22	2.14	0.61
12:LE:80:ASN:C	12:LE:80:ASN:HD22	2.08	0.61
1:L1:71:A:OP2	6:L6:164:LYS:NZ	2.34	0.61
35:SM:84:MET:HE1	35:SM:137:THR:HG22	1.83	0.61
31:SH:22:VAL:O	31:SH:25:THR:OG1	2.16	0.61
4:L4:212:ASP:OD1	4:L4:216:ASN:N	2.34	0.61
28:SC:281:ASP:OD1	28:SC:282:ALA:N	2.32	0.60
7:L7:134:GLU:N	7:L7:134:GLU:OE1	2.33	0.60
2:L2:321:C:OP2	2:L2:322:A:O2'	2.13	0.60
16:NA:349:ARG:HH12	39:ST:763:ALA:HB2	1.67	0.60
38:SS:793:GLU:OE1	38:SS:793:GLU:N	2.35	0.60
14:LG:29:ARG:HE	14:LG:41:VAL:HG22	1.66	0.60
22:NP:131:ASP:O	22:NP:135:ILE:HD12	2.01	0.60
1:L1:207:U:O2	8:L8:178:ARG:NH2	2.34	0.60
31:SH:47:ASP:OD1	31:SH:48:TYR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:SP:693:GLU:N	36:SP:693:GLU:OE1	2.35	0.60
1:L1:460:A:HO2'	4:L4:27:TYR:HH	1.49	0.60
1:L1:76:A:N7	1:L1:80:A:N6	2.49	0.60
1:L1:959:U:OP2	23:NQ:20:LYS:NZ	2.34	0.60
32:SI:819:GLU:OE1	32:SI:819:GLU:N	2.35	0.60
1:L1:1555:A:O2'	1:L1:1556:A:O4'	2.20	0.60
30:SG:125:VAL:HG21	36:SP:76:THR:HG21	1.82	0.60
1:L1:1147:A:N3	39:ST:21:GLN:NE2	2.49	0.59
28:SD:198:GLU:O	28:SD:222:GLU:N	2.35	0.59
4:L4:103:TYR:CD2	4:L4:189:LEU:HD11	2.37	0.59
7:L7:50:ASP:OD1	7:L7:51:VAL:N	2.35	0.59
18:NF:25:TRP:O	23:NQ:82:LYS:NZ	2.32	0.59
1:L1:159:U:O2'	6:L6:87:ARG:NH1	2.35	0.59
9:L9:157:ASP:OD1	9:L9:158:PHE:N	2.35	0.59
5:L5:53:VAL:HG21	5:L5:59:VAL:HA	1.83	0.59
6:L6:43:ASP:OD1	6:L6:44:GLU:N	2.35	0.59
21:NM:124:ASN:C	21:NM:124:ASN:HD22	2.08	0.59
26:SA:11:GLU:C	28:SC:232:MET:HE1	2.28	0.59
7:L7:7:LYS:NZ	7:L7:39:ARG:O	2.36	0.59
36:SP:376:LEU:O	36:SP:379:GLN:NE2	2.36	0.59
1:L1:1484:G:N2	1:L1:1606:C:O2	2.35	0.59
1:L1:162:A:H3'	1:L1:163:G:H21	1.68	0.58
1:L1:435:C:O4'	32:SI:233:ARG:NH2	2.37	0.58
1:L1:1594:G:O2'	1:L1:1600:A:N1	2.24	0.58
20:NL:263:ASN:O	20:NL:263:ASN:ND2	2.37	0.58
32:SI:56:VAL:HG23	37:SR:101:GLU:CD	2.28	0.58
32:SI:831:ARG:NH1	32:SI:835:HIS:O	2.36	0.58
1:L1:594:A:OP1	9:L9:38:ASN:ND2	2.36	0.58
1:L1:1536:G:OP1	25:NW:36:ALA:N	2.37	0.58
6:L6:18:ILE:HG21	6:L6:24:ILE:HD11	1.85	0.58
1:L1:1100:G:O2'	12:LE:74:VAL:O	2.16	0.58
11:LD:55:ASP:OD2	11:LD:58:CYS:N	2.37	0.58
32:SI:923:ASP:OD1	32:SI:924:VAL:N	2.37	0.58
36:SP:897:PHE:CZ	36:SP:901:ILE:HD11	2.39	0.58
30:SG:224:SER:OG	30:SG:229:GLU:OE1	2.21	0.58
1:L1:501:U:O2'	1:L1:502:U:OP2	2.19	0.57
1:L1:738:G:O2'	1:L1:739:G:OP1	2.22	0.57
8:L8:85:PRO:O	11:LD:11:ARG:NH1	2.36	0.57
21:NM:133:TYR:HD2	21:NM:217:LEU:HD11	1.68	0.57
1:L1:1169:G:N1	1:L1:1575:G:OP2	2.36	0.57
1:L1:273:G:OP1	36:SP:185:LYS:NZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:NM:108:ASP:OD1	21:NM:109:LYS:N	2.38	0.57
30:SG:121:LEU:HD22	36:SP:78:PRO:HB2	1.86	0.57
31:SH:219:LEU:HD11	32:SI:635:PHE:CD2	2.39	0.57
31:SH:243:ILE:HD11	31:SH:245:LEU:HD21	1.87	0.57
1:L1:1098:U:O2'	34:SL:77:GLN:O	2.22	0.57
10:LC:10:PHE:CE1	10:LC:19:VAL:HG22	2.40	0.57
32:SI:849:LEU:HD23	32:SI:896:PHE:HB3	1.87	0.57
12:LE:31:SER:O	12:LE:35:ILE:HD12	2.04	0.56
16:NA:383:ARG:NH1	35:SM:213:GLY:O	2.38	0.56
31:SH:337:VAL:N	32:SI:554:TYR:OH	2.37	0.56
32:SI:193:ARG:NH1	32:SI:197:GLU:OE2	2.38	0.56
2:L2:245:U:O4	2:L2:246:A:N6	2.38	0.56
3:L3:72:ILE:HD13	3:L3:79:TYR:CD2	2.41	0.56
4:L4:103:TYR:O	4:L4:182:TYR:OH	2.22	0.56
5:L5:140:THR:HG21	5:L5:175:LEU:CD2	2.36	0.56
31:SH:219:LEU:HD21	32:SI:635:PHE:CE2	2.40	0.56
36:SP:583:LEU:O	36:SP:586:THR:OG1	2.15	0.56
1:L1:39:A:OP1	9:L9:3:ARG:NH2	2.37	0.56
22:NP:38:LYS:NZ	22:NP:43:ASN:O	2.31	0.56
27:SB:3:TYR:O	27:SB:88:ILE:N	2.36	0.56
1:L1:1011:G:O2'	24:NS:134:GLY:O	2.19	0.56
1:L1:1608:U:OP1	10:LC:15:SER:OG	2.20	0.56
16:NA:381:LEU:O	35:SM:213:GLY:N	2.37	0.56
28:SC:253:ILE:HD13	28:SC:269:ILE:HD12	1.88	0.56
29:SF:62:GLU:OE2	30:SG:452:SER:OG	2.17	0.56
1:L1:221:A:OP2	1:L1:832:U:O2'	2.13	0.55
20:NL:156:GLN:HE21	20:NL:202:VAL:HG21	1.71	0.55
21:NM:124:ASN:O	21:NM:124:ASN:ND2	2.33	0.55
32:SI:841:THR:HG22	32:SI:842:ASN:OD1	2.06	0.55
36:SP:469:GLU:OE2	36:SP:470:ILE:N	2.40	0.55
38:SS:393:LYS:O	38:SS:397:LEU:HD13	2.06	0.55
20:NL:284:VAL:HG23	20:NL:309:ALA:HB1	1.89	0.55
1:L1:332:U:OP1	8:L8:31:ARG:NH1	2.38	0.55
3:L3:41:ARG:NH2	22:NP:36:ILE:O	2.39	0.55
24:NS:87:SER:O	24:NS:90:SER:OG	2.17	0.55
21:NM:70:LEU:HD21	21:NM:84:ILE:HD11	1.88	0.55
1:L1:406:U:O2'	6:L6:94:ARG:NH2	2.39	0.55
21:NM:122:GLU:OE2	21:NM:213:ARG:NH1	2.39	0.55
32:SI:100:ASP:OD2	32:SI:102:GLN:NE2	2.40	0.55
41:SW:167:ASP:OD1	41:SW:168:LEU:N	2.39	0.55
1:L1:388:G:OP2	1:L1:423:G:O2'	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:NW:53:GLU:O	25:NW:56:THR:OG1	2.13	0.54
1:L1:359:A:O2'	32:SI:39:MET:HE1	2.08	0.54
4:L4:98:ASN:ND2	4:L4:116:ASP:OD1	2.38	0.54
7:L7:64:VAL:HG13	7:L7:65:PRO:HD3	1.88	0.54
10:LC:101:SER:O	10:LC:105:LEU:HD23	2.06	0.54
30:SG:196:LEU:CD2	30:SG:253:THR:HG21	2.38	0.54
1:L1:705:U:HO2'	1:L1:706:A:H8	1.56	0.54
8:L8:20:GLN:NE2	8:L8:22:ARG:O	2.40	0.54
32:SI:952:PHE:HD2	32:SI:958:VAL:HG22	1.73	0.54
36:SP:749:LYS:O	36:SP:756:SER:OG	2.10	0.54
1:L1:9:U:O2'	1:L1:11:A:OP2	2.21	0.54
32:SI:996:LEU:N	32:SI:999:ASP:OD2	2.38	0.54
4:L4:230:GLU:N	4:L4:230:GLU:OE1	2.41	0.54
11:LD:94:ILE:HD12	37:SR:12:ALA:HB3	1.89	0.54
16:NA:345:LEU:HD21	32:SI:932:LEU:HD23	1.89	0.54
16:NA:356:VAL:HG21	39:ST:92:GLU:OE2	2.07	0.54
9:L9:55:ALA:O	9:L9:59:LEU:HD23	2.08	0.54
32:SI:549:ILE:HD13	32:SI:567:TRP:CE2	2.43	0.54
36:SP:615:VAL:CG2	36:SP:619:LEU:HD23	2.38	0.54
41:SW:97:ARG:NH2	41:SW:153:GLN:OE1	2.41	0.54
1:L1:512:A:OP1	9:L9:170:GLY:N	2.39	0.53
36:SP:636:ARG:O	36:SP:640:ILE:HD12	2.09	0.53
17:NB:544:ILE:HG23	32:SI:153:MET:HE1	1.91	0.53
1:L1:861:U:O2'	12:LE:56:HIS:O	2.26	0.53
1:L1:1003:A:C6	41:SW:242:MET:HE1	2.44	0.53
10:LC:51:PRO:O	10:LC:55:VAL:HG22	2.09	0.53
17:NB:594:GLU:OE2	17:NB:598:ILE:N	2.41	0.53
29:SF:52:ILE:HG22	29:SF:54:MET:SD	2.49	0.53
32:SI:164:MET:HE3	32:SI:165:PRO:HD2	1.90	0.53
1:L1:1159:C:N4	35:SM:184:GLU:OE2	2.40	0.53
1:L1:1521:G:O2'	1:L1:1523:G:OP2	2.20	0.53
2:L2:0:M7G:H82	2:L2:1:G:C1'	2.39	0.53
12:LE:80:ASN:O	12:LE:80:ASN:ND2	2.33	0.53
32:SI:93:MET:HE1	32:SI:107:VAL:HG21	1.90	0.53
1:L1:1482:C:O2'	10:LC:77:GLN:NE2	2.41	0.53
19:NG:32:ASP:OD1	19:NG:33:LEU:N	2.38	0.53
28:SC:228:GLN:O	28:SC:231:ARG:NH1	2.39	0.53
32:SI:748:ASP:OD1	32:SI:749:THR:N	2.41	0.53
7:L7:168:SER:O	7:L7:172:VAL:HG23	2.09	0.53
36:SP:864:ASP:OD1	36:SP:865:VAL:N	2.39	0.53
16:NA:409:LEU:HA	16:NA:412:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SH:219:LEU:HD11	32:SI:635:PHE:CG	2.43	0.53
7:L7:16:LEU:O	7:L7:20:VAL:HG23	2.09	0.53
32:SI:716:ARG:N	32:SI:718:MET:SD	2.83	0.53
42:SZ:444:VAL:O	42:SZ:448:GLY:N	2.41	0.53
6:L6:18:ILE:HG23	6:L6:23:ARG:HD2	1.92	0.52
30:SG:190:VAL:HG12	30:SG:196:LEU:HD23	1.90	0.52
32:SI:137:LEU:HD13	32:SI:230:MET:HE1	1.91	0.52
36:SP:963:ASP:OD1	36:SP:964:PHE:N	2.41	0.52
30:SG:321:HIS:HD1	30:SG:325:VAL:HG22	1.74	0.52
36:SP:316:LYS:O	36:SP:319:THR:OG1	2.27	0.52
17:NB:598:ILE:HG21	28:SC:98:ILE:HD13	1.90	0.52
31:SH:153:THR:O	31:SH:153:THR:HG23	2.08	0.52
6:L6:76:LEU:N	24:NS:61:GLU:OE1	2.42	0.52
30:SG:409:ASP:OD1	30:SG:410:ASP:N	2.42	0.52
7:L7:17:GLU:HA	7:L7:46:ILE:HD12	1.91	0.52
1:L1:512:A:O2'	9:L9:133:HIS:NE2	2.32	0.52
5:L5:94:THR:HG22	5:L5:114:ILE:HG13	1.91	0.52
18:NF:135:LEU:HD21	18:NF:139:TRP:CD2	2.45	0.52
30:SG:140:LEU:HD11	30:SG:568:ILE:HG21	1.91	0.52
1:L1:410:A:O3'	24:NS:11:LYS:NZ	2.42	0.52
1:L1:1463:C:O3'	39:ST:83:LYS:NZ	2.43	0.52
32:SI:925:ASN:OD1	32:SI:926:ILE:N	2.43	0.52
36:SP:389:ILE:O	36:SP:389:ILE:HG22	2.10	0.52
36:SP:922:MET:HE3	36:SP:926:LEU:HD21	1.92	0.52
25:NW:46:LYS:NZ	25:NW:69:LEU:O	2.42	0.51
39:ST:615:PRO:HA	40:SU:551:ALA:HB3	1.92	0.51
1:L1:277:U:O2'	1:L1:278:U:OP1	2.25	0.51
1:L1:1473:U:OP2	5:L5:189:THR:OG1	2.24	0.51
1:L1:201:G:O3'	36:SP:946:LYS:NZ	2.43	0.51
29:SF:22:ASP:OD1	30:SG:342:ARG:NH2	2.43	0.51
30:SG:134:ARG:NH2	30:SG:535:GLU:OE1	2.43	0.51
36:SP:615:VAL:HG23	36:SP:619:LEU:HD23	1.93	0.51
36:SP:806:THR:HG1	36:SP:820:THR:HG1	1.53	0.51
38:SS:411:LYS:HE3	38:SS:411:LYS:HA	1.92	0.51
19:NG:136:ARG:O	41:SW:248:VAL:HG11	2.10	0.51
1:L1:1230:A:N3	1:L1:1258:U:N3	2.57	0.51
8:L8:109:PHE:CE2	8:L8:183:ILE:HD11	2.45	0.51
13:LF:27:VAL:HG21	13:LF:40:LEU:HD21	1.92	0.51
29:SF:52:ILE:CG2	29:SF:67:LEU:HD23	2.36	0.51
4:L4:95:THR:HG22	13:LF:16:PRO:HG2	1.92	0.51
23:NQ:35:VAL:CG1	23:NQ:63:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SG:196:LEU:HD21	30:SG:253:THR:HG21	1.90	0.51
1:L1:75:U:O2'	36:SP:3:LYS:O	2.26	0.51
1:L1:392:G:P	8:L8:24:LYS:HZ1	2.30	0.51
29:SF:21:LEU:HD12	29:SF:90:ALA:HB3	1.93	0.51
1:L1:1126:G:N7	24:NS:107:ARG:NH1	2.59	0.51
36:SP:374:LEU:HD23	36:SP:411:PHE:CE2	2.45	0.51
1:L1:1120:U:OP2	24:NS:88:LYS:NZ	2.34	0.51
31:SH:283:ILE:HD12	32:SI:631:ILE:HG21	1.93	0.51
1:L1:129:U:N3	1:L1:265:A:OP1	2.40	0.51
1:L1:473:A:OP1	9:L9:44:ARG:NH1	2.38	0.51
30:SG:185:LEU:HD13	30:SG:527:VAL:HG11	1.92	0.51
31:SH:61:ASN:HA	39:ST:108:LYS:HZ1	1.76	0.51
1:L1:1777:G:OP1	20:NL:235:ASN:ND2	2.39	0.50
17:NB:555:ASN:OD1	17:NB:556:LYS:N	2.44	0.50
28:SC:123:ILE:O	28:SC:141:TYR:N	2.44	0.50
32:SI:927:GLU:N	32:SI:927:GLU:OE1	2.44	0.50
34:SL:68:ASP:OD1	38:SS:439:ARG:NH2	2.43	0.50
1:L1:1524:A:N3	1:L1:1590:G:O2'	2.34	0.50
4:L4:111:VAL:HG23	4:L4:111:VAL:O	2.11	0.50
7:L7:144:VAL:HG23	12:LE:49:GLU:OE1	2.11	0.50
32:SI:56:VAL:HG23	37:SR:101:GLU:OE1	2.11	0.50
36:SP:476:LEU:HD21	36:SP:508:PHE:CE1	2.46	0.50
29:SF:21:LEU:HD11	29:SF:87:LEU:HA	1.94	0.50
38:SS:387:MET:HE2	38:SS:387:MET:N	2.27	0.50
36:SP:752:THR:O	36:SP:752:THR:HG23	2.11	0.50
5:L5:140:THR:HG23	5:L5:171:ALA:HB1	1.94	0.50
22:NP:37:VAL:HG21	22:NP:100:ILE:HD11	1.93	0.50
28:SC:151:LEU:HD12	28:SC:151:LEU:H	1.77	0.50
1:L1:612:U:OP2	1:L1:613:G:O2'	2.28	0.50
30:SG:323:ASP:OD1	30:SG:324:ILE:N	2.39	0.50
12:LE:105:THR:HG23	12:LE:105:THR:O	2.10	0.50
32:SI:952:PHE:CD2	32:SI:958:VAL:HG22	2.47	0.50
36:SP:183:HIS:CD2	36:SP:188:LEU:HD12	2.46	0.50
1:L1:48:G:OP1	24:NS:7:ARG:NH2	2.43	0.50
23:NQ:35:VAL:HG11	23:NQ:63:LEU:HD12	1.94	0.50
36:SP:748:SER:O	36:SP:751:SER:OG	2.29	0.50
1:L1:58:U:O2'	1:L1:451:A:N3	2.44	0.49
1:L1:259:U:OP1	8:L8:75:LYS:NZ	2.38	0.49
31:SH:109:PHE:HE2	31:SH:303:ILE:HD12	1.78	0.49
41:SW:117:TYR:O	41:SW:121:VAL:HG12	2.11	0.49
5:L5:33:VAL:HG13	10:LC:53:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:NL:69:ASN:O	20:NL:73:ARG:NE	2.38	0.49
2:L2:0:M7G:H82	2:L2:1:G:O4'	2.12	0.49
31:SH:65:ILE:HD11	39:ST:112:VAL:HG22	1.94	0.49
36:SP:126:GLU:N	36:SP:126:GLU:OE1	2.45	0.49
36:SP:897:PHE:CE1	36:SP:901:ILE:HD11	2.47	0.49
36:SP:480:TYR:CE1	36:SP:484:ILE:HD11	2.47	0.49
39:ST:760:LYS:O	39:ST:763:ALA:HB3	2.12	0.49
1:L1:209:U:O3'	8:L8:170:SER:OG	2.28	0.49
17:NB:439:ASP:OD1	17:NB:440:ILE:N	2.45	0.49
17:NB:572:ALA:O	17:NB:576:LEU:HD23	2.13	0.49
31:SH:15:GLN:NE2	32:SI:607:ASP:OD1	2.46	0.49
31:SH:25:THR:OG1	31:SH:106:LEU:HD21	2.12	0.49
1:L1:976:G:OP1	18:NF:109:LYS:NZ	2.46	0.49
3:L3:30:TYR:O	3:L3:33:THR:OG1	2.31	0.49
7:L7:38:LEU:CD2	7:L7:77:LEU:HD21	2.42	0.49
30:SG:168:ASN:O	30:SG:172:PHE:N	2.42	0.49
36:SP:71:GLU:OE2	36:SP:75:GLN:NE2	2.43	0.49
5:L5:123:VAL:HG13	25:NW:102:THR:HG22	1.94	0.49
32:SI:549:ILE:O	32:SI:553:ILE:HD12	2.13	0.49
34:SL:138:ASP:OD1	34:SL:139:ASP:N	2.46	0.49
4:L4:54:TYR:O	13:LF:15:ASN:ND2	2.46	0.49
5:L5:140:THR:HG21	5:L5:175:LEU:HD23	1.95	0.49
16:NA:340:LEU:CD1	16:NA:345:LEU:HD22	2.42	0.49
28:SC:273:ALA:HB3	28:SC:312:ASP:OD2	2.13	0.49
