



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:46 AM UTC

PDB ID : 8FKU / pdb_00008fku
EMDB ID : EMD-29257
Title : Human nucleolar pre-60S ribosomal subunit (State C2)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.82 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

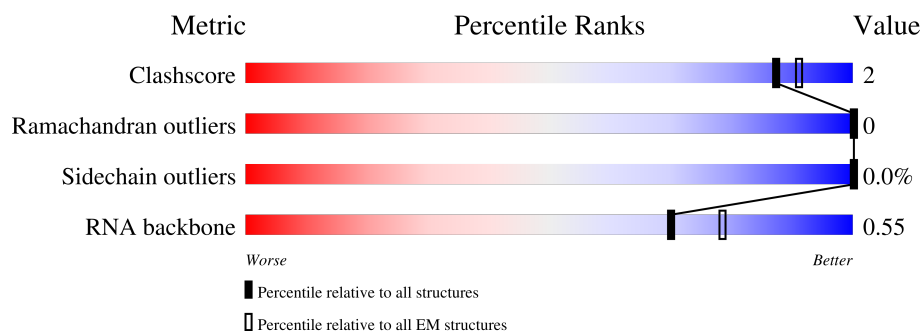
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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.



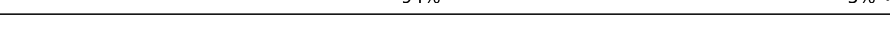
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	BA	165	88% 8% .
2	BB	217	98% .
3	L1	157	79% 16% . .
4	L2	1167	5% . 94%
5	L3	5070	35% 8% . 57%
6	L6	211	51% 6% 43%
7	L7	203	95% . .

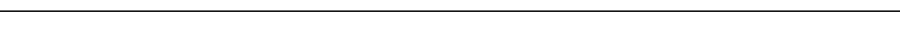
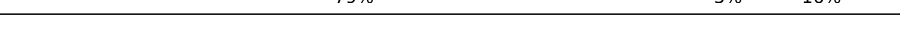
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Mol	Chain	Length	Quality of chain
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LE	160	
14	LG	140	
15	LH	156	
16	LI	145	
17	LK	148	
18	LL	137	
19	LN	403	
20	LQ	135	
21	LS	123	
22	LT	110	
23	LU	105	
24	LW	97	
25	NB	549	
26	NF	260	
27	NH	180	
28	NI	881	
29	NK	129	
30	SA	427	
31	SC	288	
32	SD	248	

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Mol	Chain	Length	Quality of chain
33	SE	266	
34	SG	192	
35	SH	293	
36	SI	255	
37	SJ	847	
38	SK	245	
39	SL	490	
40	SM	588	
41	SN	306	
42	SO	353	
43	SQ	239	
44	SR	634	
45	SS	746	
46	ST	365	
47	SV	163	
48	SW	670	
49	SY	812	
50	SZ	178	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 125869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	160	Total	C	N	O	S	0	0
			1208	749	226	229	4		

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	BB	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L1	152	Total	C	N	O	P	0	0
			3234	1443	571	1068	152		

- Molecule 4 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L2	69	Total	C	N	O	P	0	0
			1468	653	263	483	69		

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L3	2185	Total	C	N	O	P	0	0
			46844	20860	8575	15224	2185		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	120	Total	C	N	O	S	0	0
			998	625	218	154	1		

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 8 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 9 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L9	183	Total	C	N	O	S	0	0
			1546	974	325	243	4		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LA	138	Total	C	N	O	S	0	0
			1106	693	208	197	8		

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 12 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 13 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	113	Total	C	N	O	S	0	0
			747	461	143	142	1		

- Molecule 14 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 15 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LH	133	Total	C	N	O	S	0	0
			813	499	172	142			

- Molecule 16 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 17 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LK	108	Total	C	N	O	S	0	0
			642	388	137	115	2		

- Molecule 18 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LL	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 19 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LN	358	Total	C	N	O	S	0	0
			2884	1834	531	506	13		

- Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 21 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 22 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 23 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	102	Total	C	N	O	S	1	0
			840	526	180	129	5		

- Molecule 24 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LW	74	Total	C	N	O	S	0	0
			612	379	134	94	5		

- Molecule 25 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NB	67	Total	C	N	O	S	0	0
			569	355	119	92	3		

- Molecule 26 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NF	205	Total	C	N	O	S	0	0
			1684	1074	319	282	9		

- Molecule 27 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NH	180	Total	C	N	O	S	0	0
			1441	925	245	263	8		

- Molecule 28 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	NI	598	Total	C	N	O	S	0	0
			3866	2387	736	737	6		

- Molecule 29 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 30 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 31 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SC	203	Total	C	N	O	S	0	0
			1627	1049	306	270	2		

- Molecule 32 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 33 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SE	185	Total	C	N	O	S	0	0
			1491	946	289	252	4		

- Molecule 34 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SG	190	Total	C	N	O	S	1	0
			1526	961	287	272	6		

- Molecule 35 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SH	150	Total	C	N	O	S	0	0
			1267	819	224	220	4		

- Molecule 36 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SI	228	Total	C	N	O	S	1	0
			1887	1224	352	307	4		

- Molecule 37 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SJ	101	Total	C	N	O	S	0	0
			855	537	165	152	1		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 39 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 40 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SM	453	Total	C	N	O	S	0	0
			3735	2408	667	648	12		

- Molecule 41 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SN	173	Total	C	N	O	S	0	0
			1350	849	251	243	7		

- Molecule 42 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SO	296	Total	C	N	O	S	0	0
			2460	1583	446	416	15		

- Molecule 43 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 44 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SR	449	Total	C	N	O	S	0	0
			3695	2352	651	675	17		

- Molecule 45 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SS	256	Total	C	N	O	P S	0	0
			2116	1337	375	394	2 8		

- Molecule 46 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	ST	116	Total	C	N	O	S	0	0
			787	489	152	144	2		

- Molecule 47 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SV	137	Total	C	N	O	S	0	0
			1171	745	227	189	10		

- Molecule 48 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SW	444	Total	C	N	O	S	0	0
			3549	2282	605	645	17		

- Molecule 49 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SY	378	Total	C	N	O	S	0	0
			2985	1887	533	550	15		

- Molecule 50 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

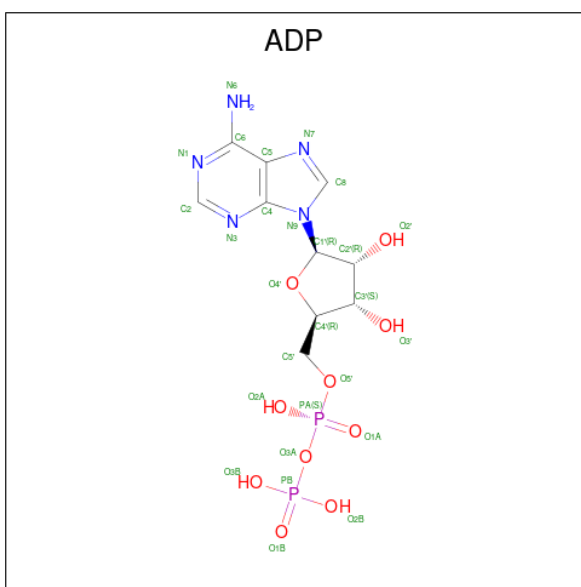
- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	L1	4	Total	Mg	0
			4	4	
51	L2	1	Total	Mg	0
			1	1	
51	L3	46	Total	Mg	0
			46	46	
51	L9	1	Total	Mg	0
			1	1	
51	LQ	1	Total	Mg	0
			1	1	
51	LT	1	Total	Mg	0
			1	1	
51	NI	1	Total	Mg	0
			1	1	
51	SA	1	Total	Mg	0
			1	1	
51	SO	1	Total	Mg	0
			1	1	
51	SR	1	Total	Mg	0
			1	1	

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

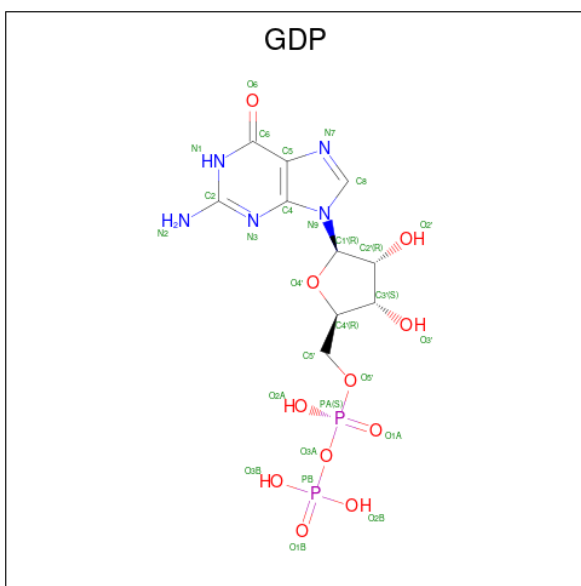
Mol	Chain	Residues	Atoms		AltConf
52	LW	1	Total	Zn	0
			1	1	
52	SV	1	Total	Zn	0
			1	1	

- Molecule 53 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
53	NI	1	Total	C	N	O	P	0
			27	10	5	10	2	

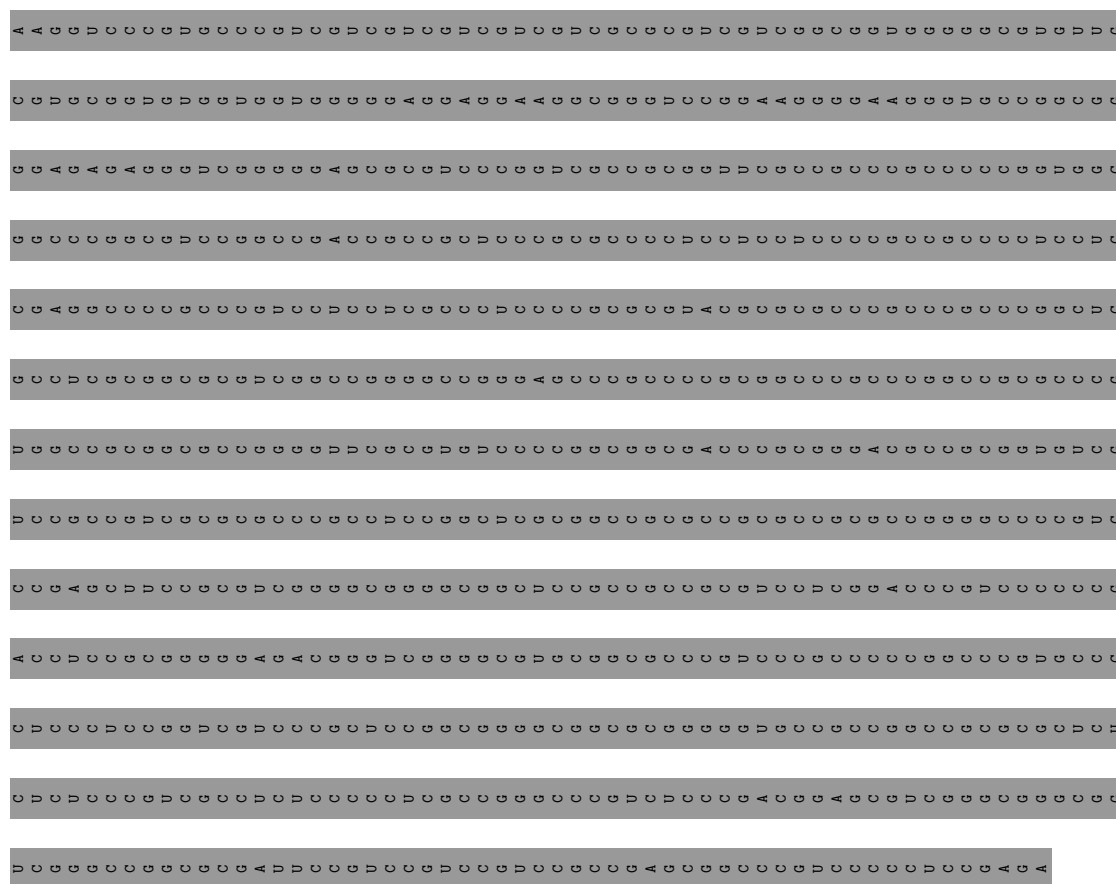
- Molecule 54 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

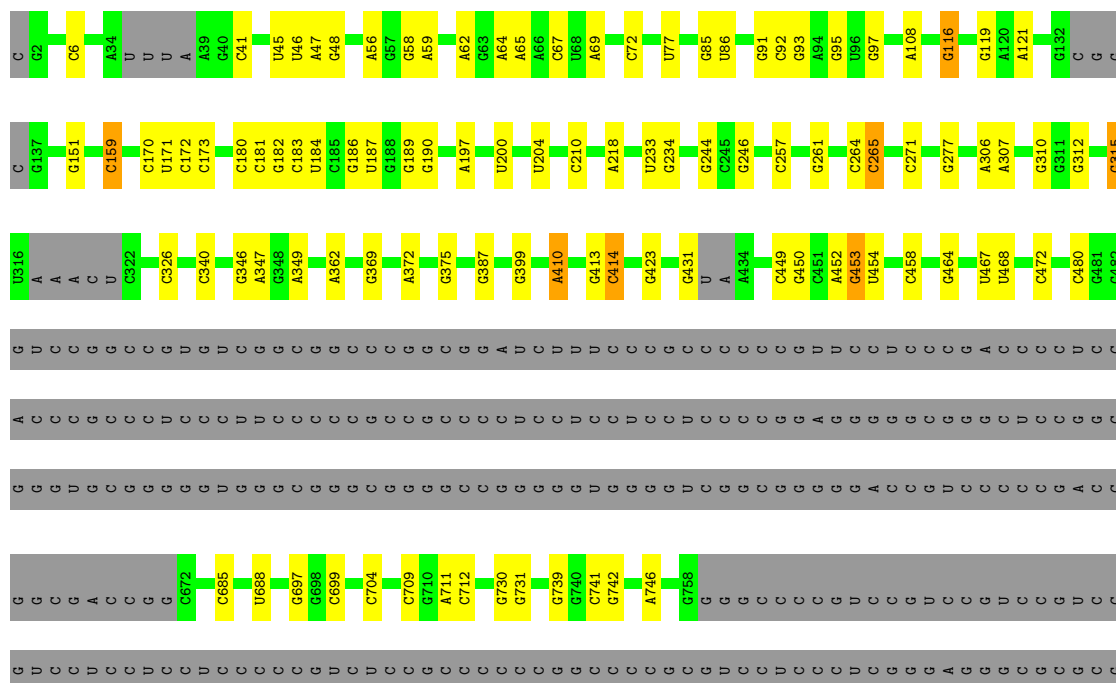
- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
55	SR	1	Total	K	0
			1	1	



