



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:40 PM UTC

PDB ID : 8I9V / pdb_00008i9v
EMDB ID : EMD-35285
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- State Dbp10-2
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
Resolution : 3.10 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:

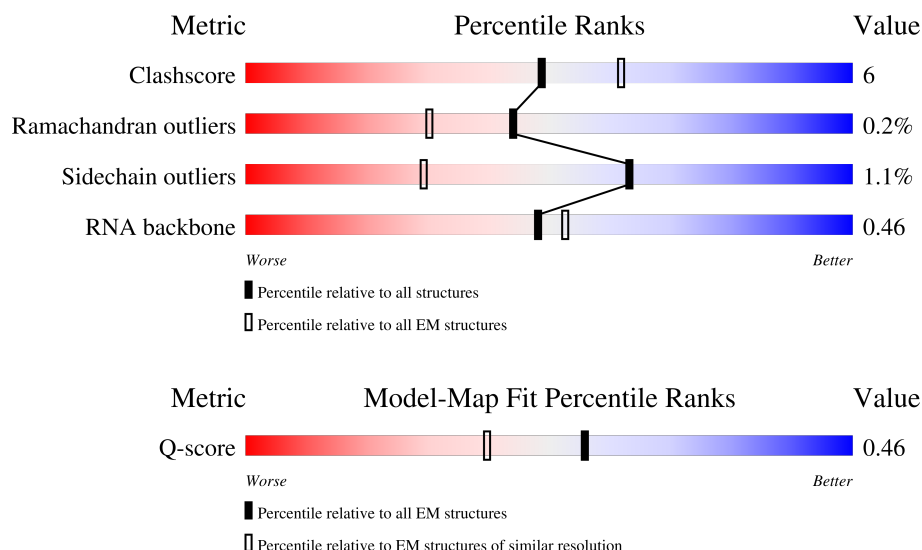
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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.



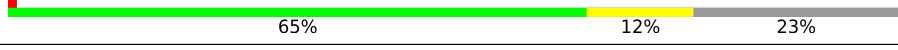
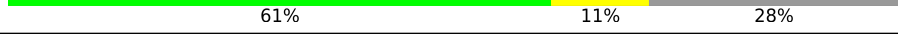
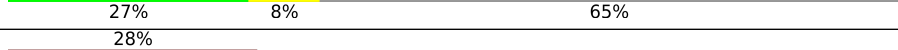
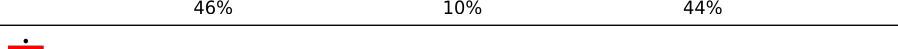
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	C1	3341	
2	C2	256	
3	C3	161	

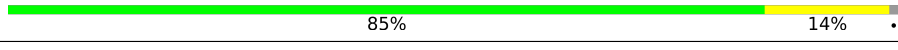
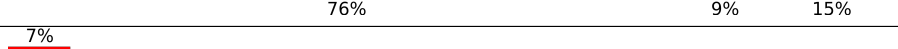
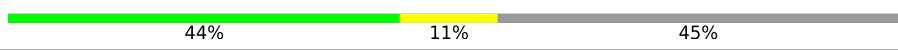
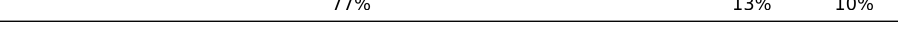
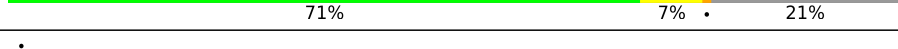
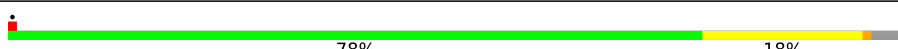
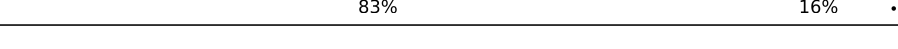
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Mol	Chain	Length	Quality of chain
4	CA	316	
5	CB	391	
6	CC	801	
7	CE	598	
8	CF	270	
9	CG	184	
10	CH	661	
11	CI	414	
12	CJ	679	
13	CK	261	
14	CL	558	
15	CM	249	
15	LF	249	
16	CN	246	
17	CO	120	
18	CP	751	
19	CQ	225	
20	CR	237	
21	CS	834	
22	CT	688	
23	CU	451	
24	CX	203	
25	CY	788	
26	Cz	123	
27	Cb	924	

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Mol	Chain	Length	Quality of chain
28	LB	392	
29	LC	365	
30	LE	200	
31	LG	262	
32	LH	192	
33	LK	165	
34	LL	213	
35	LM	142	
36	LN	203	
37	LO	204	
38	LP	187	
39	LQ	213	
40	LS	174	
41	LT	160	
42	LV	139	
43	LX	156	
44	LY	138	
45	Ld	120	
46	Le	131	
47	Lf	109	
48	Lh	935	
49	Li	110	
50	Lj	95	
51	Lq	217	
52	Cc	282	

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Mol	Chain	Length	Quality of chain
53	Cd	436	67%12%22%
54	Ce	336	49%8%42%
55	Cf	570	9%90%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 138001 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	2152	Total	C	N	O	P	0	0
			46025	20547	8331	14995	2152		

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	158	Total	C	N	O	P	0	0
			3359	1502	593	1106	158		

- Molecule 3 is a RNA chain called RNA (161-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C3	98	Total	C	N	O	P	0	0
			2097	933	381	685	98		

- Molecule 4 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CA	260	Total	C	N	O	S	0	0
			2144	1371	393	373	7		

- Molecule 5 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CB	260	Total	C	N	O	S	0	0
			2063	1322	367	371	3		

- Molecule 6 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CC	289	Total	C	N	O	S	0	0
			2388	1520	399	462	7		

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CE	463	Total	C	N	O	S	0	0
			3673	2352	643	667	11		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 8 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CF	245	Total	C	N	O	S	0	0
			1945	1222	352	362	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CG	177	Total	C	N	O	S	0	0
			1396	884	247	253	12		

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CH	476	Total	C	N	O	S	0	0
			3851	2451	669	716	15		

- Molecule 11 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CJ	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CK	232	Total	C	N	O	S	0	0
			1855	1165	363	323	4		

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CL	390	Total	C	N	O		0	0
			2173	1307	446	420			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CM	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
15	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	3		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 17 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	324	Total	C	N	O	S	0	0
			2535	1618	445	457	15		

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	112	Total	C	N	O	S	0	0
			960	607	195	148	10		

- Molecule 20 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CS	298	Total	C	N	O	S	0	0
			1750	1072	330	347	1		

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CT	458	Total	C	N	O		0	0
			2269	1353	458	458			

- Molecule 23 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

- Molecule 24 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CX	88	Total	C	N	O	S	0	0
			701	435	128	135	3		

- Molecule 25 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	CY	324	Total	C	N	O		
			1608	960	324	324	0	0

- Molecule 26 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Cz	70	Total	C	N	O	S		
			592	368	120	101	3	0	0

- Molecule 27 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Cb	642	Total	C	N	O	S		
			5058	3216	918	911	13	0	0

- Molecule 28 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LB	341	Total	C	N	O	S		
			2708	1721	493	482	12	0	0

- Molecule 29 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LC	362	Total	C	N	O	S		
			2752	1738	526	479	9	0	0

- Molecule 30 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LE	170	Total	C	N	O	S		
			1338	861	241	233	3	0	0

- Molecule 31 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	196	Total	C	N	O	S		
			1583	1021	287	270	5	0	0

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 33 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LK	146	Total	C	N	O	S	0	0
			1112	701	203	206	2		

- Molecule 34 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 35 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 36 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 37 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 38 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	154	Total	C	N	O	S	0	0
			1212	758	233	218	3		

- Molecule 39 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LX	22	Total	C	N	O		
			148	91	31	26	0	0

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 45 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ld	109	Total	C	N	O	S	0	0
			890	563	171	155	1		

- Molecule 46 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Le	131	Total	C	N	O	S	0	0
			1055	663	213	172	7		

- Molecule 47 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 48 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lh	121	Total	C	N	O	S	0	0
			995	633	196	166			

- Molecule 49 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 50 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 51 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lq	207	Total	C	N	O	S	0	0
			1600	1016	285	291	8		

- Molecule 52 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Cc	236	Total	C	N	O	S	0	0
			1898	1208	337	343	10		

- Molecule 53 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Cd	342	Total	C	N	O	S	0	0
			2763	1743	533	483	4		

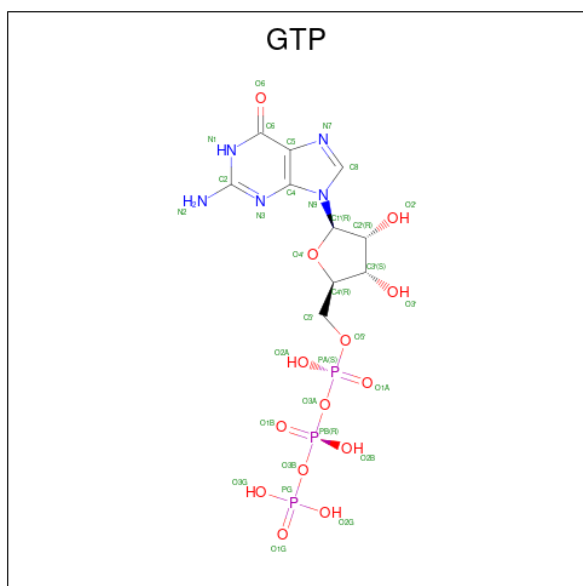
- Molecule 54 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ce	194	Total	C	N	O	S	0	0
			1609	1020	304	276	9		

- Molecule 55 is a protein called 60S ribosome biogenesis protein Rrp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Cf	59	Total	C	N	O		0	0
			513	310	111	92			

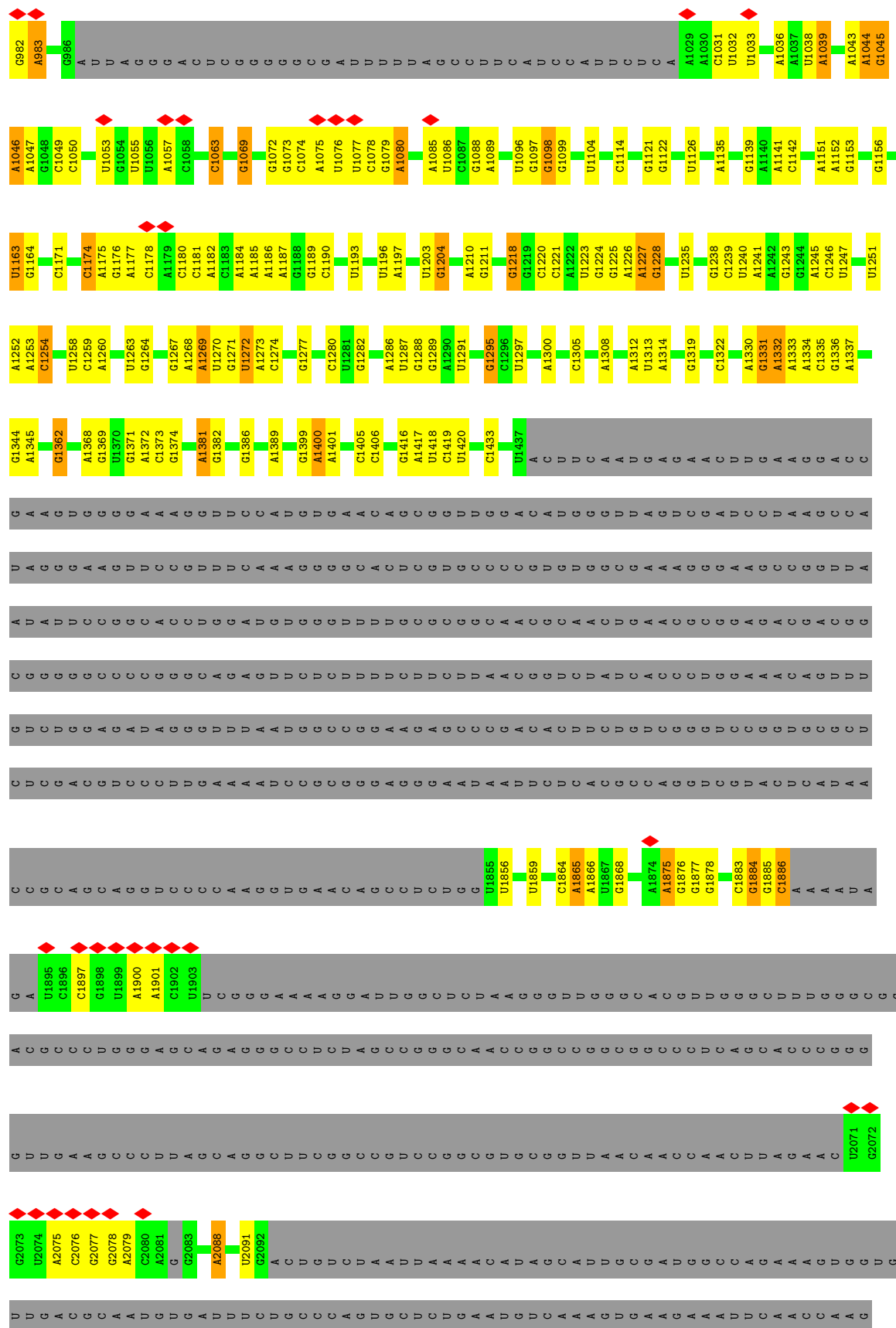
- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

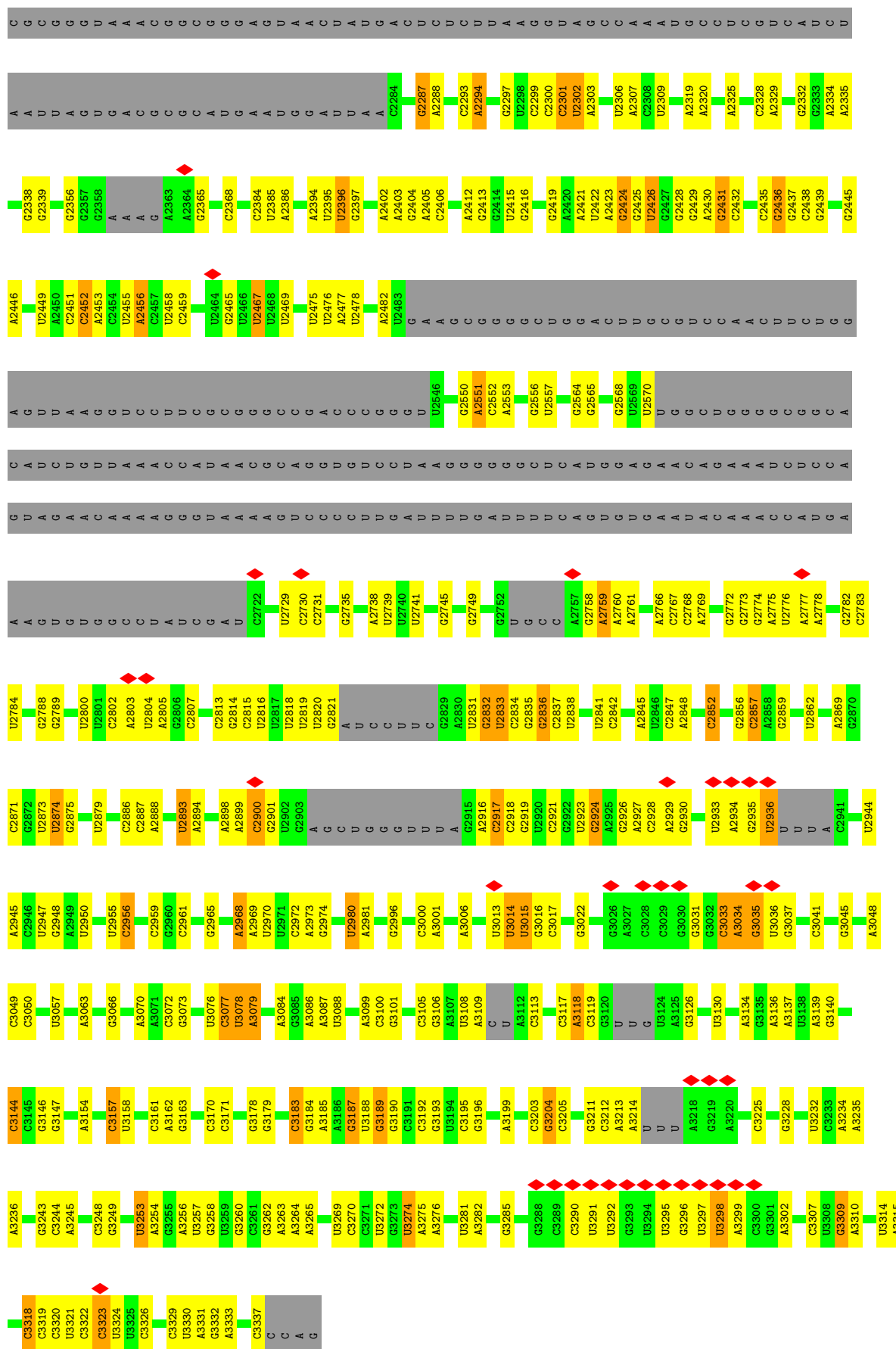


Mol	Chain	Residues	Atoms					AltConf
56	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	

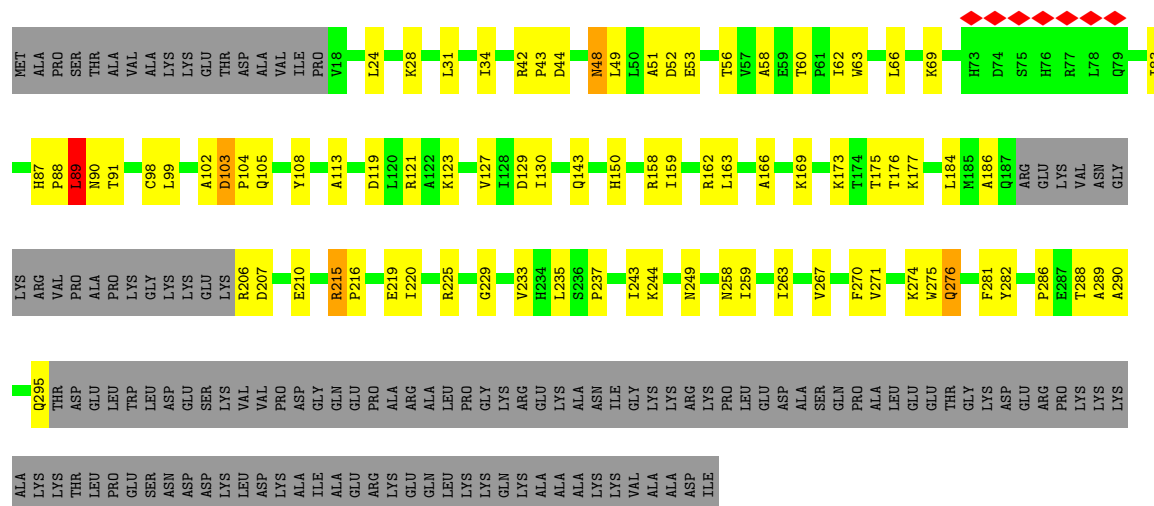
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	CQ	1	Total	Zn	0
			1	1	
57	Lj	1	Total	Zn	0
			1	1	
57	Ce	1	Total	Zn	0
			1	1	

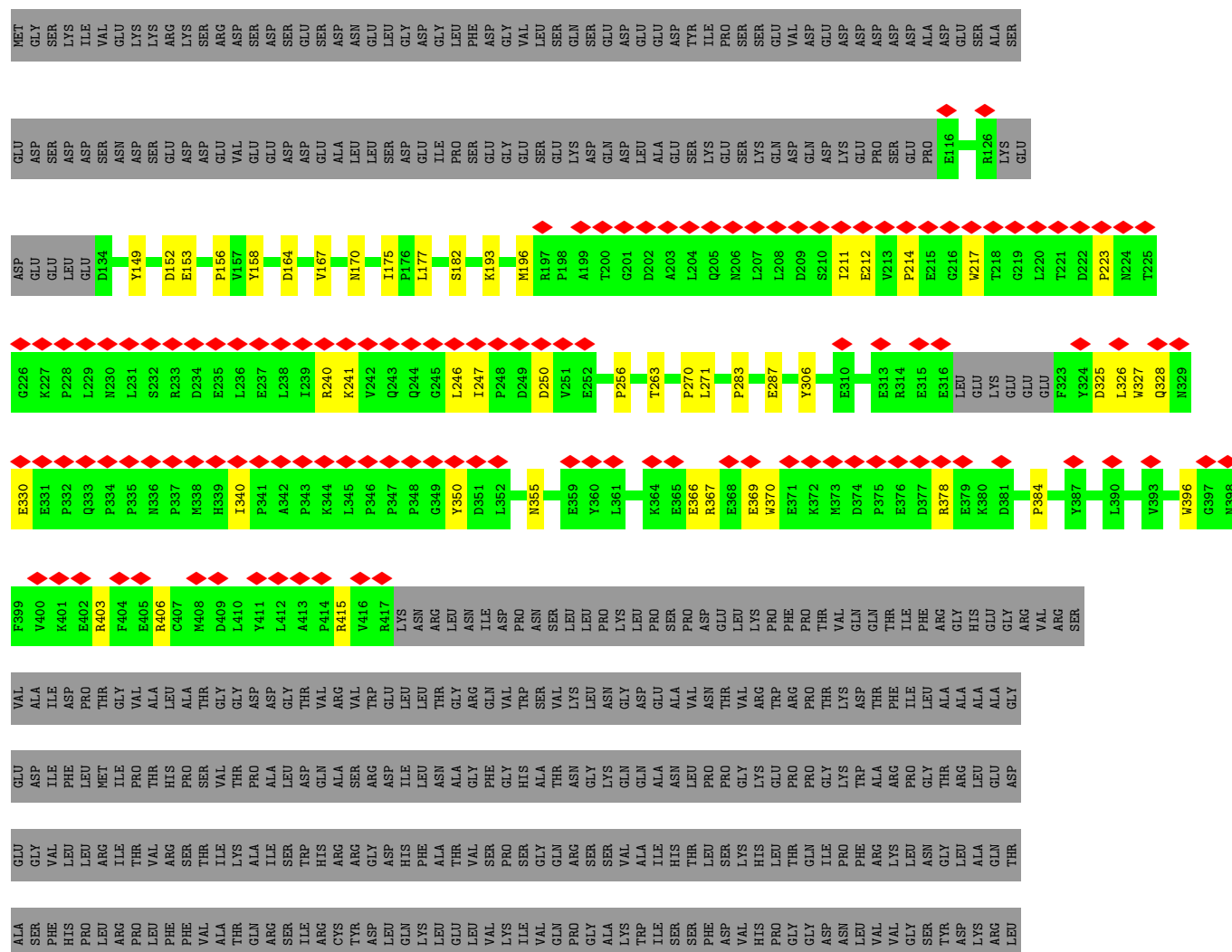


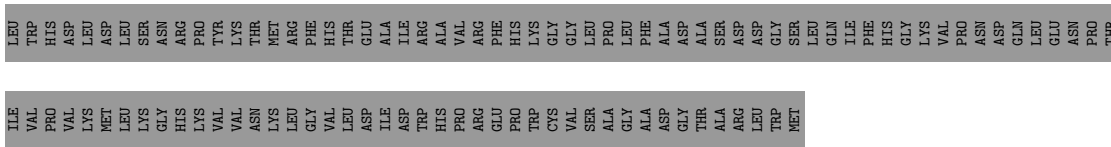




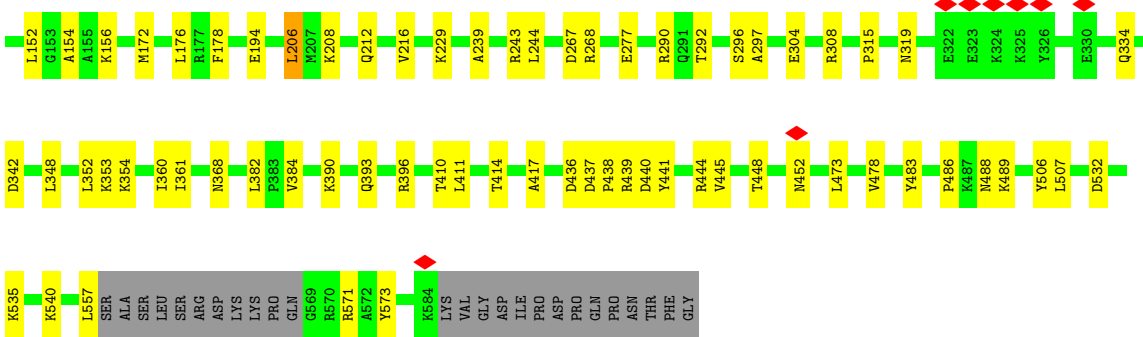
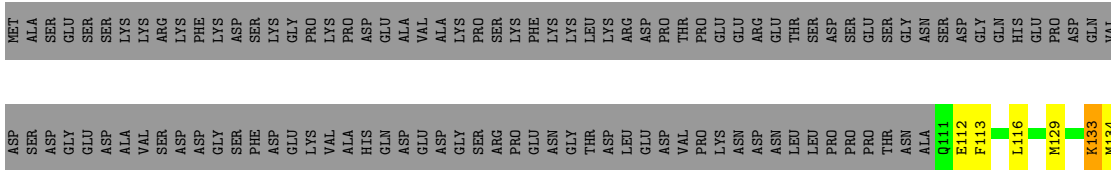


• Molecule 6: Ribosome biogenesis protein ERB1

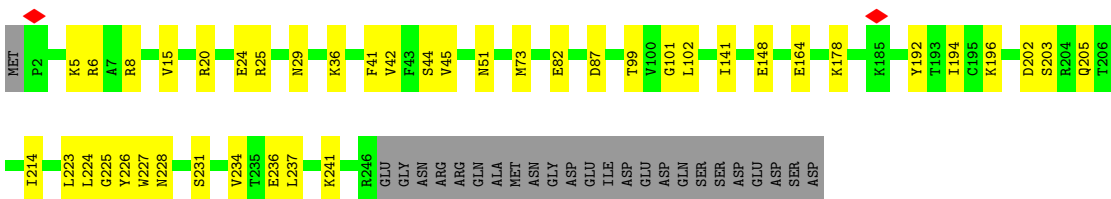
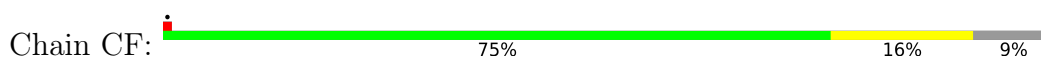




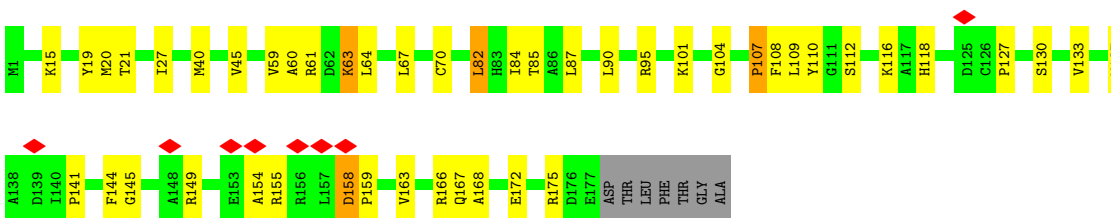
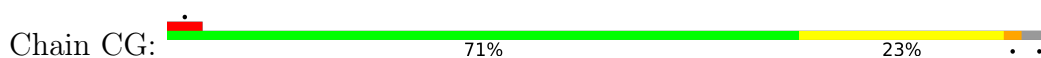
- Molecule 7: RNA helicase