1:L1:125:U:OP1	6:L6:201:GLN:NE2	2.41	0.48
11:LD:76:VAL:HG21	11:LD:87:ARG:HB2	1.94	0.48
29:SF:93:VAL:O	30:SG:552:TRP:NE1	2.45	0.48
32:SI:993:ASP:OD1	32:SI:994:LYS:N	2.46	0.48
34:SL:130:CYS:SG	34:SL:144:ARG:NH2	2.86	0.48
36:SP:356:ASP:OD2	36:SP:357:LYS:N	2.45	0.48
36:SP:481:TRP:HA	36:SP:484:ILE:HD12	1.95	0.48
1:L1:637:C:O2	7:L7:114:ARG:NH2	2.47	0.48
32:SI:549:ILE:HD13	32:SI:567:TRP:NE1	2.28	0.48
25:NW:92:ILE:CD1	25:NW:102:THR:HG23	2.43	0.48
36:SP:374:LEU:O	36:SP:378:HIS:N	2.44	0.48
36:SP:398:GLN:NE2	36:SP:438:GLU:OE1	2.46	0.48
24:NS:848:GLU:HA	24:NS:879:ALA:HB1	1.95	0.48
30:SG:333:MET:HE3	30:SG:335:ARG:HD2	1.96	0.48
36:SP:279:TRP:CE3	36:SP:282:ILE:HD11	2.49	0.48
36:SP:519:VAL:O	36:SP:523:LEU:HD23	2.14	0.48
1:L1:447:U:OP1	4:L4:49:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:738:G:OP1	4:L4:200:ARG:NH2	2.42	0.48
5:L5:83:ARG:HD2	5:L5:83:ARG:O	2.14	0.48
36:SP:881:LEU:HD11	36:SP:924:TYR:CD2	2.47	0.48
41:SW:113:TRP:HA	41:SW:116:ILE:HG22	1.96	0.48
24:NS:124:THR:HG22	24:NS:124:THR:O	2.12	0.48
1:L1:433:C:N4	1:L1:436:A:OP1	2.47	0.48
1:L1:647:G:N2	1:L1:687:G:H22	2.12	0.48
19:NG:31:THR:OG1	19:NG:32:ASP:N	2.46	0.48
24:NS:22:GLU:OE2	24:NS:25:ARG:NH1	2.46	0.48
20:NL:178:ASN:OD1	20:NL:182:TRP:NE1	2.46	0.48
34:SL:103:MET:HE1	34:SL:117:LEU:HD12	1.95	0.48
28:SC:225:ARG:NH2	28:SC:246:GLN:OE1	2.47	0.48
5:L5:92:ARG:NH2	5:L5:169:ASN:OD1	2.42	0.47
22:NP:36:ILE:O	22:NP:36:ILE:HG22	2.14	0.47
25:NW:75:LEU:HA	25:NW:78:ILE:HG22	1.96	0.47
36:SP:334:ASN:O	36:SP:337:THR:OG1	2.28	0.47
1:L1:1488:G:H3'	1:L1:1515:A:H61	1.80	0.47
16:NA:349:ARG:NH1	39:ST:763:ALA:HB2	2.28	0.47
30:SG:125:VAL:HG21	36:SP:76:THR:CG2	2.44	0.47
35:SM:99:ARG:NH2	35:SM:172:MET:HE3	2.29	0.47
1:L1:334:G:O6	8:L8:5:ARG:NH2	2.46	0.47
11:LD:123:VAL:CG2	11:LD:139:VAL:HG13	2.44	0.47
28:SC:146:PRO:HA	28:SC:152:ALA:HB3	1.96	0.47
36:SP:370:ASP:OD1	36:SP:370:ASP:N	2.46	0.47
5:L5:93:LEU:HD23	5:L5:172:ILE:HG23	1.97	0.47
6:L6:57:ASP:OD1	6:L6:60:GLY:N	2.47	0.47
35:SM:106:GLU:OE2	35:SM:173:ARG:N	2.44	0.47
1:L1:428:A:N3	1:L1:440:U:O2'	2.39	0.47
17:NB:580:ARG:NH2	34:SL:48:SER:O	2.44	0.47
32:SI:99:ASN:OD1	32:SI:100:ASP:N	2.47	0.47
1:L1:545:A:O4'	1:L1:594:A:N6	2.47	0.47
22:NP:31:PRO:HG2	22:NP:34:VAL:HG13	1.95	0.47
30:SG:454:GLU:O	30:SG:460:ARG:NE	2.43	0.47
36:SP:932:ARG:O	36:SP:935:VAL:HG22	2.14	0.47
1:L1:129:U:O4'	1:L1:264:G:N1	2.47	0.47
1:L1:740:A:OP1	11:LD:43:LYS:NZ	2.48	0.47
1:L1:1605:G:O3'	35:SM:124:MET:HE1	2.14	0.47
2:L2:82:G:O2'	2:L2:83:A:OP2	2.29	0.47
2:L2:247:U:O2'	30:SG:151:ARG:NH2	2.48	0.47
6:L6:120:GLU:N	6:L6:120:GLU:OE1	2.46	0.47
12:LE:111:MET:HE2	12:LE:116:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:NB:594:GLU:OE1	28:SC:156:MET:HE1	2.14	0.47
21:NM:124:ASN:C	21:NM:124:ASN:ND2	2.72	0.47
28:SC:295:GLU:OE2	34:SL:129:SER:OG	2.15	0.47
30:SG:252:VAL:HG22	30:SG:260:LEU:HD11	1.96	0.47
36:SP:10:SER:O	36:SP:15:ARG:NH2	2.46	0.47
30:SG:152:VAL:HG12	30:SG:562:GLY:HA2	1.97	0.47
1:L1:560:U:OP2	35:SM:282:ARG:NH2	2.47	0.47
1:L1:564:G:H1'	1:L1:1596:C:H42	1.80	0.47
1:L1:935:U:OP2	1:L1:1075:C:O2'	2.22	0.47
20:NL:59:VAL:HG23	20:NL:80:ASN:OD1	2.14	0.47
29:SF:20:ILE:HG21	29:SF:53:ILE:HD13	1.97	0.47
36:SP:84:ASP:OD1	36:SP:85:LYS:N	2.47	0.46
36:SP:259:LEU:HD23	36:SP:263:LEU:HD13	1.98	0.46
12:LE:23:ARG:O	12:LE:65:LEU:N	2.47	0.46
12:LE:7:LEU:O	12:LE:11:LEU:HD23	2.15	0.46
30:SG:304:ILE:HD11	30:SG:338:THR:HG21	1.97	0.46
32:SI:830:ARG:NH1	37:SR:138:GLU:OE2	2.48	0.46
39:ST:92:GLU:O	39:ST:96:LYS:N	2.43	0.46
1:L1:532:U:OP1	9:L9:132:ARG:NH2	2.48	0.46
16:NA:356:VAL:HG11	39:ST:92:GLU:OE1	2.15	0.46
17:NB:576:LEU:HD21	34:SL:52:PHE:CE1	2.51	0.46
32:SI:313:TYR:CZ	32:SI:317:LEU:HD11	2.50	0.46
36:SP:280:MET:HE2	36:SP:320:THR:HG23	1.97	0.46
36:SP:472:ASP:O	36:SP:476:LEU:HD23	2.15	0.46
2:L2:79:G:O2'	2:L2:328:A:N1	2.40	0.46
6:L6:159:ARG:NH2	6:L6:170:THR:OG1	2.48	0.46
32:SI:248:ARG:HA	32:SI:358:MET:HE3	1.96	0.46
36:SP:670:LEU:HD22	36:SP:681:VAL:HG11	1.96	0.46
38:SS:791:TRP:CH2	41:SW:130:MET:HE1	2.50	0.46
1:L1:1107:G:OP2	32:SI:18:LYS:NZ	2.49	0.46
5:L5:136:ALA:O	5:L5:140:THR:HG22	2.16	0.46
6:L6:122:GLU:OE2	6:L6:122:GLU:N	2.47	0.46
7:L7:63:PRO:O	7:L7:67:LEU:N	2.47	0.46
18:NF:87:ASP:OD1	18:NF:87:ASP:N	2.48	0.46
30:SG:417:SER:OG	30:SG:418:ASP:N	2.49	0.46
1:L1:802:G:H21	12:LE:107:SER:HB2	1.80	0.46
30:SG:447:SER:OG	30:SG:449:ASN:OD1	2.32	0.46
31:SH:314:ASN:OD1	31:SH:315:LYS:N	2.49	0.46
32:SI:956:MET:CE	39:ST:752:MET:HE3	2.46	0.46
36:SP:375:THR:HG22	36:SP:411:PHE:HE1	1.80	0.46
1:L1:545:A:H61	1:L1:594:A:H5''	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LC:43:ILE:HD12	10:LC:43:ILE:H	1.81	0.46
25:NW:43:ASP:O	25:NW:47:TYR:N	2.43	0.46
28:SC:103:GLU:N	28:SC:103:GLU:OE1	2.49	0.46
36:SP:397:PHE:CE2	36:SP:401:LEU:HD11	2.51	0.46
36:SP:512:ASP:OD1	36:SP:515:THR:HG23	2.16	0.46
1:L1:931:C:O2'	21:NM:118:GLN:O	2.32	0.46
1:L1:904:G:N2	1:L1:1000:C:C2	2.82	0.45
1:L1:931:C:OP1	21:NM:116:LYS:NZ	2.36	0.45
2:L2:113:G:O6	29:SF:42:LYS:NZ	2.40	0.45
10:LC:49:TYR:HB3	10:LC:53:LEU:HD13	1.98	0.45
27:SB:114:LEU:O	27:SB:118:ARG:N	2.45	0.45
29:SF:8:ALA:HB2	29:SF:61:ILE:HD11	1.97	0.45
24:NS:114:ILE:HG22	24:NS:118:GLN:HE22	1.81	0.45
1:L1:165:G:O3'	36:SP:636:ARG:NH2	2.50	0.45
6:L6:78:THR:O	6:L6:81:VAL:HG22	2.17	0.45
16:NA:384:ARG:CZ	35:SM:83:ILE:HD12	2.46	0.45
31:SH:110:SER:OG	31:SH:112:LYS:O	2.30	0.45
36:SP:137:ASP:O	36:SP:140:ILE:HG22	2.17	0.45
36:SP:200:VAL:HG21	36:SP:235:LEU:HD21	1.98	0.45
1:L1:779:U:O4	13:LF:8:ARG:NH2	2.47	0.45
6:L6:5:ILE:HD13	6:L6:16:PHE:CD2	2.52	0.45
8:L8:36:THR:OG1	8:L8:57:ALA:O	2.28	0.45
12:LE:55:ASP:OD2	23:NQ:26:GLN:NE2	2.49	0.45
16:NA:401:SER:O	41:SW:218:ASN:ND2	2.48	0.45
17:NB:557:ASP:OD1	17:NB:558:ASN:N	2.49	0.45
36:SP:796:ILE:HD11	36:SP:831:PHE:CE2	2.52	0.45
36:SP:963:ASP:O	36:SP:966:SER:OG	2.20	0.45
1:L1:819:G:O2'	1:L1:821:U:OP2	2.35	0.45
1:L1:903:U:O2'	1:L1:905:A:N7	2.45	0.45
1:L1:1088:A:N3	38:SS:403:LYS:NZ	2.64	0.45
3:L3:57:ARG:N	3:L3:60:GLU:OE1	2.50	0.45
20:NL:318:SER:O	24:NS:124:THR:HG23	2.16	0.45
22:NP:105:LEU:HD23	22:NP:122:ARG:HD3	1.97	0.45
24:NS:101:ILE:HG13	32:SI:726:LEU:HD13	1.99	0.45
28:SC:198:GLU:OE2	28:SC:200:SER:N	2.50	0.45
32:SI:968:THR:HG22	32:SI:1001:VAL:HG12	1.98	0.45
1:L1:31:C:OP1	37:SR:140:LYS:NZ	2.40	0.45
6:L6:142:ARG:O	6:L6:146:GLY:N	2.49	0.45
7:L7:73:VAL:HG22	7:L7:73:VAL:O	2.16	0.45
19:NG:48:VAL:HG21	19:NG:59:ALA:HB2	1.98	0.45
32:SI:898:GLY:N	32:SI:915:ALA:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:113:U:HO2'	1:L1:115:G:HO2'	1.62	0.45
12:LE:104:LEU:HD23	12:LE:125:ILE:HA	1.98	0.45
23:NQ:62:ILE:HD11	23:NQ:64:CYS:O	2.17	0.45
28:SD:165:ALA:HB1	28:SD:166:PRO:HD2	1.99	0.45
16:NA:350:THR:HG23	16:NA:351:ALA:N	2.32	0.45
34:SL:98:ILE:HG23	34:SL:102:VAL:HG23	1.99	0.45
41:SW:129:ARG:O	41:SW:138:GLU:N	2.45	0.45
1:L1:614:C:OP1	37:SR:3:LYS:NZ	2.34	0.45
1:L1:1583:A:N3	5:L5:76:ARG:NH1	2.64	0.45
26:SA:219:LEU:O	26:SA:223:ILE:N	2.42	0.45
39:ST:25:LYS:O	39:ST:26:SER:OG	2.17	0.45
41:SW:126:LEU:HB3	41:SW:139:LEU:HD11	1.99	0.45
6:L6:216:LEU:HD23	6:L6:220:LYS:HD3	1.99	0.44
9:L9:23:ARG:O	9:L9:26:ALA:N	2.50	0.44
24:NS:87:SER:N	24:NS:90:SER:OG	2.50	0.44
29:SF:21:LEU:HD12	29:SF:90:ALA:CB	2.47	0.44
1:L1:610:G:O2'	1:L1:613:G:O2'	2.35	0.44
16:NA:410:ALA:HB2	41:SW:173:ALA:HB2	1.99	0.44
20:NL:179:VAL:O	20:NL:183:ALA:N	2.51	0.44
32:SI:127:ALA:O	32:SI:131:ILE:HD12	2.17	0.44
36:SP:70:ILE:O	36:SP:70:ILE:HG22	2.15	0.44
41:SW:137:VAL:HG21	41:SW:159:ILE:HG21	1.98	0.44
1:L1:867:G:O6	1:L1:962:C:N4	2.51	0.44
21:NM:181:LEU:HD23	21:NM:181:LEU:C	2.43	0.44
24:NS:1258:THR:O	24:NS:1261:GLY:N	2.50	0.44
36:SP:546:GLU:O	36:SP:549:LYS:NZ	2.40	0.44
32:SI:134:ILE:HD13	32:SI:811:VAL:HG22	1.99	0.44
32:SI:931:LYS:HB2	32:SI:1006:TRP:CZ3	2.53	0.44
3:L3:73:MET:HE3	3:L3:73:MET:O	2.17	0.44
8:L8:158:SER:O	8:L8:161:SER:OG	2.20	0.44
28:SC:236:MET:SD	28:SC:236:MET:N	2.90	0.44
32:SI:207:LEU:HD12	32:SI:215:TYR:CG	2.53	0.44
38:SS:386:LEU:HA	38:SS:389:ARG:HD2	2.00	0.44
34:SL:122:ASP:OD2	34:SL:124:ARG:NH2	2.51	0.44
12:LE:37:PHE:CZ	12:LE:103:ILE:HD12	2.52	0.44
32:SI:553:ILE:HD12	32:SI:553:ILE:H	1.83	0.44
34:SL:103:MET:HE3	34:SL:106:LEU:HB2	1.99	0.44
36:SP:267:SER:O	36:SP:313:ARG:NH2	2.50	0.44
1:L1:1082:C:HO2'	1:L1:1083:G:P	2.40	0.44
16:NA:409:LEU:HD11	41:SW:173:ALA:HB3	2.00	0.44
19:NG:18:ARG:HE	19:NG:31:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SC:312:ASP:CG	28:SC:312:ASP:O	2.60	0.44
1:L1:60:U:OP2	36:SP:12:LYS:NZ	2.28	0.44
3:L3:72:ILE:HD13	3:L3:79:TYR:HD2	1.83	0.44
36:SP:372:LYS:O	36:SP:375:THR:OG1	2.35	0.44
9:L9:151:ASP:OD2	9:L9:152:SER:N	2.50	0.43
32:SI:207:LEU:HD12	32:SI:215:TYR:CD1	2.54	0.43
1:L1:1059:U:H4'	1:L1:1059:U:OP2	2.18	0.43
1:L1:1148:C:O4'	39:ST:21:GLN:NE2	2.44	0.43
35:SM:288:ASP:OD1	35:SM:289:TYR:N	2.51	0.43
36:SP:294:VAL:O	36:SP:297:VAL:HG12	2.18	0.43
36:SP:922:MET:O	36:SP:926:LEU:HD23	2.18	0.43
38:SS:413:LEU:C	38:SS:413:LEU:HD23	2.43	0.43
21:NM:89:ASP:CG	21:NM:228:LEU:HD13	2.43	0.43
24:NS:83:THR:HG23	24:NS:83:THR:O	2.17	0.43
26:SA:21:LYS:N	26:SA:47:LEU:O	2.51	0.43
32:SI:90:VAL:O	32:SI:94:THR:OG1	2.22	0.43
39:ST:388:LEU:O	39:ST:392:LYS:N	2.52	0.43
28:SC:268:VAL:C	28:SC:269:ILE:HD13	2.44	0.43
30:SG:129:GLN:O	30:SG:131:ARG:N	2.51	0.43
36:SP:170:LEU:HD13	36:SP:203:CYS:SG	2.59	0.43
36:SP:325:GLU:OE2	36:SP:328:ARG:NH1	2.51	0.43
36:SP:668:GLY:O	36:SP:671:THR:OG1	2.35	0.43
1:L1:68:A:OP1	6:L6:160:ARG:NH2	2.49	0.43
1:L1:1492:A:O2'	1:L1:1493:A:O5'	2.35	0.43
31:SH:32:LYS:HD2	31:SH:75:ILE:HD11	2.00	0.43
36:SP:335:LYS:O	36:SP:339:LEU:HD23	2.19	0.43
9:L9:31:ALA:O	9:L9:35:GLY:N	2.52	0.43
20:NL:37:HIS:ND1	20:NL:198:PRO:O	2.48	0.43
21:NM:203:ASP:OD1	21:NM:204:ILE:N	2.51	0.43
30:SG:304:ILE:CD1	30:SG:338:THR:HG21	2.48	0.43
30:SG:538:ARG:HE	30:SG:540:LEU:HD21	1.83	0.43
34:SL:59:ILE:HG23	34:SL:59:ILE:O	2.18	0.43
1:L1:390:G:O3'	24:NS:19:LYS:NZ	2.52	0.43
1:L1:1178:G:N7	39:ST:753:LYS:NZ	2.45	0.43
11:LD:22:ASN:HB3	11:LD:25:VAL:HG12	2.01	0.43
21:NM:89:ASP:OD2	21:NM:228:LEU:HD13	2.19	0.43
32:SI:838:ILE:HD12	32:SI:874:TYR:HB3	2.01	0.43
36:SP:5:ARG:O	36:SP:7:THR:N	2.44	0.43
29:SF:5:ASN:O	30:SG:462:ARG:NH1	2.52	0.43
1:L1:153:G:O6	13:LF:128:LYS:NZ	2.52	0.43
17:NB:544:ILE:HG23	32:SI:153:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SI:100:ASP:O	32:SI:359:SER:OG	2.35	0.43
32:SI:310:THR:HG23	32:SI:313:TYR:H	1.84	0.43
34:SL:72:ILE:HG22	34:SL:76:ILE:HD12	2.00	0.43
36:SP:701:LEU:HD21	36:SP:795:ASP:HB3	2.01	0.43
21:NM:104:ASP:OD1	21:NM:105:PHE:N	2.48	0.42
22:NP:100:ILE:O	22:NP:104:VAL:HG23	2.19	0.42
25:NW:40:VAL:O	25:NW:40:VAL:HG12	2.19	0.42
30:SG:424:LEU:HD21	30:SG:501:ILE:HD11	2.01	0.42
1:L1:451:A:N6	1:L1:453:U:O2	2.52	0.42
1:L1:738:G:HO2'	1:L1:739:G:P	2.42	0.42
17:NB:546:LYS:HE3	17:NB:546:LYS:HA	1.99	0.42
35:SM:100:LEU:HD22	35:SM:144:GLU:CG	2.49	0.42
10:LC:50:GLU:OE1	10:LC:50:GLU:N	2.52	0.42
22:NP:103:LYS:NZ	22:NP:106:GLN:OE1	2.32	0.42
28:SC:306:LEU:HD21	28:SC:315:ILE:HG13	2.01	0.42
30:SG:419:ASN:ND2	30:SG:421:ASN:OD1	2.51	0.42
30:SG:455:THR:O	30:SG:460:ARG:NH2	2.52	0.42
32:SI:631:ILE:O	32:SI:631:ILE:HG22	2.19	0.42
38:SS:386:LEU:C	38:SS:387:MET:HE2	2.44	0.42
1:L1:474:A:OP1	9:L9:145:SER:OG	2.35	0.42
1:L1:684:A:H2'	1:L1:685:A:C8	2.54	0.42