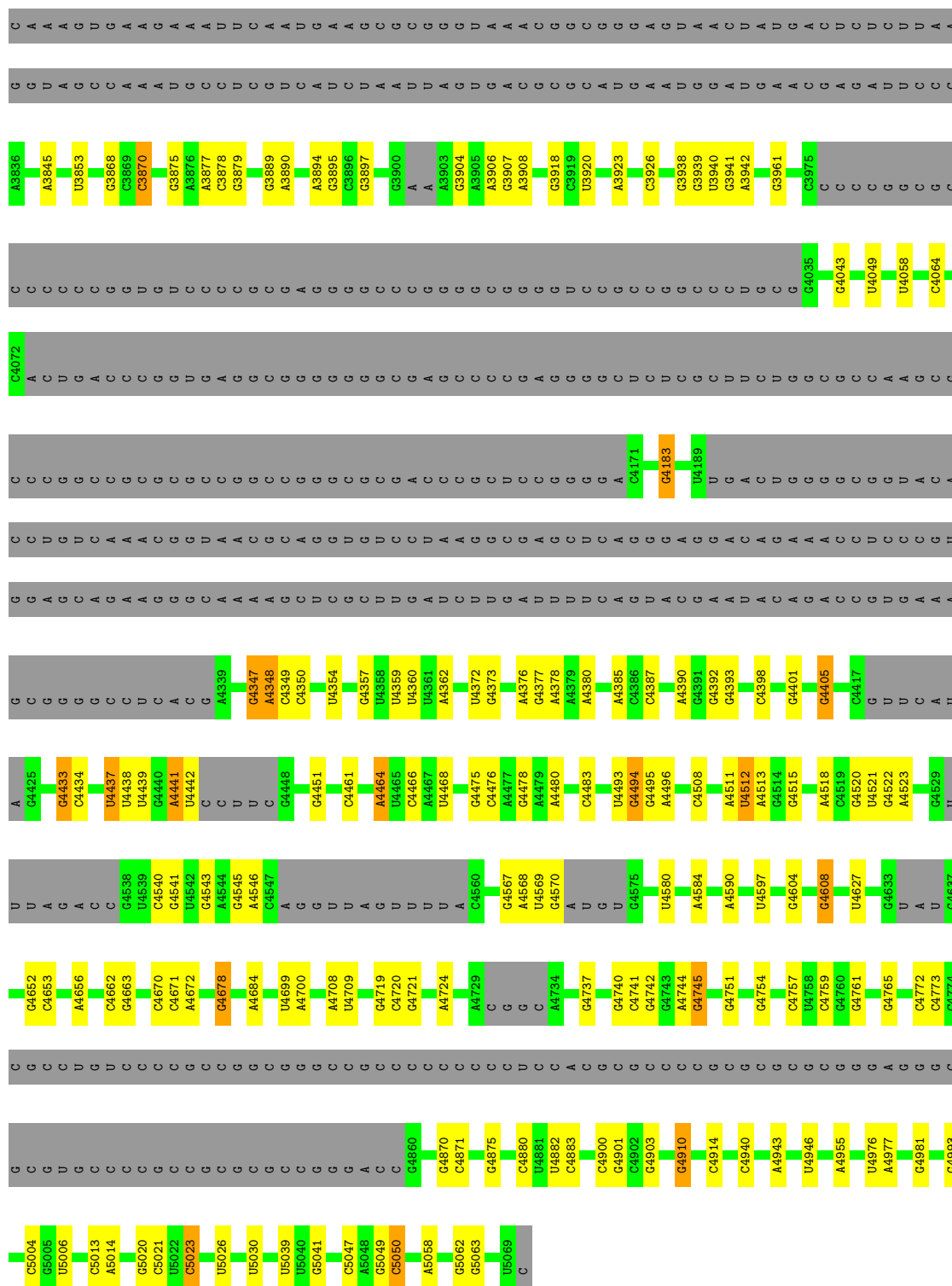
- Molecule 5: 28S rRNA

Chain L3:









• Molecule 6: 60S ribosomal protein L13

Chain L6:

51%

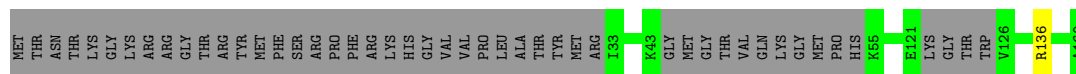
6%

43%



- Molecule 13: 60S ribosomal protein L21

Chain LE:  70% 29%



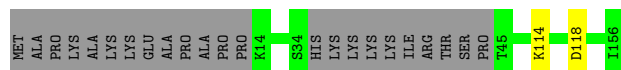
- Molecule 14: 60S ribosomal protein L23

Chain LG:  87% 9%



- Molecule 15: 60S ribosomal protein L23a

Chain LH:  84% 15%



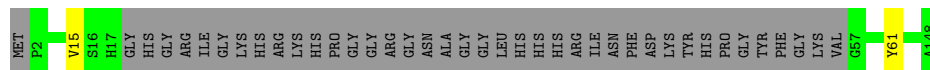
- Molecule 16: 60S ribosomal protein L26

Chain LI:  87% 6% 8%



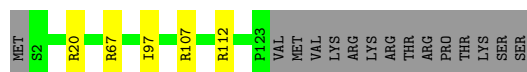
- Molecule 17: 60S ribosomal protein L27a

Chain LK:  72% 27%



- Molecule 18: 60S ribosomal protein L28

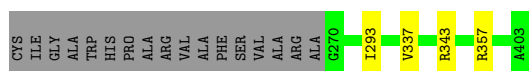
Chain LL:  85% 11%



- Molecule 19: 60S ribosomal protein L3

Chain LN:  84% 11%





- Molecule 20: 60S ribosomal protein L32

Chain LQ: 91% 5%



- Molecule 21: 60S ribosomal protein L35

Chain LS: 95% 2%



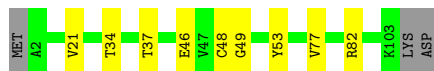
- Molecule 22: 60S ribosomal protein L35a

Chain LT: 94% 5%



- Molecule 23: 60S ribosomal protein L36

Chain LU: 89% 9%



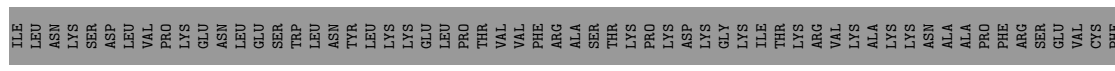
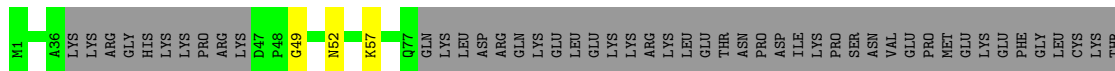
- Molecule 24: 60S ribosomal protein L37

Chain LW: 71% 5% 24%



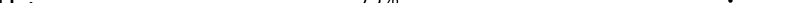
- Molecule 25: Guanine nucleotide-binding protein-like 3

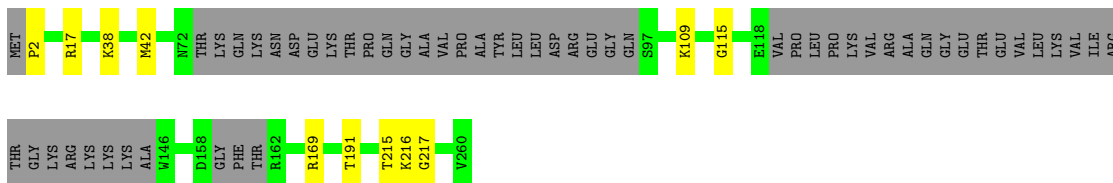
Chain NB: 12% 88% 2%



[illegible]

- Molecule 26: Ribosome biogenesis protein NSA2 homolog

Chain NF:  75% . 21%



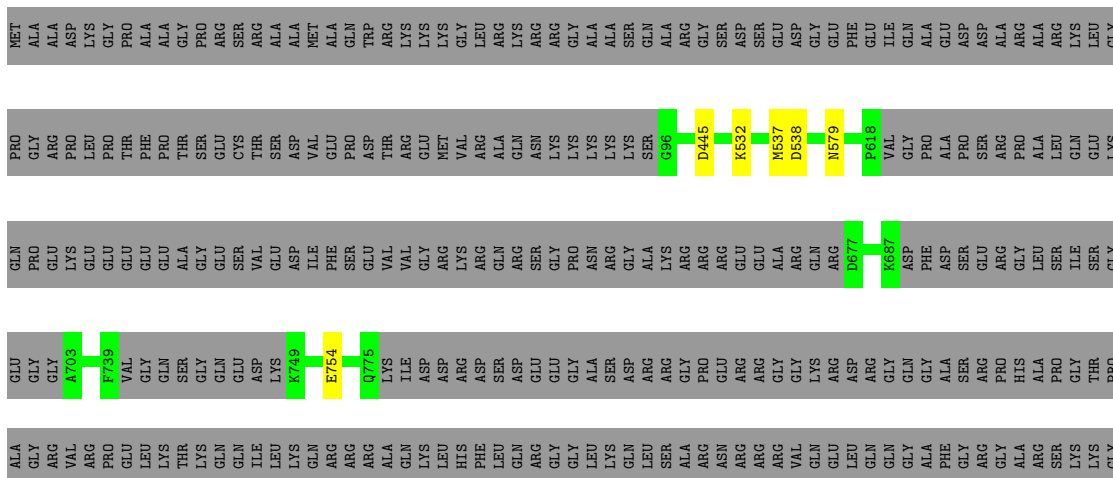
- Molecule 27: 60S ribosome subunit biogenesis protein NIP7 homolog

Chain NH: 88% 12%



- Molecule 28: ATP-dependent RNA helicase DDX54

Chain NI: 67% 32%



NET	PRO	LYS	GLY	LYS	ALA	LYS	LYS	VAL	VAL	ALA	PRO	ALA	ALA	PRO	PRO	ALA	ALA	VAL	VAL	LYS	LYS	VAL	VAL	ASN	LEU	PHE	GLY	LYS	ARG	PRO	PRO	LYS	ASN	ASN	PHE	GLY	ILE	GLY	GLN	ASP	ILE	GLN	PRO	LYS	ARG	ASP	LEU	THR	ARG	PHE	VAL	856	857	858	161
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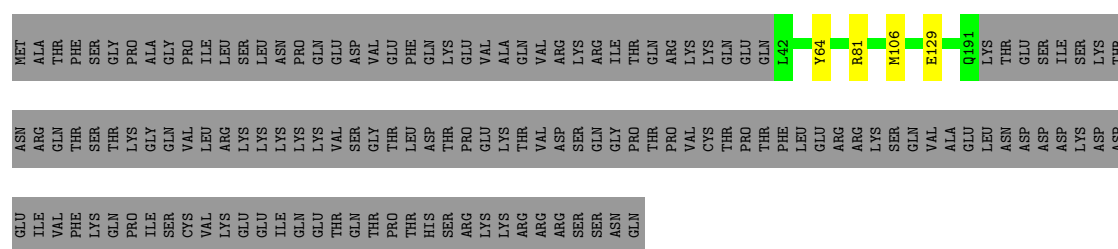
- Molecule 34: 60S ribosomal protein L9

Chain SG: 93% 6%



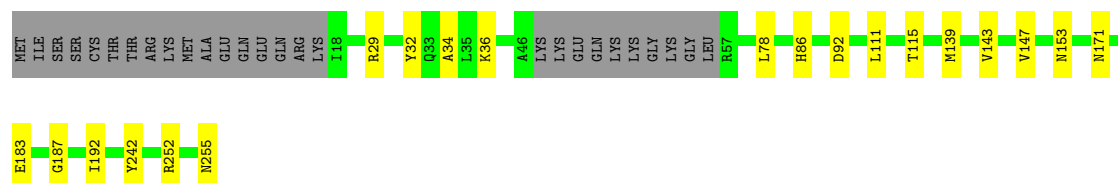
- Molecule 35: MKI67 FHA domain-interacting nucleolar phosphoprotein