- Molecule 8: Ribosome assembly factor mrt4

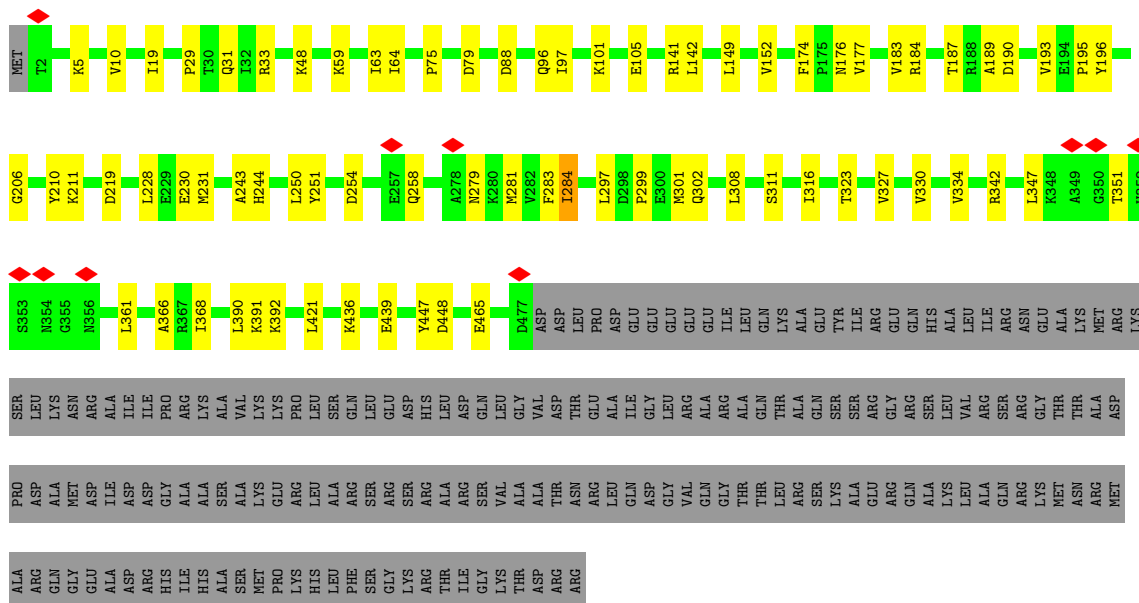


- Molecule 9: 60S ribosome subunit biogenesis protein NIP7

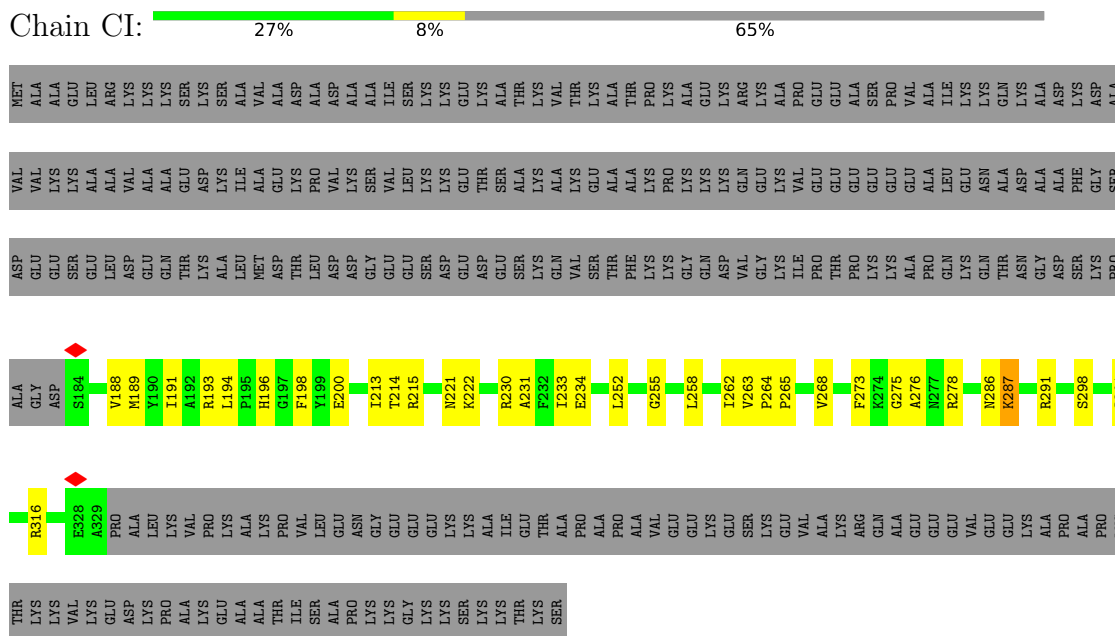


- Molecule 10: Nucleolar GTP-binding protein 1

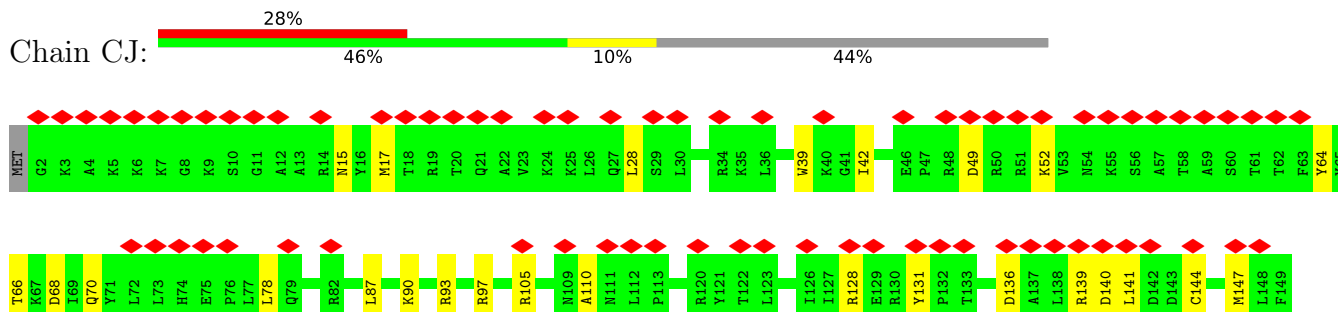


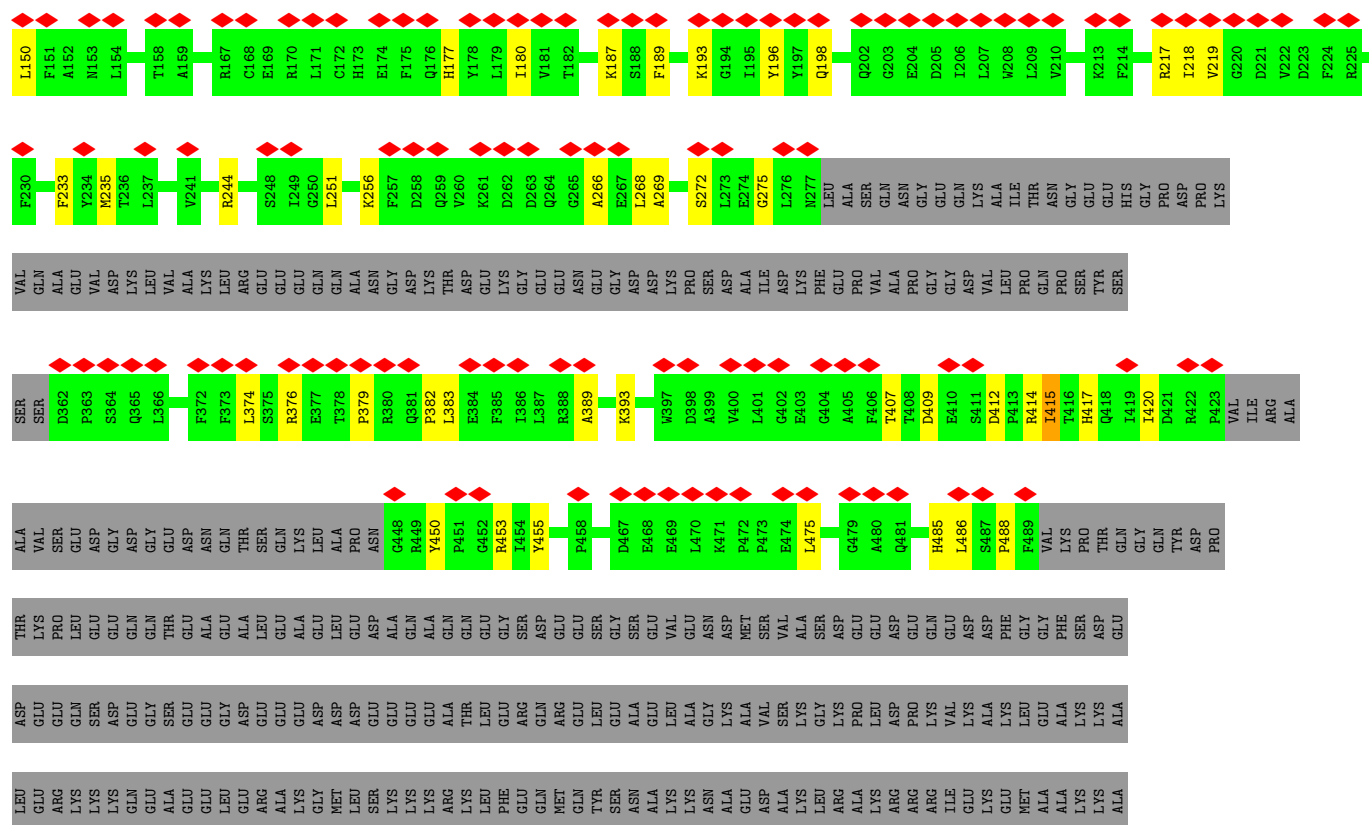


- Molecule 11: Putative RNA-binding protein

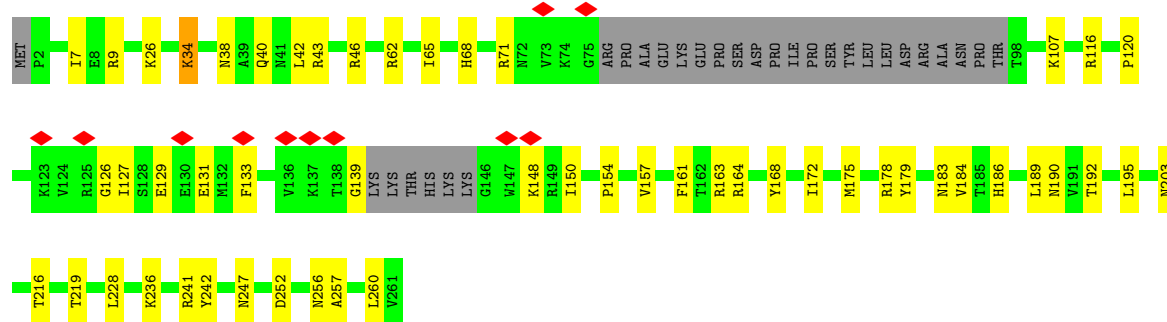


- Molecule 12: Pescadillo homolog



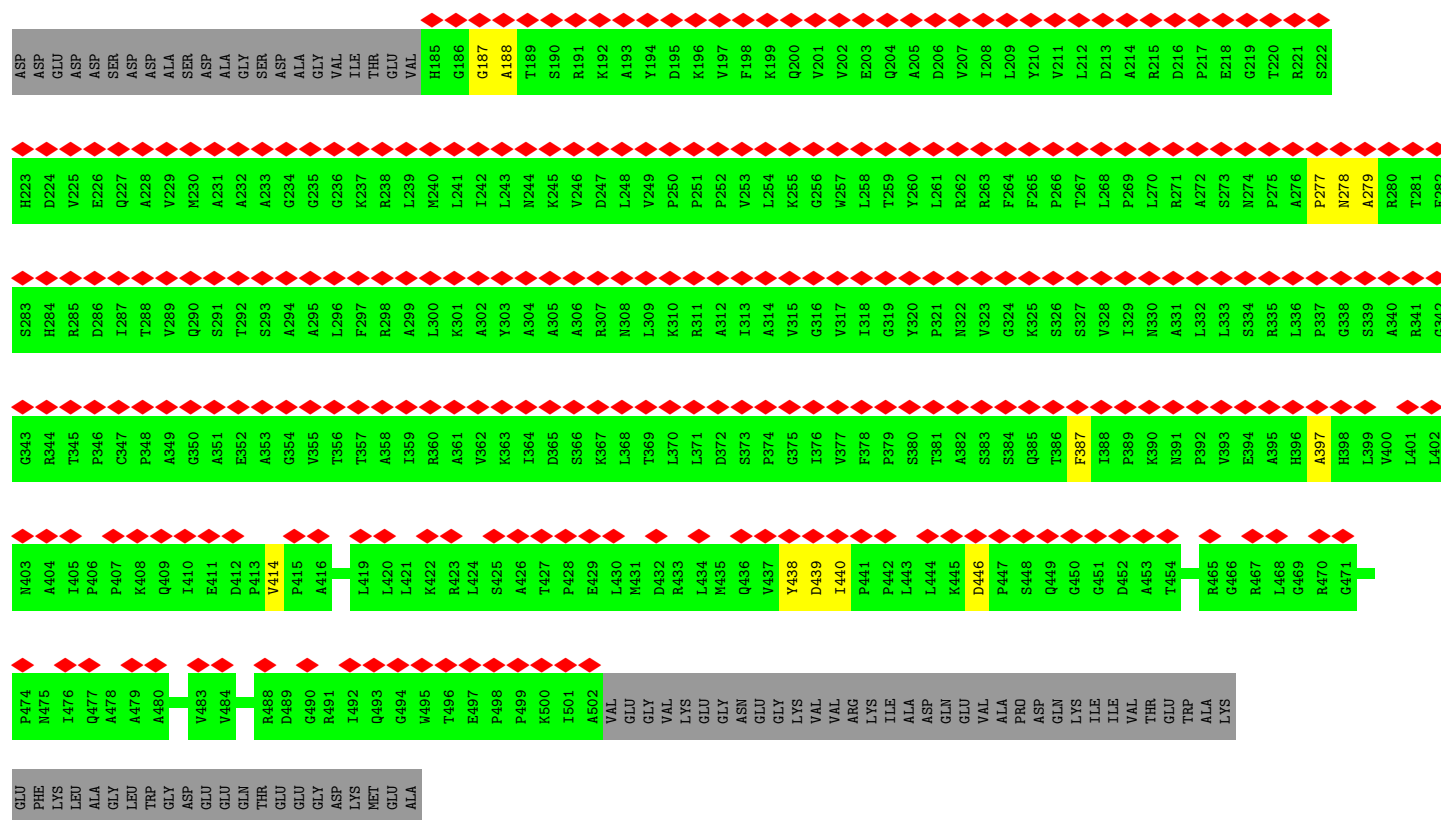


• Molecule 13: Ribosome biogenesis protein NSA2 homolog

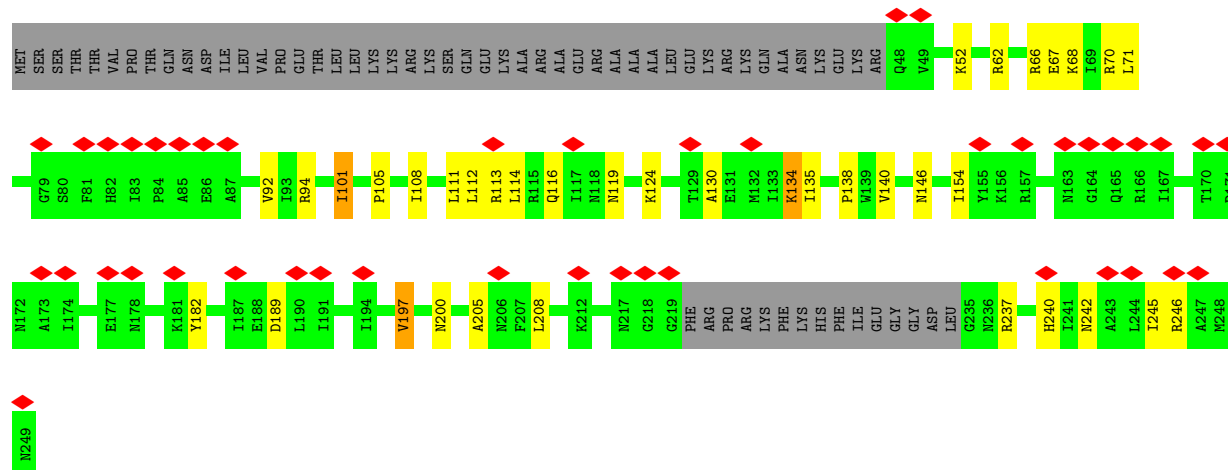


• Molecule 14: Putative GTP binding protein

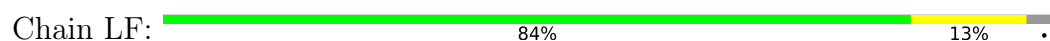


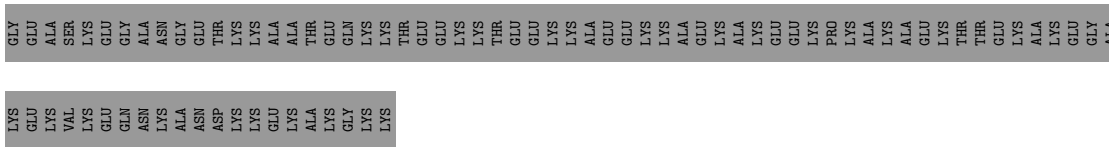


- Molecule 15: 60S ribosomal protein l7-like protein

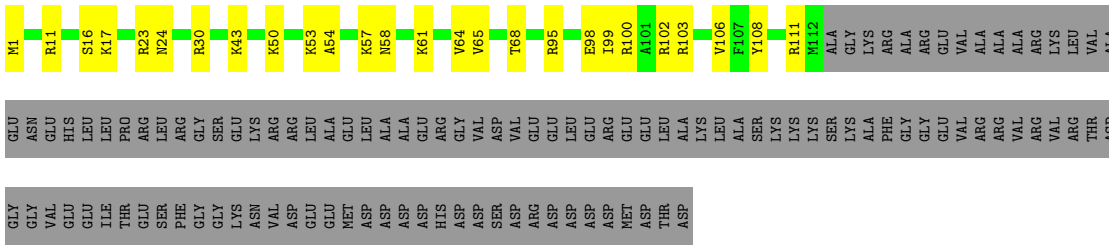
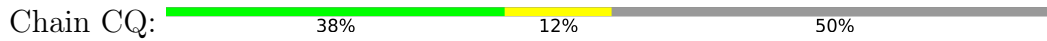


- Molecule 15: 60S ribosomal protein l7-like protein

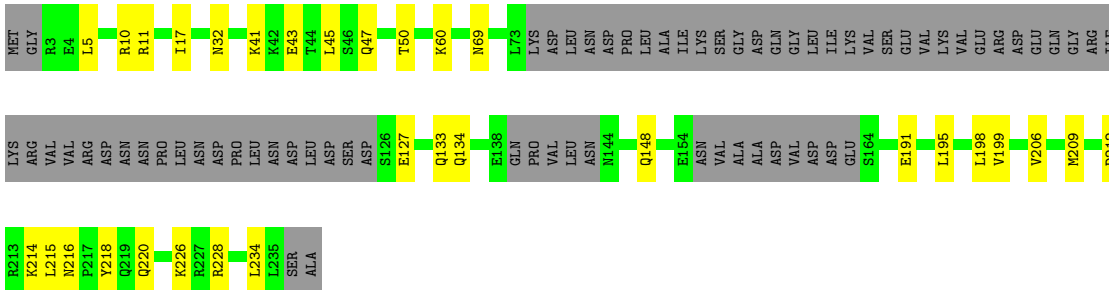




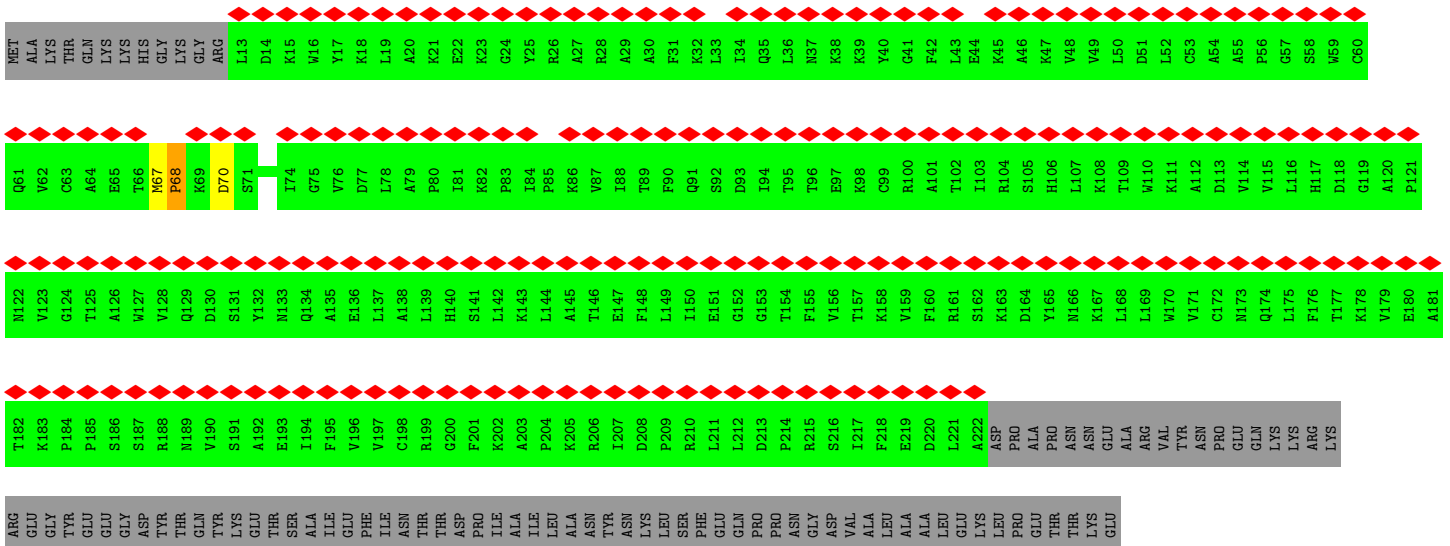
- Molecule 19: Ribosome biogenesis protein RLP24

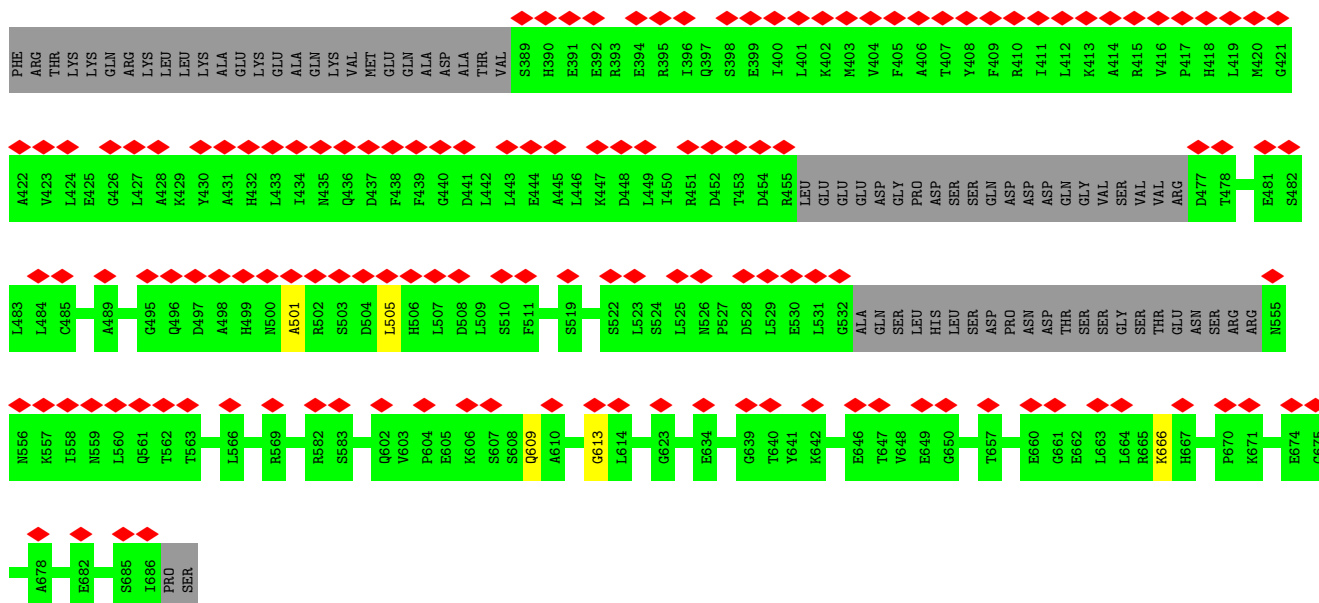


- Molecule 20: Nucleolar protein 16

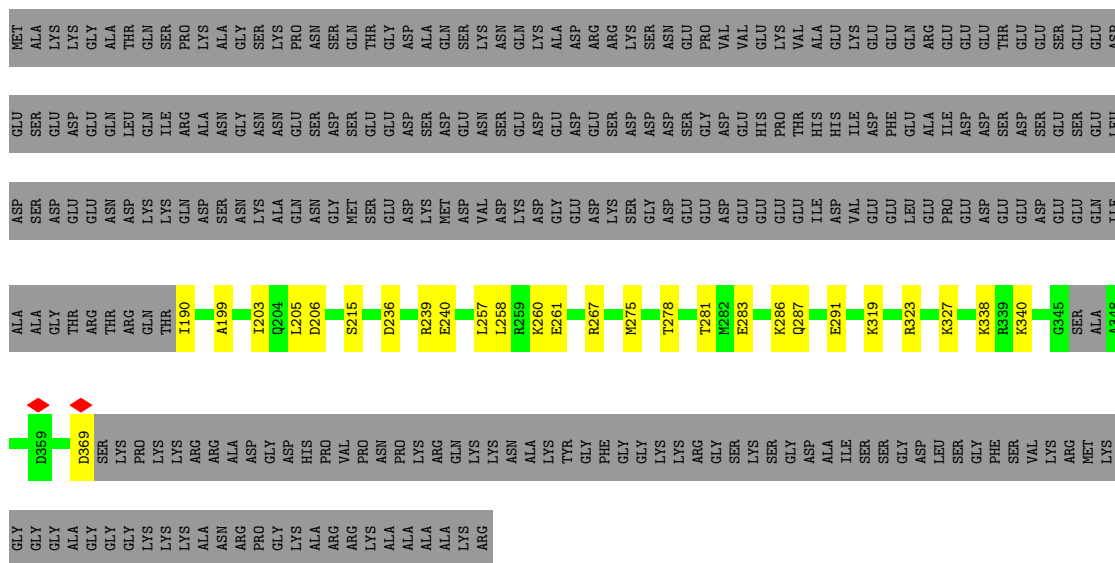


- Molecule 21: AdoMet-dependent rRNA methyltransferase SPB1

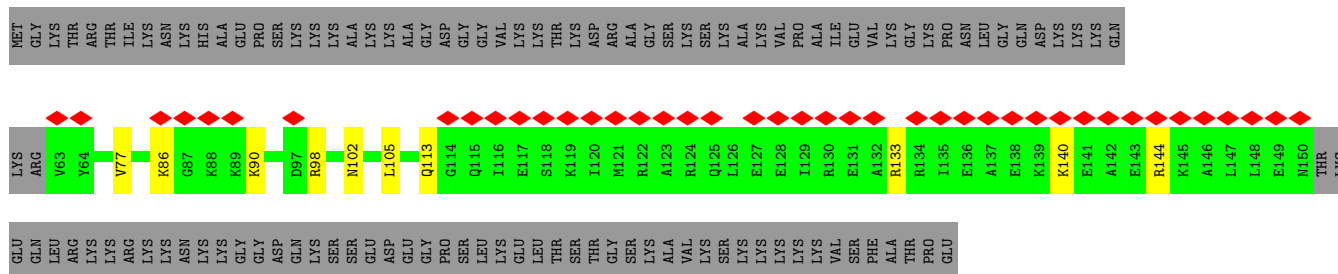
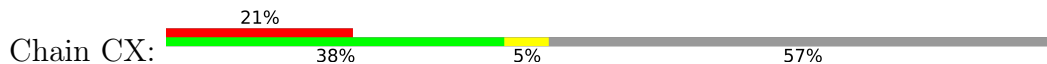




- Molecule 23: rRNA-processing protein EBP2

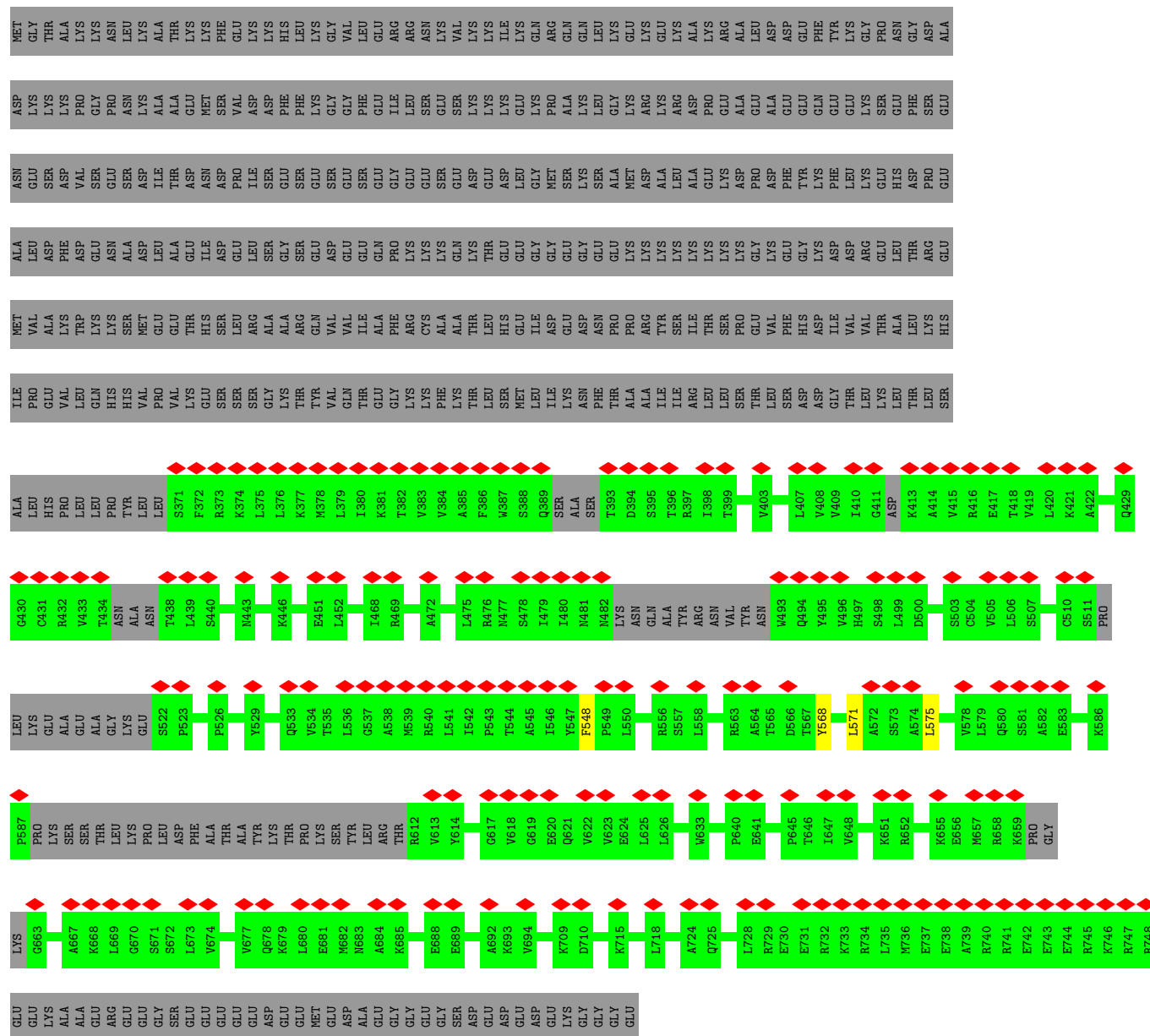


- Molecule 24: 60S ribosomal subunit-like protein



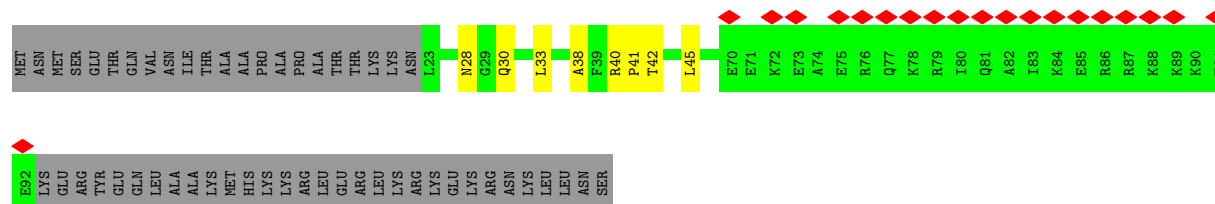
• Molecule 25: Putative NOC2 family protein