6:L6:18:ILE:HG21	6:L6:24:ILE:CD1	2.50	0.42
19:NG:30:VAL:HG11	19:NG:71:CYS:SG	2.59	0.42
21:NM:103:MET:SD	21:NM:104:ASP:N	2.92	0.42
30:SG:321:HIS:ND1	30:SG:325:VAL:HG22	2.33	0.42
5:L5:140:THR:HG21	5:L5:175:LEU:HD21	2.01	0.42
28:SC:151:LEU:HD11	28:SC:241:PHE:HE2	1.80	0.42
30:SG:477:SER:OG	30:SG:521:VAL:O	2.30	0.42
32:SI:131:ILE:HD11	32:SI:809:PRO:HG3	2.01	0.42
1:L1:68:A:OP1	6:L6:160:ARG:NH1	2.50	0.42
1:L1:871:G:H2'	1:L1:872:G:C8	2.55	0.42
4:L4:141:THR:OG1	4:L4:143:ASP:OD1	2.32	0.42
5:L5:140:THR:HG23	5:L5:171:ALA:CB	2.49	0.42
11:LD:10:GLU:OE2	11:LD:10:GLU:N	2.52	0.42
19:NG:22:SER:OG	19:NG:23:PHE:N	2.52	0.42
36:SP:362:PHE:HB3	36:SP:381:LEU:HD11	2.01	0.42
6:L6:5:ILE:HD13	6:L6:16:PHE:HD2	1.85	0.42
9:L9:86:LEU:HD23	9:L9:87:SER:O	2.20	0.42
16:NA:362:THR:O	16:NA:366:GLU:HG2	2.20	0.42
19:NG:83:ILE:HD12	19:NG:94:PRO:HG3	2.02	0.42
21:NM:29:TRP:CH2	21:NM:47:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SC:198:GLU:O	28:SC:222:GLU:N	2.52	0.42
31:SH:191:ILE:HD12	31:SH:219:LEU:CD2	2.50	0.42
37:SR:68:ILE:HD11	39:ST:785:VAL:HG22	2.02	0.42
41:SW:117:TYR:N	41:SW:118:PRO:CD	2.83	0.42
1:L1:359:A:H1'	32:SI:39:MET:HE1	2.01	0.42
31:SH:281:GLU:CG	32:SI:621:LEU:HD22	2.50	0.42
36:SP:406:GLU:OE1	36:SP:406:GLU:N	2.46	0.42
1:L1:80:A:OP1	36:SP:4:GLN:NE2	2.53	0.42
1:L1:738:G:O2'	1:L1:739:G:P	2.78	0.42
8:L8:11:ARG:NH1	8:L8:15:GLY:O	2.50	0.42
9:L9:169:PRO:O	9:L9:174:ARG:NH1	2.53	0.42
32:SI:93:MET:CE	32:SI:107:VAL:HG21	2.49	0.42
36:SP:486:PHE:O	36:SP:489:SER:OG	2.28	0.42
1:L1:241:U:H5'	6:L6:216:LEU:HD11	2.02	0.42
1:L1:789:A:OP1	4:L4:108:ARG:NH1	2.53	0.42
1:L1:1568:C:HO2'	1:L1:1569:A:P	2.42	0.42
1:L1:1568:C:O2'	1:L1:1569:A:P	2.78	0.42
1:L1:1798:U:H2'	1:L1:1799:U:O4'	2.20	0.42
5:L5:96:SER:OG	5:L5:176:THR:HG21	2.19	0.42
36:SP:371:VAL:O	36:SP:375:THR:HG23	2.19	0.42
36:SP:575:MET:HE1	36:SP:607:LEU:CD1	2.49	0.42
36:SP:907:GLU:OE1	36:SP:908:ASN:N	2.52	0.42
1:L1:258:C:O2	8:L8:178:ARG:NH1	2.51	0.41
1:L1:358:U:OP2	24:NS:2:GLY:N	2.53	0.41
3:L3:11:PHE:CD2	25:NW:41:ILE:HD11	2.55	0.41
4:L4:64:ILE:HG13	13:LF:18:LEU:HD21	2.02	0.41
16:NA:356:VAL:HG21	39:ST:92:GLU:CD	2.45	0.41
21:NM:171:ILE:O	21:NM:174:LYS:N	2.52	0.41
30:SG:364:GLU:O	30:SG:368:LEU:HD23	2.20	0.41
30:SG:405:VAL:HG23	30:SG:415:THR:HG22	2.02	0.41
36:SP:458:ILE:HG22	36:SP:491:LEU:HD21	2.02	0.41
36:SP:635:ALA:HB1	36:SP:676:PRO:HG2	2.02	0.41
37:SR:26:GLU:OE1	37:SR:26:GLU:N	2.48	0.41
3:L3:41:ARG:NH1	22:NP:38:LYS:HD2	2.35	0.41
9:L9:53:ARG:HB2	34:SL:91:LEU:HD21	2.02	0.41
24:NS:17:MET:HG3	24:NS:81:LEU:HD11	2.02	0.41
34:SL:172:LEU:HD23	34:SL:183:GLU:OE2	2.20	0.41
38:SS:382:LEU:O	38:SS:386:LEU:HD23	2.19	0.41
7:L7:159:VAL:HG23	7:L7:185:ILE:HG21	2.02	0.41
8:L8:60:ILE:HG21	8:L8:179:CYS:SG	2.60	0.41
18:NF:13:SER:OG	18:NF:14:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:NS:104:GLN:HG3	32:SI:726:LEU:HD22	2.02	0.41
1:L1:85:A:N3	1:L1:148:A:O2'	2.48	0.41
1:L1:1220:C:O2'	42:SZ:379:LYS:O	2.33	0.41
10:LC:97:VAL:HG12	10:LC:98:ASP:N	2.36	0.41
16:NA:335:ARG:NE	16:NA:340:LEU:HD23	2.35	0.41
28:SC:127:GLU:O	28:SC:137:THR:N	2.53	0.41
32:SI:838:ILE:HD12	32:SI:874:TYR:CB	2.50	0.41
36:SP:307:ASP:OD1	36:SP:308:ALA:N	2.51	0.41
36:SP:362:PHE:CG	36:SP:381:LEU:HD11	2.56	0.41
36:SP:793:PHE:HA	36:SP:796:ILE:HG22	2.02	0.41
36:SP:881:LEU:HD21	36:SP:920:VAL:HG12	2.01	0.41
1:L1:753:A:OP2	4:L4:187:ARG:NH2	2.54	0.41
4:L4:118:GLU:OE2	4:L4:237:SER:OG	2.37	0.41
7:L7:152:VAL:HG21	7:L7:181:ILE:HD11	2.02	0.41
9:L9:23:ARG:O	9:L9:27:GLU:OE1	2.38	0.41
17:NB:602:LEU:HD13	34:SL:42:ARG:HB2	2.02	0.41
23:NQ:34:ASP:OD2	23:NQ:82:LYS:HD3	2.21	0.41
1:L1:1502:G:N7	22:NP:102:ARG:NH2	2.69	0.41
4:L4:246:LEU:HB3	4:L4:250:GLU:CD	2.46	0.41
36:SP:926:LEU:HD12	36:SP:964:PHE:HB2	2.03	0.41
5:L5:178:GLY:HA3	5:L5:209:TYR:CD2	2.56	0.41
21:NM:171:ILE:O	21:NM:175:GLU:OE1	2.39	0.41
24:NS:114:ILE:O	24:NS:118:GLN:NE2	2.54	0.41
31:SH:180:MET:HB2	31:SH:301:MET:HE2	2.02	0.41
1:L1:447:U:H2'	1:L1:448:C:O4'	2.21	0.41
7:L7:70:PHE:O	7:L7:74:GLN:N	2.54	0.41
8:L8:78:ILE:HG23	8:L8:102:VAL:HG21	2.03	0.41
12:LE:8:ALA:HB2	12:LE:74:VAL:HG21	2.02	0.41
13:LF:63:GLN:NE2	13:LF:68:LYS:HE3	2.35	0.41
30:SG:347:MET:HE3	30:SG:356:ARG:HH22	1.86	0.41
31:SH:188:ILE:HD11	32:SI:635:PHE:CZ	2.56	0.41
35:SM:113:ASN:OD1	35:SM:211:ASN:ND2	2.51	0.41
1:L1:854:U:O4	1:L1:855:A:N6	2.54	0.41
21:NM:43:VAL:HG22	21:NM:43:VAL:O	2.21	0.41
21:NM:98:THR:O	21:NM:232:HIS:NE2	2.50	0.41
30:SG:429:LYS:HD2	30:SG:433:ILE:HG22	2.03	0.41
32:SI:157:ASN:O	32:SI:161:HIS:ND1	2.54	0.41
35:SM:106:GLU:O	35:SM:110:LEU:HD23	2.21	0.41
36:SP:262:ALA:HB1	36:SP:272:VAL:HG22	2.03	0.41
36:SP:479:ILE:HD12	36:SP:479:ILE:H	1.86	0.41
13:LF:73:GLY:C	13:LF:74:LEU:HD22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:NG:123:SER:O	19:NG:124:ASP:OD1	2.39	0.41
20:NL:153:LEU:HD12	20:NL:209:LEU:HD13	2.03	0.41
20:NL:221:ASN:CB	24:NS:124:THR:HG21	2.51	0.41
24:NS:497:LEU:O	24:NS:501:MET:N	2.51	0.41
28:SC:171:LEU:HD13	28:SC:234:ILE:HD13	2.02	0.41
30:SG:138:ASP:OD1	30:SG:139:LYS:N	2.53	0.41
30:SG:156:ASN:HA	30:SG:544:ALA:HB1	2.02	0.41
30:SG:509:GLU:N	30:SG:509:GLU:OE1	2.53	0.41
31:SH:81:ILE:HD11	31:SH:106:LEU:HD22	2.03	0.41
35:SM:273:VAL:O	35:SM:273:VAL:HG13	2.20	0.41
1:L1:105:A:OP1	8:L8:18:ARG:NH1	2.51	0.40
12:LE:50:PHE:HB3	12:LE:63:VAL:HG23	2.01	0.40
16:NA:403:VAL:HG22	16:NA:404:LYS:N	2.36	0.40
30:SG:253:THR:O	30:SG:260:LEU:HD12	2.20	0.40
36:SP:366:ILE:O	36:SP:407:ARG:NH1	2.54	0.40
1:L1:317:C:H5''	24:NS:30:GLN:HG3	2.02	0.40
1:L1:705:U:O2'	1:L1:706:A:O4'	2.37	0.40
17:NB:601:GLY:O	34:SL:42:ARG:N	2.53	0.40
18:NF:132:VAL:HG12	18:NF:132:VAL:O	2.21	0.40
24:NS:1242:LYS:O	41:SW:111:ASN:ND2	2.53	0.40
25:NW:56:THR:O	25:NW:103:ARG:NH1	2.55	0.40
30:SG:77:GLU:OE1	30:SG:120:ARG:NH2	2.55	0.40
36:SP:276:SER:HA	36:SP:320:THR:HG21	2.03	0.40
41:SW:202:ILE:HG23	41:SW:226:LEU:CD2	2.42	0.40
1:L1:105:A:O5'	8:L8:18:ARG:NH2	2.55	0.40
12:LE:47:ILE:HD11	12:LE:69:LEU:HD12	2.02	0.40
29:SF:44:LEU:O	29:SF:74:LYS:NZ	2.53	0.40
31:SH:181:HIS:HE2	32:SI:761:GLN:CD	2.27	0.40
31:SH:283:ILE:CD1	32:SI:631:ILE:HG21	2.50	0.40
34:SL:161:LYS:HG2	34:SL:172:LEU:HD21	2.04	0.40
36:SP:425:TRP:HB2	36:SP:457:PHE:HE2	1.86	0.40
36:SP:426:GLN:OE1	36:SP:426:GLN:N	2.52	0.40
36:SP:504:ILE:HD12	36:SP:519:VAL:HG22	2.02	0.40
36:SP:854:LEU:HB3	36:SP:873:LEU:HD21	2.02	0.40
39:ST:25:LYS:C	39:ST:26:SER:HG	2.20	0.40
6:L6:216:LEU:HD23	6:L6:220:LYS:CD	2.52	0.40
7:L7:154:LEU:HD23	7:L7:162:ILE:HD12	2.03	0.40
11:LD:110:HIS:O	11:LD:138:ASN:ND2	2.48	0.40
16:NA:384:ARG:NH2	35:SM:79:ALA:O	2.47	0.40
19:NG:76:ILE:H	19:NG:76:ILE:HD12	1.86	0.40
32:SI:941:ILE:HD12	32:SI:946:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SI:958:VAL:CG1	32:SI:979:ALA:HB2	2.52	0.40
16:NA:379:ASP:OD1	16:NA:379:ASP:N	2.49	0.40
30:SG:241:THR:HG21	30:SG:285:SER:HA	2.04	0.40
36:SP:773:LEU:O	36:SP:776:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L3	96/146 (66%)	94 (98%)	2 (2%)	0	100	100
4	L4	256/261 (98%)	250 (98%)	6 (2%)	0	100	100
5	L5	193/225 (86%)	191 (99%)	2 (1%)	0	100	100
6	L6	225/236 (95%)	223 (99%)	2 (1%)	0	100	100
7	L7	184/190 (97%)	182 (99%)	2 (1%)	0	100	100
8	L8	177/200 (88%)	173 (98%)	4 (2%)	0	100	100
9	L9	179/197 (91%)	179 (100%)	0	0	100	100
10	LC	118/143 (82%)	118 (100%)	0	0	100	100
11	LD	136/156 (87%)	132 (97%)	4 (3%)	0	100	100
12	LE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
13	LF	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
14	LG	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
16	NA	106/593 (18%)	105 (99%)	1 (1%)	0	100	100
17	NB	80/610 (13%)	80 (100%)	0	0	100	100
18	NF	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
19	NG	125/137 (91%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	NL	281/318 (88%)	280 (100%)	1 (0%)	0	100	100
21	NM	207/255 (81%)	201 (97%)	6 (3%)	0	100	100
22	NP	130/144 (90%)	128 (98%)	2 (2%)	0	100	100
23	NQ	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
24	NS	877/1267 (69%)	866 (99%)	11 (1%)	0	100	100
25	NW	67/108 (62%)	66 (98%)	1 (2%)	0	100	100
26	SA	379/504 (75%)	375 (99%)	4 (1%)	0	100	100
27	SB	401/511 (78%)	394 (98%)	7 (2%)	0	100	100
28	SC	234/327 (72%)	228 (97%)	6 (3%)	0	100	100
28	SD	234/327 (72%)	232 (99%)	2 (1%)	0	100	100
29	SE	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
29	SF	119/126 (94%)	115 (97%)	4 (3%)	0	100	100
30	SG	452/573 (79%)	444 (98%)	8 (2%)	0	100	100
31	SH	358/367 (98%)	349 (98%)	9 (2%)	0	100	100
32	SI	696/1183 (59%)	683 (98%)	13 (2%)	0	100	100
33	SJ	207/252 (82%)	204 (99%)	3 (1%)	0	100	100
33	SK	225/252 (89%)	222 (99%)	3 (1%)	0	100	100
34	SL	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
35	SM	217/290 (75%)	215 (99%)	2 (1%)	0	100	100
36	SP	935/2493 (38%)	915 (98%)	20 (2%)	0	100	100
37	SR	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
38	SS	142/899 (16%)	138 (97%)	4 (3%)	0	100	100
39	ST	555/810 (68%)	552 (100%)	3 (0%)	0	100	100
40	SU	524/552 (95%)	521 (99%)	3 (1%)	0	100	100
41	SW	180/274 (66%)	177 (98%)	3 (2%)	0	100	100
42	SZ	255/483 (53%)	251 (98%)	4 (2%)	0	100	100
All	All	10485/16434 (64%)	10327 (98%)	158 (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	L3	90/129 (70%)	90 (100%)	0	100	100
4	L4	220/222 (99%)	220 (100%)	0	100	100
5	L5	170/191 (89%)	170 (100%)	0	100	100
6	L6	194/201 (96%)	194 (100%)	0	100	100
7	L7	166/170 (98%)	166 (100%)	0	100	100
8	L8	145/161 (90%)	145 (100%)	0	100	100
9	L9	156/166 (94%)	156 (100%)	0	100	100
10	LC	100/119 (84%)	100 (100%)	0	100	100
11	LD	125/137 (91%)	125 (100%)	0	100	100
12	LE	110/111 (99%)	109 (99%)	1 (1%)	70	76
13	LF	109/113 (96%)	109 (100%)	0	100	100
14	LG	55/60 (92%)	55 (100%)	0	100	100
16	NA	103/535 (19%)	103 (100%)	0	100	100
17	NB	73/538 (14%)	73 (100%)	0	100	100
18	NF	127/128 (99%)	127 (100%)	0	100	100
19	NG	96/105 (91%)	96 (100%)	0	100	100
20	NL	255/283 (90%)	254 (100%)	1 (0%)	84	84
21	NM	189/224 (84%)	188 (100%)	1 (0%)	81	82
22	NP	107/116 (92%)	107 (100%)	0	100	100
23	NQ	68/71 (96%)	68 (100%)	0	100	100
24	NS	160/1140 (14%)	160 (100%)	0	100	100
25	NW	60/89 (67%)	60 (100%)	0	100	100
26	SA	10/435 (2%)	10 (100%)	0	100	100
27	SB	7/433 (2%)	7 (100%)	0	100	100
28	SC	198/240 (82%)	198 (100%)	0	100	100
28	SD	14/240 (6%)	14 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	SE	7/104 (7%)	7 (100%)	0	100	100
29	SF	100/104 (96%)	100 (100%)	0	100	100
30	SG	398/503 (79%)	398 (100%)	0	100	100
31	SH	307/312 (98%)	307 (100%)	0	100	100
32	SI	621/1039 (60%)	621 (100%)	0	100	100
33	SJ	9/222 (4%)	9 (100%)	0	100	100
33	SK	12/222 (5%)	12 (100%)	0	100	100
34	SL	131/169 (78%)	131 (100%)	0	100	100
35	SM	194/258 (75%)	194 (100%)	0	100	100
36	SP	881/2307 (38%)	881 (100%)	0	100	100
37	SR	113/120 (94%)	113 (100%)	0	100	100
38	SS	108/807 (13%)	108 (100%)	0	100	100
39	ST	132/732 (18%)	132 (100%)	0	100	100
40	SU	27/506 (5%)	27 (100%)	0	100	100
41	SW	159/238 (67%)	159 (100%)	0	100	100
42	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	6320/14424 (44%)	6317 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	LE	80	ASN
20	NL	263	ASN
21	NM	124	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	L3	78	HIS
4	L4	50	ASN
4	L4	69	HIS
4	L4	112	HIS
4	L4	142	HIS
4	L4	216	ASN
5	L5	44	ASN