Chain SH: 50% 49%



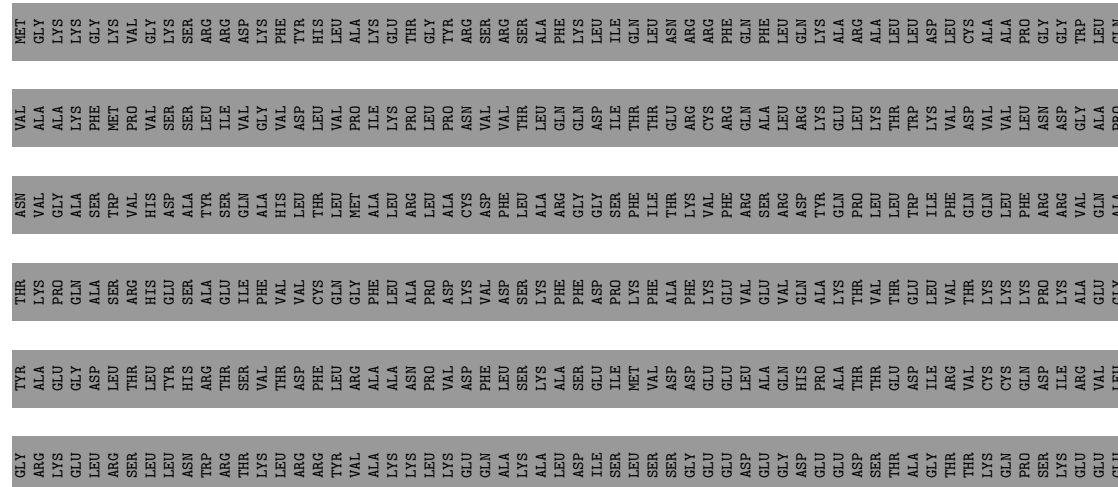
- Molecule 36: 60S ribosomal protein L7-like 1

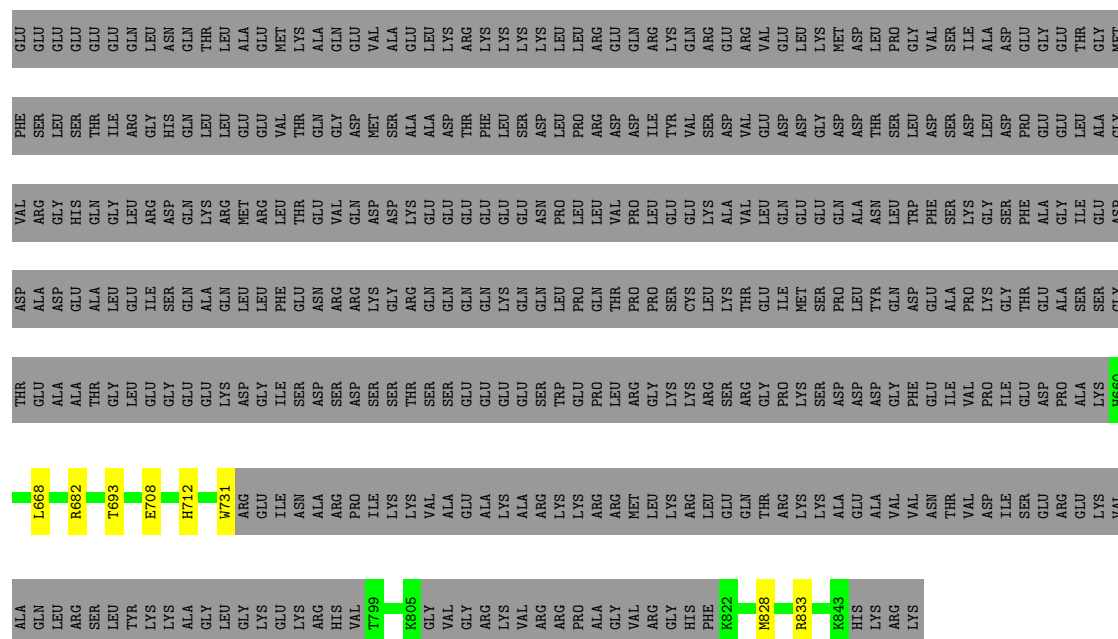
Chain SI: 82% 8% 11%



- Molecule 37: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

Chain SJ: 11% 88%





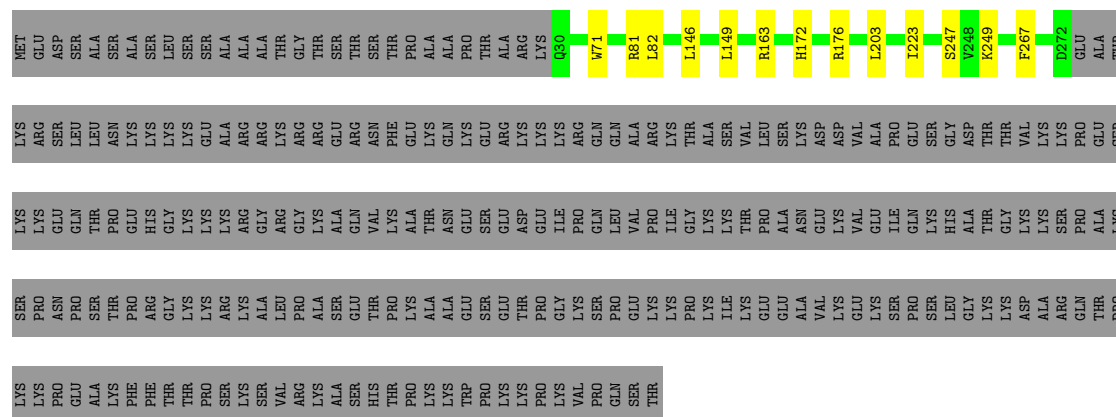
• Molecule 38: Eukaryotic translation initiation factor 6

Chain SK:



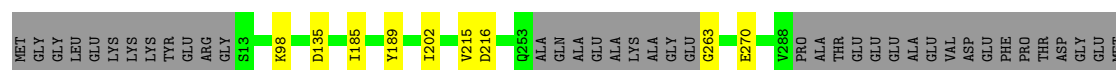
• Molecule 39: Ribosomal L1 domain-containing protein 1

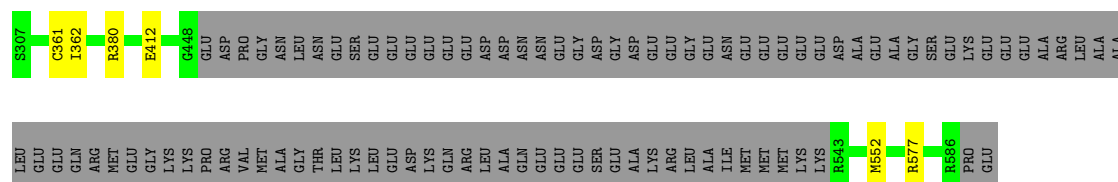
Chain SL:



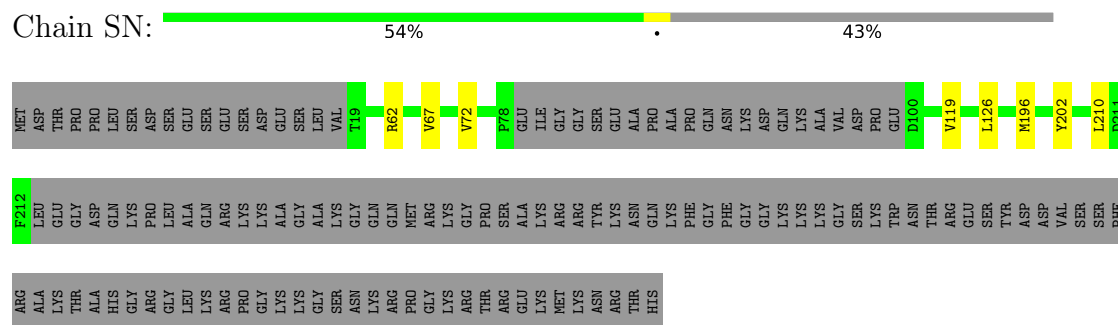
• Molecule 40: Pescadillo homolog

Chain SM:

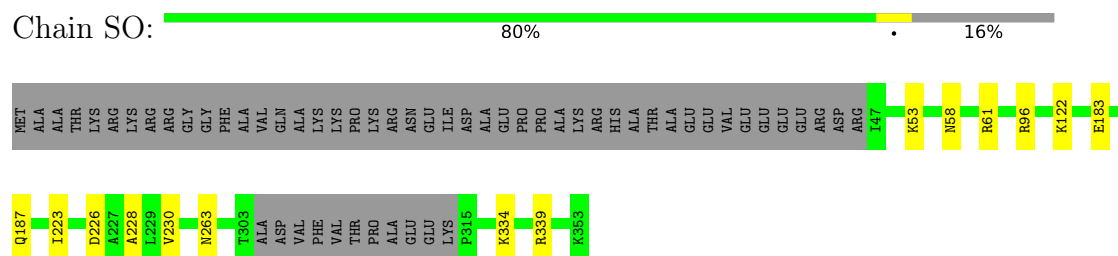




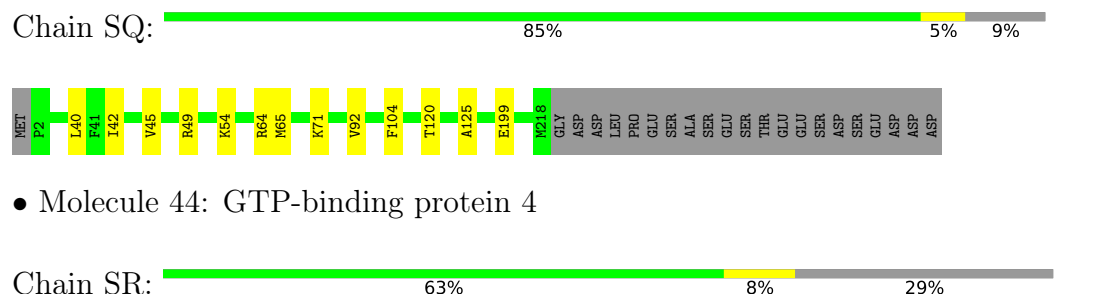
• Molecule 41: Probable rRNA-processing protein EBP2



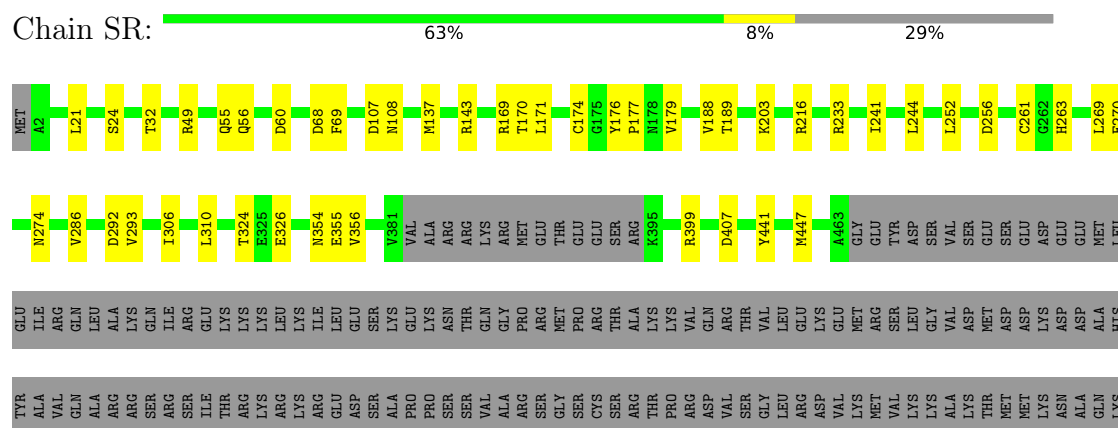
• Molecule 42: Ribosome biogenesis protein BRX1 homolog

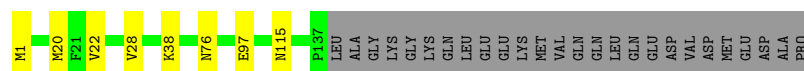


• Molecule 43: mRNA turnover protein 4 homolog



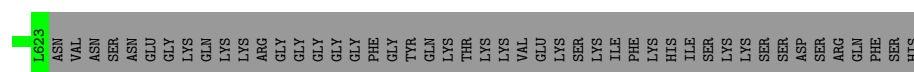
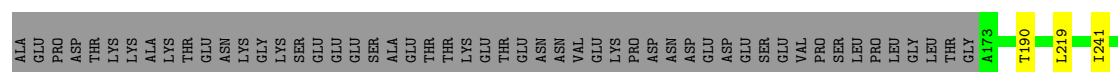
• Molecule 44: GTP-binding protein 4





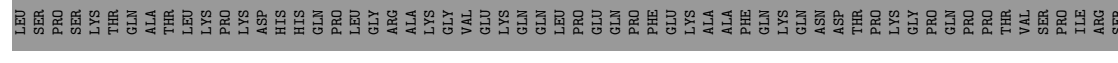
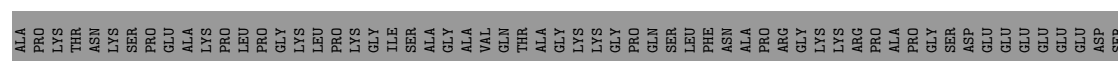
• Molecule 48: ATP-dependent RNA helicase DDX18

Chain SW: 62% 34%

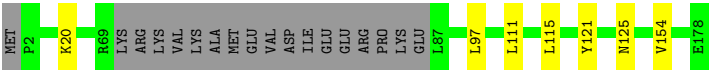
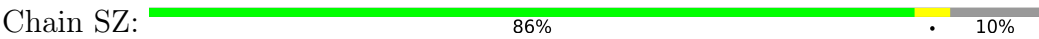