Chain CY:  22% 41% 59%

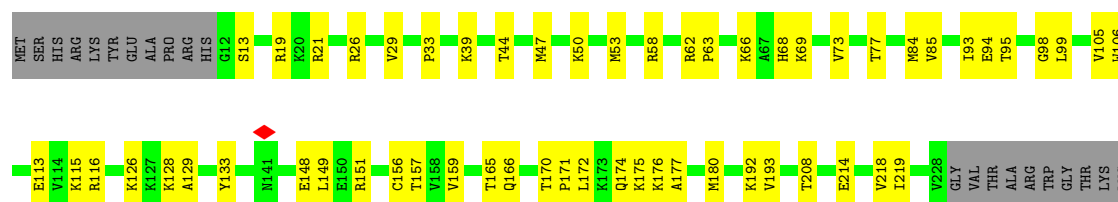


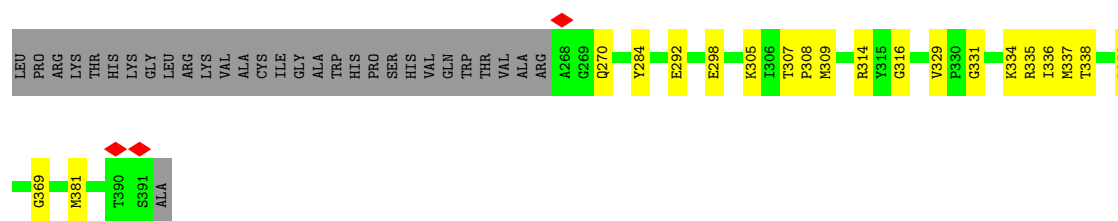
• Molecule 26: rRNA-processing protein

Chain Cz:  16% 50% 7% 43%



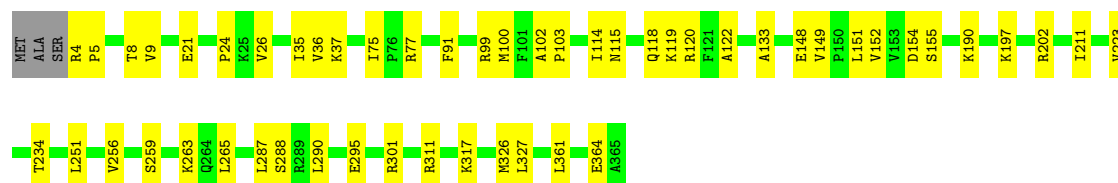
Chain Cb:





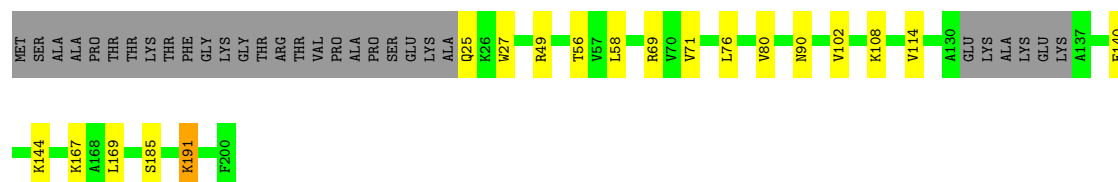
- Molecule 29: 60S ribosomal protein L4-like protein

Chain LC: 85% 14% .



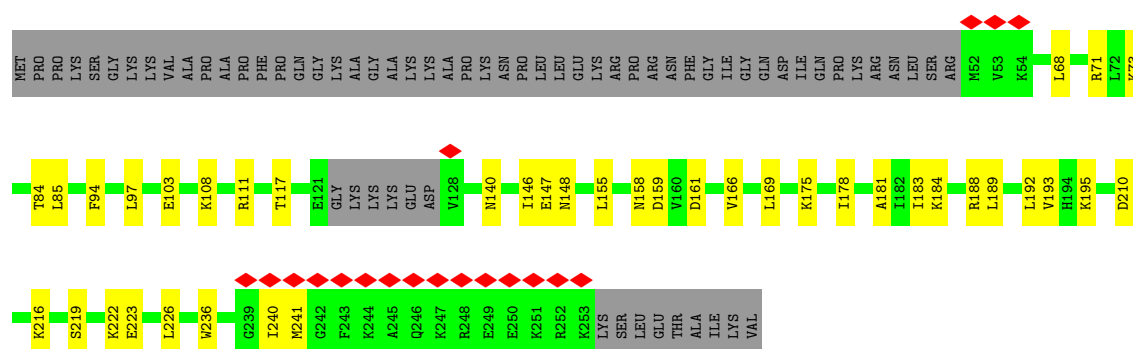
- Molecule 30: 60S ribosomal protein L6

Chain LE: 76% 9% 15%



- Molecule 31: 60S ribosomal protein L8

Chain LG: 7% 60% 15% 25%



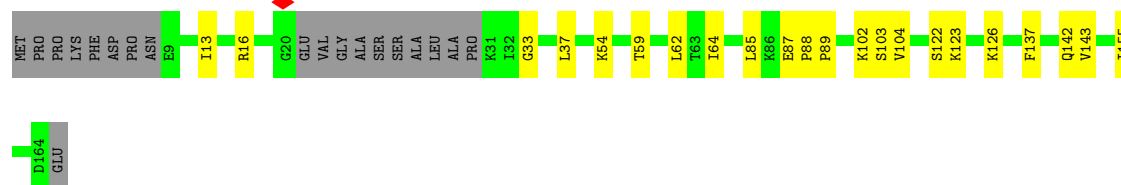
- Molecule 32: 60S ribosomal protein 19-like protein

Chain LH: 88% 11% ..

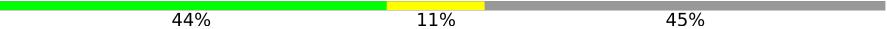


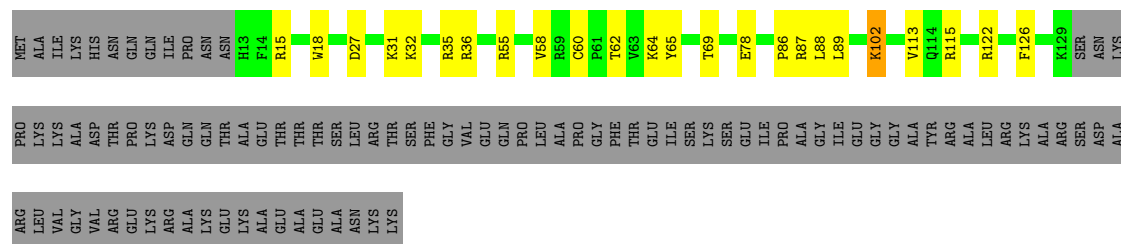
- Molecule 33: 60S ribosomal protein L12-like protein

Chain LK:  75% 13% 12%



- Molecule 34: 60S ribosomal protein L13

Chain LL:  44% 11% 45%



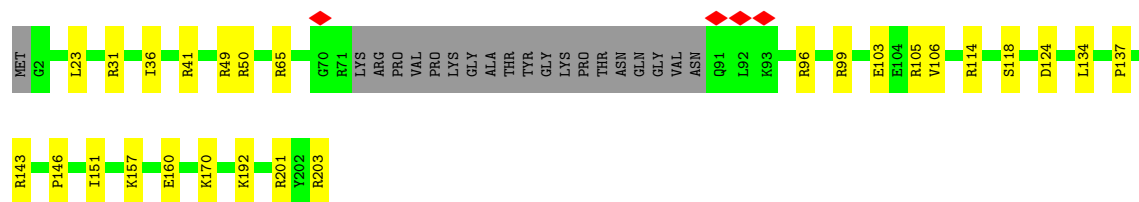
- Molecule 35: 60S ribosomal protein L14-like protein

Chain LM:  79% 18% .

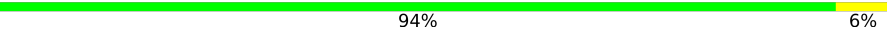


- Molecule 36: Ribosomal protein L15

Chain LN:  77% 13% 10%



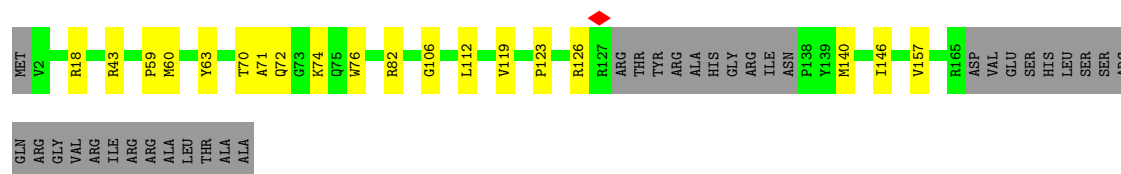
- Molecule 37: 60S ribosomal protein L16-like protein

Chain LO:  94% 6%

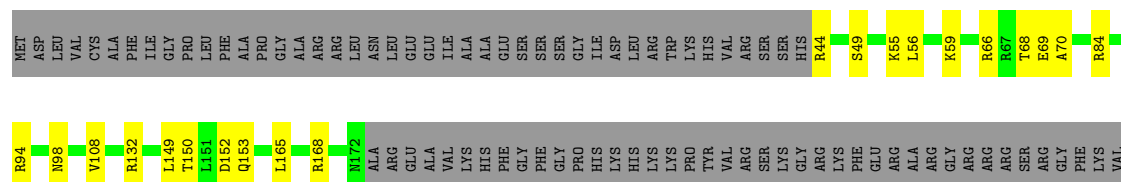


- Molecule 38: 60S ribosomal protein l17-like protein

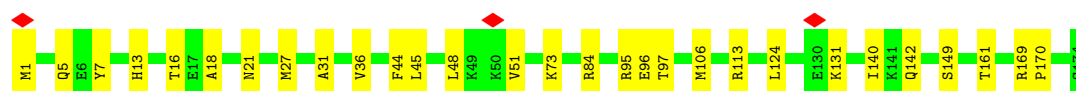
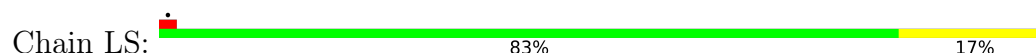
Chain LP:  72% 10% 18%



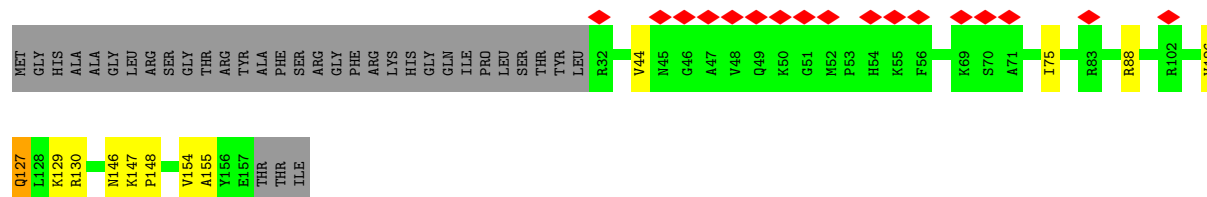
- Molecule 39: Ribosomal protein L18-like protein



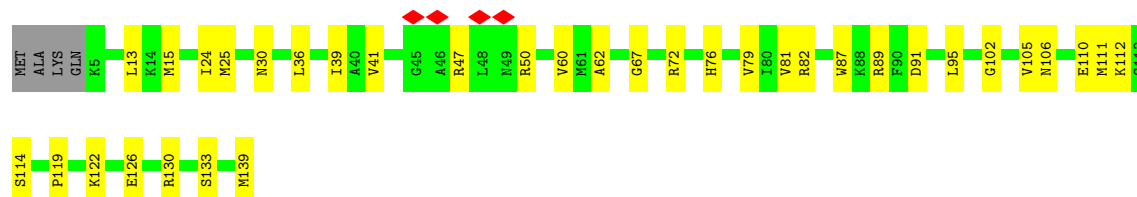
- Molecule 40: 60S ribosomal protein L20



- Molecule 41: 60S ribosomal protein l21-like protein

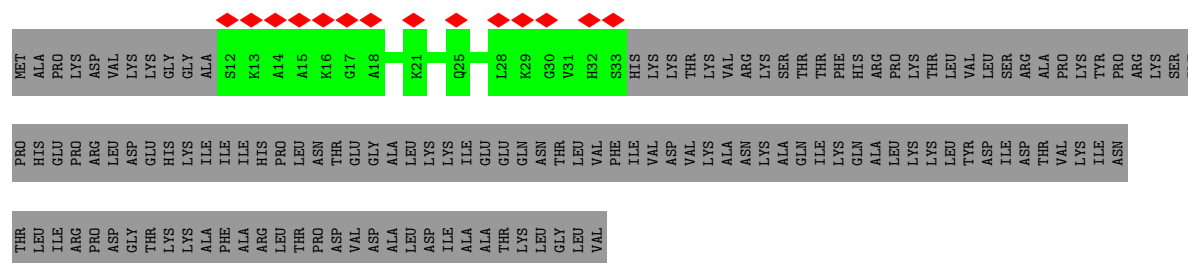


- Molecule 42: 60S ribosomal protein l23-like protein

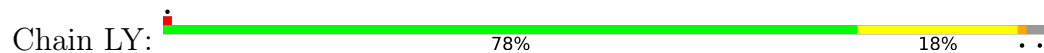


- Molecule 43: 60S ribosomal protein L25-like protein

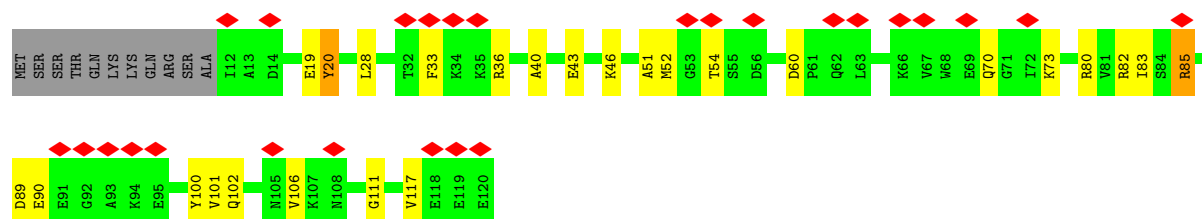




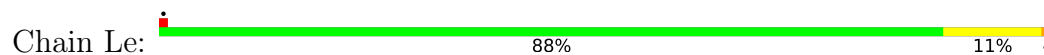
- Molecule 44: 60S ribosomal protein L26-like protein



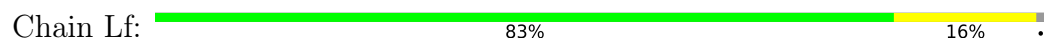
- Molecule 45: Putative 60S ribosomal protein



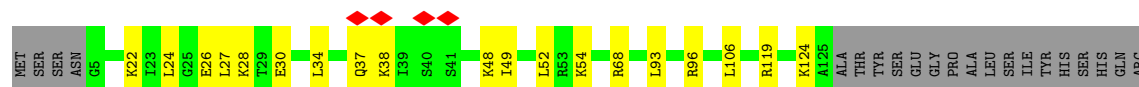
- Molecule 46: 60S ribosomal protein L32-like protein

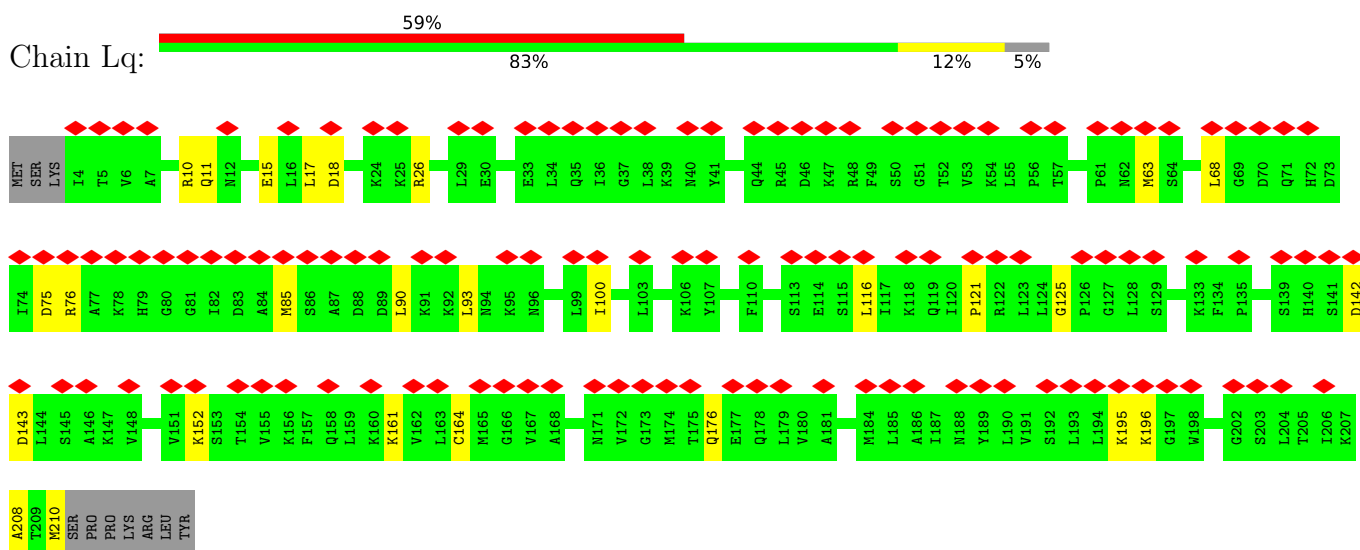


- Molecule 47: 60S ribosomal protein l33-like protein

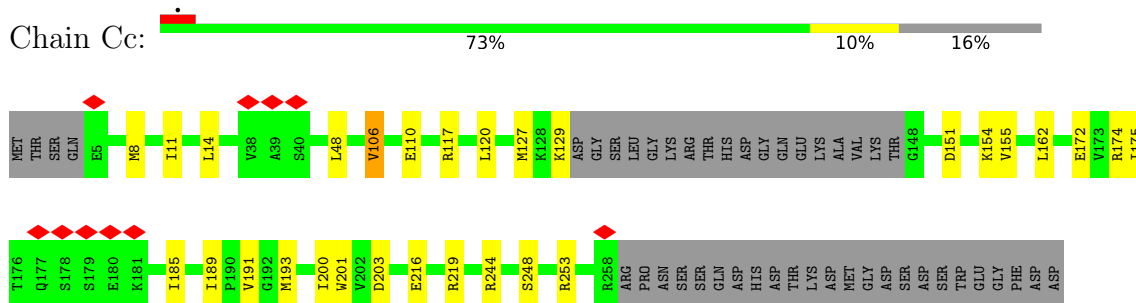


- Molecule 48: dolichyl-diphosphooligosaccharide--protein glycotransferase

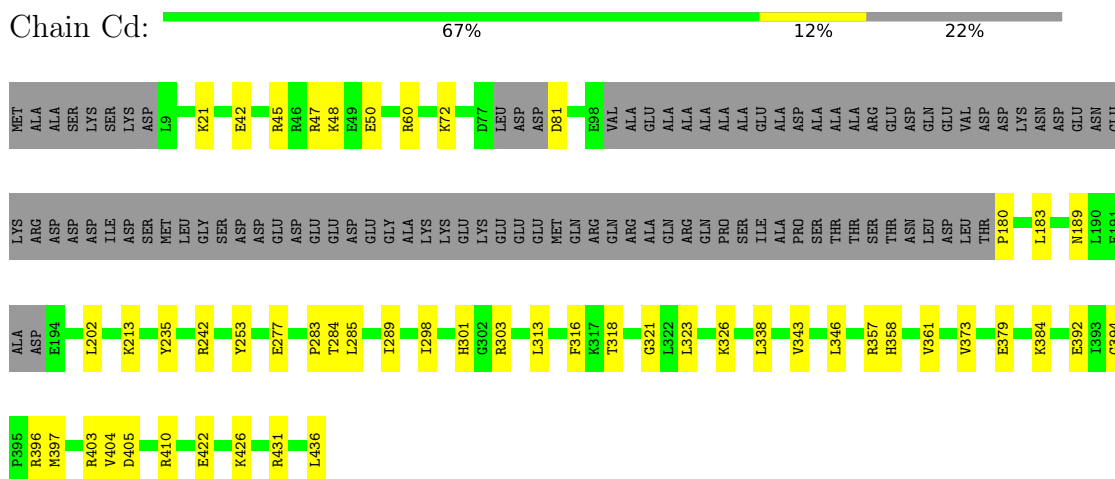




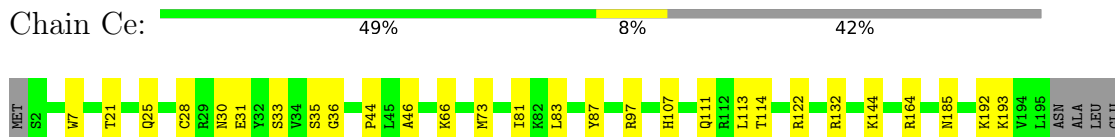
- Molecule 52: Ribosomal RNA-processing protein 1



- Molecule 53: Brix domain-containing protein



- Molecule 54: Protein MAK16



- Molecule 55: 60S ribosome biogenesis protein Rrp14

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16465	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.458	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

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	C1	0.22	0/51490	0.36	0/80245
2	C2	0.19	0/3754	0.32	0/5846
3	C3	0.19	0/2342	0.38	0/3649
4	CA	0.22	0/2190	0.57	2/2940 (0.1%)
5	CB	0.33	0/2109	0.72	1/2866 (0.0%)
6	CC	0.18	0/2459	0.44	0/3350
7	CE	0.21	0/3743	0.53	2/5045 (0.0%)
8	CF	0.19	0/1982	0.53	0/2671
9	CG	0.24	0/1422	0.63	3/1920 (0.2%)
10	CH	0.28	0/3927	0.61	1/5307 (0.0%)
11	CI	0.22	0/1225	0.61	1/1645 (0.1%)
12	CJ	0.16	0/3189	0.40	0/4309
13	CK	0.22	0/1885	0.54	1/2529 (0.0%)
14	CL	0.14	0/2178	0.39	0/2983
15	CM	0.23	0/1555	0.65	1/2091 (0.0%)
15	LF	0.20	0/2004	0.47	0/2686
16	CN	0.20	0/1881	0.53	0/2560
17	CO	0.18	0/470	0.42	0/619
18	CP	0.24	0/2594	0.62	2/3514 (0.1%)
19	CQ	0.22	0/981	0.62	1/1301 (0.1%)
20	CR	0.22	0/1369	0.47	0/1828
21	CS	0.21	0/1762	0.43	0/2417
22	CT	0.33	0/2264	0.61	0/3149
23	CU	0.24	0/1428	0.60	1/1910 (0.1%)
24	CX	0.17	0/705	0.51	0/938
25	CY	0.36	0/1600	0.62	0/2220
26	Cz	0.18	0/598	0.42	0/785
27	Cb	0.24	0/5150	0.59	2/6936 (0.0%)
28	LB	0.25	0/2760	0.54	1/3701 (0.0%)
29	LC	0.23	0/2809	0.45	0/3787
30	LE	0.19	0/1363	0.43	0/1833
31	LG	0.23	0/1606	0.53	0/2149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LH	0.20	0/1516	0.48	0/2038
33	LK	0.24	0/1124	0.65	0/1507
34	LL	0.39	0/983	0.59	0/1318
35	LM	0.19	0/1120	0.41	0/1507
36	LN	0.21	0/1595	0.42	0/2132
37	LO	0.21	0/1652	0.45	0/2215
38	LP	0.26	0/1231	0.46	0/1658
39	LQ	0.20	0/1033	0.45	0/1391
40	LS	0.22	0/1468	0.49	0/1975
41	LT	0.19	0/1033	0.53	0/1389
42	LV	0.25	0/1013	0.45	0/1361
43	LX	0.10	0/148	0.40	0/194
44	LY	0.21	0/1079	0.45	0/1443
45	Ld	0.19	0/904	0.48	0/1209
46	Le	0.20	0/1073	0.40	0/1431
47	Lf	0.23	0/883	0.47	0/1187
48	Lh	0.18	0/1006	0.44	0/1338
49	Li	0.19	0/738	0.39	0/971
50	Lj	0.28	0/606	0.46	0/803
51	Lq	0.16	0/1621	0.45	0/2180
52	Cc	0.21	0/1934	0.48	0/2614
53	Cd	0.26	0/2818	0.52	0/3786
54	Ce	0.22	0/1638	0.44	0/2196
55	Cf	0.15	0/514	0.38	0/669
All	All	0.23	0/145524	0.46	19/208241 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	LB	171	PRO	CA-N-CD	-9.51	98.69	112.00
10	CH	195	PRO	CA-N-CD	-8.05	100.72	112.00
18	CP	568	PRO	CA-N-CD	-7.82	101.06	112.00
4	CA	148	GLN	CA-C-N	6.75	129.78	120.39
4	CA	148	GLN	C-N-CA	6.75	129.78	120.39
9	CG	107	PRO	CA-N-CD	-6.72	102.59	112.00
23	CU	275	MET	CB-CG-SD	5.93	130.50	112.70
7	CE	478	VAL	CB-CA-C	5.85	116.07	110.16
15	CM	101	ILE	CB-CA-C	5.78	115.00	109.33
19	CQ	64	VAL	N-CA-C	-5.76	107.88	113.53
9	CG	63	LYS	N-CA-C	-5.74	107.52	114.75
13	CK	120	PRO	CA-N-CD	-5.72	103.99	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Cb	207	MET	CB-CG-SD	5.60	129.50	112.70
5	CB	215	ARG	CA-CB-CG	5.54	125.19	114.10
18	CP	340	VAL	N-CA-C	-5.53	108.46	113.71
11	CI	200	GLU	CA-CB-CG	5.24	124.58	114.10
7	CE	133	LYS	CA-CB-CG	5.22	124.54	114.10
27	Cb	201	GLU	N-CA-C	-5.18	107.61	114.04
9	CG	20	MET	CB-CG-SD	5.12	128.04	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	46025	0	23207	422	0
2	C2	3359	0	1698	26	0
3	C3	2097	0	1065	36	0
4	CA	2144	0	2178	48	0
5	CB	2063	0	2131	56	0
6	CC	2388	0	2301	39	0
7	CE	3673	0	3778	46	0
8	CF	1945	0	1965	31	0
9	CG	1396	0	1420	32	0
10	CH	3851	0	3894	56	0
11	CI	1196	0	1202	25	0
12	CJ	3109	0	3122	47	0
13	CK	1855	0	1952	36	0
14	CL	2173	0	1423	11	0
15	CM	1525	0	1604	22	0
15	LF	1967	0	2080	23	0
16	CN	1856	0	1856	30	0
17	CO	468	0	503	7	0
18	CP	2535	0	2549	58	0
19	CQ	960	0	1000	19	0
20	CR	1354	0	1400	22	0
21	CS	1750	0	1195	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CT	2269	0	1022	6	0
23	CU	1415	0	1457	21	0
24	CX	701	0	742	7	0
25	CY	1608	0	719	2	0
26	Cz	592	0	640	8	0
27	Cb	5058	0	5223	83	0
28	LB	2708	0	2811	55	0
29	LC	2752	0	2878	37	0
30	LE	1338	0	1423	13	0
31	LG	1583	0	1722	30	0
32	LH	1496	0	1575	16	0
33	LK	1112	0	1190	14	0
34	LL	964	0	1041	17	0
35	LM	1101	0	1170	16	0
36	LN	1563	0	1618	19	0
37	LO	1618	0	1714	13	0
38	LP	1212	0	1250	11	0
39	LQ	1021	0	1118	15	0
40	LS	1433	0	1496	20	0
41	LT	1014	0	1073	9	0
42	LV	995	0	1055	23	0
43	LX	148	0	163	0	0
44	LY	1065	0	1156	19	0
45	Ld	890	0	940	16	0
46	Le	1055	0	1133	11	0
47	Lf	862	0	891	12	0
48	Lh	995	0	1110	15	0
49	Li	731	0	797	12	0
50	Lj	595	0	625	7	0
51	Lq	1600	0	1703	18	0
52	Cc	1898	0	1931	19	0
53	Cd	2763	0	2859	38	0
54	Ce	1609	0	1681	17	0
55	Cf	513	0	556	5	0
56	CH	32	0	12	1	0
57	CQ	1	0	0	0	0
57	Ce	1	0	0	0	0
57	Lj	1	0	0	0	0
All	All	138001	0	112017	1433	0