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Mol	Chain	Res	Type
5	L5	200	ASN
5	L5	224	ASN
7	L7	150	GLN
8	L8	44	HIS
11	LD	98	ASN
13	LF	113	ASN
20	NL	46	GLN
21	NM	124	ASN
22	NP	93	HIS
23	NQ	5	GLN
24	NS	16	HIS
24	NS	104	GLN
30	SG	128	GLN
30	SG	181	ASN
30	SG	547	HIS
31	SH	234	ASN
32	SI	55	HIS
32	SI	162	HIS
32	SI	878	HIS
32	SI	1037	GLN
34	SL	143	HIS
34	SL	147	GLN
35	SM	102	GLN
36	SP	4	GLN
36	SP	46	HIS
36	SP	183	HIS
36	SP	207	ASN
36	SP	493	ASN
36	SP	577	HIS
36	SP	712	ASN
36	SP	840	ASN
36	SP	908	ASN
37	SR	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1385/1803 (76%)	275 (19%)	9 (0%)
15	N2	4/5 (80%)	2 (50%)	0
2	L2	81/334 (24%)	11 (13%)	0
All	All	1470/2142 (68%)	288 (19%)	9 (0%)

All (288) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	9	U
1	L1	10	G
1	L1	15	U
1	L1	21	U
1	L1	22	A
1	L1	34	G
1	L1	46	A
1	L1	47	A
1	L1	60	U
1	L1	65	A
1	L1	68	A
1	L1	73	U
1	L1	74	U
1	L1	75	U
1	L1	76	A
1	L1	77	U
1	L1	78	A
1	L1	104	A
1	L1	114	C
1	L1	116	U
1	L1	127	G
1	L1	129	U
1	L1	140	A
1	L1	144	U
1	L1	145	A
1	L1	159	U
1	L1	166	C
1	L1	179	A
1	L1	194	U
1	L1	195	G
1	L1	199	G
1	L1	202	A
1	L1	205	U
1	L1	215	A
1	L1	216	U
1	L1	217	A
1	L1	232	U
1	L1	233	C
1	L1	235	G
1	L1	240	U
1	L1	241	U
1	L1	250	C