• Molecule 49: Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase

Chain SY: 42% 53%



• Molecule 50: Nucleolar protein 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48037	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	BA	0.17	0/1224	0.33	0/1651
2	BB	0.17	0/1056	0.36	0/1472
3	L1	0.33	0/3611	0.31	0/5623
4	L2	0.29	0/1634	0.32	0/2538
5	L3	0.29	0/52370	0.31	0/81617
6	L6	0.31	0/1020	0.42	0/1367
7	L7	0.31	0/1666	0.40	0/2228
8	L8	0.29	0/1133	0.38	0/1516
9	L9	0.34	0/1584	0.41	0/2117
10	LA	0.19	0/1127	0.36	0/1511
11	LB	0.30	0/1239	0.36	0/1658
12	LC	0.30	0/1501	0.38	0/2013
13	LE	0.15	0/755	0.33	0/1021
14	LG	0.21	0/1007	0.37	0/1350
15	LH	0.16	0/818	0.31	0/1111
16	LI	0.30	0/1132	0.42	0/1504
17	LK	0.17	0/648	0.38	0/880
18	LL	0.28	0/995	0.35	0/1334
19	LN	0.27	0/2938	0.38	0/3923
20	LQ	0.30	0/1071	0.36	0/1429
21	LS	0.24	0/1023	0.34	0/1351
22	LT	0.34	0/895	0.41	0/1198
23	LU	0.27	0/854	0.37	0/1129
24	LW	0.28	0/626	0.46	0/829
25	NB	0.23	0/576	0.36	0/757
26	NF	0.22	0/1715	0.32	0/2282
27	NH	0.28	0/1473	0.42	0/1988
28	NI	0.13	0/3906	0.26	0/5329
29	NK	0.20	0/587	0.36	0/767
30	SA	0.29	0/2907	0.38	0/3905
31	SC	0.22	0/1657	0.36	0/2226
32	SD	0.28	0/1905	0.37	0/2539

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SE	0.30	0/1517	0.38	0/2046
34	SG	0.25	0/1548	0.36	0/2081
35	SH	0.27	0/1298	0.33	0/1742
36	SI	0.24	0/1930	0.33	0/2595
37	SJ	0.21	0/868	0.38	0/1153
38	SK	0.27	0/1877	0.39	0/2554
39	SL	0.25	0/1994	0.38	0/2684
40	SM	0.23	0/3819	0.30	0/5139
41	SN	0.18	0/1368	0.29	0/1830
42	SO	0.25	0/2521	0.36	0/3384
43	SQ	0.17	0/1817	0.32	0/2435
44	SR	0.26	0/3768	0.37	0/5086
45	SS	0.23	0/2159	0.34	0/2932
46	ST	0.16	0/795	0.30	0/1072
47	SV	0.27	0/1194	0.41	0/1582
48	SW	0.22	0/3620	0.33	0/4886
49	SY	0.26	0/3046	0.35	0/4117
50	SZ	0.23	0/1364	0.32	0/1826
All	All	0.27	0/133156	0.34	0/191307

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 [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	BA	1208	0	1257	9	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	9	0
4	L2	1468	0	755	7	0
5	L3	46844	0	23704	139	0
6	L6	998	0	1067	10	0
7	L7	1634	0	1779	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L8	1111	0	1174	3	0
9	L9	1546	0	1585	6	0
10	LA	1106	0	1130	9	0
11	LB	1223	0	1330	9	0
12	LC	1461	0	1502	15	0
13	LE	747	0	599	2	0
14	LG	993	0	1050	7	0
15	LH	813	0	640	1	0
16	LI	1115	0	1205	7	0
17	LK	642	0	455	2	0
18	LL	980	0	1041	5	0
19	LN	2884	0	3000	14	0
20	LQ	1053	0	1147	5	0
21	LS	1015	0	1148	5	0
22	LT	876	0	912	8	0
23	LU	840	0	930	8	0
24	LW	612	0	640	5	0
25	NB	569	0	625	2	0
26	NF	1684	0	1792	12	0
27	NH	1441	0	1448	20	0
28	NI	3866	0	3171	6	0
29	NK	581	0	656	5	0
30	SA	2853	0	3028	15	0
31	SC	1627	0	1771	17	0
32	SD	1870	0	1996	6	0
33	SE	1491	0	1592	9	0
34	SG	1526	0	1614	6	0
35	SH	1267	0	1291	3	0
36	SI	1887	0	2011	17	0
37	SJ	855	0	876	8	0
38	SK	1852	0	1828	19	0
39	SL	1960	0	2052	10	0
40	SM	3735	0	3830	14	0
41	SN	1350	0	1345	5	0
42	SO	2460	0	2551	12	0
43	SQ	1778	0	1817	8	0
44	SR	3695	0	3753	34	0
45	SS	2116	0	2028	17	0
46	ST	787	0	698	7	0
47	SV	1171	0	1232	8	0
48	SW	3549	0	3628	20	0
49	SY	2985	0	3004	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	SZ	1338	0	1352	5	0
51	L1	4	0	0	0	0
51	L2	1	0	0	0	0
51	L3	46	0	0	0	0
51	L9	1	0	0	0	0
51	LQ	1	0	0	0	0
51	LT	1	0	0	0	0
51	NI	1	0	0	0	0
51	SA	1	0	0	0	0
51	SO	1	0	0	0	0
51	SR	1	0	0	0	0
52	LW	1	0	0	0	0
52	SV	1	0	0	0	0
53	NI	27	0	12	0	0
54	SR	28	0	12	0	0
55	SR	1	0	0	0	0
All	All	125869	0	101166	441	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 2.