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

All (1433) 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:C1:788:A:N6	1:C1:915:G:H1	1.47	1.11
1:C1:1055:U:C4	1:C1:1063:C:N4	2.22	1.06
1:C1:1055:U:O4	1:C1:1063:C:C4	2.10	1.04
3:C3:69:G:H1	3:C3:132:U:H3	0.99	0.94
3:C3:38:G:H1	3:C3:43:U:H3	0.96	0.93
1:C1:1204:G:HO2'	1:C1:1267:G:H1	1.01	0.93
1:C1:2848:A:N6	1:C1:2871:C:H42	1.66	0.93
21:CS:68:PRO:HA	27:Cb:820:HIS:HA	1.53	0.89
1:C1:2848:A:H61	1:C1:2871:C:N4	1.69	0.88
1:C1:2735:G:H1	1:C1:2741:U:H3	0.86	0.85
1:C1:2404:G:H1	1:C1:2467:U:H3	1.25	0.85
1:C1:2848:A:H61	1:C1:2871:C:H42	0.89	0.85
1:C1:91:G:H21	1:C1:95:A:H62	1.26	0.84
1:C1:788:A:H62	1:C1:915:G:H1	0.83	0.82
1:C1:526:G:N2	1:C1:544:U:C2	2.49	0.81
18:CP:535:LYS:HD3	18:CP:584:ILE:HD11	1.61	0.81
1:C1:1055:U:C4	1:C1:1063:C:C4	2.66	0.80
1:C1:3319:C:H4'	28:LB:316:GLY:HA2	1.66	0.77
46:Le:70:SER:HG	46:Le:72:HIS:HD1	1.35	0.75
3:C3:62:G:N7	11:CI:278:ARG:NH2	2.35	0.73
1:C1:974:G:H1	1:C1:1038:U:H3	0.81	0.73
1:C1:796:G:H1	1:C1:906:A:H61	1.39	0.71
27:Cb:17:ILE:HG23	27:Cb:448:LYS:HZ1	1.56	0.70
4:CA:243:ILE:HG22	4:CA:244:ILE:HG22	1.73	0.70
4:CA:91:PHE:HB3	4:CA:103:TRP:HB2	1.74	0.69
4:CA:137:ARG:HH12	4:CA:167:GLN:HG2	1.58	0.69
9:CG:19:TYR:HB3	9:CG:90:LEU:HD11	1.73	0.69
7:CE:129:MET:HE1	7:CE:206:LEU:HD22	1.75	0.69
15:CM:146:ASN:HD21	15:CM:246:ARG:HH12	1.40	0.69
12:CJ:376:ARG:HH21	15:CM:189:ASP:HA	1.58	0.68
1:C1:2927:A:O2'	9:CG:149:ARG:NH2	2.26	0.68
6:CC:325:ASP:HB3	6:CC:328:GLN:HG3	1.74	0.68
1:C1:1055:U:O4	1:C1:1063:C:N3	2.27	0.68
1:C1:1046:A:N1	1:C1:1074:C:N3	2.41	0.67
18:CP:537:VAL:H	18:CP:582:LYS:HZ1	1.42	0.67
1:C1:2848:A:N1	1:C1:2871:C:N3	2.42	0.67
12:CJ:87:LEU:HD21	12:CJ:110:ALA:HA	1.77	0.67
1:C1:3183:C:N3	17:CO:93:ARG:NH1	2.43	0.67
10:CH:258:GLN:HE22	33:LK:33:GLY:HA3	1.59	0.67
15:CM:70:ARG:HH12	15:CM:138:PRO:HD3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1053:U:H3	1:C1:1069:G:H1	1.43	0.66
5:CB:215:ARG:HH21	5:CB:220:ILE:HG12	1.59	0.66
52:Cc:216:GLU:HA	52:Cc:219:ARG:HH12	1.59	0.66
18:CP:521:GLU:OE2	18:CP:565:ARG:NH1	2.27	0.66
8:CF:5:LYS:NZ	8:CF:6:ARG:O	2.29	0.66
35:LM:35:ASP:OD2	35:LM:38:ARG:NH1	2.28	0.66
10:CH:299:PRO:HA	10:CH:302:GLN:HG2	1.76	0.66
4:CA:78:CYS:SG	4:CA:249:SER:OG	2.53	0.66
18:CP:508:ILE:HB	18:CP:581:PHE:HB2	1.77	0.66
8:CF:194:ILE:O	8:CF:205:GLN:NE2	2.29	0.65
10:CH:439:GLU:OE2	19:CQ:1:MET:N	2.27	0.65
13:CK:175:MET:SD	13:CK:178:ARG:NH1	2.68	0.65
29:LC:155:SER:HG	29:LC:259:SER:HG	1.41	0.65
44:LY:30:MET:HB3	44:LY:100:PRO:HG2	1.76	0.65
1:C1:788:A:N6	1:C1:915:G:N1	2.32	0.65
39:LQ:68:THR:HG22	39:LQ:70:ALA:H	1.60	0.65
19:CQ:95:ARG:NH1	19:CQ:98:GLU:OE2	2.29	0.65
35:LM:106:GLN:HA	35:LM:109:ARG:HG2	1.78	0.65
3:C3:71:U:C2	3:C3:131:G:N1	2.65	0.65
32:LH:17:LYS:NZ	35:LM:3:GLU:OE1	2.30	0.65
7:CE:334:GLN:NE2	7:CE:441:TYR:OH	2.30	0.65
10:CH:183:VAL:HG21	10:CH:219:ASP:HB2	1.78	0.65
33:LK:85:LEU:HD21	33:LK:104:VAL:HG22	1.79	0.65
1:C1:2924:G:O6	9:CG:15:LYS:NZ	2.30	0.65
3:C3:71:U:O2	3:C3:131:G:C2	2.50	0.65
6:CC:325:ASP:OD1	12:CJ:244:ARG:NH1	2.30	0.64
1:C1:83:C:HO2'	1:C1:687:C:HO2'	1.42	0.64
1:C1:3188:U:OP2	17:CO:93:ARG:NH2	2.31	0.64
4:CA:121:HIS:HB2	4:CA:237:ARG:HB3	1.78	0.64
27:Cb:423:THR:OG1	27:Cb:424:ASP:N	2.30	0.64
27:Cb:491:LEU:HB3	27:Cb:568:GLY:HA3	1.80	0.64
41:LT:127:GLN:NE2	41:LT:129:LYS:O	2.29	0.64
5:CB:58:ALA:HA	5:CB:249:ASN:HB3	1.79	0.64
2:C2:39:G:C2	2:C2:105:A:C2	2.85	0.63
28:LB:331:GLY:HA3	28:LB:337:MET:HE1	1.80	0.63
9:CG:101:LYS:HA	9:CG:137:MET:HE1	1.79	0.63
1:C1:690:G:N7	4:CA:282:ARG:NH2	2.44	0.63
1:C1:1046:A:N6	1:C1:1074:C:O2	2.32	0.63
10:CH:29:PRO:O	10:CH:48:LYS:NZ	2.31	0.63
44:LY:51:LYS:NZ	44:LY:70:THR:O	2.32	0.63
47:Lf:15:HIS:NE2	47:Lf:30:SER:OG	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CP:383:ARG:NH2	18:CP:448:GLY:O	2.32	0.62
6:CC:270:PRO:HB3	31:LG:148:ASN:HA	1.81	0.62
16:CN:126:GLU:OE1	16:CN:139:ARG:NH1	2.32	0.62
1:C1:2965:G:H4'	37:LO:67:PRO:HB2	1.82	0.62
5:CB:119:ASP:HB2	5:CB:225:ARG:HH12	1.64	0.62
1:C1:1080:A:OP2	41:LT:130:ARG:NH1	2.33	0.62
8:CF:25:ARG:O	8:CF:29:ASN:ND2	2.29	0.62
16:CN:12:GLU:OE2	42:LV:130:ARG:NH2	2.31	0.62
19:CQ:17:LYS:NZ	28:LB:369:GLY:O	2.33	0.62
53:CD:42:GLU:OE1	53:CD:45:ARG:NH2	2.32	0.62
24:CX:140:LYS:HB3	24:CX:144:ARG:HH21	1.64	0.62
1:C1:663:G:N7	39:LQ:132:ARG:NH2	2.48	0.62
13:CK:242:TYR:HB3	13:CK:260:LEU:HD12	1.81	0.62
29:LC:290:LEU:HD21	39:LQ:152:ASP:HB2	1.82	0.62
40:LS:31:ALA:HB1	40:LS:36:VAL:HG13	1.80	0.62
1:C1:2302:U:H2'	1:C1:2303:A:H8	1.64	0.62
7:CE:112:GLU:HG2	7:CE:133:LYS:HA	1.82	0.62
1:C1:974:G:O6	1:C1:1038:U:O4	2.18	0.61
5:CB:175:THR:HG22	5:CB:177:LYS:H	1.63	0.61
36:LN:114:ARG:NH1	36:LN:151:ILE:O	2.33	0.61
1:C1:1372:A:N6	1:C1:1400:A:O2'	2.33	0.61
15:CM:124:LYS:HD3	15:CM:197:VAL:HG21	1.82	0.61
1:C1:608:A:OP1	47:Lf:62:ARG:NH2	2.33	0.61
1:C1:1239:C:H42	1:C1:1243:G:N2	1.98	0.61
18:CP:460:SER:O	18:CP:475:ARG:NH1	2.33	0.61
45:Ld:89:ASP:OD1	45:Ld:90:GLU:N	2.31	0.61
4:CA:33:LYS:HE3	6:CC:156:PRO:HD2	1.82	0.61
10:CH:250:LEU:HD21	10:CH:334:VAL:HG21	1.83	0.61
18:CP:485:HIS:O	18:CP:489:GLN:NE2	2.33	0.61
1:C1:385:U:O2'	44:LY:86:ARG:NH2	2.34	0.61
1:C1:1153:G:OP2	15:LF:223:ARG:NH1	2.32	0.61
1:C1:2959:C:OP1	28:LB:26:ARG:NH1	2.33	0.61
18:CP:488:LYS:HG3	18:CP:523:VAL:HG13	1.82	0.61
42:LV:30:ASN:HD21	42:LV:114:SER:HB2	1.66	0.61
2:C2:55:U:OP1	20:CR:11:ARG:NH1	2.33	0.61
9:CG:104:GLY:HA3	9:CG:118:HIS:HB3	1.83	0.61
1:C1:2478:U:O4	1:C1:2550:G:N2	2.34	0.61
1:C1:596:G:OP2	29:LC:317:LYS:NZ	2.34	0.60
1:C1:796:G:H1	1:C1:906:A:N6	1.98	0.60
1:C1:2425:G:N1	1:C1:2455:U:N3	2.49	0.60
1:C1:3298:U:H2'	1:C1:3299:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1171:C:N3	1:C1:1297:U:O2	2.34	0.60
1:C1:1274:C:OP1	13:CK:62:ARG:NH2	2.32	0.60
6:CC:340:ILE:O	6:CC:415:ARG:NH1	2.34	0.60
13:CK:260:LEU:HD22	23:CU:338:LYS:HE3	1.84	0.60
4:CA:192:ARG:NH1	23:CU:240:GLU:OE1	2.35	0.60
29:LC:91:PHE:O	29:LC:99:ARG:NH2	2.35	0.60
54:Ce:33:SER:OG	54:Ce:35:SER:O	2.20	0.60
1:C1:1104:U:OP2	14:CL:33:ARG:NH1	2.34	0.60
47:Lf:34:ILE:HG23	47:Lf:102:ILE:HD13	1.84	0.60
9:CG:110:TYR:O	13:CK:163:ARG:NH1	2.33	0.60
27:Cb:148:MET:HE2	27:Cb:163:ALA:HB2	1.84	0.60
18:CP:491:LEU:HD11	18:CP:581:PHE:HE2	1.67	0.60
33:LK:37:LEU:HD21	33:LK:64:ILE:HG12	1.83	0.60
52:Cc:8:MET:HE3	52:Cc:11:ILE:HD11	1.83	0.60
9:CG:40:MET:HB2	9:CG:45:VAL:HG12	1.84	0.60
7:CE:440:ASP:OD1	7:CE:444:ARG:NE	2.28	0.59
27:Cb:161:ALA:HA	27:Cb:212:ASP:HA	1.83	0.59
36:LN:99:ARG:NH1	36:LN:118:SER:O	2.34	0.59
23:CU:236:ASP:OD1	23:CU:239:ARG:NH2	2.35	0.59
41:LT:75:ILE:HG12	41:LT:88:ARG:HG2	1.84	0.59
53:Cd:318:THR:H	53:Cd:436:LEU:HD22	1.67	0.59
20:CR:50:THR:OG1	20:CR:69:ASN:O	2.15	0.59
27:Cb:127:ARG:HG2	27:Cb:151:ARG:HH22	1.66	0.59
1:C1:2820:U:N3	10:CH:88:ASP:OD2	2.34	0.59
1:C1:264:G:H1'	49:Li:91:ARG:HH12	1.67	0.59
5:CB:103:ASP:HB3	5:CB:104:PRO:HD2	1.85	0.59
10:CH:97:ILE:HG13	10:CH:142:LEU:HD21	1.83	0.59
22:CT:609:GLN:O	22:CT:613:GLY:N	2.30	0.59
1:C1:2088:A:O3'	19:CQ:43:LYS:NZ	2.33	0.59
4:CA:105:SER:HB2	4:CA:112:THR:HG23	1.84	0.59
16:CN:107:VAL:HG23	16:CN:108:ILE:HG13	1.85	0.59
27:Cb:493:ARG:HE	27:Cb:571:GLN:HG2	1.68	0.59
27:Cb:588:ASP:HA	27:Cb:591:LEU:HB3	1.85	0.59
27:Cb:813:PHE:HZ	27:Cb:825:LEU:HD11	1.67	0.59
1:C1:2933:U:H2'	1:C1:2934:A:H8	1.68	0.58
10:CH:190:ASP:OD2	13:CK:9:ARG:NH2	2.36	0.58
33:LK:54:LYS:NZ	33:LK:87:GLU:OE2	2.35	0.58
1:C1:1139:G:OP2	15:LF:100:LYS:NZ	2.35	0.58
8:CF:227:TRP:HB2	8:CF:234:VAL:HG12	1.84	0.58
19:CQ:61:LYS:HG3	19:CQ:111:ARG:HH12	1.67	0.58
5:CB:60:THR:HB	5:CB:286:PRO:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Cz:42:THR:HG23	26:Cz:45:LEU:HD12	1.84	0.58
11:Cl:196:HIS:O	15:CM:62:ARG:NH2	2.33	0.58
12:CJ:376:ARG:NH2	15:CM:189:ASP:OD1	2.36	0.58
1:C1:2813:C:H2'	1:C1:2814:G:H8	1.67	0.58
1:C1:3184:G:H5'	1:C1:3187:G:H21	1.68	0.58
15:CM:113:ARG:NH2	15:CM:205:ALA:O	2.36	0.58
18:CP:277:ASN:HB2	18:CP:473:THR:HA	1.84	0.58
1:C1:121:A:O2'	31:LG:108:LYS:NZ	2.36	0.58
1:C1:143:G:N7	31:LG:140:ASN:ND2	2.52	0.58
1:C1:1239:C:H42	1:C1:1243:G:H22	1.50	0.58
8:CF:44:SER:HB3	8:CF:224:LEU:HD21	1.85	0.58
19:CQ:16:SER:HB3	28:LB:73:VAL:HG21	1.84	0.58
53:Cd:289:ILE:HG12	53:Cd:397:MET:HE2	1.86	0.58
53:Cd:410:ARG:NH2	53:Cd:422:GLU:OE2	2.36	0.58
1:C1:116:A:OP1	49:Li:45:ARG:NH1	2.29	0.58
5:CB:83:ILE:HD11	5:CB:270:PHE:HE2	1.69	0.58
30:LE:69:ARG:NH1	30:LE:185:SER:OG	2.36	0.58
32:LH:23:ARG:NH1	32:LH:41:ILE:O	2.37	0.58
34:LL:27:ASP:OD2	34:LL:31:LYS:NZ	2.37	0.58
1:C1:253:U:O4	7:CE:390:LYS:NZ	2.35	0.58
19:CQ:54:ALA:O	19:CQ:58:ASN:ND2	2.36	0.58
32:LH:34:LEU:HD13	32:LH:78:MET:HG2	1.85	0.58
1:C1:243:G:N2	20:CR:191:GLU:OE1	2.37	0.58
16:CN:112:ASP:H	16:CN:156:ASN:HD21	1.52	0.58
1:C1:342:C:OP1	20:CR:10:ARG:NH2	2.35	0.57
13:CK:42:LEU:HD22	13:CK:46:ARG:HE	1.69	0.57
18:CP:484:PRO:HA	18:CP:487:GLN:HG3	1.86	0.57
27:Cb:222:LEU:HD21	27:Cb:257:GLU:HB3	1.85	0.57
27:Cb:228:MET:HE2	27:Cb:230:LEU:HD13	1.85	0.57
29:LC:21:GLU:OE2	29:LC:263:LYS:NZ	2.37	0.57
29:LC:100:MET:HE2	29:LC:103:PRO:HA	1.86	0.57
1:C1:3001:A:H4'	28:LB:13:SER:HB2	1.86	0.57
6:CC:370:TRP:HE1	6:CC:378:ARG:HG2	1.69	0.57
16:CN:116:LEU:HD11	16:CN:177:LEU:HD21	1.86	0.57
28:LB:66:LYS:HZ1	42:LV:13:LEU:H	1.51	0.57
29:LC:288:SER:HB3	52:Cc:106:VAL:HG21	1.85	0.57
7:CE:438:PRO:HB2	7:CE:439:ARG:HH12	1.69	0.57
54:Cc:81:ILE:HG21	54:Cc:97:ARG:HE	1.68	0.57
1:C1:105:C:OP1	20:CR:60:LYS:NZ	2.36	0.57
1:C1:1046:A:N6	1:C1:1074:C:C2	2.64	0.57
1:C1:3045:G:OP1	28:LB:314:ARG:NH2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LH:14:GLU:HA	35:LM:2:ALA:HB2	1.85	0.57
4:CA:244:ILE:HD12	4:CA:257:GLU:HG3	1.87	0.57
12:CJ:90:LYS:HA	12:CJ:93:ARG:HG2	1.87	0.57
39:LQ:94:ARG:O	39:LQ:98:ASN:ND2	2.37	0.57
4:CA:245:ILE:HB	4:CA:256:TYR:HB3	1.86	0.57
10:CH:251:TYR:HB3	10:CH:284:ILE:HG22	1.86	0.57
12:CJ:180:ILE:HA	12:CJ:389:ALA:HA	1.86	0.57
27:Cb:244:ASP:OD2	27:Cb:428:ARG:NH2	2.37	0.57
34:LL:55:ARG:O	34:LL:115:ARG:NH1	2.37	0.57
39:LQ:49:SER:O	39:LQ:55:LYS:NZ	2.37	0.57
1:C1:694:U:O2'	1:C1:735:G:N3	2.38	0.57
5:CB:105:GLN:HB2	5:CB:129:ASP:HB2	1.85	0.57
1:C1:263:C:O2	49:Li:91:ARG:NH2	2.38	0.57
4:CA:88:ASN:OD1	4:CA:106:LYS:NZ	2.37	0.57
8:CF:164:GLU:OE2	8:CF:207:ARG:NH2	2.38	0.57
20:CR:195:LEU:HD11	20:CR:228:ARG:HG2	1.87	0.57
1:C1:705:G:OP2	1:C1:705:G:N2	2.38	0.57
1:C1:1865:A:N3	1:C1:3035:G:N2	2.52	0.57
7:CE:154:ALA:HB3	7:CE:319:ASN:HA	1.86	0.57
9:CG:104:GLY:HA2	9:CG:107:PRO:HG2	1.87	0.57
44:LY:34:LEU:HD23	44:LY:38:LEU:HB3	1.87	0.57
10:CH:243:ALA:O	27:Cb:587:ARG:NH2	2.38	0.56
11:CI:188:VAL:HG21	11:CI:268:VAL:HG21	1.86	0.56
3:C3:5:C:H2'	5:CB:162:ARG:HH12	1.68	0.56
12:CJ:414:ARG:O	12:CJ:414:ARG:NE	2.39	0.56
1:C1:1371:G:O6	29:LC:190:LYS:NZ	2.38	0.56
1:C1:2436:G:N2	1:C1:2437:G:O6	2.37	0.56
27:Cb:15:VAL:HG13	27:Cb:448:LYS:HE3	1.87	0.56
1:C1:695:G:H5'	1:C1:735:G:H21	1.70	0.56
1:C1:978:A:N6	1:C1:1032:U:O4	2.38	0.56
1:C1:1331:G:O6	52:Cc:244:ARG:NH2	2.38	0.56
6:CC:158:TYR:HE2	6:CC:164:ASP:HB2	1.70	0.56
1:C1:1228:G:O6	1:C1:1258:U:O4	2.24	0.56
42:LV:67:GLY:O	42:LV:72:ARG:NH2	2.39	0.56
1:C1:2424:G:O6	1:C1:2455:U:O2	2.23	0.56
5:CB:48:ASN:HD22	5:CB:51:ALA:HB3	1.69	0.56
27:Cb:212:ASP:OD2	27:Cb:212:ASP:N	2.36	0.56
27:Cb:401:ASP:OD2	42:LV:72:ARG:NH1	2.33	0.56
31:LG:71:ARG:NH1	31:LG:240:ILE:O	2.38	0.56
31:LG:84:THR:HG21	31:LG:158:ASN:HD22	1.70	0.56
51:Lq:63:MET:HG2	51:Lq:152:LYS:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:780:G:H2'	1:C1:782:A:H62	1.71	0.56
15:LF:108:ILE:HG23	15:LF:132:MET:HE3	1.88	0.56
40:LS:21:ASN:ND2	41:LT:146:ASN:OD1	2.39	0.56
18:CP:337:TRP:CD1	18:CP:338:SER:HG	2.24	0.56
1:C1:1259:C:H2'	1:C1:1260:A:H8	1.71	0.56
1:C1:3314:U:H2'	1:C1:3318:C:H41	1.71	0.56
53:Cd:50:GLU:OE2	53:Cd:60:ARG:NH1	2.39	0.56
1:C1:3158:U:OP2	35:LM:128:ARG:NH2	2.39	0.56
7:CE:290:ARG:NH1	7:CE:292:THR:OG1	2.39	0.56
31:LG:210:ASP:OD1	31:LG:210:ASP:N	2.38	0.56
48:Lh:34:LEU:HD13	48:Lh:37:GLN:HE21	1.71	0.56
1:C1:289:A:O2'	49:Li:42:GLN:NE2	2.37	0.55
3:C3:17:G:H2'	3:C3:18:G:C8	2.41	0.55
34:LL:122:ARG:HG3	48:Lh:124:LYS:HB2	1.88	0.55
13:CK:203:ASN:ND2	13:CK:219:THR:OG1	2.39	0.55
29:LC:115:ASN:HB2	29:LC:118:GLN:HG3	1.87	0.55
5:CB:103:ASP:OD2	5:CB:206:ARG:NH1	2.39	0.55
9:CG:87:LEU:HD21	9:CG:141:PRO:HB2	1.88	0.55
35:LM:30:ILE:HD13	35:LM:39:VAL:HG21	1.88	0.55
52:Cc:172:GLU:OE2	52:Cc:174:ARG:NH2	2.40	0.55
1:C1:323:G:H5''	20:CR:5:LEU:HD22	1.88	0.55
1:C1:976:U:N3	1:C1:1036:A:C8	2.74	0.55
4:CA:170:LYS:HB3	6:CC:167:VAL:HG21	1.88	0.55
10:CH:368:ILE:HD13	16:CN:238:LYS:HG3	1.88	0.55
45:Ld:19:GLU:HB3	45:Ld:80:ARG:HD2	1.89	0.55
51:Lq:68:LEU:HB3	51:Lq:116:LEU:HD23	1.88	0.55
6:CC:170:ASN:ND2	6:CC:223:PRO:O	2.37	0.55
6:CC:355:ASN:H	12:CJ:485:HIS:HE1	1.54	0.55
6:CC:403:ARG:HH21	6:CC:406:ARG:HH22	1.54	0.55
9:CG:15:LYS:HZ3	9:CG:82:LEU:HD22	1.70	0.55
18:CP:521:GLU:OE1	18:CP:548:PHE:N	2.39	0.55
27:Cb:162:ARG:HA	27:Cb:235:ILE:HA	1.87	0.55
1:C1:2431:G:H21	1:C1:2432:C:H41	1.55	0.55
4:CA:196:ILE:HG23	4:CA:229:ILE:HD11	1.89	0.55
5:CB:158:ARG:HG2	5:CB:159:ILE:HD13	1.89	0.55
12:CJ:217:ARG:NH2	12:CJ:219:VAL:O	2.36	0.55
12:CJ:412:ASP:O	12:CJ:453:ARG:NH1	2.39	0.55
20:CR:43:GLU:HB3	20:CR:47:GLN:HG3	1.88	0.55
42:LV:25:MET:HE3	42:LV:102:GLY:HA3	1.89	0.55
45:Ld:82:ARG:HH11	45:Ld:117:VAL:HG21	1.72	0.55
1:C1:679:A:OP1	36:LN:201:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1218:G:N3	1:C1:1227:A:C5	2.74	0.55
1:C1:2729:U:C4	1:C1:2731:C:N4	2.75	0.55
1:C1:2874:U:C6	1:C1:2893:U:H2'	2.42	0.55
6:CC:263:THR:OG1	49:Li:55:GLU:OE1	2.23	0.55
16:CN:173:LEU:HD22	16:CN:181:LEU:HD11	1.89	0.55
18:CP:384:CYS:HB2	18:CP:408:ILE:HD12	1.88	0.55
18:CP:535:LYS:HG2	18:CP:582:LYS:HB2	1.87	0.55
25:CY:571:LEU:O	25:CY:575:LEU:N	2.36	0.55
46:Le:114:LYS:O	54:Ce:122:ARG:NH1	2.39	0.55
53:Cd:384:LYS:O	54:Ce:193:LYS:NZ	2.40	0.55
1:C1:374:U:OP2	53:Cd:47:ARG:NH2	2.40	0.55
18:CP:498:CYS:SG	18:CP:499:ASN:N	2.79	0.55
1:C1:507:G:OP1	15:LF:73:ARG:NH2	2.39	0.55
1:C1:2091:U:C2	1:C1:2287:G:N1	2.75	0.55
7:CE:304:GLU:HB3	7:CE:308:ARG:HH21	1.71	0.55
46:Le:97:ILE:HG21	46:Le:106:ARG:HG2	1.89	0.55
53:Cd:81:ASP:OD1	53:Cd:81:ASP:N	2.39	0.55
1:C1:695:G:N2	1:C1:698:A:OP2	2.39	0.54
3:C3:65:G:O2'	3:C3:142:A:OP1	2.22	0.54
4:CA:106:LYS:HB2	4:CA:110:GLY:HA3	1.89	0.54
12:CJ:256:LYS:HE3	12:CJ:272:SER:HB3	1.88	0.54
42:LV:106:ASN:OD1	42:LV:110:GLU:N	2.35	0.54
1:C1:2934:A:OP1	55:Cf:532:ARG:NH1	2.37	0.54
8:CF:82:GLU:N	8:CF:82:GLU:OE1	2.41	0.54
12:CJ:450:TYR:N	12:CJ:455:TYR:OH	2.41	0.54
27:Cb:159:PHE:HA	27:Cb:210:ASN:HD21	1.72	0.54
28:LB:94:GLU:HB2	28:LB:157:THR:HG21	1.89	0.54
29:LC:301:ARG:NH2	39:LQ:66:ARG:O	2.40	0.54
34:LL:86:PRO:HG2	34:LL:89:LEU:HB3	1.89	0.54
1:C1:588:C:H4'	29:LC:327:LEU:HD23	1.90	0.54
5:CB:263:ILE:HG23	5:CB:281:PHE:HE2	1.72	0.54
29:LC:295:GLU:HG2	52:Cc:191:VAL:HG13	1.88	0.54
33:LK:13:ILE:HB	33:LK:62:LEU:HB2	1.88	0.54
1:C1:674:U:OP2	34:LL:36:ARG:NH2	2.41	0.54
1:C1:3309:G:N2	28:LB:381:MET:O	2.41	0.54
3:C3:25:U:H3	5:CB:173:LYS:HG3	1.70	0.54
11:CI:213:ILE:HD13	11:CI:233:ILE:HD11	1.90	0.54
11:CI:214:THR:HG22	11:CI:215:ARG:HG2	1.89	0.54
55:Cf:511:GLU:HA	55:Cf:514:LYS:HE3	1.89	0.54
2:C2:48:A:O2'	2:C2:51:G:N2	2.41	0.54
2:C2:63:G:HO2'	48:Lh:54:LYS:HZ2	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:35:ARG:HB2	4:CA:86:CYS:HA	1.90	0.54
16:CN:97:ILE:HG22	16:CN:128:ILE:HD11	1.89	0.54
5:CB:31:LEU:HA	5:CB:34:ILE:HD12	1.90	0.54
5:CB:235:LEU:HD11	5:CB:270:PHE:HB3	1.90	0.54
32:LH:89:LYS:HB2	32:LH:185:GLU:HB3	1.88	0.54
44:LY:2:LYS:HD2	44:LY:7:VAL:HG13	1.89	0.54
53:CD:180:PRO:HG2	53:CD:183:LEU:HB3	1.90	0.54
1:C1:1046:A:N1	1:C1:1074:C:C4	2.76	0.54
1:C1:2996:G:OP1	28:LB:62:ARG:NH1	2.41	0.54
18:CP:334:VAL:HG13	18:CP:337:TRP:HE1	1.73	0.54
15:LF:94:ARG:HB2	15:LF:114:LEU:HD13	1.90	0.54
38:LP:126:ARG:HD3	38:LP:140:MET:HE1	1.89	0.54
1:C1:430:A:OP2	1:C1:606:G:N2	2.35	0.54
28:LB:58:ARG:NH1	28:LB:284:TYR:OH	2.41	0.54
1:C1:83:C:O2'	1:C1:687:C:O2'	2.19	0.54
2:C2:127:U:O2	12:CJ:15:ASN:ND2	2.41	0.54
51:LQ:76:ARG:HH12	51:LQ:143:ASP:HA	1.73	0.54
5:CB:282:TYR:HB3	5:CB:290:ALA:HB1	1.90	0.53
26:CZ:41:PRO:HG2	32:LH:62:ARG:HH12	1.73	0.53
1:C1:36:C:H4'	1:C1:789:A:H2	1.73	0.53
1:C1:37:U:O2	34:LL:15:ARG:NH2	2.39	0.53
1:C1:1331:G:H3'	15:LF:21:LYS:HE3	1.89	0.53
7:CE:239:ALA:HB3	7:CE:244:LEU:HD22	1.89	0.53
8:CF:45:VAL:O	8:CF:99:THR:OG1	2.26	0.53
29:LC:133:ALA:HA	29:LC:149:VAL:HG21	1.90	0.53
1:C1:3269:U:H5''	28:LB:309:MET:HE2	1.91	0.53
2:C2:40:A:OP2	2:C2:103:G:N1	2.36	0.53
6:CC:271:LEU:HD12	31:LG:147:GLU:HG2	1.90	0.53
28:LB:47:MET:H	28:LB:84:MET:HE3	1.73	0.53
42:LV:15:MET:HB2	42:LV:87:TRP:HB2	1.90	0.53
1:C1:2888:A:H5'	27:Cb:3:LYS:HB2	1.91	0.53
29:LC:8:THR:OG1	29:LC:148:GLU:OE1	2.27	0.53
15:LF:169:LEU:HA	15:LF:174:ILE:HD11	1.90	0.53
40:LS:27:MET:HE1	40:LS:44:PHE:HB2	1.91	0.53
1:C1:2395:U:H3'	1:C1:2396:U:H2'	1.90	0.53
1:C1:2424:G:O6	1:C1:2455:U:C2	2.62	0.53
1:C1:2973:A:H2'	1:C1:2974:G:H8	1.74	0.53
3:C3:58:A:H5''	11:CI:230:ARG:HH11	1.74	0.53
15:CM:113:ARG:NH2	15:CM:208:LEU:O	2.37	0.53
27:Cb:200:LEU:HD13	27:Cb:220:ARG:HE	1.74	0.53
1:C1:6:A:O5'	12:CJ:93:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:724:C:O2	39:LQ:168:ARG:NE	2.40	0.53
5:CB:99:LEU:HD22	5:CB:127:VAL:HG22	1.90	0.53
6:CC:211:ILE:HG22	6:CC:212:GLU:HG3	1.91	0.53