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Mol	Chain	Res	Type
1	L1	260	U
1	L1	261	U
1	L1	265	A
1	L1	275	C
1	L1	276	C
1	L1	278	U
1	L1	279	G
1	L1	280	U
1	L1	290	G
1	L1	299	A
1	L1	304	U
1	L1	314	C
1	L1	316	A
1	L1	322	G
1	L1	333	A
1	L1	337	G
1	L1	338	C
1	L1	344	A
1	L1	352	A
1	L1	359	A
1	L1	360	A
1	L1	361	C
1	L1	400	A
1	L1	401	A
1	L1	402	C
1	L1	404	G
1	L1	423	G
1	L1	424	C
1	L1	425	A
1	L1	426	G
1	L1	437	A
1	L1	438	A
1	L1	439	U
1	L1	444	C
1	L1	460	A
1	L1	467	G
1	L1	477	A
1	L1	486	G
1	L1	502	U
1	L1	505	A
1	L1	507	U
1	L1	511	A

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Mol	Chain	Res	Type
1	L1	515	A
1	L1	519	C
1	L1	520	A
1	L1	532	U
1	L1	534	A
1	L1	540	G
1	L1	542	A
1	L1	545	A
1	L1	563	U
1	L1	564	G
1	L1	565	C
1	L1	570	A
1	L1	578	U
1	L1	594	A
1	L1	595	G
1	L1	611	U
1	L1	619	A
1	L1	623	A
1	L1	624	G
1	L1	629	U
1	L1	639	U
1	L1	640	U
1	L1	649	U
1	L1	650	U
1	L1	685	A
1	L1	687	G
1	L1	690	G
1	L1	691	C
1	L1	696	C
1	L1	697	C
1	L1	710	U
1	L1	711	U
1	L1	739	G
1	L1	743	U
1	L1	752	A
1	L1	765	G
1	L1	766	U
1	L1	771	A
1	L1	774	A
1	L1	775	G
1	L1	782	U
1	L1	783	G

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Mol	Chain	Res	Type
1	L1	784	C
1	L1	789	A
1	L1	794	U
1	L1	803	A
1	L1	811	A
1	L1	812	A
1	L1	815	G
1	L1	821	U
1	L1	824	G
1	L1	830	U
1	L1	833	U
1	L1	834	G
1	L1	835	U
1	L1	863	A
1	L1	881	A
1	L1	886	U
1	L1	898	A
1	L1	904	G
1	L1	907	A
1	L1	913	G
1	L1	926	A
1	L1	934	C
1	L1	935	U
1	L1	944	A
1	L1	945	U
1	L1	960	U
1	L1	966	A
1	L1	969	C
1	L1	973	A
1	L1	992	A
1	L1	1005	A
1	L1	1007	C
1	L1	1011	G
1	L1	1026	A
1	L1	1028	C
1	L1	1029	U
1	L1	1030	A
1	L1	1032	G
1	L1	1043	A
1	L1	1051	G
1	L1	1052	U
1	L1	1053	G