All (441) 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)
39:SL:82:LEU:HD13	39:SL:203:LEU:HD13	1.41	1.00
5:L3:183:C:OP2	42:SO:334:LYS:NZ	2.03	0.91
5:L3:5063:G:O6	19:LN:124:LYS:NZ	2.09	0.86
5:L3:458:C:O2'	31:SC:110:ARG:NH2	2.09	0.85
5:L3:4946:U:HO2'	22:LT:2:SER:HG	1.14	0.82
30:SA:340:ILE:HG21	31:SC:50:LEU:HD13	1.60	0.82
50:SZ:111:LEU:HD11	50:SZ:115:LEU:HD23	1.60	0.82
1:BA:16:ARG:NH2	5:L3:1975:G:O2'	2.12	0.82
4:L2:53:G:OP2	35:SH:81:ARG:NH1	2.15	0.80
3:L1:75:G:OP2	16:LI:74:TYR:OH	1.98	0.80
48:SW:190:THR:HG23	48:SW:274:LEU:HD21	1.62	0.80
5:L3:4678:G:OP1	29:NK:14:ARG:NH1	2.16	0.79
4:L2:10:U:OP2	39:SL:163:ARG:NH2	2.16	0.78
27:NH:22:GLU:OE1	46:ST:276:ASN:ND2	2.15	0.78
5:L3:1238:A:OP2	31:SC:60:SER:OG	2.01	0.78
5:L3:3890:A:OP2	5:L3:4570:G:N2	2.16	0.78
48:SW:249:ARG:NH1	48:SW:250:ASN:OD1	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:NF:17:ARG:NH1	34:SG:180:TYR:OH	2.17	0.77
5:L3:5039:U:O3'	47:SV:115:ASN:ND2	2.18	0.77
12:LC:125:GLN:NE2	12:LC:127:MET:SD	2.57	0.77
5:L3:4508:C:O2	14:LG:46:LYS:NZ	2.18	0.77
5:L3:453:G:N2	5:L3:1293:G:O6	2.19	0.75
38:SK:119:PRO:O	38:SK:139:ARG:NH2	2.19	0.75
40:SM:135:ASP:OD2	45:SS:304:LYS:NZ	2.20	0.74
22:LT:33:VAL:HG23	22:LT:38:GLU:HB2	1.70	0.74
5:L3:72:C:N3	6:L6:60:ARG:NH1	2.35	0.73
43:SQ:120:THR:OG1	43:SQ:199:GLU:OE1	2.05	0.73
5:L3:2361:G:O6	10:LA:25:HIS:ND1	2.21	0.73
5:L3:2045:G:O6	5:L3:3870:C:O2'	2.05	0.73
42:SO:61:ARG:NH1	45:SS:128:ASP:OD2	2.22	0.73
9:L9:20:ARG:NH2	37:SJ:693:THR:O	2.22	0.73
5:L3:62:A:N3	5:L3:77:U:O2'	2.22	0.73
5:L3:184:U:O2'	5:L3:189:G:OP2	2.06	0.73
5:L3:4441:A:N6	28:NI:445:ASP:O	2.21	0.72
5:L3:1280:C:O2'	30:SA:321:ASN:OD1	2.08	0.72
19:LN:357:ARG:NE	44:SR:407:ASP:OD1	2.23	0.71
5:L3:151:G:OP2	9:L9:4:TYR:OH	2.08	0.71
44:SR:169:ARG:NH1	44:SR:216:ARG:O	2.24	0.71
10:LA:36:ILE:HD11	10:LA:48:LEU:HD21	1.72	0.70
5:L3:2574:G:O2'	5:L3:2575:U:OP1	2.09	0.70
39:SL:82:LEU:CD1	39:SL:203:LEU:HD13	2.20	0.70
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.09	0.70
5:L3:1524:A:O2'	5:L3:1525:A:O5'	2.07	0.70
28:NI:579:ASN:O	44:SR:203:LYS:NZ	2.25	0.70
5:L3:1369:C:OP2	5:L3:1370:G:O2'	2.04	0.69
3:L1:93:C:OP1	24:LW:76:HIS:NE2	2.23	0.69
14:LG:111:GLU:OE1	14:LG:131:ARG:NH1	2.26	0.69
5:L3:1983:A:N1	28:NI:579:ASN:ND2	2.41	0.68
5:L3:306:A:OP1	23:LU:53:TYR:OH	2.11	0.68
19:LN:107:ALA:HB2	19:LN:201:LEU:HD22	1.74	0.68
18:LL:20:ARG:NH1	20:LQ:78:LEU:O	2.26	0.68
10:LA:40:HIS:NE2	10:LA:110:ASP:O	2.27	0.68
44:SR:441:TYR:OH	47:SV:97:GLU:OE2	2.12	0.67
18:LL:20:ARG:NH2	20:LQ:84:GLU:OE2	2.29	0.66
5:L3:4354:U:OP1	49:SY:530:TYR:OH	2.12	0.66
26:NF:109:LYS:HD2	49:SY:236:LEU:HD11	1.77	0.66
43:SQ:64:ARG:NH1	43:SQ:65:MET:O	2.29	0.66
5:L3:1502:G:OP1	11:LB:65:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1883:G:OP1	20:LQ:47:ARG:NH1	2.28	0.65
5:L3:4478:G:N2	5:L3:4608:G:O2'	2.29	0.65
5:L3:1659:U:H2'	17:LK:15:VAL:HG23	1.79	0.65
5:L3:4437:U:O2'	44:SR:143:ARG:NH2	2.30	0.65
5:L3:47:A:OP2	6:L6:20:ARG:NH2	2.29	0.65
24:LW:15:THR:HG23	24:LW:16:HIS:ND1	2.12	0.65
42:SO:223:ILE:HD11	42:SO:230:VAL:HG23	1.78	0.65
44:SR:176:TYR:HH	44:SR:263:HIS:CE1	2.15	0.65
39:SL:223:ILE:HD12	39:SL:223:ILE:H	1.62	0.65
33:SE:106:THR:OG1	33:SE:109:GLU:OE2	2.06	0.65
43:SQ:49:ARG:NH1	43:SQ:125:ALA:O	2.30	0.64
5:L3:1508:A:OP1	30:SA:110:ARG:NH2	2.30	0.64
42:SO:122:LYS:NZ	42:SO:263:ASN:OD1	2.30	0.64
38:SK:228:GLN:OE1	38:SK:228:GLN:N	2.32	0.63
5:L3:4468:U:HO2'	29:NK:2:ALA:N	1.97	0.62
5:L3:4662:C:O2'	5:L3:5004:C:OP1	2.16	0.62
5:L3:4910:G:N2	7:L7:106:ASP:O	2.33	0.62
30:SA:204:ARG:NH1	30:SA:205:ARG:O	2.33	0.62
21:LS:80:PRO:HD2	21:LS:83:LEU:HD12	1.80	0.61
40:SM:189:TYR:CZ	40:SM:202:ILE:HD12	2.35	0.61
4:L2:13:C:OP1	36:SI:86:HIS:NE2	2.31	0.61
36:SI:153:ASN:ND2	40:SM:263:GLY:O	2.34	0.61
36:SI:92:ASP:OD1	36:SI:242:TYR:OH	2.18	0.61
5:L3:1524:A:HO2'	5:L3:1525:A:P	2.24	0.61
49:SY:532:LEU:HD23	49:SY:537:VAL:HG23	1.82	0.61
5:L3:977:C:OP1	31:SC:59:ARG:NH2	2.34	0.61
38:SK:174:SER:O	38:SK:178:GLN:N	2.32	0.61
5:L3:4946:U:O2'	22:LT:2:SER:OG	2.00	0.61
41:SN:202:TYR:CZ	41:SN:210:LEU:HD11	2.35	0.61
44:SR:174:CYS:SG	44:SR:244:LEU:HD21	2.41	0.61
5:L3:1961:G:N7	43:SQ:71:LYS:NZ	2.42	0.60
5:L3:2083:C:OP2	11:LB:14:ARG:NH2	2.33	0.60
5:L3:375:G:OP2	24:LW:52:LYS:NZ	2.25	0.60
5:L3:244:G:O6	50:SZ:20:LYS:NZ	2.34	0.60
19:LN:86:VAL:HG13	19:LN:162:VAL:HG13	1.84	0.60
14:LG:27:ASN:OD1	14:LG:28:CYS:N	2.35	0.59
36:SI:143:VAL:O	36:SI:147:VAL:HG12	2.01	0.59
30:SA:339:THR:HG22	30:SA:342:ARG:HH22	1.67	0.59
14:LG:49:LEU:HG	14:LG:52:LEU:HD12	1.84	0.59
31:SC:133:PHE:O	31:SC:138:ARG:NH2	2.36	0.59
16:LI:34:LEU:HD22	16:LI:44:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:453:G:N1	5:L3:1293:G:N7	2.46	0.59
19:LN:219:VAL:HG11	19:LN:337:VAL:CG2	2.31	0.59
5:L3:4183:G:N7	27:NH:1:MET:N	2.51	0.59
23:LU:21:VAL:HG21	48:SW:321:GLY:HA3	1.85	0.58
23:LU:46:GLU:OE1	45:SS:227:PHE:N	2.34	0.58
45:SS:198:ASP:OD1	45:SS:199:GLU:N	2.36	0.58
5:L3:4597:U:O2'	44:SR:399:ARG:NH2	2.35	0.58
44:SR:270:GLU:O	44:SR:274:ASN:ND2	2.31	0.58
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.03	0.58
3:L1:102:G:OP2	3:L1:104:A:O2'	2.21	0.58
5:L3:4940:C:OP1	31:SC:156:ARG:NH1	2.36	0.58
39:SL:81:ARG:C	39:SL:82:LEU:HD12	2.28	0.58
5:L3:121:A:OP1	33:SE:110:LYS:NZ	2.35	0.58
44:SR:107:ASP:OD1	44:SR:108:ASN:N	2.36	0.58
5:L3:182:G:N7	42:SO:339:ARG:NH1	2.51	0.58
32:SD:105:VAL:HG13	32:SD:136:VAL:HG12	1.86	0.58
5:L3:4493:U:O2'	5:L3:4494:G:O5'	2.22	0.58
25:NB:52:ASN:OD1	25:NB:57:LYS:NZ	2.36	0.58
5:L3:423:G:N3	10:LA:118:GLN:NE2	2.53	0.57
38:SK:175:SER:O	38:SK:178:GLN:NE2	2.37	0.57
4:L2:93:C:HO2'	4:L2:94:U:P	2.28	0.57
5:L3:4663:G:OP2	47:SV:38:LYS:NZ	2.35	0.57
6:L6:62:PRO:O	6:L6:63:THR:OG1	2.18	0.57
14:LG:42:VAL:HG13	14:LG:45:ILE:HG22	1.86	0.57
44:SR:188:VAL:HG23	44:SR:189:THR:HG23	1.87	0.56
32:SD:171:ASP:OD2	32:SD:172:ASN:N	2.38	0.56
48:SW:241:ILE:HG13	48:SW:304:ILE:HD11	1.87	0.56
5:L3:1921:C:O2'	12:LC:160:ARG:NH2	2.38	0.56
35:SH:64:TYR:OH	35:SH:106:MET:HE1	2.06	0.56
5:L3:4903:G:OP2	29:NK:84:LYS:NZ	2.30	0.56
36:SI:252:ARG:NH1	40:SM:270:GLU:OE1	2.39	0.56
10:LA:6:LEU:HD12	10:LA:116:HIS:CD2	2.41	0.56
27:NH:8:GLU:OE1	46:ST:252:ARG:NH1	2.38	0.56
44:SR:269:LEU:HD12	44:SR:306:ILE:HG23	1.86	0.56
27:NH:66:LEU:CD2	49:SY:438:ILE:HG23	2.37	0.55
12:LC:17:LEU:HD21	13:LE:136:ARG:NH1	2.22	0.55
49:SY:555:ARG:O	49:SY:558:ARG:NH1	2.34	0.55
5:L3:265:C:N4	50:SZ:154:VAL:HG21	2.22	0.55
12:LC:95:ARG:NH1	12:LC:113:MET:SD	2.79	0.55
22:LT:33:VAL:HG23	22:LT:38:GLU:CB	2.35	0.55
26:NF:115:GLY:O	28:NI:532:LYS:NZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SA:124:ILE:HG21	30:SA:264:TYR:OH	2.06	0.55
5:L3:346:G:OP1	16:LI:8:THR:HG23	2.06	0.55
7:L7:190:ASP:OD1	7:L7:191:LYS:N	2.39	0.55
5:L3:4362:A:OP1	49:SY:486:ARG:NH1	2.39	0.55
34:SG:140:GLN:NE2	34:SG:143:GLU:OE2	2.40	0.55
5:L3:67:C:OP2	5:L3:312:G:N2	2.40	0.54
23:LU:46:GLU:OE1	45:SS:228:SER:N	2.39	0.54
5:L3:2044:U:N3	7:L7:63:ASN:OD1	2.40	0.54
5:L3:5039:U:O2'	47:SV:115:ASN:ND2	2.40	0.54
21:LS:37:THR:HG23	21:LS:37:THR:O	2.08	0.54
48:SW:335:ALA:O	48:SW:339:LEU:HD23	2.09	0.53
5:L3:2079:G:OP2	20:LQ:64:LYS:NZ	2.41	0.53
48:SW:241:ILE:HD11	48:SW:254:VAL:HG23	1.89	0.53
12:LC:95:ARG:NH2	12:LC:112:ASP:OD2	2.40	0.53
5:L3:4724:A:O2'	19:LN:104:THR:HG22	2.09	0.53
27:NH:51:ILE:HD13	49:SY:411:VAL:HG22	1.90	0.53
5:L3:1996:C:O2	43:SQ:54:LYS:NZ	2.42	0.53
1:BA:138:SER:OG	5:L3:1976:G:N3	2.42	0.53
12:LC:17:LEU:HD21	13:LE:136:ARG:HH11	1.74	0.53
28:NI:537:MET:HE3	28:NI:538:ASP:H	1.74	0.53
31:SC:161:ARG:O	31:SC:182:ASN:ND2	2.41	0.53
3:L1:83:C:H42	16:LI:50:ARG:NH1	2.06	0.53
5:L3:3961:G:O2'	5:L3:4043:G:N2	2.41	0.53
21:LS:91:MET:HE1	24:LW:78:PHE:CD2	2.44	0.52
32:SD:41:MET:HE2	32:SD:41:MET:N	2.23	0.52
27:NH:52:MET:HE1	46:ST:258:PHE:CE1	2.45	0.52
12:LC:99:ASP:OD2	12:LC:100:LEU:N	2.41	0.52
5:L3:410:A:O2'	5:L3:414:C:O2'	2.11	0.52
27:NH:57:ASN:HD22	49:SY:451:VAL:HG12	1.74	0.52
41:SN:62:ARG:NH1	42:SO:58:ASN:OD1	2.43	0.52
27:NH:52:MET:HE1	46:ST:258:PHE:HE1	1.75	0.52
30:SA:211:TYR:OH	30:SA:218:ILE:HD11	2.10	0.52
39:SL:149:LEU:HD21	39:SL:176:ARG:HG3	1.92	0.52
48:SW:289:SER:OG	48:SW:294:GLU:OE2	2.28	0.52
38:SK:132:VAL:HG12	38:SK:133:LEU:HD23	1.92	0.52
30:SA:335:MET:O	30:SA:339:THR:HG23	2.10	0.52
33:SE:229:ARG:NH1	33:SE:230:TYR:OH	2.42	0.52
3:L1:84:A:N6	3:L1:87:G:O6	2.44	0.51
5:L3:2851:G:N2	28:NI:754:GLU:O	2.42	0.51
49:SY:540:VAL:HG22	49:SY:541:PRO:HD2	1.92	0.51
34:SG:86:LEU:HD22	34:SG:188:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SR:56:GLN:NE2	44:SR:60:ASP:OD2	2.44	0.51
5:L3:116:G:O2'	45:SS:239:ARG:NH1	2.43	0.51
5:L3:1284:G:O4'	31:SC:130:LYS:NZ	2.38	0.51
9:L9:61:ILE:HG21	9:L9:131:GLU:OE2	2.11	0.51
5:L3:45:U:O2'	6:L6:14:PHE:O	2.28	0.50
5:L3:4387:C:O3'	26:NF:169:ARG:NH2	2.42	0.50
5:L3:4910:G:H4'	19:LN:95:THR:HG22	1.93	0.50
38:SK:222:PHE:O	38:SK:224:LEU:N	2.43	0.50
3:L1:62:A:OP1	21:LS:52:LYS:NZ	2.44	0.50
31:SC:50:LEU:HD12	31:SC:51:VAL:N	2.26	0.50
38:SK:107:VAL:HG13	38:SK:118:HIS:HB2	1.93	0.50
41:SN:67:VAL:HG22	41:SN:126:LEU:HD13	1.94	0.50
5:L3:315:G:N7	42:SO:96:ARG:NH2	2.59	0.50
38:SK:122:ASP:OD1	38:SK:125:THR:OG1	2.30	0.50
14:LG:96:LEU:HD11	47:SV:22:VAL:HG23	1.94	0.50
33:SE:132:ARG:NH2	45:SS:245:SER:O	2.45	0.50
4:L2:93:C:O2'	4:L2:94:U:O5'	2.18	0.50
44:SR:447:MET:SD	44:SR:447:MET:N	2.85	0.49
1:BA:105:THR:HG22	1:BA:108:GLU:OE2	2.13	0.49
42:SO:223:ILE:HD11	42:SO:230:VAL:CG2	2.43	0.49
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.44	0.49
11:LB:124:ASP:OD1	11:LB:125:GLN:N	2.44	0.49
36:SI:192:ILE:HD12	45:SS:351:ARG:HH11	1.77	0.49
23:LU:48:CYS:SG	23:LU:49:GLY:N	2.85	0.49
38:SK:98:GLU:OE2	47:SV:76:ASN:ND2	2.43	0.49
5:L3:1726:U:H5'	32:SD:135:ILE:HD11	1.94	0.49
5:L3:4434:C:O4'	26:NF:191:THR:HG23	2.12	0.49
12:LC:76:LYS:NZ	12:LC:100:LEU:O	2.34	0.49
27:NH:58:ILE:HD11	49:SY:413:LEU:HD11	1.94	0.49
12:LC:69:GLU:OE1	12:LC:76:LYS:NZ	2.45	0.49
23:LU:77:VAL:HG11	23:LU:82:ARG:HB3	1.95	0.49
43:SQ:42:ILE:HD11	43:SQ:92:VAL:HG13	1.93	0.49
43:SQ:45:VAL:HG23	43:SQ:45:VAL:O	2.13	0.49
1:BA:105:THR:HG23	1:BA:108:GLU:H	1.78	0.49
5:L3:1950:U:O2'	12:LC:116:ARG:NH1	2.45	0.49
36:SI:183:GLU:O	36:SI:187:GLY:N	2.46	0.49
45:SS:150:VAL:HG13	45:SS:150:VAL:O	2.13	0.49
5:L3:709:C:OP1	22:LT:89:ARG:NH2	2.45	0.48
6:L6:127:PHE:HZ	50:SZ:97:LEU:HD22	1.77	0.48
1:BA:95:GLN:HB2	1:BA:98:ILE:HD11	1.94	0.48
44:SR:68:ASP:OD1	44:SR:69:PHE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1284:G:N3	31:SC:130:LYS:NZ	2.53	0.48
27:NH:69:CYS:O	27:NH:84:THR:OG1	2.22	0.48
36:SI:29:ARG:NH1	45:SS:369:ASP:OD1	2.45	0.48
44:SR:256:ASP:OD2	44:SR:261:CYS:N	2.40	0.48
5:L3:4543:G:N7	27:NH:15:LYS:NZ	2.49	0.48
34:SG:36:ARG:NH1	34:SG:152:GLU:OE2	2.47	0.48
5:L3:4993:G:H22	5:L3:5058:A:H2	1.61	0.48
43:SQ:40:LEU:HD12	43:SQ:104:PHE:CE2	2.49	0.48
4:L2:91:C:OP2	39:SL:176:ARG:NH2	2.47	0.48
5:L3:1328:G:O2'	5:L3:2349:A:OP1	2.32	0.48
23:LU:34:THR:OG1	23:LU:37:THR:HG22	2.14	0.48
42:SO:53:LYS:NZ	45:SS:155:ASP:OD2	2.43	0.47
50:SZ:121:TYR:O	50:SZ:125:ASN:ND2	2.46	0.47
40:SM:412:GLU:OE1	40:SM:412:GLU:N	2.46	0.47
4:L2:99:G:N2	35:SH:129:GLU:OE1	2.47	0.47
5:L3:159:C:O2	6:L6:88:LYS:NZ	2.32	0.47
14:LG:112:MET:SD	14:LG:117:ILE:HD11	2.54	0.47
5:L3:2000:G:O2'	5:L3:2017:A:N1	2.41	0.47
5:L3:5047:C:O2'	5:L3:5050:C:OP2	2.25	0.47
19:LN:219:VAL:HG11	19:LN:337:VAL:HG21	1.95	0.47
27:NH:135:SER:OG	27:NH:136:MET:N	2.47	0.47
33:SE:143:VAL:HG11	33:SE:201:THR:HG21	1.96	0.47
38:SK:2:ALA:CB	38:SK:215:LEU:HD11	2.45	0.47
49:SY:532:LEU:HD11	49:SY:539:LEU:HD23	1.97	0.47
5:L3:5021:C:O2	5:L3:5023:C:N4	2.47	0.47
40:SM:215:VAL:HG23	45:SS:364:PHE:CG	2.50	0.47
5:L3:4483:C:H5''	44:SR:21:LEU:HD13	1.97	0.47
5:L3:369:G:N2	5:L3:372:A:OP2	2.41	0.46
5:L3:4347:G:O2'	5:L3:4348:A:O5'	2.30	0.46
38:SK:61:ARG:O	38:SK:105:GLY:N	2.47	0.46
27:NH:114:LEU:O	27:NH:117:GLY:N	2.47	0.46
29:NK:9:TRP:CH2	29:NK:13:MET:HE3	2.50	0.46
29:NK:9:TRP:CZ2	29:NK:13:MET:HE3	2.50	0.46
30:SA:192:GLY:O	30:SA:195:LYS:NZ	2.47	0.46
49:SY:321:ARG:NE	49:SY:343:LYS:O	2.40	0.46
49:SY:429:LEU:HD12	49:SY:439:ILE:HD11	1.96	0.46
27:NH:58:ILE:HD11	49:SY:413:LEU:CD1	2.46	0.46
47:SV:20:MET:HE3	47:SV:28:VAL:HG11	1.98	0.46
22:LT:33:VAL:HG13	22:LT:33:VAL:O	2.16	0.46
36:SI:115:THR:HG23	36:SI:139:MET:HG2	1.97	0.46
49:SY:532:LEU:HD21	49:SY:539:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LA:36:ILE:HD12	10:LA:91:LEU:HD13	1.97	0.46
33:SE:58:PRO:HG2	33:SE:61:ILE:HD12	1.97	0.46
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.48	0.46
49:SY:417:ALA:O	49:SY:441:HIS:NE2	2.49	0.46
5:L3:2340:C:H4'	30:SA:42:THR:HG23	1.97	0.46
16:LI:50:ARG:NH2	16:LI:51:LYS:O	2.49	0.46
20:LQ:84:GLU:O	20:LQ:87:VAL:HG22	2.16	0.46
36:SI:252:ARG:NH2	40:SM:270:GLU:OE2	2.49	0.46
5:L3:480:C:OP1	18:LL:67:ARG:NH1	2.50	0.46
5:L3:1325:C:O2	37:SJ:833:ARG:NH1	2.45	0.46
38:SK:71:LEU:HD21	38:SK:132:VAL:HG11	1.96	0.46
44:SR:292:ASP:OD1	44:SR:293:VAL:N	2.46	0.46
40:SM:577:ARG:HE	40:SM:577:ARG:HA	1.81	0.45
44:SR:356:VAL:HG12	44:SR:356:VAL:O	2.16	0.45
30:SA:69:THR:HB	37:SJ:828:MET:HE2	1.98	0.45
5:L3:5047:C:O2	5:L3:5049:G:O2'	2.20	0.45
31:SC:214:ASP:OD1	31:SC:215:ALA:N	2.48	0.45
5:L3:3923:A:OP2	5:L3:4377:G:O2'	2.26	0.45
9:L9:31:ARG:NH1	37:SJ:708:GLU:OE1	2.49	0.45
49:SY:283:PHE:HE2	49:SY:484:ILE:HD12	1.82	0.45
44:SR:233:ARG:NH1	44:SR:241:ILE:HD11	2.30	0.45
39:SL:146:LEU:HD21	39:SL:172:HIS:CD2	2.51	0.45
27:NH:163:VAL:HG12	27:NH:164:PHE:O	2.17	0.45
5:L3:180:C:N3	42:SO:339:ARG:NH1	2.64	0.45
22:LT:2:SER:N	31:SC:274:VAL:HG11	2.31	0.45
27:NH:66:LEU:HD23	49:SY:438:ILE:HG23	1.97	0.45
36:SI:29:ARG:NH1	45:SS:373:CYS:SG	2.90	0.45
5:L3:4464:A:N7	44:SR:32:THR:OG1	2.42	0.45
5:L3:4493:U:C2'	5:L3:4494:G:O5'	2.65	0.45
27:NH:29:ASP:OD1	46:ST:269:LEU:HD11	2.17	0.45
33:SE:135:VAL:HG22	33:SE:136:LEU:N	2.32	0.45
36:SI:78:LEU:HD13	36:SI:111:LEU:HD23	1.99	0.45
48:SW:590:TYR:CD2	48:SW:604:LEU:HD11	2.52	0.45
5:L3:1354:A:HO2'	17:LK:61:TYR:HH	1.64	0.44
12:LC:81:TRP:NE1	12:LC:92:ASN:OD1	2.48	0.44
46:ST:232:VAL:O	46:ST:232:VAL:HG12	2.17	0.44
5:L3:4745:G:H22	5:L3:4955:A:H2	1.65	0.44
40:SM:185:ILE:HD11	45:SS:342:PHE:CD2	2.53	0.44
32:SD:219:GLY:O	32:SD:246:ARG:NH2	2.51	0.44
44:SR:171:LEU:HD23	44:SR:252:LEU:HD11	2.00	0.44
30:SA:14:LYS:HE3	30:SA:14:LYS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LU:21:VAL:HG21	48:SW:321:GLY:CA	2.48	0.44
44:SR:179:VAL:HG22	44:SR:179:VAL:O	2.18	0.44
5:L3:85:G:O2'	5:L3:86:U:OP2	2.36	0.44
5:L3:85:G:O2'	5:L3:97:G:O6	2.29	0.44
9:L9:126:THR:HG21	37:SJ:712:HIS:HD2	1.81	0.44
9:L9:126:THR:HG21	37:SJ:712:HIS:CD2	2.53	0.44
19:LN:57:VAL:HG12	19:LN:73:VAL:HG22	1.98	0.44
38:SK:73:PRO:O	38:SK:76:THR:HG22	2.17	0.44
48:SW:397:VAL:HG22	48:SW:398:ASP:H	1.83	0.44
49:SY:565:SER:O	49:SY:567:ARG:NH1	2.51	0.44
39:SL:249:LYS:HE3	39:SL:267:PHE:CE1	2.52	0.44
12:LC:82:LEU:HD12	12:LC:124:ILE:HG23	1.99	0.43
12:LC:92:ASN:ND2	25:NB:49:GLY:O	2.50	0.43
19:LN:293:ILE:HG23	19:LN:293:ILE:O	2.18	0.43
38:SK:123:ARG:HD2	38:SK:123:ARG:N	2.32	0.43
48:SW:351:ILE:HG23	48:SW:358:ARG:HH22	1.82	0.43
8:L8:81:ASP:OD2	8:L8:84:THR:HG22	2.19	0.43
44:SR:354:ASN:OD1	44:SR:355:GLU:N	2.51	0.43
5:L3:911:U:H2'	5:L3:912:G:O4'	2.17	0.43
16:LI:38:LEU:HD22	16:LI:42:TYR:HE2	1.84	0.43
21:LS:91:MET:HE1	24:LW:78:PHE:CE2	2.53	0.43
34:SG:105:ILE:CD1	34:SG:112:VAL:HG12	2.48	0.43
42:SO:183:GLU:OE1	42:SO:187:GLN:NE2	2.51	0.43
3:L1:83:C:O2'	3:L1:84:A:N7	2.40	0.43
12:LC:150:ILE:HG23	12:LC:150:ILE:O	2.18	0.43
31:SC:49:VAL:O	31:SC:49:VAL:HG23	2.18	0.43
6:L6:64:VAL:HA	6:L6:67:HIS:ND1	2.33	0.43
30:SA:5:ARG:NH1	30:SA:24:LEU:O	2.52	0.43
31:SC:148:THR:HG22	31:SC:200:LYS:HG2	2.00	0.43
45:SS:197:THR:HG22	45:SS:198:ASP:N	2.34	0.43
48:SW:555:TRP:CE3	48:SW:558:ILE:HD12	2.54	0.43
5:L3:46:U:OP2	5:L3:47:A:O2'	2.23	0.43
5:L3:1279:A:O2'	5:L3:1281:G:N7	2.40	0.43
18:LL:112:ARG:NH2	31:SC:120:ASP:OD2	2.46	0.43
5:L3:2486:G:OP2	36:SI:36:LYS:NZ	2.38	0.43
42:SO:226:ASP:O	42:SO:228:ALA:N	2.51	0.43
48:SW:378:SER:OG	48:SW:379:LEU:HD12	2.19	0.43
5:L3:4977:A:O2'	19:LN:21:ARG:NH2	2.52	0.43
22:LT:54:LYS:O	22:LT:66:LYS:NZ	2.44	0.43
31:SC:278:THR:HG22	31:SC:279:ASN:N	2.34	0.43
38:SK:79:GLN:OE1	47:SV:1:MET:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1669:A:H2'	5:L3:1670:G:O4'	2.19	0.43
5:L3:4515:G:OP1	44:SR:49:ARG:NH1	2.43	0.43
5:L3:4567:G:O2'	5:L3:4981:G:N7	2.47	0.43
7:L7:202:LEU:HD11	8:L8:119:ARG:NH1	2.34	0.43
44:SR:176:TYR:CD1	44:SR:177:PRO:HD2	2.53	0.43
36:SI:255:ASN:O	36:SI:255:ASN:ND2	2.52	0.42
48:SW:327:LEU:HD22	48:SW:354:LEU:HD22	2.01	0.42
3:L1:69:U:H2'	3:L1:70:G:O4'	2.20	0.42
5:L3:4511:A:N6	19:LN:2:SER:OG	2.52	0.42
5:L3:4875:G:H2'	12:LC:169:THR:HG22	2.00	0.42
36:SI:255:ASN:HD22	36:SI:255:ASN:C	2.25	0.42
49:SY:569:PHE:HE2	49:SY:581:ILE:HD12	1.84	0.42
5:L3:1504:G:OP1	11:LB:147:GLU:OE2	2.36	0.42
16:LI:34:LEU:HD22	16:LI:44:VAL:CG2	2.49	0.42
26:NF:217:GLY:HA3	41:SN:196:MET:HE1	2.00	0.42
40:SM:361:CYS:SG	40:SM:362:ILE:N	2.93	0.42
48:SW:219:LEU:HB3	48:SW:361:MET:HG3	1.99	0.42
49:SY:388:ILE:HG21	49:SY:402:MET:SD	2.59	0.42
5:L3:4433:G:N3	26:NF:191:THR:HG21	2.35	0.42
26:NF:109:LYS:NZ	49:SY:279:SER:OG	2.52	0.42
37:SJ:668:LEU:HD12	37:SJ:731:TRP:HH2	1.83	0.42
5:L3:4493:U:HO2'	5:L3:4494:G:C4'	2.27	0.42
5:L3:4744:A:H2'	5:L3:4745:G:O4'	2.20	0.42
37:SJ:682:ARG:NH1	45:SS:127:SEP:O1P	2.49	0.42
48:SW:329:CYS:SG	48:SW:361:MET:HE1	2.60	0.42
5:L3:1427:A:C2	11:LB:138:LEU:HD23	2.55	0.42
30:SA:109:ARG:O	30:SA:109:ARG:HG2	2.20	0.42
44:SR:233:ARG:HH12	44:SR:241:ILE:HD11	1.84	0.42
36:SI:32:TYR:CE2	36:SI:34:ALA:HB2	2.55	0.42
38:SK:77:THR:HG23	38:SK:80:GLU:H	1.84	0.42
38:SK:150:SER:HA	38:SK:194:ALA:HB3	2.02	0.42
44:SR:170:THR:C	44:SR:171:LEU:HD12	2.45	0.42
5:L3:4387:C:OP1	26:NF:169:ARG:NH1	2.52	0.42
5:L3:4761:G:OP1	7:L7:37:ARG:NH2	2.47	0.42
6:L6:111:GLN:HA	6:L6:114:VAL:HG22	2.02	0.42
11:LB:70:MET:HE1	11:LB:137:VAL:HB	2.01	0.42
15:LH:114:LYS:O	15:LH:118:ASP:N	2.53	0.42
39:SL:71:TRP:N	39:SL:247:SER:O	2.43	0.42
41:SN:72:VAL:HG11	41:SN:119:VAL:HG22	2.02	0.42
49:SY:335:LEU:HD22	49:SY:346:LEU:HB3	2.02	0.42
5:L3:2484:A:O2'	40:SM:216:ASP:OD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:81:ILE:O	1:BA:85:LEU:HD23	2.20	0.41
5:L3:1833:G:N2	5:L3:1835:G:O4'	2.53	0.41
18:LL:97:ILE:HD13	18:LL:107:ARG:HA	2.03	0.41
5:L3:307:A:N3	5:L3:310:G:O2'	2.53	0.41
5:L3:1364:U:OP2	6:L6:36:ARG:NH1	2.53	0.41
5:L3:4493:U:O2'	5:L3:4494:G:O4'	2.21	0.41
5:L3:4569:U:H4'	10:LA:79:THR:HG21	2.02	0.41
44:SR:269:LEU:CD1	44:SR:306:ILE:HG23	2.50	0.41
48:SW:397:VAL:HG22	48:SW:398:ASP:N	2.36	0.41
5:L3:1457:G:O2'	11:LB:75:ARG:NH2	2.53	0.41
5:L3:1879:C:H2'	5:L3:1880:G:O4'	2.21	0.41
5:L3:4604:G:H4'	26:NF:2:PRO:HG3	2.03	0.41
27:NH:10:ARG:HA	46:ST:271:LEU:HD21	2.03	0.41
33:SE:192:ARG:HE	40:SM:98:LYS:HA	1.86	0.41
48:SW:339:LEU:HD13	48:SW:344:GLU:HB3	2.03	0.41
5:L3:2052:G:O2'	5:L3:2057:A:N1	2.53	0.41
7:L7:189:ILE:HD12	8:L8:119:ARG:HE	1.84	0.41
10:LA:36:ILE:CD1	10:LA:91:LEU:HD13	2.50	0.41
19:LN:222:VAL:O	19:LN:343:ARG:NH1	2.53	0.41
3:L1:46:G:O2'	3:L1:61:A:N1	2.50	0.41
44:SR:286:VAL:HG21	44:SR:310:LEU:HD23	2.03	0.41
5:L3:4359:U:O2'	5:L3:4360:U:O4'	2.37	0.41
30:SA:100:ARG:HB3	30:SA:100:ARG:CZ	2.51	0.41
36:SI:192:ILE:HD11	40:SM:380:ARG:HE	1.85	0.41
5:L3:1364:U:OP2	6:L6:36:ARG:NH2	2.52	0.41
26:NF:215:THR:HG22	26:NF:216:LYS:N	2.35	0.41
44:SR:55:GLN:HA	44:SR:137:MET:HE1	2.03	0.41
10:LA:41:ILE:HD11	10:LA:99:GLU:CG	2.51	0.41
33:SE:157:ILE:HB	33:SE:183:ILE:HD13	2.03	0.41
34:SG:41:ILE:HG22	34:SG:43:VAL:HG13	2.02	0.41
38:SK:19:LEU:HB3	38:SK:198:VAL:HG22	2.03	0.41
1:BA:41:LYS:NZ	1:BA:45:ASP:OD2	2.54	0.40
5:L3:711:A:H2'	5:L3:712:C:C6	2.56	0.40
5:L3:2043:A:O2'	5:L3:4461:C:O2	2.39	0.40
48:SW:423:ASN:O	48:SW:428:LEU:HD11	2.21	0.40
49:SY:532:LEU:HD21	49:SY:539:LEU:HD23	2.03	0.40
5:L3:1501:C:H2'	11:LB:68:ARG:NH1	2.36	0.40
5:L3:3918:G:OP1	27:NH:72:LYS:NZ	2.50	0.40
27:NH:176:GLU:HA	27:NH:176:GLU:OE1	2.21	0.40
32:SD:147:LEU:O	32:SD:151:ASN:ND2	2.54	0.40
40:SM:552:MET:HE2	40:SM:552:MET:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SY:354:PRO:O	49:SY:358:THR:HG23	2.21	0.40
26:NF:38:LYS:HE2	26:NF:42:MET:HE1	2.02	0.40
38:SK:101:LEU:HB3	38:SK:107:VAL:HG21	2.02	0.40
44:SR:55:GLN:CA	44:SR:137:MET:HE1	2.51	0.40
45:SS:272:ARG:NE	45:SS:273:PRO:O	2.54	0.40
48:SW:274:LEU:O	48:SW:274:LEU:HD23	2.22	0.40
49:SY:335:LEU:HD21	49:SY:348:VAL:HG22	2.03	0.40
1:BA:58:ILE:HD11	1:BA:73:VAL:CG1	2.52	0.40
5:L3:688:U:O3'	31:SC:107:VAL:HG12	2.22	0.40
5:L3:4405:G:O6	44:SR:24:SER:OG	2.38	0.40
44:SR:324:THR:O	44:SR:326:GLU:N	2.52	0.40
5:L3:1354:A:N1	5:L3:1385:G:O2'	2.54	0.40
5:L3:4493:U:C5	5:L3:4512:U:H2'	2.57	0.40
5:L3:4580:U:O2'	19:LN:182:GLU:OE2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	158/165 (96%)	156 (99%)	2 (1%)	0	100	100
2	BB	211/217 (97%)	207 (98%)	4 (2%)	0	100	100
6	L6	118/211 (56%)	116 (98%)	2 (2%)	0	100	100
7	L7	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
8	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
9	L9	179/204 (88%)	179 (100%)	0	0	100	100
10	LA	134/184 (73%)	133 (99%)	1 (1%)	0	100	100
11	LB	149/188 (79%)	148 (99%)	1 (1%)	0	100	100
12	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LE	107/160 (67%)	104 (97%)	3 (3%)	0	100	100
14	LG	132/140 (94%)	131 (99%)	1 (1%)	0	100	100
15	LH	129/156 (83%)	128 (99%)	1 (1%)	0	100	100
16	LI	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
17	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
18	LL	120/137 (88%)	120 (100%)	0	0	100	100
19	LN	352/403 (87%)	347 (99%)	5 (1%)	0	100	100
20	LQ	126/135 (93%)	126 (100%)	0	0	100	100
21	LS	120/123 (98%)	120 (100%)	0	0	100	100
22	LT	107/110 (97%)	107 (100%)	0	0	100	100
23	LU	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
24	LW	72/97 (74%)	71 (99%)	1 (1%)	0	100	100
25	NB	63/549 (12%)	61 (97%)	2 (3%)	0	100	100
26	NF	197/260 (76%)	193 (98%)	4 (2%)	0	100	100
27	NH	178/180 (99%)	177 (99%)	1 (1%)	0	100	100
28	NI	590/881 (67%)	587 (100%)	3 (0%)	0	100	100
29	NK	63/129 (49%)	63 (100%)	0	0	100	100
30	SA	356/427 (83%)	350 (98%)	6 (2%)	0	100	100
31	SC	197/288 (68%)	191 (97%)	6 (3%)	0	100	100
32	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
33	SE	183/266 (69%)	180 (98%)	3 (2%)	0	100	100
34	SG	189/192 (98%)	187 (99%)	2 (1%)	0	100	100
35	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
36	SI	225/255 (88%)	220 (98%)	5 (2%)	0	100	100
37	SJ	95/847 (11%)	95 (100%)	0	0	100	100
38	SK	242/245 (99%)	232 (96%)	10 (4%)	0	100	100
39	SL	241/490 (49%)	233 (97%)	8 (3%)	0	100	100
40	SM	445/588 (76%)	443 (100%)	2 (0%)	0	100	100
41	SN	169/306 (55%)	169 (100%)	0	0	100	100
42	SO	292/353 (83%)	286 (98%)	6 (2%)	0	100	100
43	SQ	216/239 (90%)	212 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	SR	445/634 (70%)	436 (98%)	9 (2%)	0	100	100
45	SS	250/746 (34%)	242 (97%)	8 (3%)	0	100	100
46	ST	112/365 (31%)	109 (97%)	3 (3%)	0	100	100
47	SV	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
48	SW	440/670 (66%)	428 (97%)	12 (3%)	0	100	100
49	SY	376/812 (46%)	372 (99%)	4 (1%)	0	100	100
50	SZ	156/178 (88%)	154 (99%)	2 (1%)	0	100	100
All	All	9281/14226 (65%)	9137 (98%)	144 (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	
1	BA	132/137 (96%)	132 (100%)	0	100	100
6	L6	104/177 (59%)	104 (100%)	0	100	100
7	L7	171/174 (98%)	171 (100%)	0	100	100
8	L8	115/161 (71%)	115 (100%)	0	100	100
9	L9	155/172 (90%)	155 (100%)	0	100	100
10	LA	121/163 (74%)	121 (100%)	0	100	100
11	LB	136/165 (82%)	136 (100%)	0	100	100
12	LC	157/157 (100%)	157 (100%)	0	100	100
13	LE	51/140 (36%)	51 (100%)	0	100	100
14	LG	102/107 (95%)	102 (100%)	0	100	100
15	LH	39/133 (29%)	39 (100%)	0	100	100
16	LI	124/135 (92%)	124 (100%)	0	100	100
17	LK	29/121 (24%)	29 (100%)	0	100	100
18	LL	106/121 (88%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LN	313/348 (90%)	313 (100%)	0	100	100
20	LQ	114/121 (94%)	114 (100%)	0	100	100
21	LS	109/110 (99%)	109 (100%)	0	100	100
22	LT	88/89 (99%)	88 (100%)	0	100	100
23	LU	87/89 (98%)	87 (100%)	0	100	100
24	LW	63/80 (79%)	63 (100%)	0	100	100
25	NB	61/485 (13%)	61 (100%)	0	100	100
26	NF	182/228 (80%)	182 (100%)	0	100	100
27	NH	155/155 (100%)	155 (100%)	0	100	100
28	NI	267/730 (37%)	267 (100%)	0	100	100
29	NK	61/115 (53%)	61 (100%)	0	100	100
30	SA	298/348 (86%)	298 (100%)	0	100	100
31	SC	180/252 (71%)	180 (100%)	0	100	100
32	SD	194/215 (90%)	194 (100%)	0	100	100
33	SE	158/223 (71%)	158 (100%)	0	100	100
34	SG	170/171 (99%)	170 (100%)	0	100	100
35	SH	140/274 (51%)	140 (100%)	0	100	100
36	SI	205/228 (90%)	204 (100%)	1 (0%)	81	93
37	SJ	91/733 (12%)	91 (100%)	0	100	100
38	SK	212/213 (100%)	212 (100%)	0	100	100
39	SL	226/437 (52%)	226 (100%)	0	100	100
40	SM	401/509 (79%)	401 (100%)	0	100	100
41	SN	133/260 (51%)	133 (100%)	0	100	100
42	SO	274/319 (86%)	274 (100%)	0	100	100
43	SQ	195/214 (91%)	195 (100%)	0	100	100
44	SR	410/574 (71%)	410 (100%)	0	100	100
45	SS	227/648 (35%)	227 (100%)	0	100	100
46	ST	60/300 (20%)	60 (100%)	0	100	100
47	SV	127/149 (85%)	127 (100%)	0	100	100
48	SW	393/591 (66%)	393 (100%)	0	100	100
49	SY	325/685 (47%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	7602/12114 (63%)	7601 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	SI	171	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
6	L6	15	HIS
7	L7	26	GLN
7	L7	42	ASN
7	L7	173	GLN
7	L7	199	HIS
8	L8	34	ASN
9	L9	145	ASN
10	LA	10	ASN
10	LA	97	ASN
11	LB	7	HIS
12	LC	37	HIS
12	LC	108	GLN
16	LI	127	GLN
17	LK	14	HIS
19	LN	3	HIS
19	LN	184	GLN
19	LN	302	ASN
19	LN	354	GLN
21	LS	20	GLN
22	LT	99	HIS
23	LU	26	HIS
23	LU	36	HIS
25	NB	16	HIS
26	NF	33	HIS
27	NH	175	HIS
29	NK	89	GLN
29	NK	98	ASN
30	SA	310	HIS
30	SA	329	ASN
30	SA	347	HIS