8:CF:42:VAL:HG13	8:CF:224:LEU:HB2	1.90	0.53
15:CM:105:PRO:HA	15:CM:108:ILE:HG22	1.89	0.53
1:C1:642:C:H2'	1:C1:643:A:H8	1.74	0.53
1:C1:983:A:N1	1:C1:1032:U:O2'	2.40	0.53
8:CF:228:ASN:HB3	8:CF:231:SER:HB3	1.89	0.53
10:CH:279:ASN:OD1	10:CH:279:ASN:N	2.41	0.53
12:CJ:189:PHE:HB3	12:CJ:196:TYR:HB2	1.90	0.53
13:CK:116:ARG:NH1	18:CP:273:TYR:OH	2.41	0.53
22:CT:666:LYS:O	25:CY:568:TYR:N	2.42	0.53
27:Cb:324:ILE:HA	27:Cb:328:ILE:HB	1.90	0.53
35:LM:33:ILE:HA	35:LM:39:VAL:HG23	1.88	0.53
38:LP:106:GLY:O	54:Ce:164:ARG:NH2	2.42	0.53
1:C1:92:G:H5'	1:C1:93:C:H5''	1.90	0.53
1:C1:297:U:OP2	4:CA:96:LYS:NZ	2.39	0.53
10:CH:342:ARG:NH2	27:Cb:519:GLU:OE2	2.41	0.53
18:CP:580:LYS:HG2	18:CP:582:LYS:HZ2	1.73	0.53
2:C2:133:C:H2'	2:C2:134:G:H8	1.74	0.53
5:CB:44:ASP:OD1	5:CB:44:ASP:N	2.41	0.53
10:CH:210:TYR:CZ	10:CH:211:LYS:HE2	2.44	0.53
13:CK:127:ILE:HD12	13:CK:131:GLU:HG3	1.91	0.53
1:C1:661:G:O6	39:LQ:84:ARG:NH2	2.36	0.53
1:C1:1055:U:O4	1:C1:1063:C:N4	2.24	0.53
1:C1:340:C:O2	1:C1:344:A:O2'	2.27	0.52
1:C1:734:C:H2'	1:C1:735:G:H8	1.73	0.52
1:C1:2886:C:O2'	27:Cb:4:ARG:NH2	2.41	0.52
1:C1:3033:C:OP2	45:Ld:73:LYS:NZ	2.43	0.52
2:C2:103:G:OP2	2:C2:105:A:O2'	2.25	0.52
9:CG:85:THR:HG23	18:CP:426:HIS:HB3	1.90	0.52
10:CH:390:LEU:HD11	16:CN:43:GLN:HB2	1.91	0.52
13:CK:154:PRO:HB3	13:CK:179:TYR:HE2	1.74	0.52
30:LE:25:GLN:NE2	30:LE:27:TRP:O	2.42	0.52
1:C1:2944:U:H2'	1:C1:2945:A:H8	1.75	0.52
1:C1:36:C:O2'	1:C1:915:G:N3	2.40	0.52
1:C1:1263:U:H2'	1:C1:1264:G:H8	1.75	0.52
1:C1:2475:U:O2	1:C1:2551:A:C6	2.63	0.52
5:CB:88:PRO:HB3	5:CB:229:GLY:HA3	1.90	0.52
7:CE:113:PHE:HD1	7:CE:134:MET:HE2	1.74	0.52
7:CE:342:ASP:OD2	7:CE:540:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Cb:297:ALA:HB1	27:Cb:300:LYS:HB2	1.91	0.52
30:LE:56:THR:OG1	30:LE:108:LYS:NZ	2.43	0.52
15:LF:216:PRO:HD3	15:LF:248:MET:HE3	1.91	0.52
5:CB:83:ILE:HD11	5:CB:270:PHE:CE2	2.44	0.52
1:C1:2426:U:O2'	51:Lq:164:CYS:SG	2.59	0.52
7:CE:152:LEU:HD23	7:CE:315:PRO:HB3	1.92	0.52
14:CL:5:ILE:HD13	37:LO:53:LEU:HD12	1.92	0.52
17:CO:37:LEU:HD22	28:LB:208:THR:HB	1.92	0.52
28:LB:50:LYS:HD3	28:LB:337:MET:HE3	1.92	0.52
1:C1:403:U:H2'	1:C1:404:G:H8	1.74	0.52
15:CM:182:TYR:O	15:CM:200:ASN:ND2	2.42	0.52
15:LF:104:LYS:HD3	15:LF:135:ILE:HD13	1.91	0.52
46:Le:24:ASP:OD1	46:Le:24:ASP:N	2.36	0.52
1:C1:3157:C:OP1	35:LM:132:ARG:NH2	2.33	0.52
5:CB:275:TRP:HZ3	5:CB:295:GLN:HB3	1.75	0.52
10:CH:176:ASN:ND2	10:CH:196:TYR:O	2.30	0.52
1:C1:230:A:H2'	1:C1:231:A:C8	2.44	0.52
4:CA:38:VAL:HG12	4:CA:90:LEU:HB3	1.92	0.52
5:CB:42:ARG:HD3	5:CB:43:PRO:HD2	1.90	0.52
7:CE:393:GLN:HG2	7:CE:396:ARG:HH21	1.74	0.52
7:CE:506:TYR:HD2	7:CE:507:LEU:HD12	1.75	0.52
1:C1:370:A:H4'	44:LY:90:THR:HG22	1.92	0.52
1:C1:597:G:N7	29:LC:311:ARG:NH2	2.57	0.52
9:CG:112:SER:HB2	13:CK:139:GLY:HA3	1.92	0.52
13:CK:236:LYS:HZ3	18:CP:474:ASN:HB3	1.74	0.52
31:LG:222:LYS:HG3	31:LG:226:LEU:HD12	1.92	0.52
42:LV:105:VAL:HA	42:LV:111:MET:HA	1.91	0.52
53:Cd:284:THR:HB	53:Cd:405:ASP:HB2	1.91	0.52
4:CA:244:ILE:HD11	4:CA:254:ILE:HD12	1.92	0.52
24:CX:98:ARG:NH1	24:CX:102:ASN:OD1	2.42	0.52
27:Cb:600:GLN:O	27:Cb:625:ARG:NH1	2.43	0.52
27:Cb:798:GLY:HA3	27:Cb:804:ILE:HD12	1.93	0.52
1:C1:1239:C:N4	1:C1:1243:G:H22	2.06	0.51
1:C1:2857:C:O2'	1:C1:2859:G:OP2	2.27	0.51
29:LC:364:GLU:OE2	41:LT:147:LYS:NZ	2.42	0.51
1:C1:3076:U:OP2	26:Cz:28:ASN:ND2	2.41	0.51
1:C1:2436:G:O3'	1:C1:2438:C:N4	2.43	0.51
1:C1:2947:U:OP1	37:LO:66:ASN:ND2	2.44	0.51
16:CN:22:SER:HB3	16:CN:67:ARG:HG3	1.91	0.51
16:CN:109:VAL:HB	16:CN:149:GLY:HA2	1.91	0.51
15:LF:155:TYR:OH	15:LF:188:GLU:OE2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:350:G:N2	1:C1:353:A:OP2	2.37	0.51
1:C1:704:C:OP1	1:C1:732:A:O2'	2.26	0.51
1:C1:2936:U:H5''	55:Cf:526:LYS:HD3	1.92	0.51
6:CC:182:SER:HB2	24:CX:133:ARG:HH22	1.75	0.51
46:Le:10:ILE:HA	46:Le:64:THR:HG21	1.92	0.51
47:Lf:47:LEU:HD11	47:Lf:76:PRO:HD3	1.92	0.51
53:Cd:298:ILE:HD11	53:Cd:396:ARG:HG3	1.93	0.51
4:CA:109:ASN:ND2	6:CC:153:GLU:OE2	2.43	0.51
5:CB:42:ARG:HG3	5:CB:44:ASP:H	1.75	0.51
8:CF:236:GLU:O	8:CF:241:LYS:NZ	2.39	0.51
10:CH:79:ASP:OD2	10:CH:244:HIS:NE2	2.40	0.51
28:LB:26:ARG:HG3	28:LB:336:ILE:HD13	1.91	0.51
1:C1:1218:G:C2	1:C1:1227:A:C5	2.98	0.51
1:C1:1877:G:H2'	1:C1:1878:G:C8	2.45	0.51
1:C1:50:U:H2'	1:C1:51:A:H8	1.76	0.51
1:C1:653:G:OP1	36:LN:203:ARG:NH2	2.42	0.51
1:C1:2735:G:O6	1:C1:2741:U:O4	2.29	0.51
1:C1:2873:U:HO2'	1:C1:2893:U:HO2'	1.59	0.51
5:CB:216:PRO:HB2	5:CB:219:GLU:HG2	1.91	0.51
27:Cb:131:VAL:HG23	27:Cb:270:LEU:HD22	1.91	0.51
8:CF:141:ILE:HD11	8:CF:178:LYS:HD2	1.93	0.51
12:CJ:28:LEU:HD11	12:CJ:78:LEU:HD12	1.92	0.51
12:CJ:251:LEU:HG	12:CJ:275:GLY:HA2	1.92	0.51
18:CP:317:ARG:NH2	18:CP:341:GLY:O	2.44	0.51
15:LF:221:ARG:NH1	15:LF:232:GLY:O	2.42	0.51
5:CB:281:PHE:HB2	5:CB:295:GLN:HE22	1.76	0.51
7:CE:194:GLU:OE1	7:CE:194:GLU:N	2.42	0.51
31:LG:155:LEU:HD23	31:LG:183:ILE:HD13	1.93	0.51
38:LP:60:MET:HE3	38:LP:82:ARG:HB2	1.91	0.51
1:C1:213:G:C6	1:C1:1371:G:C2	2.99	0.51
3:C3:13:C:H2'	3:C3:14:C:H2'	1.91	0.51
27:Cb:130:VAL:HB	27:Cb:269:LEU:HD22	1.92	0.51
27:Cb:190:LYS:NZ	27:Cb:209:THR:O	2.43	0.51
1:C1:1218:G:C2	1:C1:1227:A:C6	2.99	0.50
18:CP:270:ILE:HD13	18:CP:285:LEU:HD21	1.93	0.50
28:LB:53:MET:HG2	28:LB:77:THR:HA	1.93	0.50
1:C1:432:U:OP2	53:Cd:235:TYR:OH	2.29	0.50
1:C1:1288:G:O6	1:C1:2328:C:O2'	2.29	0.50
1:C1:1875:A:H2'	1:C1:1876:G:C8	2.45	0.50
6:CC:177:LEU:HD11	6:CC:223:PRO:HA	1.93	0.50
13:CK:184:VAL:HG12	13:CK:257:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Cb:95:MET:HE1	27:Cb:121:ILE:HD12	1.91	0.50
27:Cb:432:ILE:HG13	27:Cb:456:ARG:HD2	1.93	0.50
1:C1:137:C:OP1	12:CJ:105:ARG:NH2	2.40	0.50
1:C1:385:U:OP1	53:Cd:72:LYS:NZ	2.45	0.50
1:C1:2368:C:H5''	23:CU:323:ARG:HH12	1.76	0.50
6:CC:196:MET:SD	6:CC:196:MET:N	2.84	0.50
7:CE:384:VAL:HG23	7:CE:410:THR:HB	1.94	0.50
23:CU:206:ASP:OD1	23:CU:206:ASP:N	2.45	0.50
31:LG:159:ASP:N	31:LG:159:ASP:OD1	2.42	0.50
46:Le:130:GLU:OE2	53:Cd:403:ARG:NH2	2.44	0.50
1:C1:2973:A:H2'	1:C1:2974:G:C8	2.47	0.50
13:CK:68:HIS:HA	13:CK:71:ARG:HG2	1.93	0.50
13:CK:247:ASN:ND2	13:CK:252:ASP:OD2	2.44	0.50
23:CU:267:ARG:NH2	24:CX:77:VAL:O	2.44	0.50
27:Cb:180:VAL:HG11	27:Cb:191:THR:HG21	1.93	0.50
27:Cb:182:GLU:O	27:Cb:185:LYS:NZ	2.45	0.50
1:C1:66:A:N6	1:C1:76:G:H1'	2.26	0.50
1:C1:1269:A:O2'	26:Cz:40:ARG:NH1	2.42	0.50
1:C1:1332:A:H2'	1:C1:1333:A:C8	2.47	0.50
1:C1:3015:U:N3	1:C1:3036:U:O2	2.42	0.50
51:Lq:93:LEU:HB3	51:Lq:100:ILE:HD12	1.91	0.50
1:C1:3234:A:H5''	28:LB:128:LYS:HE3	1.92	0.50
10:CH:230:GLU:OE1	10:CH:230:GLU:N	2.45	0.50
23:CU:283:GLU:O	23:CU:286:LYS:N	2.45	0.50
15:LF:67:GLU:HA	15:LF:70:ARG:HG2	1.93	0.50
31:LG:85:LEU:HD11	31:LG:183:ILE:HG22	1.93	0.50
33:LK:54:LYS:HE3	33:LK:89:PRO:HB3	1.92	0.50
42:LV:79:VAL:HG23	42:LV:105:VAL:HG11	1.93	0.50
1:C1:2076:C:H2'	1:C1:2077:G:H8	1.75	0.50
3:C3:1:C:N4	11:CI:252:LEU:O	2.44	0.50
8:CF:73:MET:HE3	8:CF:102:LEU:HG	1.94	0.50
11:CI:255:GLY:O	31:LG:216:LYS:NZ	2.42	0.50
27:Cb:191:THR:HG22	27:Cb:213:ILE:HB	1.93	0.50
29:LC:24:PRO:HG2	29:LC:265:LEU:HD23	1.93	0.50
38:LP:70:THR:HG23	38:LP:72:GLN:H	1.77	0.50
51:Lq:76:ARG:NH1	51:Lq:142:ASP:O	2.45	0.50
1:C1:1171:C:H42	1:C1:1297:U:H1'	1.77	0.50
1:C1:1417:A:H5''	1:C1:1418:U:H5''	1.92	0.50
6:CC:214:PRO:HD2	6:CC:217:TRP:HB2	1.94	0.50
7:CE:216:VAL:O	7:CE:229:LYS:NZ	2.45	0.50
18:CP:307:VAL:HG22	27:Cb:716:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LB:170:THR:HG22	28:LB:172:LEU:HG	1.94	0.50
1:C1:2821:G:N2	10:CH:64:ILE:O	2.42	0.50
5:CB:143:GLN:NE2	5:CB:166:ALA:O	2.45	0.50
9:CG:109:LEU:HD11	18:CP:355:PRO:HB3	1.94	0.50
12:CJ:187:LYS:HD3	12:CJ:488:PRO:HB2	1.94	0.50
29:LC:9:VAL:HA	29:LC:152:VAL:HG23	1.93	0.50
1:C1:1277:G:OP1	40:LS:84:ARG:NE	2.45	0.49
1:C1:2832:G:N3	1:C1:2833:U:O2'	2.45	0.49
17:CO:36:LYS:HB3	28:LB:208:THR:HG22	1.92	0.49
27:Cb:165:VAL:HB	27:Cb:215:ILE:HG22	1.93	0.49
30:LE:140:GLU:O	30:LE:144:LYS:NZ	2.39	0.49
48:Lh:93:LEU:HD22	48:Lh:96:ARG:HH21	1.76	0.49
52:Cc:11:ILE:HA	52:Cc:14:LEU:HD12	1.94	0.49
53:Cd:45:ARG:HA	53:Cd:48:LYS:HZ2	1.77	0.49
1:C1:3307:C:OP1	19:CQ:111:ARG:NH2	2.41	0.49
5:CB:186:ALA:HA	5:CB:215:ARG:HB2	1.94	0.49
9:CG:60:ALA:HB3	9:CG:63:LYS:HB3	1.93	0.49
9:CG:155:ARG:O	9:CG:155:ARG:NH1	2.45	0.49
28:LB:149:LEU:HD12	28:LB:193:VAL:HG13	1.94	0.49
36:LN:146:PRO:HG2	48:Lh:106:LEU:HD13	1.93	0.49
3:C3:26:U:H5''	5:CB:169:LYS:HG3	1.94	0.49
13:CK:157:VAL:HG21	13:CK:178:ARG:HH21	1.77	0.49
51:Lq:121:PRO:HA	51:Lq:125:GLY:HA3	1.94	0.49
1:C1:2091:U:N3	1:C1:2287:G:N1	2.61	0.49
10:CH:96:GLN:HE21	10:CH:141:ARG:HH12	1.58	0.49
10:CH:187:THR:HG21	10:CH:206:GLY:HA3	1.95	0.49
29:LC:151:LEU:HD23	29:LC:256:VAL:HG12	1.93	0.49
32:LH:89:LYS:O	32:LH:184:SER:OG	2.29	0.49
1:C1:260:A:OP1	36:LN:50:ARG:NH1	2.46	0.49
1:C1:331:C:OP1	1:C1:1362:G:O2'	2.30	0.49
1:C1:2815:C:O2'	13:CK:183:ASN:OD1	2.25	0.49
1:C1:2898:A:OP2	1:C1:2900:C:O2'	2.26	0.49
6:CC:366:GLU:OE1	6:CC:366:GLU:N	2.37	0.49
10:CH:19:ILE:HG21	10:CH:59:LYS:HE2	1.94	0.49
13:CK:129:GLU:OE2	13:CK:164:ARG:NH1	2.45	0.49
22:CT:218:LEU:O	22:CT:222:ALA:N	2.43	0.49
23:CU:340:LYS:NZ	23:CU:369:ASP:OD1	2.44	0.49
53:Cd:373:VAL:HA	53:Cd:379:GLU:HA	1.94	0.49
4:CA:35:ARG:H	4:CA:87:ASN:HD21	1.59	0.49
23:CU:239:ARG:NH1	23:CU:240:GLU:OE2	2.45	0.49
29:LC:154:ASP:N	29:LC:154:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LH:9:THR:HG23	32:LH:52:VAL:HG13	1.95	0.49
34:LL:126:PHE:O	48:Lh:119:ARG:NH1	2.46	0.49
53:Cd:298:ILE:O	53:Cd:301:HIS:ND1	2.46	0.49
1:C1:258:C:O2	49:Li:39:LYS:NZ	2.38	0.49
1:C1:703:A:OP1	1:C1:733:C:O2'	2.31	0.49
1:C1:944:G:H2'	1:C1:945:G:C8	2.47	0.49
1:C1:2814:G:H21	13:CK:192:THR:HG21	1.77	0.49
1:C1:2918:C:H2'	1:C1:2919:G:H8	1.76	0.49
6:CC:283:PRO:HB2	20:CR:218:TYR:HE2	1.77	0.49
10:CH:31:GLN:OE1	10:CH:33:ARG:NH1	2.46	0.49
10:CH:439:GLU:OE2	16:CN:79:GLN:NE2	2.45	0.49
18:CP:520:ASN:HB3	18:CP:577:PHE:CD1	2.47	0.49
27:Cb:323:HIS:HD2	27:Cb:509:LEU:HD22	1.77	0.49
53:Cd:338:LEU:HD22	54:Ce:185:ASN:HD21	1.78	0.49
1:C1:781:G:H22	29:LC:102:ALA:HA	1.78	0.49
1:C1:1218:G:N1	1:C1:1227:A:N6	2.61	0.49
1:C1:3118:A:OP1	53:Cd:301:HIS:NE2	2.40	0.49
3:C3:49:G:OP1	5:CB:176:THR:N	2.45	0.49
8:CF:225:GLY:HA2	8:CF:237:LEU:HG	1.94	0.49
12:CJ:136:ASP:HA	12:CJ:139:ARG:HD2	1.95	0.49
12:CJ:407:THR:OG1	12:CJ:409:ASP:OD1	2.27	0.49
13:CK:126:GLY:HA3	13:CK:161:PHE:HB2	1.94	0.49
18:CP:383:ARG:HH12	18:CP:447:ILE:HG21	1.77	0.49
18:CP:516:CYS:O	18:CP:520:ASN:ND2	2.45	0.49
28:LB:63:PRO:HA	28:LB:68:HIS:HD1	1.77	0.49
31:LG:146:ILE:HB	31:LG:178:ILE:HD13	1.94	0.49
1:C1:19:U:H2'	1:C1:20:A:C8	2.47	0.49
1:C1:910:A:O2'	50:Lj:49:TRP:O	2.28	0.49
1:C1:2395:U:OP2	1:C1:2396:U:O2'	2.28	0.49
3:C3:25:U:H2'	5:CB:169:LYS:HG2	1.93	0.49
23:CU:319:LYS:O	23:CU:323:ARG:HG3	2.12	0.49
27:Cb:835:ASN:OD1	27:Cb:838:ARG:NH2	2.46	0.49
28:LB:335:ARG:HB3	28:LB:337:MET:HE2	1.94	0.49
35:LM:88:TYR:HD2	35:LM:90:VAL:HG12	1.77	0.49
37:LO:36:VAL:HB	37:LO:106:VAL:HG12	1.93	0.49
53:Cd:189:ASN:HD21	53:Cd:283:PRO:HD3	1.78	0.49
53:Cd:321:GLY:HA3	53:Cd:436:LEU:HD23	1.95	0.49
1:C1:1218:G:C2	1:C1:1227:A:N6	2.80	0.49
1:C1:1280:C:O2	13:CK:40:GLN:NE2	2.45	0.49
5:CB:52:ASP:O	5:CB:56:THR:OG1	2.23	0.49
6:CC:256:PRO:O	31:LG:236:TRP:NE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CM:94:ARG:HG3	15:CM:114:LEU:HB3	1.95	0.49
20:CR:133:GLN:HE22	34:LL:113:VAL:HG11	1.76	0.49
27:Cb:134:ALA:HA	27:Cb:295:LEU:HD12	1.95	0.49
29:LC:326:MET:HE1	15:LF:155:TYR:CZ	2.48	0.49
46:Le:13:LYS:NZ	46:Le:59:GLY:O	2.45	0.49
48:Lh:24:LEU:O	48:Lh:28:LYS:NZ	2.46	0.49
4:CA:111:PRO:HG2	23:CU:203:ILE:HD11	1.93	0.48
6:CC:152:ASP:O	7:CE:573:TYR:OH	2.31	0.48
6:CC:287:GLU:OE1	31:LG:111:ARG:NH2	2.46	0.48
7:CE:441:TYR:O	7:CE:445:VAL:HG22	2.13	0.48
27:Cb:228:MET:HA	27:Cb:813:PHE:CD1	2.47	0.48
27:Cb:228:MET:HA	27:Cb:813:PHE:HD1	1.77	0.48
30:LE:108:LYS:HB2	30:LE:108:LYS:HZ3	1.77	0.48
1:C1:2091:U:N3	1:C1:2287:G:C6	2.81	0.48
1:C1:2852:C:H1'	1:C1:3063:A:H2	1.77	0.48
2:C2:71:A:OP1	44:LY:27:ARG:NH1	2.46	0.48
27:Cb:396:VAL:HA	27:Cb:400:LEU:HD22	1.93	0.48
28:LB:29:VAL:HA	28:LB:219:ILE:HD13	1.95	0.48
31:LG:103:GLU:OE2	31:LG:111:ARG:NH1	2.45	0.48
1:C1:3136:A:H2'	1:C1:3137:A:H8	1.78	0.48
14:CL:38:LEU:HD23	14:CL:41:LYS:HD2	1.94	0.48
42:LV:91:ASP:OD1	42:LV:91:ASP:N	2.41	0.48
1:C1:35:A:H2'	1:C1:36:C:H6	1.79	0.48
1:C1:553:U:H2'	1:C1:554:G:H8	1.78	0.48
1:C1:916:U:H2'	1:C1:917:A:C8	2.48	0.48
7:CE:438:PRO:HA	7:CE:441:TYR:HB3	1.94	0.48
12:CJ:374:LEU:HD22	12:CJ:383:LEU:HD13	1.96	0.48
22:CT:259:ARG:O	22:CT:263:LEU:N	2.45	0.48
27:Cb:174:LEU:HA	27:Cb:177:LEU:HB3	1.95	0.48
15:LF:184:ILE:HG23	15:LF:189:ASP:HB3	1.95	0.48
35:LM:130:GLU:HB3	37:LO:187:ALA:HB1	1.95	0.48
39:LQ:150:THR:OG1	39:LQ:152:ASP:OD1	2.28	0.48
44:LY:34:LEU:HD11	44:LY:47:ILE:HG12	1.95	0.48
45:Ld:33:PHE:HD1	45:Ld:73:LYS:HB2	1.79	0.48
1:C1:63:A:N3	1:C1:78:U:O2'	2.42	0.48
1:C1:324:C:H4'	50:Lj:71:PRO:HB3	1.96	0.48
3:C3:71:U:C2	3:C3:131:G:C2	3.01	0.48
4:CA:194:TYR:HB3	4:CA:231:LEU:HB3	1.95	0.48
7:CE:296:SER:OG	7:CE:297:ALA:N	2.47	0.48
16:CN:74:THR:HB	16:CN:98:GLU:HA	1.95	0.48
23:CU:278:THR:HG23	23:CU:281:THR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Ld:36:ARG:NH1	45:Ld:73:LYS:O	2.42	0.48
6:CC:367:ARG:NH1	6:CC:384:PRO:O	2.41	0.48
18:CP:402:MET:HE2	18:CP:402:MET:HB3	1.68	0.48
27:Cb:243:ALA:HA	27:Cb:246:LEU:HD12	1.94	0.48
34:LL:60:CYS:HB2	34:LL:65:TYR:O	2.13	0.48
51:Lq:75:ASP:OD1	51:Lq:75:ASP:N	2.46	0.48
1:C1:247:A:H2'	1:C1:248:G:H8	1.79	0.48
1:C1:3253:U:O5'	28:LB:174:GLN:NE2	2.47	0.48
5:CB:24:LEU:HD12	5:CB:28:LYS:HZ3	1.78	0.48
15:CM:130:ALA:O	15:CM:134:LYS:N	2.46	0.48
15:LF:15:PRO:HB3	52:Cc:110:GLU:HG2	1.95	0.48
44:LY:43:ASN:ND2	44:LY:126:GLU:OE2	2.43	0.48
1:C1:662:C:O2'	1:C1:666:U:OP1	2.29	0.48
1:C1:672:G:N7	34:LL:32:LYS:NZ	2.61	0.48
1:C1:672:G:OP2	34:LL:35:ARG:NH2	2.39	0.48
1:C1:1038:U:H2'	1:C1:1039:A:C8	2.49	0.48
1:C1:1264:G:H4'	8:CF:99:THR:HG22	1.95	0.48
1:C1:2319:A:H2'	1:C1:2320:A:H8	1.79	0.48
1:C1:2328:C:H2'	1:C1:2329:A:H8	1.79	0.48
4:CA:32:ASN:HB3	4:CA:166:PRO:HB3	1.96	0.48
11:CI:193:ARG:HB2	11:CI:258:LEU:HA	1.96	0.48
16:CN:85:ARG:NH2	16:CN:89:PRO:O	2.46	0.48
27:Cb:332:PRO:HD3	27:Cb:367:HIS:CE1	2.48	0.48
51:Lq:85:MET:HE2	51:Lq:90:LEU:HG	1.94	0.48
53:Cd:316:PHE:HA	53:Cd:436:LEU:HD21	1.95	0.48
1:C1:745:U:O2	1:C1:749:C:N3	2.46	0.48
3:C3:68:G:H2'	3:C3:69:G:H8	1.78	0.48
5:CB:69:LYS:NZ	5:CB:276:GLN:O	2.45	0.48
9:CG:145:GLY:HA2	9:CG:167:GLN:HB2	1.95	0.48
13:CK:186:HIS:CD2	13:CK:228:LEU:HD11	2.49	0.48
18:CP:320:LEU:HD13	18:CP:361:HIS:HB3	1.96	0.48
28:LB:115:LYS:NZ	28:LB:129:ALA:O	2.47	0.48
1:C1:2404:G:H2'	1:C1:2405:A:H8	1.79	0.48
1:C1:2729:U:O4	1:C1:2745:G:O6	2.31	0.48
8:CF:223:LEU:HB3	8:CF:237:LEU:HD12	1.95	0.48
9:CG:133:VAL:HG22	9:CG:144:PHE:HB3	1.96	0.48
12:CJ:379:PRO:HB2	12:CJ:382:PRO:HD2	1.95	0.48
51:Lq:17:LEU:HA	51:Lq:18:ASP:HA	1.59	0.48
11:CI:298:SER:HB2	11:CI:301:GLN:HG3	1.96	0.47
12:CJ:177:HIS:HA	12:CJ:180:ILE:HG12	1.95	0.47
53:Cd:285:LEU:HG	53:Cd:404:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:72:SER:OG	4:CA:73:ARG:N	2.47	0.47
4:CA:254:ILE:HG22	23:CU:190:ILE:HD11	1.96	0.47
5:CB:207:ASP:HB3	5:CB:210:GLU:HB3	1.95	0.47
20:CR:198:LEU:HD22	20:CR:209:MET:HB3	1.96	0.47
33:LK:16:ARG:HA	33:LK:59:THR:HA	1.95	0.47
54:Ce:44:PRO:O	54:Ce:66:LYS:NZ	2.32	0.47
1:C1:421:U:O2'	47:Lf:90:PRO:O	2.31	0.47
1:C1:2416:G:O6	1:C1:2446:A:N1	2.47	0.47
4:CA:46:TYR:OH	4:CA:47:ARG:NH2	2.46	0.47
30:LE:49:ARG:NH1	47:Lf:109:ILE:O	2.47	0.47
35:LM:5:ASN:OD1	35:LM:5:ASN:N	2.46	0.47
44:LY:69:VAL:HG22	44:LY:81:VAL:HG12	1.96	0.47
45:Ld:54:THR:HB	45:Ld:85:ARG:HH12	1.79	0.47
47:Lf:74:THR:HG21	47:Lf:86:LYS:HD3	1.97	0.47
53:Cd:242:ARG:NH2	54:Ce:132:ARG:O	2.47	0.47
1:C1:369:C:O2'	1:C1:383:G:N2	2.46	0.47
1:C1:934:G:H3'	1:C1:1098:G:N2	2.28	0.47
1:C1:1885:G:H5''	1:C1:1886:C:H5	1.78	0.47
1:C1:2385:U:H3	1:C1:2565:G:H1	1.61	0.47
5:CB:108:TYR:HE2	5:CB:184:LEU:HD13	1.79	0.47
12:CJ:39:TRP:HD1	12:CJ:233:PHE:HB2	1.79	0.47
20:CR:127:GLU:HB2	20:CR:134:GLN:HE22	1.80	0.47
1:C1:638:G:O2'	1:C1:1417:A:OP1	2.33	0.47
1:C1:1308:A:O2'	47:Lf:79:ASN:OD1	2.31	0.47
1:C1:2980:U:H2'	1:C1:2981:A:H8	1.79	0.47
1:C1:3315:A:O2'	1:C1:3318:C:OP2	2.27	0.47
4:CA:139:ILE:HG13	4:CA:176:ILE:HD11	1.96	0.47
10:CH:448:ASP:OD1	10:CH:448:ASP:N	2.48	0.47
15:CM:111:LEU:HD23	15:CM:112:LEU:HD23	1.96	0.47
21:CS:68:PRO:C	21:CS:70:ASP:H	2.22	0.47
1:C1:727:C:H2'	1:C1:728:A:H8	1.80	0.47
1:C1:1272:U:H2'	1:C1:1273:A:C8	2.49	0.47
1:C1:2788:G:H2'	1:C1:2789:G:C8	2.50	0.47
5:CB:49:LEU:HG	7:CE:483:TYR:HB3	1.95	0.47
11:CI:221:ASN:OD1	11:CI:222:LYS:N	2.48	0.47
19:CQ:68:THR:HG21	19:CQ:100:ARG:HB2	1.96	0.47
28:LB:172:LEU:HD22	28:LB:334:LYS:HG2	1.96	0.47
1:C1:155:G:H2'	1:C1:156:G:C8	2.50	0.47
1:C1:574:G:H2'	1:C1:575:A:H8	1.79	0.47
1:C1:2738:A:H5'	51:Lq:161:LYS:HE2	1.96	0.47
1:C1:2921:C:N4	1:C1:2927:A:N6	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CG:67:LEU:HB2	18:CP:434:ILE:HG23	1.96	0.47
10:CH:10:VAL:HG21	10:CH:63:ILE:HD12	1.96	0.47
12:CJ:266:ALA:HB1	12:CJ:269:ALA:HB3	1.95	0.47
18:CP:334:VAL:HG21	27:Cb:716:MET:HE3	1.97	0.47
27:Cb:107:ARG:HH11	27:Cb:185:LYS:HE2	1.80	0.47
27:Cb:456:ARG:O	27:Cb:459:ARG:NH2	2.48	0.47
33:LK:104:VAL:HB	33:LK:143:VAL:HG22	1.96	0.47
51:Lq:195:LYS:HE2	51:Lq:196:LYS:HE2	1.95	0.47