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Mol	Chain	Res	Type
1	L1	1054	U
1	L1	1058	U
1	L1	1059	U
1	L1	1060	U
1	L1	1062	A
1	L1	1076	A
1	L1	1081	A
1	L1	1082	C
1	L1	1083	G
1	L1	1092	A
1	L1	1093	A
1	L1	1096	C
1	L1	1098	U
1	L1	1099	U
1	L1	1100	G
1	L1	1109	G
1	L1	1114	G
1	L1	1119	G
1	L1	1122	G
1	L1	1128	C
1	L1	1129	U
1	L1	1130	G
1	L1	1131	A
1	L1	1158	C
1	L1	1160	A
1	L1	1167	G
1	L1	1179	G
1	L1	1189	A
1	L1	1191	U
1	L1	1192	C
1	L1	1193	A
1	L1	1197	C
1	L1	1200	G
1	L1	1202	A
1	L1	1207	C
1	L1	1208	A
1	L1	1218	G
1	L1	1220	C
1	L1	1227	A
1	L1	1228	G
1	L1	1230	A
1	L1	1232	U

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Mol	Chain	Res	Type
1	L1	1256	A
1	L1	1267	G
1	L1	1268	G
1	L1	1269	U
1	L1	1270	G
1	L1	1436	A
1	L1	1437	U
1	L1	1438	G
1	L1	1440	C
1	L1	1465	C
1	L1	1471	A
1	L1	1483	A
1	L1	1490	C
1	L1	1491	U
1	L1	1492	A
1	L1	1493	A
1	L1	1496	U
1	L1	1506	G
1	L1	1514	U
1	L1	1515	A
1	L1	1516	A
1	L1	1521	G
1	L1	1523	G
1	L1	1524	A
1	L1	1535	U
1	L1	1537	C
1	L1	1542	G
1	L1	1548	G
1	L1	1553	G
1	L1	1554	U
1	L1	1555	A
1	L1	1556	A
1	L1	1557	U
1	L1	1559	A
1	L1	1569	A
1	L1	1570	A
1	L1	1579	U
1	L1	1584	G
1	L1	1590	G
1	L1	1595	U
1	L1	1599	C
1	L1	1600	A

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Mol	Chain	Res	Type
1	L1	1601	G
1	L1	1617	U
1	L1	1618	C
1	L1	1619	C
1	L1	1624	C
1	L1	1628	U
1	L1	1645	G
1	L1	1651	A
1	L1	1653	C
1	L1	1755	A
1	L1	1772	C
1	L1	1780	G
1	L1	1781	A
1	L1	1782	A
1	L1	1783	C
1	L1	1784	C
1	L1	1792	G
1	L1	1794	A
1	L1	1795	U
1	L1	1800	A
1	L1	1801	A
1	L1	1802	A
1	L1	1803	G
2	L2	2	U
2	L2	10	C
2	L2	13	C
2	L2	14	A
2	L2	15	U
2	L2	16	A
2	L2	88	U
2	L2	118	A
2	L2	324	U
2	L2	325	C
2	L2	329	C
15	N2	7	U
15	N2	10	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	240	U
1	L1	277	U

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Mol	Chain	Res	Type
1	L1	278	U
1	L1	738	G
1	L1	1051	G
1	L1	1082	C
1	L1	1491	U
1	L1	1555	A
1	L1	1568	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	SEP	SS	423	38	8,9,10	1.62	1 (12%)	7,12,14	1.37	1 (14%)

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
38	SEP	SS	423	38	-	4/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	SS	423	SEP	P-O1P	3.53	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	SS	423	SEP	OG-CB-CA	2.98	111.05	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	SS	423	SEP	CB-OG-P-O1P
38	SS	423	SEP	CB-OG-P-O2P
38	SS	423	SEP	CB-OG-P-O3P
38	SS	423	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 49 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	$\# Z > 2$
45	GTP	SI	2001	43	33,34,34	1.83	4 (12%)	50,54,54	1.48	7 (14%)

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
45	GTP	SI	2001	43	-	3/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	SI	2001	GTP	C5-N7	6.73	1.52	1.39
45	SI	2001	GTP	C8-N9	-4.20	1.28	1.37
45	SI	2001	GTP	C4-N9	-3.85	1.28	1.38
45	SI	2001	GTP	C4-N3	2.25	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	SI	2001	GTP	C8-N9-C4	7.20	119.53	106.03
45	SI	2001	GTP	N9-C4-N3	2.69	131.33	125.95
45	SI	2001	GTP	C6-C5-N7	2.44	134.73	130.29
45	SI	2001	GTP	C1'-N9-C8	-2.35	120.04	126.73
45	SI	2001	GTP	C8-N7-C5	-2.15	100.43	104.26
45	SI	2001	GTP	C5-C4-N9	-2.13	101.84	105.66
45	SI	2001	GTP	C1'-N9-C4	-2.05	120.43	126.49

There are no chirality outliers.

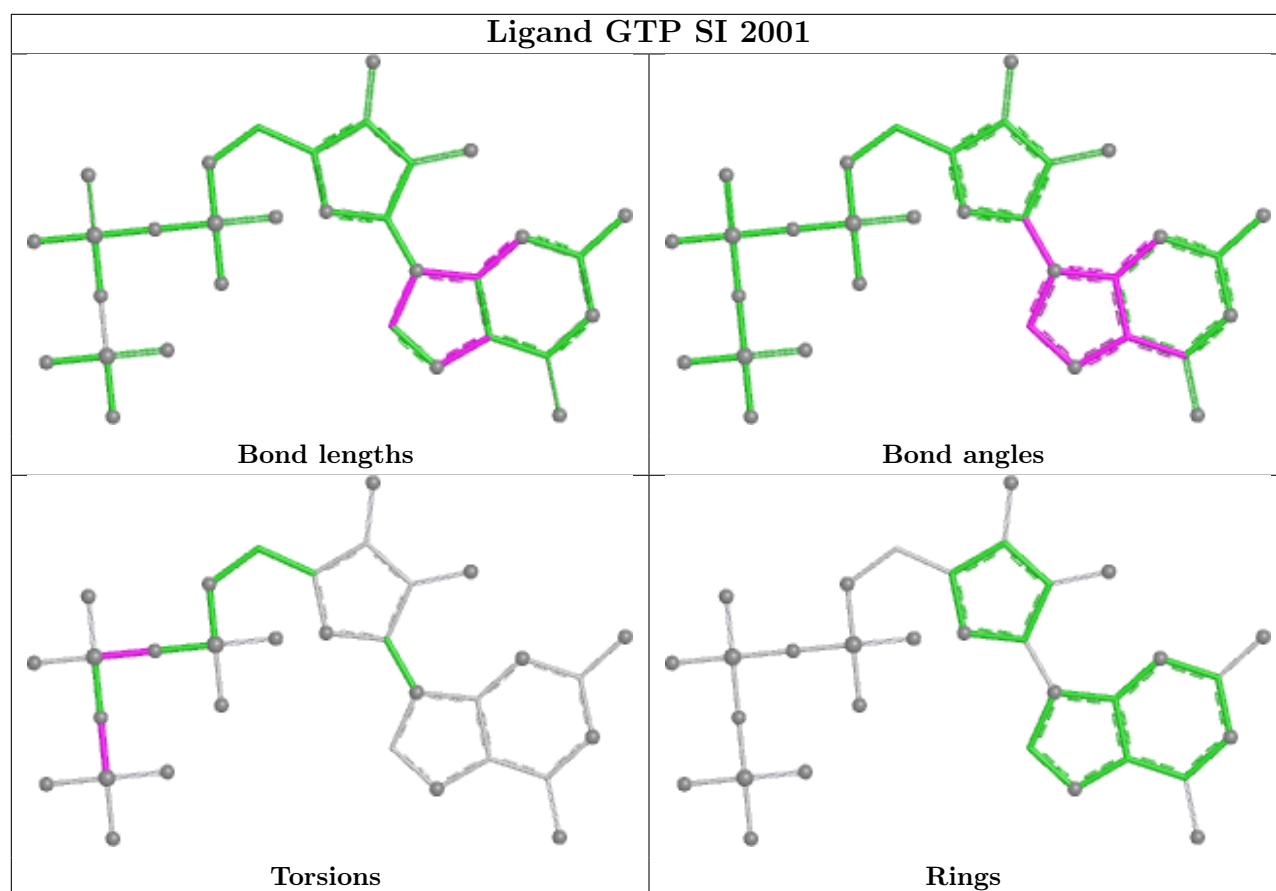
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	SI	2001	GTP	PB-O3B-PG-O2G
45	SI	2001	GTP	PA-O3A-PB-O1B
45	SI	2001	GTP	PB-O3B-PG-O3G

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.

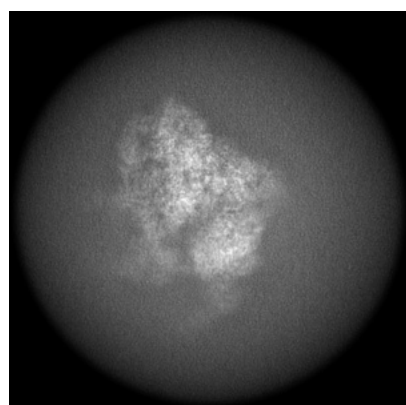
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49089. These allow visual inspection of the internal detail of the map and identification of artifacts.

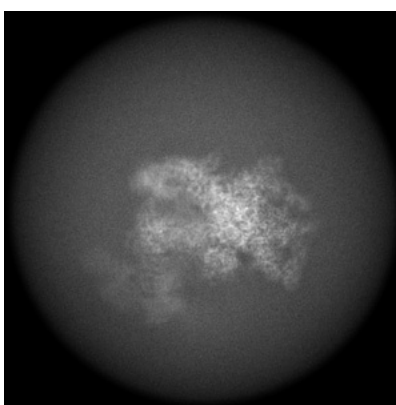
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

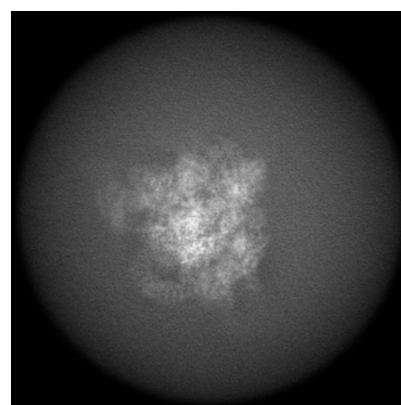
6.1.1 Primary map



X



Y

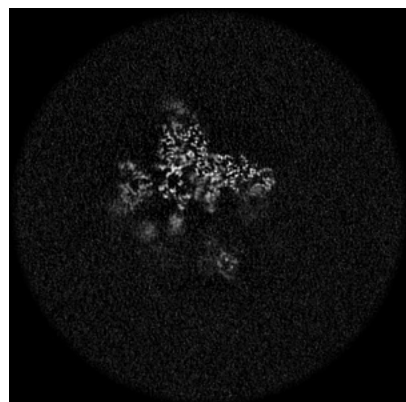


Z

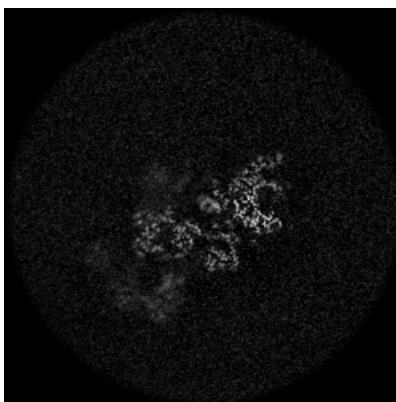
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

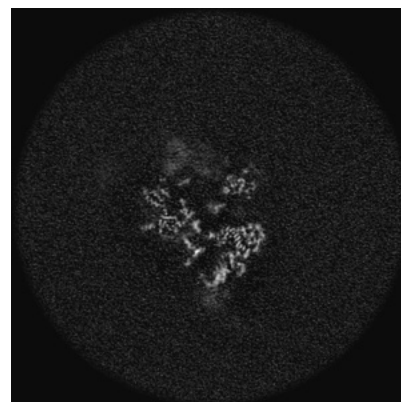
6.2.1 Primary map



X Index: 252



Y Index: 252

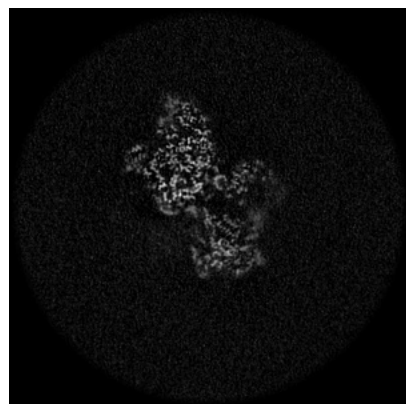


Z Index: 252

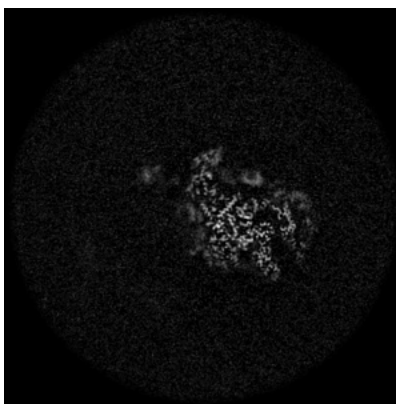
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