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Mol	Chain	Res	Type
31	SC	136	HIS
31	SC	190	HIS
32	SD	24	ASN
32	SD	80	ASN
32	SD	192	HIS
32	SD	235	ASN
33	SE	149	ASN
34	SG	140	GLN
34	SG	163	GLN
36	SI	94	HIS
36	SI	207	HIS
36	SI	225	HIS
36	SI	255	ASN
37	SJ	712	HIS
37	SJ	726	HIS
39	SL	218	HIS
39	SL	225	HIS
40	SM	28	GLN
40	SM	154	HIS
40	SM	211	HIS
40	SM	376	GLN
40	SM	572	HIS
44	SR	37	HIS
44	SR	45	HIS
44	SR	128	GLN
44	SR	157	HIS
44	SR	167	ASN
44	SR	209	HIS
44	SR	246	HIS
45	SS	234	HIS
45	SS	310	HIS
47	SV	115	ASN
47	SV	129	GLN
47	SV	132	HIS
48	SW	328	GLN
48	SW	402	GLN
48	SW	525	HIS
48	SW	593	HIS
49	SY	244	GLN
49	SY	256	GLN
49	SY	268	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	19 (12%)	0
4	L2	65/1167 (5%)	10 (15%)	0
5	L3	2146/5070 (42%)	296 (13%)	6 (0%)
All	All	2361/6394 (36%)	325 (13%)	6 (0%)