14:CL:37:LYS:HG2	14:CL:41:LYS:HE3	1.97	0.47
22:CT:501:ALA:O	22:CT:505:LEU:N	2.46	0.47
23:CU:257:LEU:O	23:CU:260:LYS:NZ	2.48	0.47
27:Cb:604:PHE:HB2	27:Cb:621:VAL:HG21	1.95	0.47
1:C1:231:A:H2'	1:C1:232:G:C8	2.49	0.47
1:C1:1196:U:H2'	1:C1:1197:A:C8	2.50	0.47
6:CC:263:THR:HG23	31:LG:175:LYS:HB2	1.97	0.47
18:CP:321:ALA:O	18:CP:325:ILE:HG13	2.15	0.47
27:Cb:129:ASP:HB3	27:Cb:287:LEU:HD23	1.97	0.47
27:Cb:135:ARG:HH12	27:Cb:459:ARG:CZ	2.27	0.47
34:LL:78:GLU:OE1	49:Li:29:ARG:NH1	2.48	0.47
36:LN:114:ARG:HD3	36:LN:137:PRO:HG3	1.96	0.47
1:C1:2300:C:H2'	1:C1:2301:C:C6	2.50	0.47
4:CA:82:GLU:O	49:Li:76:LYS:NZ	2.48	0.47
5:CB:288:THR:OG1	5:CB:289:ALA:N	2.45	0.47
6:CC:366:GLU:HA	6:CC:369:GLU:HB2	1.97	0.47
8:CF:87:ASP:O	8:CF:227:TRP:NE1	2.48	0.47
40:LS:13:HIS:HD2	40:LS:51:VAL:HG12	1.79	0.47
42:LV:76:HIS:CE1	42:LV:112:LYS:NZ	2.83	0.47
1:C1:562:U:H2'	1:C1:563:A:H8	1.80	0.46
1:C1:3195:C:H2'	1:C1:3196:G:H8	1.80	0.46
12:CJ:17:MET:O	12:CJ:64:TYR:N	2.47	0.46
20:CR:206:VAL:HG21	20:CR:226:LYS:HE2	1.97	0.46
28:LB:21:ARG:HG3	28:LB:270:GLN:HG2	1.96	0.46
2:C2:63:G:H22	2:C2:97:A:H2	1.63	0.46
7:CE:348:LEU:HD23	7:CE:352:LEU:HD13	1.96	0.46
44:LY:31:SER:HA	44:LY:48:PRO:HA	1.97	0.46
45:Ld:60:ASP:OD2	45:Ld:100:TYR:OH	2.27	0.46
1:C1:2874:U:H2'	1:C1:2875:G:O4'	2.15	0.46
2:C2:154:C:H2'	2:C2:155:A:C8	2.51	0.46
10:CH:308:LEU:O	10:CH:311:SER:OG	2.30	0.46
18:CP:376:LEU:HD11	18:CP:452:ARG:HB3	1.97	0.46
18:CP:455:LEU:HD21	18:CP:457:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Cb:237:TYR:HD2	27:Cb:267:GLN:HB3	1.80	0.46
44:LY:44:VAL:HG21	44:LY:118:LEU:HG	1.97	0.46
48:Lh:22:LYS:O	48:Lh:26:GLU:HG3	2.16	0.46
52:Cc:120:LEU:HD11	52:Cc:162:LEU:HD21	1.96	0.46
52:Cc:151:ASP:OD1	52:Cc:154:LYS:N	2.45	0.46
53:Cd:358:HIS:CE1	53:Cd:392:GLU:HG3	2.50	0.46
1:C1:361:A:OP2	53:Cd:21:LYS:NZ	2.33	0.46
1:C1:631:G:H5''	1:C1:1098:G:C8	2.50	0.46
1:C1:3072:C:OP2	32:LH:62:ARG:NH2	2.49	0.46
1:C1:3243:G:O2'	1:C1:3245:A:N6	2.49	0.46
3:C3:126:G:H2'	3:C3:127:G:H8	1.80	0.46
10:CH:436:LYS:HA	10:CH:436:LYS:HD3	1.67	0.46
13:CK:184:VAL:HG21	13:CK:195:LEU:HD12	1.97	0.46
1:C1:975:G:N2	1:C1:976:U:O4	2.49	0.46
1:C1:2385:U:H2'	1:C1:2386:A:H8	1.81	0.46
24:CX:102:ASN:HA	24:CX:105:LEU:HG	1.98	0.46
29:LC:211:ILE:HB	29:LC:234:THR:HG23	1.96	0.46
1:C1:191:A:N3	1:C1:211:G:O2'	2.46	0.46
1:C1:1163:U:O4	37:LO:22:SER:OG	2.31	0.46
1:C1:2921:C:N3	1:C1:2927:A:N1	2.63	0.46
1:C1:2972:C:OP2	17:CO:2:ALA:N	2.49	0.46
9:CG:27:ILE:HD12	24:CX:105:LEU:HD21	1.96	0.46
20:CR:198:LEU:HB3	20:CR:209:MET:HE3	1.97	0.46
30:LE:71:VAL:HG11	30:LE:169:LEU:HD21	1.97	0.46
53:Cd:357:ARG:HB3	53:Cd:394:GLY:HA3	1.97	0.46
2:C2:154:C:H5''	31:LG:184:LYS:HB3	1.98	0.46
28:LB:116:ARG:HB3	28:LB:176:LYS:HG3	1.98	0.46
29:LC:287:LEU:HD21	39:LQ:59:LYS:HB3	1.98	0.46
15:LF:32:ARG:HD2	15:LF:32:ARG:HA	1.70	0.46
38:LP:59:PRO:HG3	38:LP:76:TRP:CG	2.50	0.46
1:C1:189:G:N1	1:C1:192:A:OP2	2.46	0.46
1:C1:1049:C:H2'	1:C1:1050:C:C6	2.51	0.46
1:C1:1176:G:H2'	1:C1:1177:A:C8	2.51	0.46
1:C1:2918:C:H2'	1:C1:2919:G:C8	2.51	0.46
1:C1:3073:G:C4	26:Cz:38:ALA:HB2	2.49	0.46
1:C1:3117:C:H3'	53:Cd:303:ARG:NH1	2.30	0.46
10:CH:250:LEU:HD23	10:CH:283:PHE:HB2	1.98	0.46
15:CM:68:LYS:HB3	15:CM:68:LYS:HZ2	1.81	0.46
17:CO:92:GLY:O	28:LB:151:ARG:NH2	2.39	0.46
18:CP:465:ILE:HG21	18:CP:472:LYS:HD3	1.98	0.46
15:LF:146:ASN:OD1	15:LF:242:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Li:41:ALA:HB3	49:Li:50:ARG:HH22	1.80	0.46
1:C1:267:U:H2'	1:C1:268:A:C8	2.51	0.46
3:C3:61:A:C8	11:CI:275:GLY:HA3	2.51	0.46
5:CB:63:TRP:HE3	5:CB:244:LYS:HG2	1.81	0.46
6:CC:350:TYR:HE1	12:CJ:486:LEU:HB3	1.81	0.46
8:CF:41:PHE:CE2	8:CF:226:TYR:HB3	2.51	0.46
12:CJ:141:LEU:HA	12:CJ:144:CYS:HB3	1.97	0.46
17:CO:25:VAL:HG21	28:LB:352:LEU:HD23	1.97	0.46
21:CS:696:PHE:CE1	31:LG:68:LEU:HD21	2.51	0.46
27:Cb:148:MET:HE1	27:Cb:237:TYR:HB3	1.98	0.46
29:LC:361:LEU:HD11	41:LT:148:PRO:HG2	1.98	0.46
1:C1:1225:G:N2	1:C1:1252:A:O2'	2.46	0.46
1:C1:2432:C:C2	1:C1:2451:C:H4'	2.50	0.46
3:C3:58:A:H2	11:CI:263:VAL:HG22	1.81	0.46
8:CF:36:LYS:HB2	8:CF:36:LYS:HE3	1.60	0.46
12:CJ:15:ASN:O	12:CJ:66:THR:OG1	2.31	0.46
1:C1:643:A:H2'	1:C1:644:A:C8	2.50	0.45
1:C1:2299:C:H2'	1:C1:2300:C:C6	2.51	0.45
3:C3:71:U:N3	3:C3:131:G:N1	2.64	0.45
48:Lh:30:GLU:HG2	48:Lh:52:LEU:HD11	1.97	0.45
1:C1:526:G:N2	1:C1:544:U:O2	2.48	0.45
1:C1:975:G:H4'	1:C1:976:U:H5'	1.98	0.45
1:C1:2452:C:H4'	51:Lq:210:MET:HE1	1.98	0.45
1:C1:3189:G:H2'	1:C1:3190:G:H8	1.81	0.45
16:CN:174:SER:HB2	16:CN:181:LEU:HB2	1.98	0.45
27:Cb:321:LEU:HD21	27:Cb:371:ILE:HD13	1.97	0.45
28:LB:33:PRO:HD2	28:LB:44:THR:HG21	1.98	0.45
36:LN:106:VAL:HG11	36:LN:134:LEU:HD21	1.97	0.45
40:LS:95:ARG:HB2	40:LS:140:ILE:HD12	1.98	0.45
53:Cd:285:LEU:HD21	53:Cd:323:LEU:HD23	1.97	0.45
1:C1:31:C:H4'	36:LN:96:ARG:HG2	1.98	0.45
10:CH:436:LYS:HG3	28:LB:298:GLU:HG2	1.98	0.45
19:CQ:98:GLU:O	19:CQ:102:ARG:HG2	2.16	0.45
19:CQ:103:ARG:HA	19:CQ:106:VAL:HG12	1.98	0.45
27:Cb:181:LYS:HE2	27:Cb:181:LYS:H	1.81	0.45
32:LH:16:LEU:HD21	32:LH:83:THR:HG23	1.98	0.45
39:LQ:108:VAL:HG22	39:LQ:165:LEU:HD23	1.96	0.45
45:Ld:52:MET:O	45:Ld:85:ARG:NH2	2.50	0.45
47:Lf:15:HIS:O	47:Lf:97:GLY:N	2.41	0.45
1:C1:3188:U:H2'	1:C1:3189:G:C8	2.52	0.45
3:C3:51:C:H5''	7:CE:488:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:112:THR:OG1	4:CA:249:SER:O	2.32	0.45
16:CN:104:LEU:HA	16:CN:107:VAL:HG22	1.99	0.45
27:Cb:170:ARG:HH12	27:Cb:174:LEU:HD11	1.81	0.45
28:LB:106:TRP:HB2	28:LB:133:TYR:CE2	2.52	0.45
32:LH:18:VAL:HG11	32:LH:53:ILE:HD11	1.97	0.45
1:C1:6:A:O3'	12:CJ:97:ARG:NH2	2.44	0.45
1:C1:373:U:OP2	53:Cd:60:ARG:NH2	2.49	0.45
1:C1:631:G:H5'	1:C1:1099:G:H1'	1.97	0.45
1:C1:1295:G:O2'	1:C1:1300:A:N1	2.49	0.45
2:C2:14:C:H5''	38:LP:123:PRO:HD3	1.99	0.45
4:CA:90:LEU:HD11	4:CA:102:MET:HE2	1.99	0.45
18:CP:317:ARG:NH2	18:CP:338:SER:O	2.50	0.45
20:CR:148:GLN:OE1	34:LL:86:PRO:HB3	2.16	0.45
27:Cb:207:MET:HA	27:Cb:207:MET:HE3	1.98	0.45
28:LB:19:ARG:HA	28:LB:19:ARG:HD3	1.74	0.45
1:C1:1270:U:O5'	26:Cz:40:ARG:NH2	2.49	0.45
14:CL:187:GLY:HA2	14:CL:188:ALA:HA	1.68	0.45
27:Cb:140:LYS:HB3	27:Cb:271:PHE:HD2	1.81	0.45
40:LS:48:LEU:HD23	41:LT:155:ALA:HB2	1.99	0.45
1:C1:137:C:H2'	1:C1:138:G:O4'	2.17	0.45
1:C1:190:G:N7	54:Ce:144:LYS:NZ	2.65	0.45
1:C1:424:G:H2'	1:C1:425:A:H8	1.81	0.45
1:C1:966:U:H2'	1:C1:967:U:H6	1.81	0.45
1:C1:1121:G:H2'	1:C1:1122:G:H8	1.82	0.45
1:C1:2306:U:H2'	1:C1:2307:A:C8	2.51	0.45
1:C1:2841:U:H2'	1:C1:2842:C:H6	1.81	0.45
7:CE:488:ASN:N	7:CE:488:ASN:OD1	2.49	0.45
8:CF:51:ASN:OD1	8:CF:51:ASN:N	2.50	0.45
28:LB:218:VAL:HG11	28:LB:329:VAL:HG13	1.98	0.45
29:LC:301:ARG:HD3	39:LQ:69:GLU:HG3	1.99	0.45
45:Ld:43:GLU:HA	45:Ld:46:LYS:HB3	1.99	0.45
52:Cc:201:TRP:HE1	52:Cc:248:SER:HB3	1.81	0.45
1:C1:367:A:H1'	44:LY:86:ARG:HE	1.82	0.45
1:C1:614:C:H2'	1:C1:615:A:C8	2.51	0.45
1:C1:642:C:H2'	1:C1:643:A:C8	2.52	0.45
1:C1:708:G:H2'	1:C1:709:G:H8	1.82	0.45
1:C1:979:A:H2'	1:C1:980:G:C8	2.52	0.45
1:C1:2917:C:H2'	1:C1:2918:C:C6	2.52	0.45
18:CP:308:ILE:HD13	18:CP:308:ILE:HA	1.85	0.45
18:CP:385:LEU:HD22	18:CP:453:VAL:HB	1.99	0.45
29:LC:35:ILE:HG22	29:LC:122:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:574:G:H2'	1:C1:575:A:C8	2.52	0.45
4:CA:139:ILE:HB	4:CA:179:VAL:HG22	1.99	0.45
23:CU:287:GLN:O	23:CU:291:GLU:HG3	2.17	0.45
29:LC:24:PRO:HB2	29:LC:26:VAL:HG12	1.99	0.45
53:CD:202:LEU:HB2	53:CD:253:TYR:CD2	2.50	0.45
1:C1:603:G:H2'	1:C1:604:G:H8	1.82	0.45
1:C1:643:A:H2'	1:C1:644:A:H8	1.81	0.45
1:C1:933:A:N3	1:C1:1096:U:O2'	2.44	0.45
1:C1:3105:C:H2'	1:C1:3106:G:H8	1.82	0.45
3:C3:128:C:H2'	3:C3:129:G:H8	1.82	0.45
7:CE:361:ILE:HD13	7:CE:411:LEU:HB3	1.99	0.45
7:CE:445:VAL:HA	7:CE:448:THR:HG22	1.99	0.45
8:CF:73:MET:HE1	8:CF:101:GLY:HA2	1.98	0.45
10:CH:465:GLU:OE1	19:CQ:103:ARG:NH2	2.50	0.45
16:CN:15:VAL:HG13	16:CN:61:ARG:HG3	1.99	0.45
18:CP:321:ALA:HB2	18:CP:342:LEU:HD21	1.98	0.45
20:CR:41:LYS:HE2	20:CR:41:LYS:HB2	1.87	0.45
33:LK:126:LYS:NZ	33:LK:155:ILE:O	2.49	0.45
52:Cc:117:ARG:HH21	52:Cc:200:ILE:HG22	1.82	0.45
52:Cc:203:ASP:HB3	52:Cc:253:ARG:HH12	1.83	0.45
3:C3:69:G:O6	3:C3:132:U:O4	2.35	0.44
7:CE:360:ILE:HG22	7:CE:410:THR:HG23	1.98	0.44
20:CR:47:GLN:H	20:CR:47:GLN:HG2	1.66	0.44
40:LS:16:THR:HG22	40:LS:18:ALA:H	1.81	0.44
48:Lh:38:LYS:HD3	48:Lh:49:ILE:HG13	2.00	0.44
1:C1:553:U:H2'	1:C1:554:G:C8	2.52	0.44
1:C1:694:U:OP1	1:C1:761:A:O2'	2.34	0.44
3:C3:71:U:H3	3:C3:130:G:H1	1.64	0.44
11:CI:189:MET:HB2	11:CI:262:ILE:HD13	1.99	0.44
12:CJ:136:ASP:OD1	12:CJ:139:ARG:NH1	2.43	0.44
16:CN:187:ASN:H	16:CN:210:THR:HG22	1.81	0.44
16:CN:197:MET:HE3	16:CN:206:THR:HG22	1.99	0.44
27:Cb:163:ALA:HB3	27:Cb:213:ILE:HA	1.99	0.44
29:LC:197:LYS:HB2	29:LC:202:ARG:HH11	1.82	0.44
36:LN:96:ARG:HD2	36:LN:96:ARG:HA	1.83	0.44
55:Cf:503:LYS:HD2	55:Cf:503:LYS:HA	1.69	0.44
1:C1:3077:C:OP2	13:CK:26:LYS:NZ	2.38	0.44
5:CB:48:ASN:ND2	5:CB:51:ALA:O	2.50	0.44
8:CF:24:GLU:H	8:CF:24:GLU:HG2	1.60	0.44
8:CF:99:THR:OG1	8:CF:99:THR:O	2.35	0.44
10:CH:327:VAL:HA	10:CH:330:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LC:114:ILE:HB	29:LC:119:LYS:HD2	1.98	0.44
31:LG:193:VAL:HG12	31:LG:195:LYS:HG2	1.99	0.44
36:LN:31:ARG:O	36:LN:65:ARG:NH2	2.50	0.44
1:C1:20:A:H2'	1:C1:21:G:C8	2.52	0.44
1:C1:253:U:N3	7:CE:368:ASN:OD1	2.50	0.44
1:C1:788:A:H61	1:C1:915:G:H22	1.64	0.44
1:C1:3118:A:OP2	53:Cd:303:ARG:NH2	2.47	0.44
6:CC:403:ARG:HG3	12:CJ:150:LEU:HD22	1.98	0.44
16:CN:199:VAL:HG23	16:CN:204:ALA:HB2	1.98	0.44
49:Li:25:LYS:HE2	49:Li:25:LYS:HB2	1.66	0.44
1:C1:497:U:H2'	1:C1:498:C:C6	2.53	0.44
1:C1:978:A:H2'	1:C1:979:A:C8	2.53	0.44
1:C1:1420:U:OP1	29:LC:77:ARG:NH2	2.47	0.44
1:C1:3022:G:O6	1:C1:3034:A:N6	2.50	0.44
4:CA:35:ARG:H	4:CA:87:ASN:ND2	2.16	0.44
13:CK:236:LYS:NZ	18:CP:474:ASN:HB3	2.32	0.44
27:Cb:187:THR:OG1	27:Cb:188:ASP:N	2.50	0.44
32:LH:13:PRO:HD2	32:LH:16:LEU:HD12	1.99	0.44
34:LL:62:THR:HG23	34:LL:64:LYS:H	1.82	0.44
45:Ld:80:ARG:HG2	45:Ld:106:VAL:HG11	2.00	0.44
1:C1:1260:A:O2'	8:CF:15:VAL:O	2.35	0.44
1:C1:2735:G:N2	1:C1:2741:U:O2	2.31	0.44
5:CB:259:ILE:O	5:CB:263:ILE:HG13	2.18	0.44
7:CE:178:PHE:O	7:CE:212:GLN:NE2	2.46	0.44
7:CE:243:ARG:HH22	7:CE:557:LEU:HD22	1.83	0.44
7:CE:486:PRO:HB2	7:CE:489:LYS:HG2	1.99	0.44
12:CJ:187:LYS:HB2	12:CJ:198:GLN:HB3	1.99	0.44
12:CJ:235:MET:HE3	12:CJ:235:MET:HB3	1.83	0.44
13:CK:241:ARG:HD2	13:CK:241:ARG:HA	1.81	0.44
31:LG:166:VAL:HG12	31:LG:169:LEU:HD12	1.99	0.44
51:Lq:26:ARG:HH22	51:Lq:208:ALA:HB1	1.83	0.44
1:C1:14:U:H3	2:C2:136:G:H21	1.65	0.44
1:C1:944:G:H2'	1:C1:945:G:H8	1.81	0.44
1:C1:2078:G:H2'	1:C1:2079:A:H8	1.82	0.44
3:C3:17:G:H2'	3:C3:18:G:H8	1.81	0.44
3:C3:140:G:H3'	11:CI:291:ARG:HH12	1.83	0.44
4:CA:228:ASP:OD1	4:CA:228:ASP:N	2.46	0.44
5:CB:52:ASP:OD1	5:CB:53:GLU:N	2.51	0.44
5:CB:233:VAL:HG23	5:CB:243:ILE:HD12	2.00	0.44
18:CP:383:ARG:HG3	18:CP:407:VAL:HG13	2.00	0.44
22:CT:260:GLY:O	22:CT:264:ARG:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LB:47:MET:HE2	28:LB:180:MET:SD	2.58	0.44
51:Lq:18:ASP:OD1	51:Lq:18:ASP:N	2.49	0.44
1:C1:91:G:N2	1:C1:95:A:H62	2.05	0.44
1:C1:403:U:H2'	1:C1:404:G:C8	2.53	0.44
1:C1:1235:U:H5'	33:LK:137:PHE:HE2	1.83	0.44
1:C1:1875:A:H2'	1:C1:1876:G:H8	1.82	0.44
1:C1:2419:G:H2'	1:C1:2421:A:H62	1.83	0.44
1:C1:3187:G:O6	28:LB:151:ARG:NH1	2.42	0.44
1:C1:3275:A:H2'	1:C1:3276:A:C8	2.53	0.44
3:C3:71:U:N3	3:C3:131:G:C6	2.85	0.44
10:CH:149:LEU:HA	10:CH:152:VAL:HG22	2.00	0.44
14:CL:71:GLU:HA	14:CL:74:ILE:HD12	1.98	0.44
18:CP:333:PRO:HA	18:CP:342:LEU:HD12	1.99	0.44
18:CP:444:PRO:HB3	18:CP:497:SER:HB2	2.00	0.44
19:CQ:108:TYR:HD1	19:CQ:111:ARG:HD3	1.83	0.44
27:Cb:422:VAL:HG21	27:Cb:427:ALA:HB2	1.99	0.44
27:Cb:490:VAL:HG12	27:Cb:505:VAL:HA	1.99	0.44
1:C1:745:U:H3	1:C1:748:U:H3	1.65	0.44
1:C1:2887:C:O2'	27:Cb:3:LYS:O	2.29	0.44
4:CA:40:SER:HB3	4:CA:52:LEU:HD13	2.00	0.44
7:CE:414:THR:HG23	7:CE:417:ALA:H	1.83	0.44
12:CJ:131:TYR:OH	12:CJ:140:ASP:OD2	2.30	0.44
13:CK:133:PHE:HE2	13:CK:148:LYS:HG2	1.83	0.44
18:CP:308:ILE:HD11	18:CP:364:LEU:HD22	2.00	0.44
19:CQ:17:LYS:HA	19:CQ:17:LYS:HD2	1.78	0.44
20:CR:32:ASN:OD1	20:CR:32:ASN:N	2.51	0.44
33:LK:103:SER:OG	33:LK:142:GLN:O	2.32	0.44
35:LM:15:GLU:HB3	40:LS:149:SER:HB2	2.00	0.44
50:Lj:64:MET:HB3	50:Lj:68:SER:HB3	2.00	0.44
54:Ce:21:THR:OG1	54:Ce:25:GLN:O	2.34	0.44
1:C1:231:A:H2'	1:C1:232:G:H8	1.83	0.43
1:C1:264:G:H2'	1:C1:265:A:H8	1.82	0.43
1:C1:439:C:H2'	1:C1:440:G:C8	2.53	0.43
1:C1:749:C:H2'	1:C1:750:G:C8	2.52	0.43
3:C3:68:G:H2'	3:C3:69:G:C8	2.53	0.43
4:CA:158:LEU:HD23	4:CA:158:LEU:HA	1.87	0.43
10:CH:244:HIS:CE1	27:Cb:591:LEU:HD11	2.53	0.43
27:Cb:259:LEU:HA	27:Cb:262:LEU:HD12	2.00	0.43
40:LS:124:LEU:HD11	41:LT:154:VAL:HG12	2.00	0.43
45:Ld:28:LEU:HD11	45:Ld:40:ALA:HB2	2.00	0.43
1:C1:181:A:H3'	44:LY:45:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2076:C:H2'	1:C1:2077:G:C8	2.52	0.43
1:C1:2813:C:H2'	1:C1:2814:G:C8	2.48	0.43
4:CA:81:ALA:HB3	4:CA:107:VAL:HG11	2.00	0.43
4:CA:111:PRO:HG3	23:CU:199:ALA:HB1	1.99	0.43
5:CB:113:ALA:HA	5:CB:121:ARG:HH22	1.83	0.43
10:CH:184:ARG:NH1	10:CH:189:ALA:O	2.52	0.43
11:CI:191:ILE:HG23	11:CI:231:ALA:HB3	1.99	0.43
29:LC:36:VAL:HG21	29:LC:251:LEU:HD21	1.98	0.43
29:LC:75:ILE:HD12	29:LC:75:ILE:HA	1.90	0.43
31:LG:219:SER:O	31:LG:223:GLU:HG2	2.18	0.43
42:LV:89:ARG:CZ	42:LV:95:LEU:HD11	2.49	0.43
50:Lj:27:LEU:HA	50:Lj:34:CYS:HA	2.00	0.43
1:C1:247:A:H2'	1:C1:248:G:C8	2.52	0.43
4:CA:273:LYS:HB3	4:CA:273:LYS:HE2	1.75	0.43
5:CB:98:CYS:HB2	5:CB:150:HIS:CD2	2.53	0.43
10:CH:193:VAL:HG22	56:CH:701:GTP:H5'	2.00	0.43
13:CK:7:ILE:HD13	13:CK:7:ILE:HA	1.90	0.43
20:CR:199:VAL:HG11	20:CR:234:LEU:HD13	1.99	0.43
40:LS:131:LYS:HE3	40:LS:131:LYS:HB2	1.85	0.43
1:C1:2431:G:N1	1:C1:2438:C:N3	2.66	0.43
1:C1:3078:U:H1'	1:C1:3079:A:H5''	1.99	0.43
1:C1:3314:U:O2'	1:C1:3315:A:N7	2.52	0.43
9:CG:108:PHE:CE1	9:CG:166:ARG:HG2	2.54	0.43
12:CJ:475:LEU:HD23	12:CJ:475:LEU:HA	1.89	0.43
15:CM:67:GLU:OE2	15:CM:138:PRO:HG3	2.18	0.43
16:CN:57:ARG:NH2	42:LV:126:GLU:O	2.51	0.43
31:LG:85:LEU:HD23	31:LG:181:ALA:HB1	1.99	0.43
51:Lq:26:ARG:HG3	51:Lq:210:MET:HB3	2.01	0.43
1:C1:404:G:OP1	38:LP:63:TYR:OH	2.34	0.43
1:C1:916:U:H2'	1:C1:917:A:H8	1.83	0.43
1:C1:2458:U:H2'	1:C1:2459:C:C6	2.54	0.43
6:CC:246:LEU:HD12	6:CC:247:ILE:HG13	2.00	0.43
10:CH:281:MET:HE2	10:CH:281:MET:HB3	1.89	0.43
10:CH:447:TYR:HE2	16:CN:79:GLN:HE21	1.67	0.43
12:CJ:42:ILE:HD12	12:CJ:68:ASP:HB2	2.01	0.43
18:CP:545:LYS:HD2	18:CP:545:LYS:HA	1.71	0.43
33:LK:88:PRO:HA	33:LK:89:PRO:HD3	1.80	0.43
35:LM:19:VAL:HA	35:LM:29:ALA:HA	2.01	0.43
47:Lf:45:PHE:HZ	47:Lf:109:ILE:HD11	1.84	0.43
48:Lh:54:LYS:HA	48:Lh:54:LYS:HD3	1.78	0.43
1:C1:650:C:H2'	1:C1:651:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2570:U:N3	1:C1:2758:G:C6	2.87	0.43
5:CB:237:PRO:HB2	11:CI:286:ASN:HD21	1.84	0.43
18:CP:478:LYS:HE3	18:CP:478:LYS:HB3	1.74	0.43
19:CQ:17:LYS:O	19:CQ:30:ARG:NH2	2.44	0.43
27:Cb:136:THR:HA	27:Cb:140:LYS:NZ	2.33	0.43
27:Cb:164:LEU:HB2	27:Cb:235:ILE:HG21	2.00	0.43
30:LE:76:LEU:HB2	30:LE:80:VAL:HG23	2.00	0.43
37:LO:132:GLN:HB3	37:LO:135:ARG:HG3	1.99	0.43
45:Ld:83:ILE:HD12	45:Ld:101:VAL:HG22	2.00	0.43
51:Lq:10:ARG:HH22	51:Lq:176:GLN:HB3	1.83	0.43
51:Lq:11:GLN:NE2	51:Lq:15:GLU:OE1	2.42	0.43
54:Ce:83:LEU:HD13	54:Ce:113:LEU:HD13	2.00	0.43
1:C1:613:U:O2	1:C1:1381:A:O2'	2.31	0.43
1:C1:934:G:H3'	1:C1:1098:G:H21	1.84	0.43
1:C1:955:U:OP1	39:LQ:44:ARG:NH2	2.52	0.43
1:C1:1174:C:OP1	13:CK:43:ARG:NH1	2.48	0.43
1:C1:2836:G:H2'	1:C1:2837:C:C6	2.54	0.43
1:C1:2837:C:H2'	1:C1:2838:U:C6	2.54	0.43
11:CI:287:LYS:O	11:CI:291:ARG:HG2	2.19	0.43
14:CL:387:PHE:H	14:CL:397:ALA:HB2	1.84	0.43
16:CN:186:VAL:HG23	16:CN:193:ILE:HD12	2.01	0.43
27:Cb:230:LEU:HD12	27:Cb:230:LEU:HA	1.90	0.43
29:LC:4:ARG:HA	29:LC:5:PRO:HD3	1.90	0.43
30:LE:69:ARG:O	30:LE:90:ASN:ND2	2.52	0.43
36:LN:114:ARG:HH21	36:LN:157:LYS:HG2	1.84	0.43
52:Cc:175:ILE:HB	52:Cc:185:ILE:HB	2.00	0.43
1:C1:388:A:P	53:Cd:431:ARG:HH12	2.41	0.43
1:C1:2319:A:H2'	1:C1:2320:A:C8	2.54	0.43
1:C1:3105:C:H2'	1:C1:3106:G:C8	2.53	0.43
2:C2:9:A:H2'	2:C2:10:A:C8	2.54	0.43
2:C2:95:G:C2	50:Lj:79:ARG:HD2	2.54	0.43
3:C3:25:U:N3	5:CB:173:LYS:HG3	2.34	0.43
5:CB:52:ASP:O	5:CB:56:THR:N	2.50	0.43
5:CB:52:ASP:H	7:CE:354:LYS:NZ	2.17	0.43
10:CH:392:LYS:HB3	10:CH:392:LYS:HE3	1.72	0.43
11:CI:194:LEU:HD22	11:CI:198:PHE:HB3	2.00	0.43
23:CU:205:LEU:H	23:CU:205:LEU:HD23	1.84	0.43
27:Cb:168:PRO:HG3	27:Cb:246:LEU:HG	2.01	0.43
1:C1:2955:U:H2'	1:C1:2956:C:C6	2.53	0.43
2:C2:63:G:O2'	48:Lh:54:LYS:NZ	2.36	0.43
13:CK:203:ASN:ND2	13:CK:216:THR:OG1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LB:95:THR:OG1	28:LB:98:GLY:O	2.26	0.43
53:Cd:183:LEU:HD11	53:Cd:323:LEU:HD12	2.01	0.43
1:C1:909:C:H2'	1:C1:910:A:C8	2.54	0.43
1:C1:976:U:C2	1:C1:1036:A:N7	2.87	0.43
1:C1:3319:C:H2'	1:C1:3320:C:C6	2.53	0.43
6:CC:263:THR:HG1	49:Li:55:GLU:CD	2.27	0.43
6:CC:396:TRP:HB2	12:CJ:193:LYS:HA	2.01	0.43
6:CC:406:ARG:NH2	12:CJ:147:MET:SD	2.92	0.43
9:CG:154:ALA:HB1	9:CG:163:VAL:HG23	2.01	0.43
16:CN:121:LEU:O	16:CN:139:ARG:NH2	2.52	0.43
31:LG:189:LEU:HD23	31:LG:189:LEU:HA	1.82	0.43
1:C1:1322:C:OP2	46:Le:62:LYS:NZ	2.46	0.42
1:C1:2841:U:H2'	1:C1:2842:C:C6	2.54	0.42
5:CB:102:ALA:HA	5:CB:130:ILE:HG22	2.01	0.42