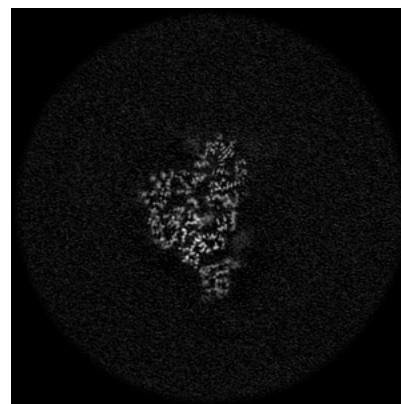
6.3.1 Primary map



X Index: 230



Y Index: 216

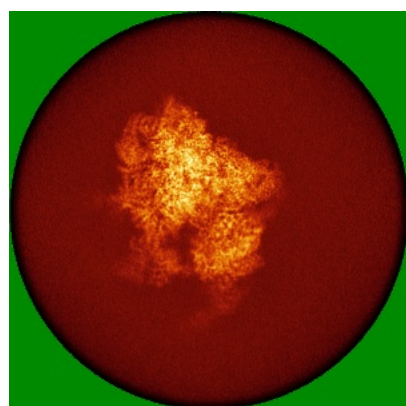


Z Index: 283

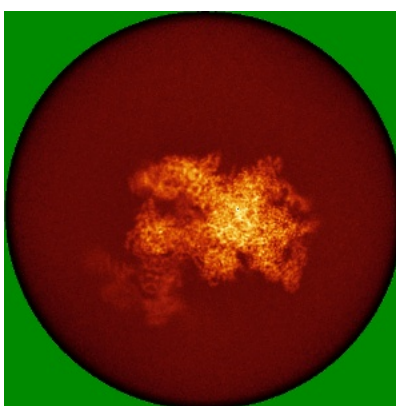
The images above show the largest variance slices of the map in three orthogonal directions.

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

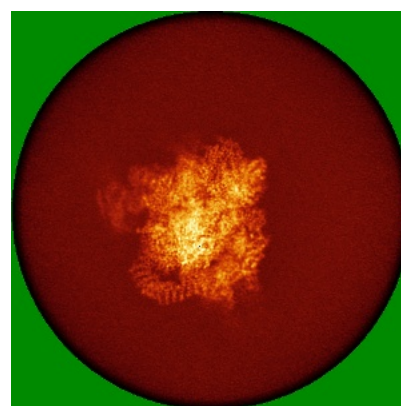
6.4.1 Primary map



X



Y

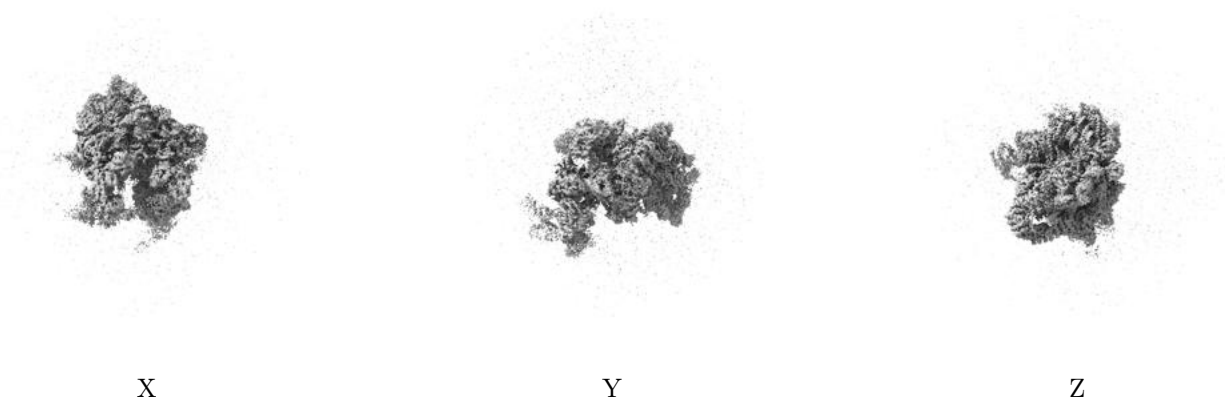


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

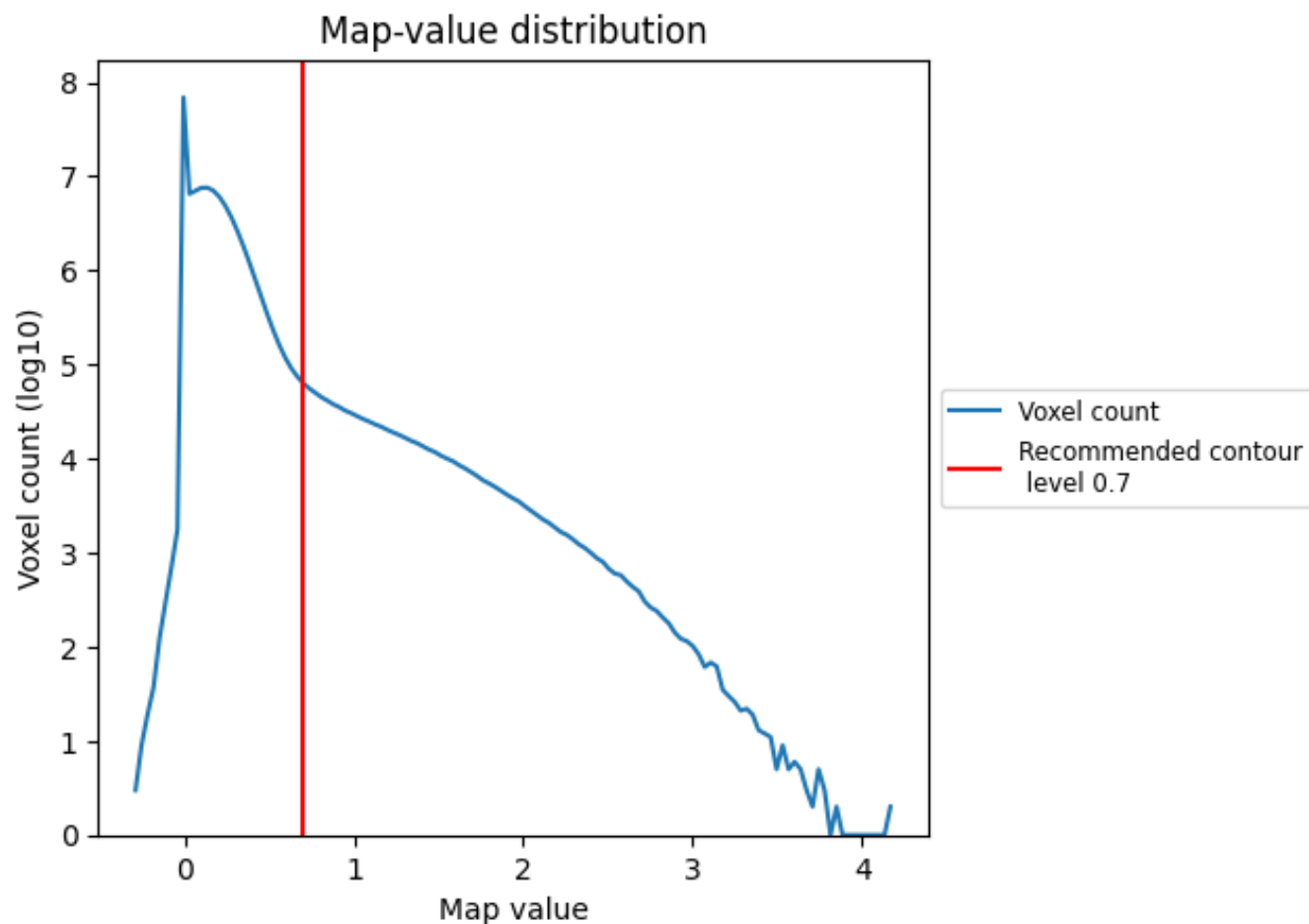
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

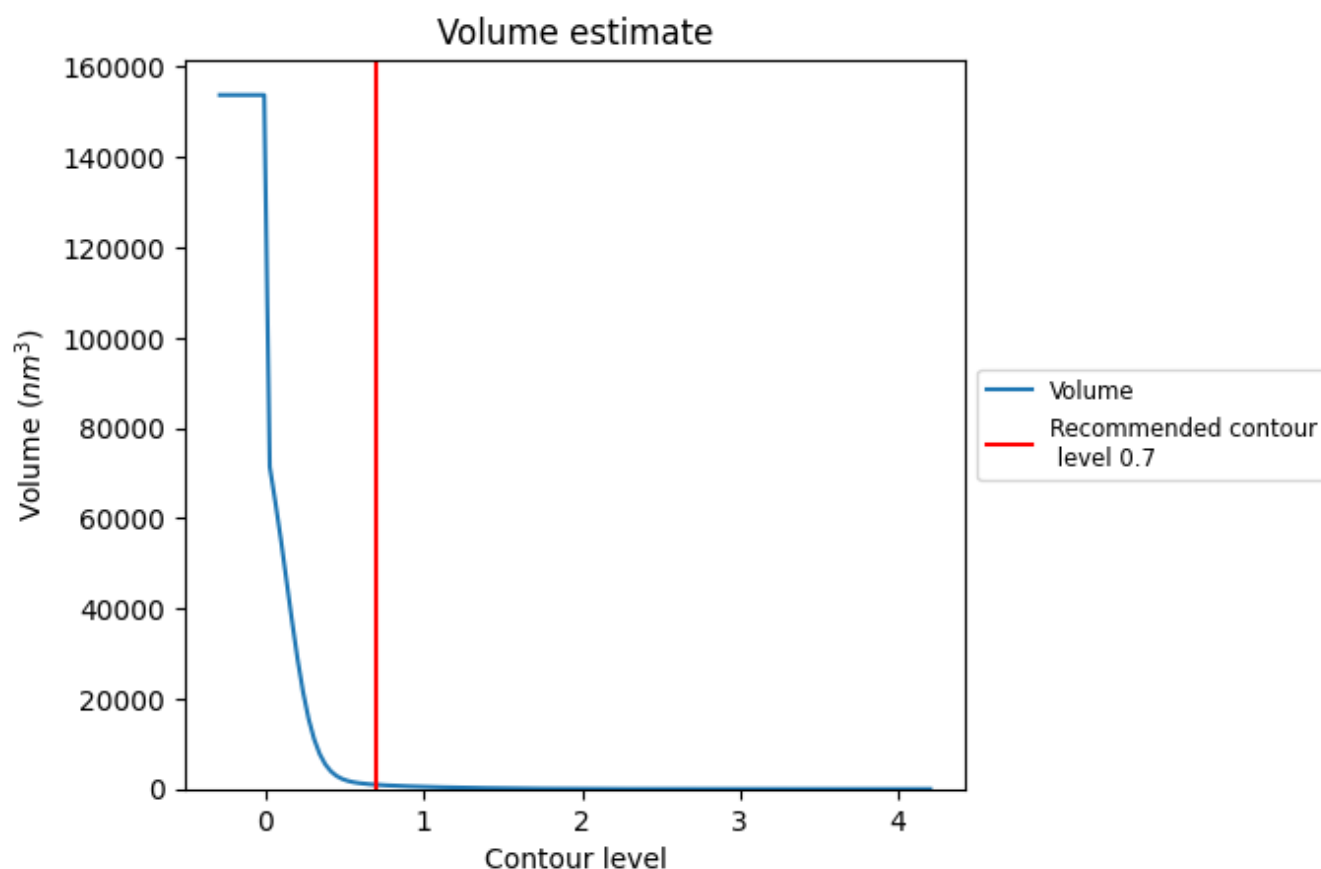
This section contains the results of statistical analysis of the map.

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.