All (325) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L1	34	U
3	L1	52	A
3	L1	54	C
3	L1	55	U
3	L1	59	A
3	L1	62	A
3	L1	63	U
3	L1	68	G
3	L1	82	A
3	L1	83	C
3	L1	84	A
3	L1	86	U
3	L1	94	G
3	L1	103	A
3	L1	105	C
3	L1	110	U
3	L1	111	U
3	L1	114	G
3	L1	156	U
4	L2	2	C
4	L2	9	A
4	L2	11	C
4	L2	48	G
4	L2	49	G
4	L2	62	U
4	L2	87	G
4	L2	94	U
4	L2	96	A
4	L2	101	A
5	L3	6	C
5	L3	41	C
5	L3	48	G
5	L3	56	A

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Mol	Chain	Res	Type
5	L3	58	G
5	L3	59	A
5	L3	64	A
5	L3	65	A
5	L3	69	A
5	L3	91	G
5	L3	92	C
5	L3	93	G
5	L3	95	G
5	L3	108	A
5	L3	116	G
5	L3	119	G
5	L3	159	C
5	L3	170	C
5	L3	171	U
5	L3	172	C
5	L3	173	C
5	L3	181	C
5	L3	186	G
5	L3	187	U
5	L3	190	G
5	L3	197	A
5	L3	200	U
5	L3	204	U
5	L3	210	C
5	L3	218	A
5	L3	233	U
5	L3	234	G
5	L3	246	G
5	L3	257	C
5	L3	261	G
5	L3	264	C
5	L3	265	C
5	L3	271	C
5	L3	277	G
5	L3	315	G
5	L3	326	C
5	L3	340	C
5	L3	347	A
5	L3	349	A
5	L3	362	A
5	L3	387	G

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Mol	Chain	Res	Type
5	L3	399	G
5	L3	410	A
5	L3	413	G
5	L3	414	C
5	L3	431	G
5	L3	449	C
5	L3	450	G
5	L3	452	A
5	L3	453	G
5	L3	454	U
5	L3	464	G
5	L3	467	U
5	L3	468	U
5	L3	472	C
5	L3	685	C
5	L3	697	G
5	L3	699	C
5	L3	704	C
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	741	C
5	L3	742	G
5	L3	746	A
5	L3	913	U
5	L3	915	A
5	L3	917	A
5	L3	926	G
5	L3	932	A
5	L3	933	G
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	956	A
5	L3	960	A
5	L3	1071	C
5	L3	1072	C
5	L3	1280	C
5	L3	1284	G
5	L3	1287	G
5	L3	1293	G
5	L3	1294	A