10:CH:75:PRO:HB2	10:CH:244:HIS:ND1	2.34	0.42
16:CN:14:GLY:O	16:CN:61:ARG:NH1	2.52	0.42
19:CQ:95:ARG:O	19:CQ:99:ILE:HG13	2.19	0.42
37:LO:66:ASN:HA	37:LO:67:PRO:HD3	1.92	0.42
46:Le:96:GLU:HG3	46:Le:122:ASN:HD21	1.84	0.42
52:Cc:129:LYS:H	52:Cc:129:LYS:HG2	1.62	0.42
52:Cc:189:ILE:HG23	52:Cc:193:MET:HE3	2.00	0.42
1:C1:194:G:OP1	1:C1:213:G:O2'	2.34	0.42
1:C1:434:G:H2'	1:C1:435:C:C6	2.53	0.42
1:C1:727:C:H2'	1:C1:728:A:C8	2.54	0.42
1:C1:796:G:H5'	50:Lj:16:HIS:CE1	2.53	0.42
1:C1:1072:G:N2	1:C1:1073:G:N2	2.67	0.42
1:C1:1884:G:N3	1:C1:2294:A:C5	2.87	0.42
1:C1:2772:G:H2'	1:C1:2773:G:H8	1.83	0.42
1:C1:3323:C:N4	1:C1:3326:C:OP2	2.53	0.42
2:C2:130:C:H2'	2:C2:131:G:C8	2.54	0.42
5:CB:89:LEU:HD13	5:CB:89:LEU:HA	1.84	0.42
7:CE:172:MET:HG2	7:CE:176:LEU:HD13	2.01	0.42
8:CF:192:TYR:HD2	8:CF:194:ILE:HG22	1.84	0.42
9:CG:172:GLU:OE1	9:CG:175:ARG:NH2	2.52	0.42
13:CK:65:ILE:HD12	13:CK:65:ILE:HA	1.82	0.42
19:CQ:24:ASN:HA	42:LV:119:PRO:HD3	2.01	0.42
19:CQ:53:LYS:HG2	19:CQ:57:LYS:HE2	2.01	0.42
28:LB:219:ILE:HB	28:LB:338:THR:HB	2.01	0.42
33:LK:122:SER:OG	33:LK:123:LYS:N	2.52	0.42
54:Ce:107:HIS:NE2	54:Ce:111:GLN:OE1	2.52	0.42
1:C1:508:G:OP1	15:LF:73:ARG:NE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3158:U:C4	35:LM:121:MET:HG3	2.54	0.42
4:CA:116:TYR:HB2	4:CA:243:ILE:HD11	2.00	0.42
5:CB:267:VAL:HA	5:CB:271:VAL:HB	2.01	0.42
5:CB:274:LYS:HB3	5:CB:275:TRP:H	1.48	0.42
7:CE:268:ARG:NH2	7:CE:436:ASP:OD1	2.44	0.42
9:CG:116:LYS:HG2	9:CG:159:PRO:HA	2.01	0.42
10:CH:101:LYS:O	10:CH:105:GLU:HG3	2.19	0.42
28:LB:113:GLU:HB2	28:LB:177:ALA:HB2	2.00	0.42
30:LE:191:LYS:NZ	37:LO:4:PHE:O	2.52	0.42
36:LN:137:PRO:O	36:LN:143:ARG:NH1	2.52	0.42
53:Cd:313:LEU:HD23	53:Cd:346:LEU:HB2	2.01	0.42
1:C1:144:U:P	36:LN:49:ARG:HH22	2.42	0.42
1:C1:2816:U:OP1	13:CK:107:LYS:NZ	2.43	0.42
1:C1:2921:C:H42	1:C1:2927:A:N6	2.18	0.42
1:C1:3274:U:H5''	19:CQ:50:LYS:HZ2	1.84	0.42
6:CC:327:TRP:HB3	6:CC:330:GLU:HB2	2.01	0.42
12:CJ:39:TRP:CD1	12:CJ:233:PHE:HB2	2.54	0.42
13:CK:247:ASN:HB3	13:CK:256:ASN:HB2	2.02	0.42
30:LE:167:LYS:HE2	30:LE:167:LYS:HB2	1.93	0.42
52:Cc:127:MET:SD	52:Cc:155:VAL:HG23	2.59	0.42
1:C1:597:G:N1	1:C1:1319:G:OP1	2.41	0.42
1:C1:1044:A:N3	41:LT:130:ARG:NH2	2.68	0.42
1:C1:2078:G:H2'	1:C1:2079:A:C8	2.55	0.42
2:C2:57:C:H4'	2:C2:63:G:N7	2.35	0.42
13:CK:34:LYS:NZ	13:CK:38:ASN:OD1	2.39	0.42
20:CR:216:ASN:HD21	20:CR:220:GLN:HG3	1.85	0.42
27:Cb:117:GLN:O	27:Cb:121:ILE:HG12	2.19	0.42
32:LH:92:TYR:HB3	32:LH:181:ILE:HG23	2.01	0.42
40:LS:1:MET:HE3	40:LS:1:MET:HB2	1.81	0.42
40:LS:106:MET:HE3	40:LS:106:MET:HB3	1.85	0.42
40:LS:140:ILE:HD13	40:LS:140:ILE:HA	1.85	0.42
53:Cd:426:LYS:H	53:Cd:426:LYS:HG2	1.70	0.42
1:C1:1210:A:OP1	8:CF:203:SER:OG	2.32	0.42
1:C1:3203:C:H2'	1:C1:3204:G:C8	2.55	0.42
2:C2:71:A:H2'	44:LY:50:ARG:NH1	2.35	0.42
8:CF:41:PHE:CD2	8:CF:226:TYR:HB3	2.55	0.42
10:CH:421:LEU:HD13	28:LB:69:LYS:HD3	2.01	0.42
28:LB:292:GLU:HA	28:LB:305:LYS:HD3	2.02	0.42
31:LG:161:ASP:HB2	36:LN:41:ARG:HH12	1.84	0.42
42:LV:41:VAL:HA	42:LV:60:VAL:HG12	2.00	0.42
49:Li:41:ALA:HB1	49:Li:46:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2556:G:H2'	1:C1:2557:U:C6	2.54	0.42
1:C1:3014:U:O2'	1:C1:3016:G:OP1	2.37	0.42
1:C1:3031:G:H5'	45:Ld:70:GLN:HE21	1.85	0.42
1:C1:3144:C:H4'	37:LO:178:ARG:HH22	1.84	0.42
10:CH:391:LYS:O	16:CN:43:GLN:NE2	2.51	0.42
15:CM:116:GLN:N	15:CM:119:ASN:HD21	2.18	0.42
18:CP:402:MET:H	18:CP:402:MET:HG2	1.68	0.42
18:CP:458:PRO:O	18:CP:487:GLN:NE2	2.48	0.42
28:LB:93:ILE:HG22	28:LB:156:CYS:HA	2.01	0.42
29:LC:148:GLU:O	29:LC:151:LEU:HB2	2.19	0.42
36:LN:31:ARG:NH1	36:LN:124:ASP:OD2	2.52	0.42
38:LP:119:VAL:HG22	38:LP:146:ILE:HG12	2.02	0.42
42:LV:47:ARG:HD2	42:LV:50:ARG:HB2	2.02	0.42
1:C1:1171:C:N3	1:C1:1297:U:C2	2.87	0.42
1:C1:3192:C:H2'	1:C1:3193:G:C8	2.55	0.42
2:C2:70:G:OP1	44:LY:120:ARG:NH2	2.53	0.42
3:C3:4:C:N3	15:CM:66:ARG:NH1	2.68	0.42
3:C3:141:U:OP2	11:CI:291:ARG:NH1	2.51	0.42
5:CB:87:HIS:ND1	5:CB:258:ASN:OD1	2.52	0.42
9:CG:59:VAL:HG11	9:CG:64:LEU:HD13	2.01	0.42
10:CH:5:LYS:HE2	10:CH:5:LYS:HB3	1.90	0.42
10:CH:63:ILE:HD11	10:CH:149:LEU:HD13	2.01	0.42
10:CH:361:LEU:HD12	10:CH:361:LEU:HA	1.92	0.42
16:CN:61:ARG:HD3	42:LV:133:SER:HA	2.01	0.42
15:LF:134:LYS:HE2	15:LF:134:LYS:HB2	1.82	0.42
32:LH:3:TYR:OH	32:LH:62:ARG:NH1	2.46	0.42
38:LP:43:ARG:HG2	38:LP:43:ARG:HH11	1.84	0.42
53:Cd:189:ASN:OD1	53:Cd:189:ASN:N	2.41	0.42
1:C1:100:A:H2'	1:C1:101:G:N3	2.34	0.42
1:C1:194:G:H2'	1:C1:195:G:H8	1.84	0.42
1:C1:399:A:C2	2:C2:17:A:H1'	2.55	0.42
1:C1:697:A:N6	1:C1:736:A:O3'	2.53	0.42
1:C1:2455:U:O2'	1:C1:2456:A:H5''	2.20	0.42
1:C1:3192:C:H2'	1:C1:3193:G:H8	1.84	0.42
1:C1:3265:A:H5'	45:Ld:111:GLY:H	1.84	0.42
9:CG:84:ILE:HG23	9:CG:168:ALA:HB1	2.00	0.42
10:CH:279:ASN:ND2	27:Cb:511:ARG:HH22	2.17	0.42
15:CM:242:ASN:HA	15:CM:245:ILE:HG22	2.02	0.42
36:LN:103:GLU:HB3	36:LN:160:GLU:HB2	2.02	0.42
44:LY:48:PRO:O	44:LY:114:ARG:NH2	2.52	0.42
1:C1:115:A:N6	1:C1:149:U:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:506:G:O3'	15:LF:66:ARG:NH2	2.53	0.42
10:CH:228:LEU:HA	10:CH:231:MET:HE2	2.02	0.42
10:CH:301:MET:SD	10:CH:301:MET:N	2.92	0.42
18:CP:495:ILE:HD12	18:CP:495:ILE:H	1.85	0.42
23:CU:319:LYS:HB2	23:CU:319:LYS:HE2	1.92	0.42
54:Ce:30:ASN:ND2	54:Ce:44:PRO:HG2	2.35	0.42
1:C1:181:A:P	44:LY:45:ARG:HH21	2.43	0.41
1:C1:713:G:C5	1:C1:723:G:C2	3.08	0.41
2:C2:97:A:OP1	48:Lh:68:ARG:NH1	2.53	0.41
4:CA:114:LYS:HB3	4:CA:243:ILE:HB	2.01	0.41
8:CF:20:ARG:HD2	8:CF:20:ARG:HA	1.79	0.41
9:CG:64:LEU:HD11	18:CP:434:ILE:HG22	2.02	0.41
18:CP:409:PHE:CE2	18:CP:434:ILE:HD12	2.55	0.41
18:CP:422:ILE:HG23	18:CP:426:HIS:CE1	2.55	0.41
23:CU:215:SER:HB3	23:CU:261:GLU:OE1	2.20	0.41
23:CU:258:LEU:HD23	23:CU:258:LEU:HA	1.88	0.41
36:LN:36:ILE:HD11	36:LN:105:ARG:HB3	2.02	0.41
1:C1:380:G:H4'	38:LP:18:ARG:HB2	2.02	0.41
1:C1:575:A:H5''	47:Lf:72:LYS:HD3	2.00	0.41
1:C1:3118:A:H2'	1:C1:3119:C:C6	2.54	0.41
6:CC:326:LEU:O	12:CJ:128:ARG:NH1	2.53	0.41
9:CG:127:PRO:HD2	9:CG:130:SER:HB3	2.01	0.41
18:CP:453:VAL:HG23	18:CP:508:ILE:HG23	2.01	0.41
28:LB:105:VAL:HG22	28:LB:148:GLU:HB3	2.02	0.41
28:LB:159:VAL:HG22	28:LB:192:LYS:HD3	2.01	0.41
31:LG:223:GLU:HG2	31:LG:223:GLU:H	1.78	0.41
36:LN:192:LYS:HE2	36:LN:192:LYS:HB3	1.74	0.41
1:C1:2944:U:H2'	1:C1:2945:A:C8	2.55	0.41
5:CB:163:LEU:HD23	5:CB:163:LEU:HA	1.85	0.41
14:CL:438:TYR:O	14:CL:440:ILE:N	2.53	0.41
18:CP:552:MET:HB2	18:CP:554:LYS:HZ2	1.86	0.41
27:Cb:833:LYS:HB2	27:Cb:836:LEU:HB2	2.02	0.41
42:LV:24:ILE:HD13	42:LV:24:ILE:HA	1.90	0.41
42:LV:82:ARG:HD3	42:LV:119:PRO:HG2	2.02	0.41
52:Cc:48:LEU:HD23	52:Cc:48:LEU:HA	1.89	0.41
1:C1:655:U:H2'	1:C1:656:U:C6	2.55	0.41
1:C1:2774:G:H2'	1:C1:2775:A:H8	1.85	0.41
1:C1:2961:C:O2'	28:LB:99:LEU:O	2.33	0.41
6:CC:241:LYS:NZ	6:CC:250:ASP:OD1	2.53	0.41
11:CI:188:VAL:O	11:CI:263:VAL:N	2.49	0.41
27:Cb:133:MET:HE3	27:Cb:275:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Cb:381:TYR:HD2	27:Cb:538:THR:HG21	1.86	0.41
28:LB:126:LYS:HE3	28:LB:126:LYS:HB3	1.96	0.41
30:LE:114:VAL:HG21	30:LE:169:LEU:HD13	2.02	0.41
35:LM:17:GLY:HA2	35:LM:72:LEU:HD22	2.02	0.41
40:LS:5:GLN:HB2	40:LS:7:TYR:CE1	2.55	0.41
50:Lj:60:GLY:HA2	50:Lj:64:MET:HE2	2.01	0.41
1:C1:3235:A:H2'	1:C1:3236:A:C8	2.55	0.41
8:CF:202:ASP:OD1	8:CF:202:ASP:N	2.42	0.41
14:CL:277:PRO:O	14:CL:279:ALA:N	2.53	0.41
15:CM:71:LEU:HD21	15:CM:135:ILE:HG23	2.02	0.41
18:CP:385:LEU:HD13	18:CP:453:VAL:HG12	2.01	0.41
20:CR:214:LYS:HG2	20:CR:215:LEU:HG	2.02	0.41
26:Cz:30:GLN:H	26:Cz:30:GLN:HG2	1.64	0.41
27:Cb:446:GLN:HB2	27:Cb:449:ILE:HG12	2.02	0.41
55:Cf:528:GLU:O	55:Cf:532:ARG:HG3	2.20	0.41
1:C1:926:C:H2'	1:C1:927:C:C6	2.55	0.41
1:C1:1088:G:H2'	1:C1:1089:A:C8	2.56	0.41
1:C1:2077:G:H2'	1:C1:2078:G:H8	1.85	0.41
4:CA:40:SER:HB2	4:CA:44:VAL:HG11	2.03	0.41
4:CA:134:LYS:O	4:CA:173:LYS:NZ	2.53	0.41
7:CE:352:LEU:HD21	7:CE:410:THR:HG21	2.03	0.41
7:CE:353:LYS:HG3	7:CE:382:LEU:HD11	2.03	0.41
12:CJ:393:LYS:HA	12:CJ:393:LYS:HD3	1.87	0.41
18:CP:324:LEU:HB3	18:CP:329:VAL:HB	2.03	0.41
27:Cb:513:GLU:HA	27:Cb:516:ASN:ND2	2.35	0.41
28:LB:39:LYS:HB3	28:LB:39:LYS:HE2	1.88	0.41
31:LG:222:LYS:HA	31:LG:226:LEU:HB2	2.03	0.41
34:LL:87:ARG:NH2	34:LL:88:LEU:HD13	2.36	0.41
40:LS:45:LEU:HD12	40:LS:45:LEU:HA	1.89	0.41
1:C1:5:G:O3'	12:CJ:93:ARG:NH2	2.47	0.41
1:C1:957:G:H2'	1:C1:958:A:H8	1.86	0.41
1:C1:1344:G:H2'	1:C1:1345:A:C8	2.56	0.41
1:C1:2759:A:N1	9:CG:61:ARG:NH2	2.47	0.41
1:C1:2836:G:H2'	1:C1:2837:C:H6	1.86	0.41
3:C3:65:G:H21	3:C3:143:A:N6	2.18	0.41
4:CA:63:ARG:HE	4:CA:63:ARG:HB2	1.54	0.41
12:CJ:49:ASP:HB3	12:CJ:52:LYS:HB2	2.02	0.41
14:CL:66:LEU:HA	14:CL:69:ARG:HG2	2.02	0.41
15:CM:92:VAL:HG22	15:CM:140:VAL:HG22	2.02	0.41
15:CM:237:ARG:HB3	15:CM:240:HIS:HB2	2.01	0.41
27:Cb:564:ILE:HD13	27:Cb:564:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LB:47:MET:HB2	28:LB:165:THR:HG21	2.03	0.41
31:LG:94:PHE:CZ	31:LG:188:ARG:HG2	2.56	0.41
34:LL:102:LYS:HE3	34:LL:102:LYS:HB2	1.74	0.41
42:LV:89:ARG:NH1	42:LV:122:LYS:HE3	2.36	0.41
54:Ce:7:TRP:HB2	54:Ce:46:ALA:HB1	2.03	0.41
1:C1:448:A:H3'	1:C1:449:U:H4'	2.03	0.41
1:C1:683:C:O2'	1:C1:684:G:N7	2.48	0.41
1:C1:966:U:H2'	1:C1:967:U:C6	2.55	0.41
9:CG:70:CYS:HB3	9:CG:85:THR:HG21	2.03	0.41
12:CJ:415:ILE:HD11	12:CJ:417:HIS:O	2.21	0.41
28:LB:85:VAL:HG23	28:LB:166:GLN:HE21	1.86	0.41
15:LF:53:ARG:HE	15:LF:53:ARG:HB2	1.69	0.41
39:LQ:149:LEU:HD23	39:LQ:153:GLN:HB3	2.03	0.41
54:Ce:31:GLU:H	54:Ce:31:GLU:HG3	1.70	0.41
1:C1:713:G:C6	1:C1:723:G:C2	3.09	0.41
1:C1:1171:C:C4	1:C1:1297:U:O2	2.74	0.41
1:C1:1251:U:H1'	1:C1:1254:C:H5	1.85	0.41
1:C1:1272:U:OP1	8:CF:8:ARG:HD2	2.21	0.41
1:C1:1305:C:H4'	40:LS:1:MET:HA	2.03	0.41
1:C1:1405:C:H2'	1:C1:1406:C:C6	2.56	0.41
1:C1:3254:A:H5''	28:LB:175:LYS:HG3	2.03	0.41
6:CC:306:TYR:HB3	31:LG:117:THR:HG21	2.02	0.41
7:CE:116:LEU:HD23	7:CE:134:MET:HE1	2.03	0.41
7:CE:277:GLU:OE1	7:CE:277:GLU:N	2.54	0.41
9:CG:21:THR:HB	9:CG:95:ARG:HB3	2.01	0.41
9:CG:158:ASP:OD1	9:CG:159:PRO:HD2	2.20	0.41
23:CU:338:LYS:HA	23:CU:338:LYS:HE2	2.03	0.41
27:Cb:270:LEU:HD21	27:Cb:279:LEU:HD21	2.03	0.41
15:LF:237:ARG:HD2	15:LF:241:ILE:HD12	2.03	0.41
31:LG:97:LEU:HB3	31:LG:192:LEU:HD11	2.02	0.41
32:LH:151:ASN:OD1	32:LH:151:ASN:N	2.54	0.41
40:LS:169:ARG:HA	40:LS:170:PRO:HD3	1.93	0.41
42:LV:36:LEU:HB3	42:LV:62:ALA:HB1	2.02	0.41
46:Le:76:LEU:HD12	46:Le:76:LEU:HA	1.95	0.41
52:Cc:203:ASP:OD1	52:Cc:203:ASP:N	2.36	0.41
1:C1:1045:G:OP2	1:C1:1045:G:N2	2.45	0.41
1:C1:2412:A:H2'	1:C1:2413:G:C8	2.55	0.41
1:C1:2437:G:H3'	1:C1:2438:C:C6	2.56	0.41
1:C1:3041:C:O2'	1:C1:3272:U:OP1	2.27	0.41
3:C3:34:C:H2'	3:C3:35:G:H8	1.86	0.41
4:CA:137:ARG:NH1	4:CA:167:GLN:HG2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CA:259:LYS:HE2	4:CA:259:LYS:HB2	1.90	0.41
20:CR:17:ILE:HD13	20:CR:17:ILE:HA	1.90	0.41
29:LC:287:LEU:HD22	39:LQ:56:LEU:HD12	2.03	0.41
40:LS:73:LYS:NZ	40:LS:97:THR:O	2.54	0.41
48:Lh:48:LYS:HB2	48:Lh:48:LYS:HE2	1.79	0.41
1:C1:603:G:H2'	1:C1:604:G:C8	2.56	0.40
1:C1:694:U:H1'	1:C1:735:G:H1'	2.04	0.40
1:C1:1185:A:H61	1:C1:1282:G:H1'	1.86	0.40
1:C1:1196:U:H2'	1:C1:1197:A:H8	1.87	0.40
1:C1:1386:G:N2	1:C1:1389:A:OP2	2.32	0.40
1:C1:2091:U:C2	1:C1:2287:G:C2	3.08	0.40
1:C1:2928:C:H5'	9:CG:149:ARG:NH2	2.36	0.40
1:C1:2947:U:H2'	1:C1:2948:G:C8	2.56	0.40
1:C1:2968:A:N1	1:C1:3000:C:O2'	2.45	0.40
1:C1:3016:G:H2'	1:C1:3017:C:C6	2.56	0.40
3:C3:56:A:H4'	11:CI:193:ARG:HE	1.86	0.40
4:CA:294:ARG:HA	4:CA:294:ARG:HD3	1.83	0.40
6:CC:149:TYR:OH	7:CE:571:ARG:NH2	2.54	0.40
7:CE:437:ASP:HB3	7:CE:440:ASP:HB3	2.03	0.40
10:CH:297:LEU:HD23	10:CH:297:LEU:H	1.86	0.40
13:CK:164:ARG:HD2	13:CK:168:TYR:O	2.20	0.40
16:CN:111:ASN:HB2	16:CN:156:ASN:ND2	2.37	0.40
27:Cb:10:PRO:HD3	27:Cb:376:LYS:HD2	2.02	0.40
32:LH:127:LYS:HB3	32:LH:127:LYS:HE3	1.90	0.40
33:LK:102:LYS:HB3	33:LK:102:LYS:HE2	1.90	0.40
35:LM:73:PRO:HG2	35:LM:76:ALA:HB2	2.03	0.40
46:Le:67:MET:HE3	46:Le:67:MET:HB2	1.88	0.40
54:Ce:28:CYS:N	54:Ce:36:GLY:O	2.40	0.40
1:C1:21:G:H3'	1:C1:22:G:H8	1.86	0.40
1:C1:202:A:O2'	1:C1:204:A:OP2	2.34	0.40
1:C1:290:U:H5''	1:C1:291:G:H5'	2.04	0.40
1:C1:1151:A:H2'	1:C1:1152:A:C8	2.56	0.40
1:C1:2403:A:H2'	1:C1:2404:G:C8	2.56	0.40
1:C1:2768:C:H2'	1:C1:2769:A:C8	2.55	0.40
2:C2:81:U:H2'	2:C2:82:U:C6	2.57	0.40
10:CH:366:ALA:HA	16:CN:167:ILE:HD11	2.03	0.40
11:CI:273:PHE:HB3	11:CI:276:ALA:HB2	2.02	0.40
24:CX:86:LYS:HA	24:CX:90:LYS:HD2	2.03	0.40
26:Cz:33:LEU:HD23	26:Cz:33:LEU:HA	1.91	0.40
42:LV:81:VAL:HG13	42:LV:82:ARG:HG3	2.03	0.40
45:Ld:20:TYR:HE2	45:Ld:51:ALA:HB1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Cd:326:LYS:HA	53:Cd:326:LYS:HD3	1.87	0.40
1:C1:683:C:OP2	29:LC:120:ARG:NH2	2.53	0.40
1:C1:780:G:O2'	34:LL:18:TRP:NE1	2.49	0.40
1:C1:1156:G:N2	37:LO:89:MET:SD	2.95	0.40
1:C1:2403:A:H2'	1:C1:2404:G:H8	1.86	0.40
1:C1:2570:U:C4	1:C1:2758:G:N1	2.89	0.40
2:C2:119:C:H5''	12:CJ:70:GLN:NE2	2.37	0.40
5:CB:48:ASN:OD1	5:CB:48:ASN:N	2.53	0.40
6:CC:240:ARG:HD3	21:CS:652:ILE:HG12	2.03	0.40
7:CE:267:ASP:OD1	7:CE:267:ASP:N	2.55	0.40
10:CH:316:ILE:HD13	10:CH:316:ILE:HA	1.97	0.40
18:CP:412:ASP:OD1	18:CP:412:ASP:N	2.54	0.40
30:LE:58:LEU:HD13	30:LE:102:VAL:HG11	2.02	0.40
37:LO:4:PHE:CZ	47:Lf:14:ARG:HG3	2.56	0.40
1:C1:1193:U:O2'	40:LS:113:ARG:NH1	2.55	0.40
1:C1:2837:C:H2'	1:C1:2838:U:H6	1.86	0.40
2:C2:70:G:H5''	44:LY:117:ILE:HD11	2.04	0.40
3:C3:38:G:O6	3:C3:43:U:O4	2.39	0.40
4:CA:308:ASP:N	4:CA:313:GLU:OE2	2.55	0.40
8:CF:148:GLU:HG3	8:CF:214:ILE:HG12	2.03	0.40
10:CH:177:VAL:HG13	10:CH:254:ASP:HB2	2.02	0.40
10:CH:297:LEU:HG	10:CH:302:GLN:OE1	2.22	0.40
15:CM:101:ILE:HD12	15:CM:101:ILE:HA	1.92	0.40
28:LB:307:THR:HA	28:LB:308:PRO:HD3	1.95	0.40
54:Ce:87:TYR:OH	54:Ce:114:THR:OG1	2.25	0.40
1:C1:1039:A:H5'	15:LF:104:LYS:NZ	2.37	0.40
7:CE:438:PRO:HB2	7:CE:439:ARG:NH1	2.34	0.40
7:CE:532:ASP:OD1	7:CE:535:LYS:HG3	2.22	0.40
10:CH:347:LEU:O	10:CH:351:THR:OG1	2.23	0.40
11:CI:188:VAL:HA	11:CI:234:GLU:OE1	2.21	0.40
11:CI:264:PRO:HA	11:CI:265:PRO:HD3	1.95	0.40
14:CL:73:ARG:NH1	14:CL:73:ARG:O	2.55	0.40
16:CN:11:ASN:HD22	16:CN:209:ASP:CG	2.29	0.40
27:Cb:151:ARG:NH2	27:Cb:267:GLN:OE1	2.54	0.40
27:Cb:388:LEU:HD23	27:Cb:388:LEU:HA	1.96	0.40
27:Cb:440:ASN:OD1	27:Cb:453:ARG:NH1	2.49	0.40
28:LB:113:GLU:H	28:LB:113:GLU:HG2	1.61	0.40
37:LO:26:LYS:HA	37:LO:26:LYS:HD2	1.78	0.40
38:LP:70:THR:OG1	38:LP:71:ALA:N	2.54	0.40
48:Lh:27:LEU:HD23	48:Lh:27:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CA	254/316 (80%)	234 (92%)	19 (8%)	1 (0%)	30	61
5	CB	256/391 (66%)	244 (95%)	10 (4%)	2 (1%)	16	47
6	CC	283/801 (35%)	272 (96%)	11 (4%)	0	100	100
7	CE	459/598 (77%)	445 (97%)	13 (3%)	1 (0%)	43	73
8	CF	243/270 (90%)	234 (96%)	9 (4%)	0	100	100
9	CG	175/184 (95%)	167 (95%)	8 (5%)	0	100	100
10	CH	474/661 (72%)	456 (96%)	18 (4%)	0	100	100
11	CI	144/414 (35%)	136 (94%)	8 (6%)	0	100	100
12	CJ	374/679 (55%)	365 (98%)	9 (2%)	0	100	100
13	CK	226/261 (87%)	216 (96%)	10 (4%)	0	100	100
14	CL	384/558 (69%)	357 (93%)	22 (6%)	5 (1%)	9	35
15	CM	183/249 (74%)	175 (96%)	8 (4%)	0	100	100
15	LF	238/249 (96%)	228 (96%)	9 (4%)	1 (0%)	30	61
16	CN	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	322/751 (43%)	307 (95%)	15 (5%)	0	100	100
19	CQ	110/225 (49%)	106 (96%)	4 (4%)	0	100	100
20	CR	159/237 (67%)	155 (98%)	4 (2%)	0	100	100
21	CS	294/834 (35%)	286 (97%)	6 (2%)	2 (1%)	18	49
22	CT	448/688 (65%)	425 (95%)	21 (5%)	2 (0%)	30	61
23	CU	174/451 (39%)	166 (95%)	8 (5%)	0	100	100
24	CX	86/203 (42%)	82 (95%)	4 (5%)	0	100	100
25	CY	308/788 (39%)	292 (95%)	15 (5%)	1 (0%)	36	67
26	Cz	68/123 (55%)	67 (98%)	1 (2%)	0	100	100
27	Cb	630/924 (68%)	597 (95%)	33 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	LB	337/392 (86%)	320 (95%)	17 (5%)	0	100	100
29	LC	360/365 (99%)	348 (97%)	12 (3%)	0	100	100
30	LE	166/200 (83%)	160 (96%)	6 (4%)	0	100	100
31	LG	192/262 (73%)	188 (98%)	4 (2%)	0	100	100
32	LH	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
33	LK	142/165 (86%)	132 (93%)	10 (7%)	0	100	100
34	LL	115/213 (54%)	109 (95%)	6 (5%)	0	100	100
35	LM	135/142 (95%)	131 (97%)	4 (3%)	0	100	100
36	LN	179/203 (88%)	174 (97%)	5 (3%)	0	100	100
37	LO	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
38	LP	150/187 (80%)	149 (99%)	1 (1%)	0	100	100
39	LQ	127/213 (60%)	123 (97%)	4 (3%)	0	100	100
40	LS	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
41	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	16	47
42	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
43	LX	20/156 (13%)	20 (100%)	0	0	100	100
44	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
45	Ld	107/120 (89%)	102 (95%)	5 (5%)	0	100	100
46	Le	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
47	Lf	106/109 (97%)	102 (96%)	3 (3%)	1 (1%)	14	44
48	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
49	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
50	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
51	Lq	205/217 (94%)	186 (91%)	19 (9%)	0	100	100
52	Cc	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
53	Cd	334/436 (77%)	323 (97%)	11 (3%)	0	100	100
54	Ce	192/336 (57%)	185 (96%)	7 (4%)	0	100	100
55	Cf	57/570 (10%)	57 (100%)	0	0	100	100
All	All	11105/18067 (62%)	10656 (96%)	432 (4%)	17 (0%)	44	73