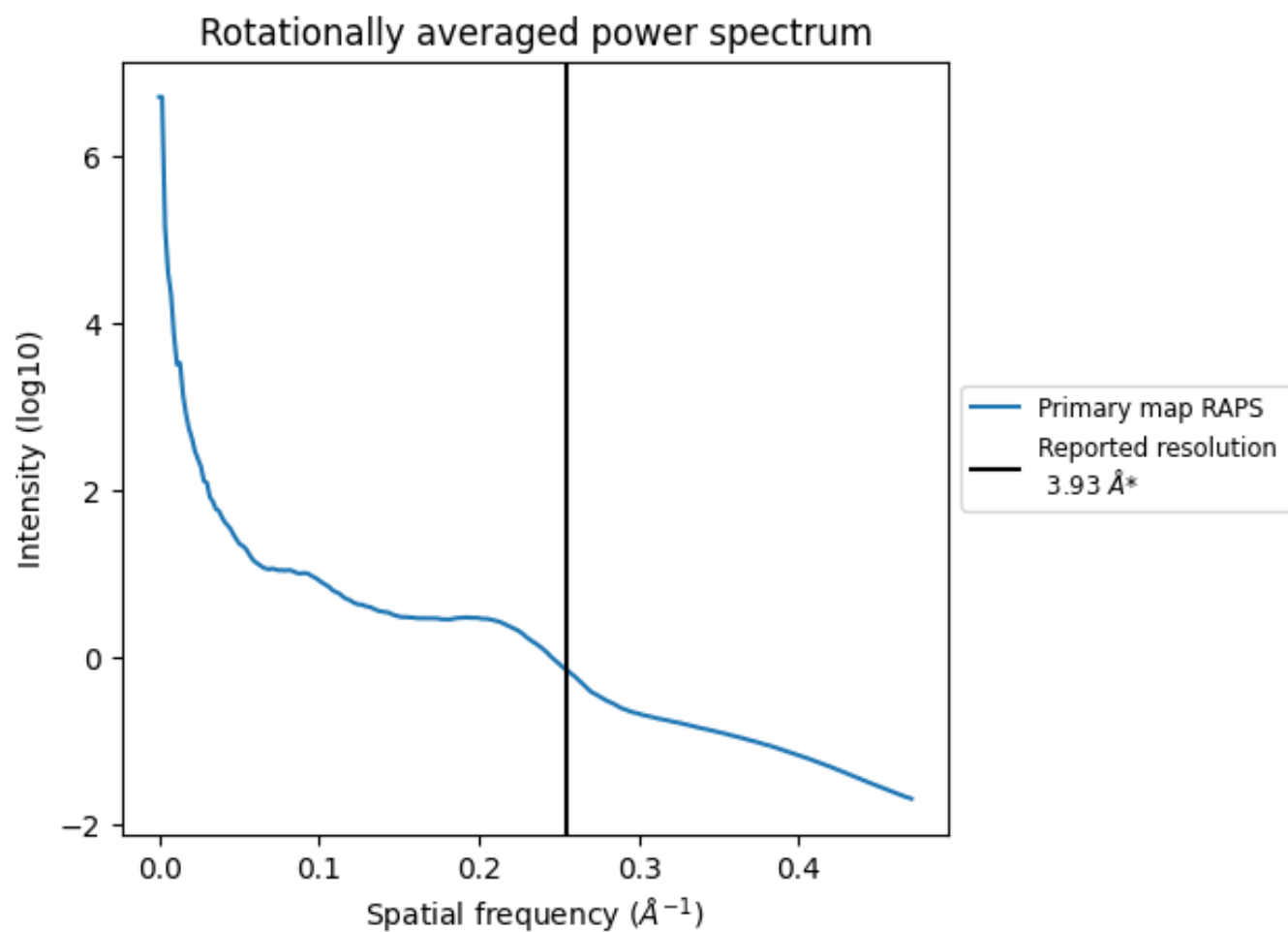
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 939 nm³; this corresponds to an approximate mass of 848 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 0.254 $\text{\AA}^{-1}$

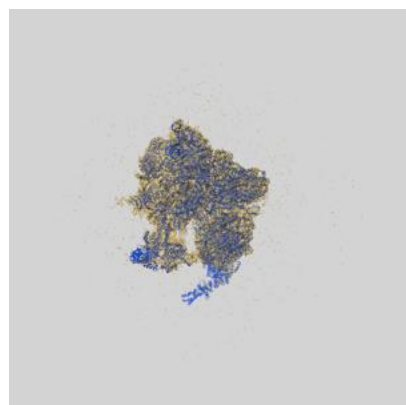
8 Fourier-Shell correlation ⓘ

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

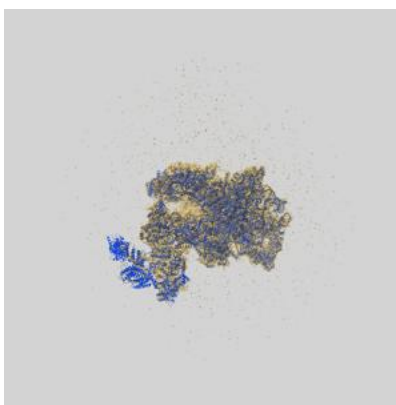
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49089 and PDB model 9N79. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

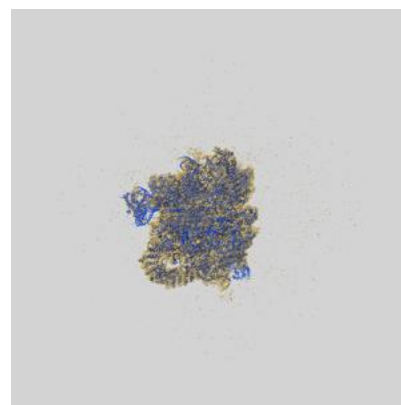
9.1 Map-model overlay [i](#)



X



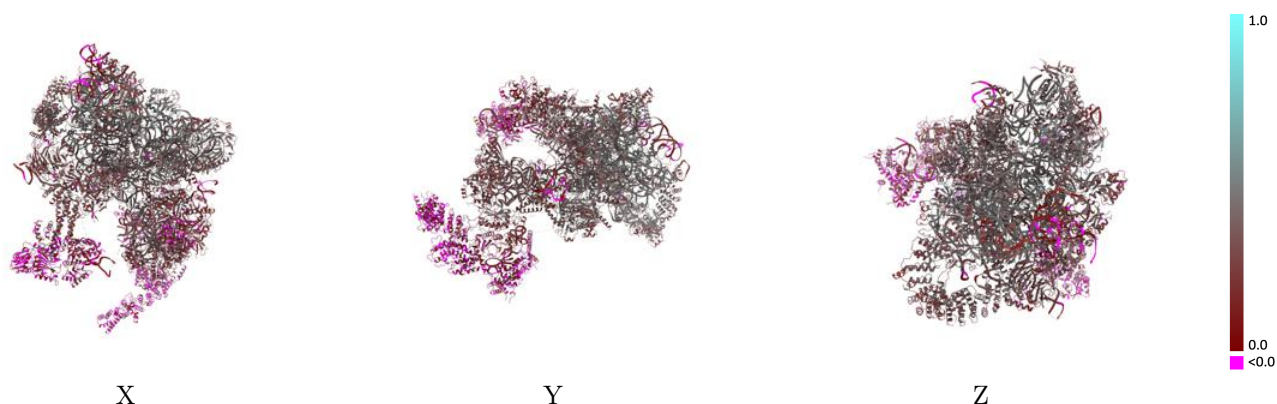
Y



Z

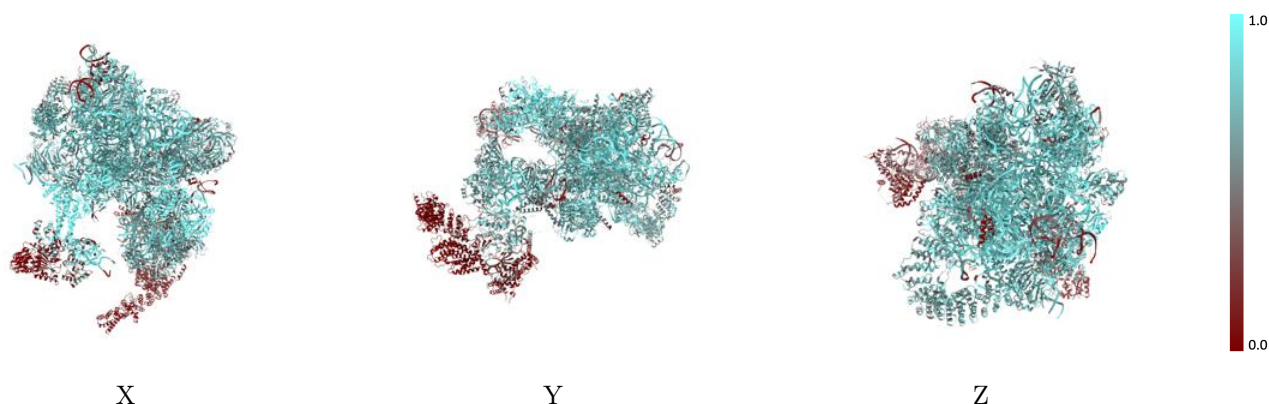
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



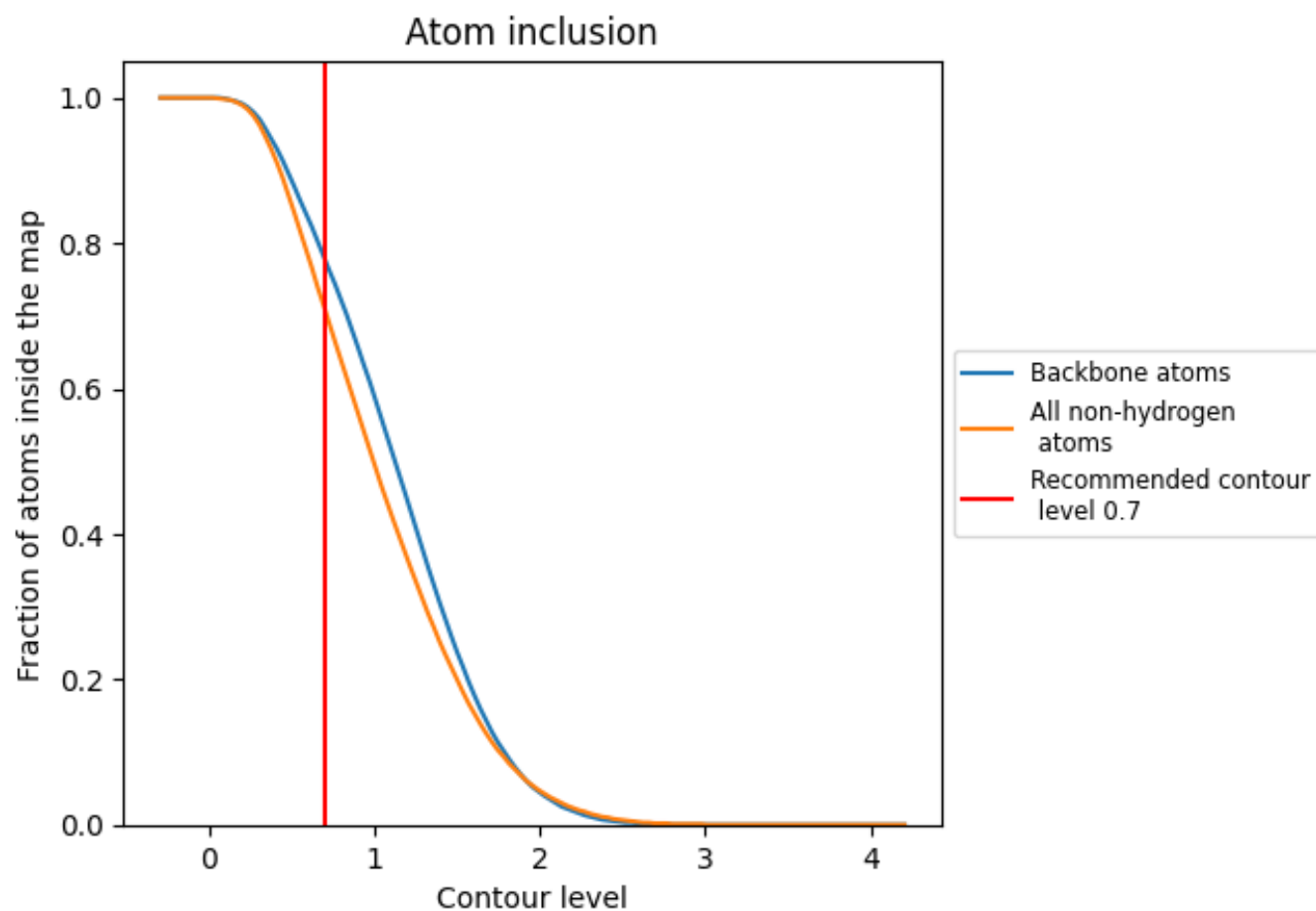
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.3240
L1	 0.8550	 0.3510
L2	 0.8380	 0.2280
L3	 0.5990	 0.2790
L4	 0.8370	 0.4500
L5	 0.6880	 0.2920
L6	 0.7690	 0.4050
L7	 0.7200	 0.3380
L8	 0.8240	 0.4430
L9	 0.8250	 0.3910
LC	 0.6750	 0.3200
LD	 0.8250	 0.4630
LE	 0.8540	 0.4130
LF	 0.8380	 0.4120
LG	 0.5830	 0.2860
N2	 0.7000	 0.2310
NA	 0.6240	 0.3340
NB	 0.6080	 0.3170
NF	 0.7390	 0.4440
NG	 0.6520	 0.4240
NL	 0.7310	 0.3960
NM	 0.6540	 0.4090
NP	 0.6890	 0.2900
NQ	 0.6490	 0.4190
NS	 0.7900	 0.2600
NW	 0.6240	 0.2870
SA	 0.8700	 0.2850
SB	 0.5130	 0.1560
SC	 0.7140	 0.3210
SD	 0.1440	 0.0530
SE	 0.4260	 0.1080
SF	 0.6890	 0.2850
SG	 0.6990	 0.2840
SH	 0.7550	 0.3990
SI	 0.7860	 0.3940



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Chain	Atom inclusion	Q-score
SJ	 0.4360	 0.1910
SK	 0.5910	 0.2950
SL	 0.7940	 0.3940
SM	 0.6680	 0.3550
SP	 0.6500	 0.3410
SR	 0.8100	 0.4150
SS	 0.7110	 0.3730
ST	 0.2080	 0.1440
SU	 0.0510	 0.0530
SW	 0.6620	 0.3740
SZ	 0.1210	 0.0640