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Mol	Chain	Res	Type
5	L3	1295	C
5	L3	1296	G
5	L3	1301	C
5	L3	1313	C
5	L3	1314	C
5	L3	1354	A
5	L3	1358	G
5	L3	1359	G
5	L3	1377	G
5	L3	1378	C
5	L3	1379	C
5	L3	1435	G
5	L3	1447	C
5	L3	1448	G
5	L3	1463	C
5	L3	1497	A
5	L3	1498	G
5	L3	1500	A
5	L3	1525	A
5	L3	1654	G
5	L3	1661	C
5	L3	1670	G
5	L3	1691	G
5	L3	1726	U
5	L3	1804	A
5	L3	1810	G
5	L3	1836	G
5	L3	1837	A
5	L3	1842	G
5	L3	1853	G
5	L3	1856	C
5	L3	1870	C
5	L3	1881	C
5	L3	1883	G
5	L3	1891	A
5	L3	1897	A
5	L3	1910	G
5	L3	1918	U
5	L3	1921	C
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C

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Mol	Chain	Res	Type
5	L3	1935	C
5	L3	1938	C
5	L3	1941	A
5	L3	1944	A
5	L3	1945	G
5	L3	1969	G
5	L3	1984	A
5	L3	1997	U
5	L3	2002	A
5	L3	2024	G
5	L3	2025	A
5	L3	2026	A
5	L3	2034	G
5	L3	2044	U
5	L3	2046	G
5	L3	2055	G
5	L3	2056	G
5	L3	2069	A
5	L3	2084	C
5	L3	2085	G
5	L3	2089	G
5	L3	2090	U
5	L3	2091	C
5	L3	2268	A
5	L3	2289	C
5	L3	2300	A
5	L3	2301	G
5	L3	2313	A
5	L3	2314	G
5	L3	2348	G
5	L3	2351	C
5	L3	2474	G
5	L3	2480	G
5	L3	2484	A
5	L3	2485	U
5	L3	2488	C
5	L3	2490	U
5	L3	2492	C
5	L3	2493	G
5	L3	2500	U
5	L3	2575	U
5	L3	2769	U

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Mol	Chain	Res	Type
5	L3	2844	A
5	L3	2845	A
5	L3	2848	G
5	L3	2852	U
5	L3	3845	A
5	L3	3853	U
5	L3	3868	G
5	L3	3870	C
5	L3	3875	G
5	L3	3877	A
5	L3	3878	C
5	L3	3879	G
5	L3	3889	G
5	L3	3894	A
5	L3	3895	G
5	L3	3897	G
5	L3	3904	G
5	L3	3906	A
5	L3	3907	G
5	L3	3908	A
5	L3	3920	U
5	L3	3926	C
5	L3	3938	G
5	L3	3939	G
5	L3	3940	U
5	L3	3941	G
5	L3	3942	A
5	L3	4049	U
5	L3	4058	U
5	L3	4064	C
5	L3	4183	G
5	L3	4348	A
5	L3	4349	C
5	L3	4350	C
5	L3	4357	G
5	L3	4372	U
5	L3	4373	G
5	L3	4376	A
5	L3	4378	A
5	L3	4380	A
5	L3	4385	A
5	L3	4390	A

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Mol	Chain	Res	Type
5	L3	4392	G
5	L3	4393	G
5	L3	4398	C
5	L3	4401	G
5	L3	4405	G
5	L3	4433	G
5	L3	4437	U
5	L3	4438	U
5	L3	4439	U
5	L3	4441	A
5	L3	4442	U
5	L3	4451	G
5	L3	4464	A
5	L3	4466	C
5	L3	4475	G
5	L3	4476	C
5	L3	4480	A
5	L3	4494	G
5	L3	4495	G
5	L3	4496	A
5	L3	4512	U
5	L3	4513	A
5	L3	4518	A
5	L3	4521	U
5	L3	4522	G
5	L3	4523	A
5	L3	4540	C
5	L3	4541	G
5	L3	4545	G
5	L3	4546	A
5	L3	4568	A
5	L3	4584	A
5	L3	4590	A
5	L3	4608	G
5	L3	4627	U
5	L3	4652	G
5	L3	4653	C
5	L3	4656	A
5	L3	4670	C
5	L3	4671	C
5	L3	4672	A
5	L3	4678	G

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Mol	Chain	Res	Type
5	L3	4684	A
5	L3	4700	A
5	L3	4708	A
5	L3	4709	U
5	L3	4719	G
5	L3	4720	C
5	L3	4721	G
5	L3	4737	G
5	L3	4740	G
5	L3	4741	C
5	L3	4742	G
5	L3	4745	G
5	L3	4751	G
5	L3	4754	G
5	L3	4757	C
5	L3	4759	C
5	L3	4765	G
5	L3	4772	C
5	L3	4773	C
5	L3	4870	G
5	L3	4871	C
5	L3	4880	C
5	L3	4882	U
5	L3	4883	C
5	L3	4900	C
5	L3	4901	G
5	L3	4910	G
5	L3	4914	C
5	L3	4943	A
5	L3	4976	U
5	L3	5006	U
5	L3	5013	C
5	L3	5014	A
5	L3	5020	G
5	L3	5023	C
5	L3	5026	U
5	L3	5030	U
5	L3	5041	G
5	L3	5050	C
5	L3	5062	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	2084	C
5	L3	2574	G
5	L3	4347	G
5	L3	4520	G
5	L3	4699	U
5	L3	5013	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	SEP	SS	126	45	8,9,10	1.54	1 (12%)	7,12,14	1.26	1 (14%)
45	SEP	SS	127	45	8,9,10	1.53	1 (12%)	7,12,14	1.34	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
45	SEP	SS	126	45	-	0/6/8/10	-
45	SEP	SS	127	45	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	SS	126	SEP	P-O1P	3.41	1.61	1.50
45	SS	127	SEP	P-O1P	3.37	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	SS	127	SEP	OG-CB-CA	2.83	110.90	108.14
45	SS	126	SEP	OG-CB-CA	2.66	110.73	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	SS	127	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	SS	127	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 61 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	GDP	SR	1001	55,51	29,30,30	3.02	13 (44%)	45,47,47	2.71	17 (37%)
53	ADP	NI	1001	51	28,29,29	1.35	5 (17%)	43,45,45	1.88	10 (23%)

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
54	GDP	SR	1001	55,51	-	1/16/32/32	0/3/3/3
53	ADP	NI	1001	51	-	1/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	SR	1001	GDP	O6-C6	8.70	1.40	1.23
54	SR	1001	GDP	C5-N7	6.48	1.52	1.39
54	SR	1001	GDP	C2-N2	4.78	1.45	1.34
54	SR	1001	GDP	PA-O3A	4.60	1.64	1.59
53	NI	1001	ADP	C5-C4	4.36	1.46	1.39
54	SR	1001	GDP	C8-N9	-4.27	1.27	1.37
54	SR	1001	GDP	C4-N9	-3.97	1.27	1.38
54	SR	1001	GDP	C5-C4	3.67	1.48	1.38
54	SR	1001	GDP	C4-N3	2.73	1.40	1.34
53	NI	1001	ADP	C5-N7	-2.45	1.34	1.39
54	SR	1001	GDP	PB-O2B	-2.44	1.45	1.54
54	SR	1001	GDP	PB-O3B	-2.44	1.45	1.54
53	NI	1001	ADP	C5-C6	2.41	1.47	1.41
53	NI	1001	ADP	C8-N7	2.30	1.36	1.31
54	SR	1001	GDP	C2'-C3'	-2.22	1.47	1.53
54	SR	1001	GDP	O4'-C1'	2.16	1.47	1.42
54	SR	1001	GDP	PA-O2A	-2.07	1.45	1.55
53	NI	1001	ADP	C4-N9	-2.01	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SR	1001	GDP	C8-N9-C4	8.10	121.21	106.03
54	SR	1001	GDP	N9-C4-N3	6.69	139.33	125.95
54	SR	1001	GDP	C5-C4-N3	-6.59	117.89	128.39
53	NI	1001	ADP	C5-C4-N3	-5.69	118.89	126.72
54	SR	1001	GDP	C2-N3-C4	5.28	121.39	112.30
54	SR	1001	GDP	C6-C5-N7	4.90	139.20	130.29
54	SR	1001	GDP	C4-C5-N7	-4.74	103.16	110.67
53	NI	1001	ADP	N3-C4-N9	4.62	135.03	127.17
53	NI	1001	ADP	N3-C2-N1	-3.86	122.74	128.58
53	NI	1001	ADP	C2-N3-C4	3.84	121.21	111.83
53	NI	1001	ADP	C4-C5-N7	-3.35	106.75	110.58
54	SR	1001	GDP	N9-C8-N7	-3.25	107.37	113.40
53	NI	1001	ADP	C4-N9-C8	3.09	108.99	105.74
54	SR	1001	GDP	O3B-PB-O3A	2.98	114.61	104.64
54	SR	1001	GDP	O2B-PB-O3A	2.94	114.49	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SR	1001	GDP	C2-N1-C6	-2.93	119.80	125.11
53	NI	1001	ADP	C5-N7-C8	2.67	107.65	103.45
54	SR	1001	GDP	C2'-C3'-C4'	2.66	107.75	102.61
54	SR	1001	GDP	C1'-N9-C8	-2.59	119.36	126.73
54	SR	1001	GDP	C3'-C2'-C1'	2.56	106.31	101.46
54	SR	1001	GDP	C5-C6-N1	2.54	119.72	113.25
53	NI	1001	ADP	N9-C8-N7	-2.40	110.53	113.94
54	SR	1001	GDP	C1'-N9-C4	-2.40	119.40	126.49
54	SR	1001	GDP	O6-C6-C5	-2.36	120.29	126.53
54	SR	1001	GDP	O2A-PA-O1A	-2.36	101.47	112.44
53	NI	1001	ADP	C6-C5-N7	2.15	136.23	132.09
53	NI	1001	ADP	C2-N1-C6	2.11	122.19	118.73

There are no chirality outliers.

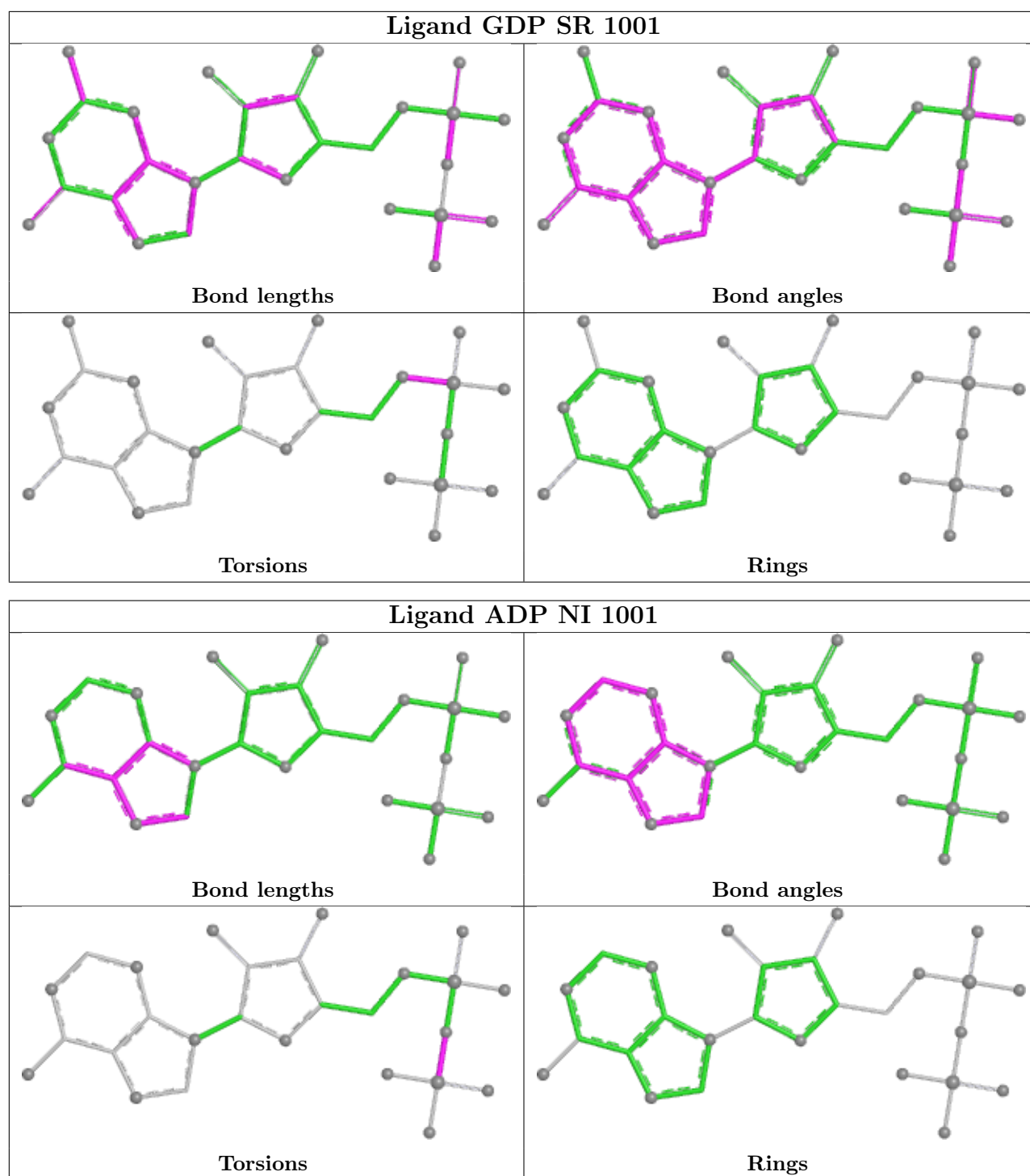
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	SR	1001	GDP	C5'-O5'-PA-O2A
53	NI	1001	ADP	PA-O3A-PB-O3B

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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29257. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.