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CA	236	PRO
5	CB	103	ASP
14	CL	414	VAL
21	CS	67	MET
22	CT	254	PRO
25	CY	548	PHE
14	CL	446	ASP
15	LF	12	ILE
47	Lf	93	ALA
14	CL	42	ASN
14	CL	278	ASN
14	CL	439	ASP
5	CB	89	LEU
7	CE	452	ASN
41	LT	44	VAL
21	CS	68	PRO
22	CT	237	PRO

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	
4	CA	231/276 (84%)	230 (100%)	1 (0%)	84	86
5	CB	222/329 (68%)	214 (96%)	8 (4%)	31	62
6	CC	266/710 (38%)	264 (99%)	2 (1%)	73	81
7	CE	398/517 (77%)	394 (99%)	4 (1%)	68	79
8	CF	214/236 (91%)	213 (100%)	1 (0%)	81	85
9	CG	150/155 (97%)	148 (99%)	2 (1%)	61	77
10	CH	424/575 (74%)	421 (99%)	3 (1%)	76	82
11	CI	121/336 (36%)	119 (98%)	2 (2%)	53	74
12	CJ	332/579 (57%)	328 (99%)	4 (1%)	63	78
13	CK	198/225 (88%)	193 (98%)	5 (2%)	42	69
14	CL	65/458 (14%)	64 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CM	161/215 (75%)	157 (98%)	4 (2%)	42	69
15	LF	206/215 (96%)	206 (100%)	0	100	100
16	CN	206/206 (100%)	205 (100%)	1 (0%)	81	85
17	CO	48/99 (48%)	48 (100%)	0	100	100
18	CP	273/632 (43%)	270 (99%)	3 (1%)	65	78
19	CQ	100/192 (52%)	97 (97%)	3 (3%)	36	65
20	CR	144/206 (70%)	142 (99%)	2 (1%)	59	76
21	CS	73/716 (10%)	73 (100%)	0	100	100
23	CU	149/376 (40%)	148 (99%)	1 (1%)	76	82
24	CX	76/172 (44%)	75 (99%)	1 (1%)	61	77
26	Cz	60/107 (56%)	60 (100%)	0	100	100
27	Cb	540/779 (69%)	534 (99%)	6 (1%)	65	78
28	LB	290/331 (88%)	289 (100%)	1 (0%)	86	87
29	LC	283/285 (99%)	281 (99%)	2 (1%)	76	82
30	LE	143/166 (86%)	142 (99%)	1 (1%)	76	82
31	LG	168/222 (76%)	166 (99%)	2 (1%)	63	78
32	LH	167/169 (99%)	166 (99%)	1 (1%)	78	83
33	LK	121/136 (89%)	121 (100%)	0	100	100
34	LL	99/176 (56%)	96 (97%)	3 (3%)	36	65
35	LM	115/117 (98%)	113 (98%)	2 (2%)	53	74
36	LN	164/180 (91%)	162 (99%)	2 (1%)	63	78
37	LO	163/163 (100%)	163 (100%)	0	100	100
38	LP	125/152 (82%)	122 (98%)	3 (2%)	43	69
39	LQ	110/178 (62%)	110 (100%)	0	100	100
40	LS	154/154 (100%)	151 (98%)	3 (2%)	50	73
41	LT	109/135 (81%)	107 (98%)	2 (2%)	51	73
42	LV	99/102 (97%)	97 (98%)	2 (2%)	48	72
43	LX	12/129 (9%)	12 (100%)	0	100	100
44	LY	117/119 (98%)	115 (98%)	2 (2%)	53	74
45	Ld	95/105 (90%)	92 (97%)	3 (3%)	34	64
46	Le	114/114 (100%)	113 (99%)	1 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Lf	89/90 (99%)	89 (100%)	0	100	100
48	Lh	108/781 (14%)	108 (100%)	0	100	100
49	Li	75/93 (81%)	75 (100%)	0	100	100
50	Lj	61/78 (78%)	60 (98%)	1 (2%)	55	75
51	Lq	179/189 (95%)	179 (100%)	0	100	100
52	Cc	204/244 (84%)	203 (100%)	1 (0%)	81	85
53	Cd	291/367 (79%)	287 (99%)	4 (1%)	59	76
54	Ce	173/297 (58%)	171 (99%)	2 (1%)	63	78
55	Cf	53/482 (11%)	53 (100%)	0	100	100
All	All	8538/14065 (61%)	8446 (99%)	92 (1%)	63	78

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CA	295	GLN
5	CB	48	ASN
5	CB	62	ILE
5	CB	66	LEU
5	CB	89	LEU
5	CB	90	ASN
5	CB	91	THR
5	CB	123	LYS
5	CB	276	GLN
6	CC	175	ILE
6	CC	193	LYS
7	CE	156	LYS
7	CE	206	LEU
7	CE	208	LYS
7	CE	473	LEU
8	CF	196	LYS
9	CG	82	LEU
9	CG	158	ASP
10	CH	174	PHE
10	CH	284	ILE
10	CH	323	THR
11	CI	287	LYS
11	CI	316	ARG
12	CJ	218	ILE
12	CJ	268	LEU

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Mol	Chain	Res	Type
12	CJ	415	ILE
12	CJ	420	ILE
13	CK	34	LYS
13	CK	150	ILE
13	CK	172	ILE
13	CK	189	LEU
13	CK	190	ASN
14	CL	19	ARG
15	CM	52	LYS
15	CM	134	LYS
15	CM	154	ILE
15	CM	197	VAL
16	CN	161	VAL
18	CP	270	ILE
18	CP	337	TRP
18	CP	576	PHE
19	CQ	11	ARG
19	CQ	23	ARG
19	CQ	65	VAL
20	CR	45	LEU
20	CR	212	ASP
23	CU	327	LYS
24	CX	113	GLN
27	Cb	121	ILE
27	Cb	212	ASP
27	Cb	214	ILE
27	Cb	255	LEU
27	Cb	305	LEU
27	Cb	562	GLU
28	LB	214	GLU
29	LC	37	LYS
29	LC	223	VAL
30	LE	191	LYS
31	LG	73	LYS
31	LG	241	MET
32	LH	41	ILE
34	LL	58	VAL
34	LL	69	THR
34	LL	102	LYS
35	LM	14	VAL
35	LM	20	LEU
36	LN	23	LEU

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Mol	Chain	Res	Type
36	LN	170	LYS
38	LP	74	LYS
38	LP	112	LEU
38	LP	157	VAL
40	LS	96	GLU
40	LS	142	GLN
40	LS	161	THR
41	LT	126	VAL
41	LT	127	GLN
42	LV	39	ILE
42	LV	139	MET
44	LY	78	VAL
44	LY	86	ARG
45	Ld	20	TYR
45	Ld	85	ARG
45	Ld	102	GLN
46	Le	64	THR
50	Lj	58	VAL
52	Cc	106	VAL
53	Cd	213	LYS
53	Cd	277	GLU
53	Cd	343	VAL
53	Cd	361	VAL
54	Ce	73	MET
54	Ce	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	CA	25	ASN
4	CA	119	ASN
4	CA	121	HIS
5	CB	47	GLN
5	CB	249	ASN
6	CC	286	ASN
7	CE	235	ASN
7	CE	280	GLN
7	CE	443	HIS
8	CF	14	GLN
9	CG	18	ASN
10	CH	226	HIS
10	CH	258	GLN

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Mol	Chain	Res	Type
10	CH	306	ASN
10	CH	389	ASN
12	CJ	485	HIS
13	CK	3	GLN
13	CK	105	GLN
13	CK	190	ASN
13	CK	203	ASN
15	CM	119	ASN
15	CM	192	HIS
16	CN	79	GLN
16	CN	156	ASN
18	CP	322	GLN
18	CP	411	ASN
18	CP	485	HIS
18	CP	489	GLN
18	CP	499	ASN
19	CQ	24	ASN
19	CQ	58	ASN
20	CR	148	GLN
20	CR	196	GLN
20	CR	216	ASN
20	CR	220	GLN
23	CU	364	ASN
26	Cz	58	GLN
27	Cb	367	HIS
27	Cb	377	HIS
27	Cb	446	GLN
28	LB	109	HIS
28	LB	183	GLN
29	LC	60	GLN
29	LC	203	HIS
29	LC	205	GLN
29	LC	250	HIS
29	LC	315	GLN
30	LE	145	GLN
15	LF	206	ASN
31	LG	62	GLN
31	LG	140	ASN
31	LG	158	ASN
31	LG	246	GLN
32	LH	44	ASN
32	LH	96	HIS

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Mol	Chain	Res	Type
32	LH	102	ASN
32	LH	142	GLN
33	LK	65	GLN
33	LK	100	HIS
34	LL	17	HIS
34	LL	25	HIS
35	LM	110	GLN
36	LN	138	ASN
37	LO	27	GLN
38	LP	49	GLN
38	LP	72	GLN
38	LP	75	GLN
38	LP	121	GLN
38	LP	142	ASN
39	LQ	86	ASN
40	LS	21	ASN
41	LT	146	ASN
42	LV	76	HIS
44	LY	56	GLN
45	Ld	29	HIS
46	Le	79	ASN
48	Lh	37	GLN
49	Li	42	GLN
52	Cc	187	GLN
52	Cc	257	ASN
53	Cd	291	ASN
53	Cd	347	HIS
53	Cd	349	GLN
54	Ce	86	ASN
54	Ce	185	ASN
55	Cf	518	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2134/3341 (63%)	480 (22%)	15 (0%)
2	C2	157/256 (61%)	30 (19%)	1 (0%)
3	C3	96/161 (59%)	34 (35%)	0
All	All	2387/3758 (63%)	544 (22%)	16 (0%)

All (544) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	A
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	67	A
1	C1	73	A
1	C1	74	G
1	C1	85	A
1	C1	91	G
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	136	C
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	163	U
1	C1	176	U
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	204	A
1	C1	205	G
1	C1	206	A

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Mol	Chain	Res	Type
1	C1	211	G
1	C1	212	A
1	C1	214	A
1	C1	225	G
1	C1	241	G
1	C1	244	U
1	C1	249	C
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	300	A
1	C1	302	U
1	C1	308	U
1	C1	309	A
1	C1	310	A
1	C1	311	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	377	A
1	C1	382	G
1	C1	384	G
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	400	A
1	C1	413	G
1	C1	414	A
1	C1	430	A
1	C1	431	C

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Mol	Chain	Res	Type
1	C1	432	U
1	C1	433	U
1	C1	445	A
1	C1	446	U
1	C1	448	A
1	C1	449	U
1	C1	450	C
1	C1	457	U
1	C1	459	U
1	C1	460	C
1	C1	467	G
1	C1	468	C
1	C1	469	A
1	C1	474	G
1	C1	484	G
1	C1	485	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	558	G
1	C1	582	A
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G
1	C1	598	A
1	C1	608	A
1	C1	623	C
1	C1	633	A
1	C1	651	A
1	C1	652	A
1	C1	664	A
1	C1	668	U

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Mol	Chain	Res	Type
1	C1	678	A
1	C1	684	G
1	C1	692	A
1	C1	693	A
1	C1	699	G
1	C1	702	A
1	C1	703	A
1	C1	706	U
1	C1	707	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	731	G
1	C1	739	C
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	767	A
1	C1	787	A
1	C1	796	G
1	C1	798	A
1	C1	907	A
1	C1	918	G
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	940	C
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	958	A
1	C1	960	C
1	C1	961	U

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Mol	Chain	Res	Type
1	C1	965	G
1	C1	973	A
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	979	A
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1043	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1063	C
1	C1	1069	G
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1097	G
1	C1	1098	G
1	C1	1114	C
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1163	U
1	C1	1164	G
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1180	C
1	C1	1181	C
1	C1	1182	A
1	C1	1184	A

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Mol	Chain	Res	Type
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1203	U
1	C1	1204	G
1	C1	1211	G
1	C1	1218	G
1	C1	1221	C
1	C1	1223	U
1	C1	1224	G
1	C1	1226	A
1	C1	1227	A
1	C1	1228	G
1	C1	1238	G
1	C1	1240	U
1	C1	1241	A
1	C1	1245	A
1	C1	1246	C
1	C1	1247	U
1	C1	1253	A
1	C1	1254	C
1	C1	1268	A
1	C1	1269	A
1	C1	1271	G
1	C1	1272	U
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1362	G

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Mol	Chain	Res	Type
1	C1	1368	A
1	C1	1369	G
1	C1	1373	C
1	C1	1374	G
1	C1	1381	A
1	C1	1382	G
1	C1	1399	G
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1433	C
1	C1	1856	U
1	C1	1859	U
1	C1	1864	C
1	C1	1865	A
1	C1	1866	A
1	C1	1868	G
1	C1	1875	A
1	C1	1883	C
1	C1	1884	G
1	C1	1886	C
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	2075	A
1	C1	2088	A
1	C1	2287	G
1	C1	2288	A
1	C1	2293	C
1	C1	2294	A
1	C1	2297	G
1	C1	2302	U
1	C1	2309	U
1	C1	2325	A
1	C1	2332	G
1	C1	2334	A
1	C1	2335	A
1	C1	2338	G
1	C1	2339	G
1	C1	2356	G
1	C1	2365	G

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Mol	Chain	Res	Type
1	C1	2384	C
1	C1	2394	A
1	C1	2396	U
1	C1	2397	G
1	C1	2402	A
1	C1	2406	C
1	C1	2415	U
1	C1	2422	U
1	C1	2423	A
1	C1	2424	G
1	C1	2426	U
1	C1	2428	G
1	C1	2429	G
1	C1	2430	A
1	C1	2431	G
1	C1	2435	C
1	C1	2436	G
1	C1	2439	G
1	C1	2445	G
1	C1	2449	U
1	C1	2452	C
1	C1	2453	A
1	C1	2456	A
1	C1	2465	G
1	C1	2467	U
1	C1	2469	U
1	C1	2476	U
1	C1	2477	A
1	C1	2482	A
1	C1	2551	A
1	C1	2552	C
1	C1	2553	A
1	C1	2564	G
1	C1	2568	G
1	C1	2730	C
1	C1	2739	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2766	A
1	C1	2767	C

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Mol	Chain	Res	Type
1	C1	2776	U
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2800	U
1	C1	2802	C
1	C1	2803	A
1	C1	2804	U
1	C1	2805	A
1	C1	2807	C
1	C1	2818	U
1	C1	2819	U
1	C1	2831	U
1	C1	2832	G
1	C1	2833	U
1	C1	2834	C
1	C1	2835	G
1	C1	2836	G
1	C1	2845	A
1	C1	2847	C
1	C1	2852	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2879	U
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2900	C
1	C1	2901	G
1	C1	2916	A
1	C1	2917	C
1	C1	2923	U
1	C1	2924	G
1	C1	2926	G
1	C1	2929	A
1	C1	2930	G
1	C1	2935	G

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Mol	Chain	Res	Type
1	C1	2936	U
1	C1	2950	U
1	C1	2956	C
1	C1	2968	A
1	C1	2969	A
1	C1	2970	U
1	C1	2980	U
1	C1	3006	A
1	C1	3013	U
1	C1	3014	U
1	C1	3015	U
1	C1	3033	C
1	C1	3034	A
1	C1	3035	G
1	C1	3037	G
1	C1	3048	A
1	C1	3049	C
1	C1	3050	C
1	C1	3057	U
1	C1	3066	G
1	C1	3070	A
1	C1	3077	C
1	C1	3079	A
1	C1	3084	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3108	U
1	C1	3109	A
1	C1	3113	C
1	C1	3118	A
1	C1	3126	G
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3144	C
1	C1	3146	G
1	C1	3147	G

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Mol	Chain	Res	Type
1	C1	3154	A
1	C1	3157	C
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3179	G
1	C1	3183	C
1	C1	3185	A
1	C1	3187	G
1	C1	3189	G
1	C1	3199	A
1	C1	3205	C
1	C1	3211	G
1	C1	3212	C
1	C1	3213	A
1	C1	3214	A
1	C1	3225	C
1	C1	3228	G
1	C1	3232	U
1	C1	3244	C
1	C1	3248	C
1	C1	3249	G
1	C1	3253	U
1	C1	3256	A
1	C1	3257	U
1	C1	3258	G
1	C1	3260	G
1	C1	3262	G
1	C1	3263	A
1	C1	3264	A
1	C1	3270	C
1	C1	3274	U
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3290	C
1	C1	3291	U
1	C1	3292	U
1	C1	3295	U

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Mol	Chain	Res	Type
1	C1	3296	G
1	C1	3297	U
1	C1	3298	U
1	C1	3302	A
1	C1	3309	G
1	C1	3310	A
1	C1	3318	C
1	C1	3321	U
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3329	C
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	34	U
2	C2	35	C
2	C2	49	G
2	C2	51	G
2	C2	53	A
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	77	A
2	C2	78	G
2	C2	81	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	100	U
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	111	A
2	C2	113	U
2	C2	124	G
2	C2	126	A

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Mol	Chain	Res	Type
2	C2	127	U
2	C2	129	C
2	C2	136	G
2	C2	152	G
2	C2	158	U
3	C3	5	C
3	C3	6	A
3	C3	7	U
3	C3	8	C
3	C3	15	U
3	C3	16	G
3	C3	17	G
3	C3	21	U
3	C3	25	U
3	C3	26	U
3	C3	31	A
3	C3	32	C
3	C3	48	G
3	C3	54	G
3	C3	55	A
3	C3	56	A
3	C3	57	A
3	C3	59	G
3	C3	60	C
3	C3	61	A
3	C3	63	U
3	C3	64	G
3	C3	68	G
3	C3	71	U
3	C3	72	C
3	C3	73	G
3	C3	75	U
3	C3	130	G
3	C3	133	G
3	C3	134	C
3	C3	137	G
3	C3	141	U
3	C3	143	A
3	C3	144	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	308	U
1	C1	519	A
1	C1	1044	A
1	C1	1046	A
1	C1	1220	C
1	C1	2301	C
1	C1	2929	A
1	C1	3078	U
1	C1	3162	A
1	C1	3204	G
1	C1	3257	U
1	C1	3263	A
1	C1	3296	G
1	C1	3297	U
2	C2	123	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	GTP	CH	701	-	33,34,34	0.89	1 (3%)	50,54,54	1.61	9 (18%)

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
56	GTP	CH	701	-	-	6/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CH	701	GTP	C2-N3	2.10	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	CH	701	GTP	C5-C4-N3	-5.11	120.26	128.39
56	CH	701	GTP	C2-N3-C4	4.62	120.27	112.30
56	CH	701	GTP	N9-C4-N3	3.35	132.65	125.95
56	CH	701	GTP	C2-N1-C6	-2.92	119.81	125.11
56	CH	701	GTP	N9-C8-N7	-2.55	108.67	113.40
56	CH	701	GTP	C5-C6-N1	2.46	119.51	113.25
56	CH	701	GTP	C8-N7-C5	2.41	108.55	104.26
56	CH	701	GTP	O6-C6-C5	-2.36	120.31	126.53
56	CH	701	GTP	C3'-C2'-C1'	2.11	105.46	101.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	CH	701	GTP	PB-O3B-PG-O2G
56	CH	701	GTP	PB-O3B-PG-O3G
56	CH	701	GTP	C5'-O5'-PA-O3A
56	CH	701	GTP	C4'-C5'-O5'-PA
56	CH	701	GTP	C5'-O5'-PA-O2A
56	CH	701	GTP	C3'-C4'-C5'-O5'

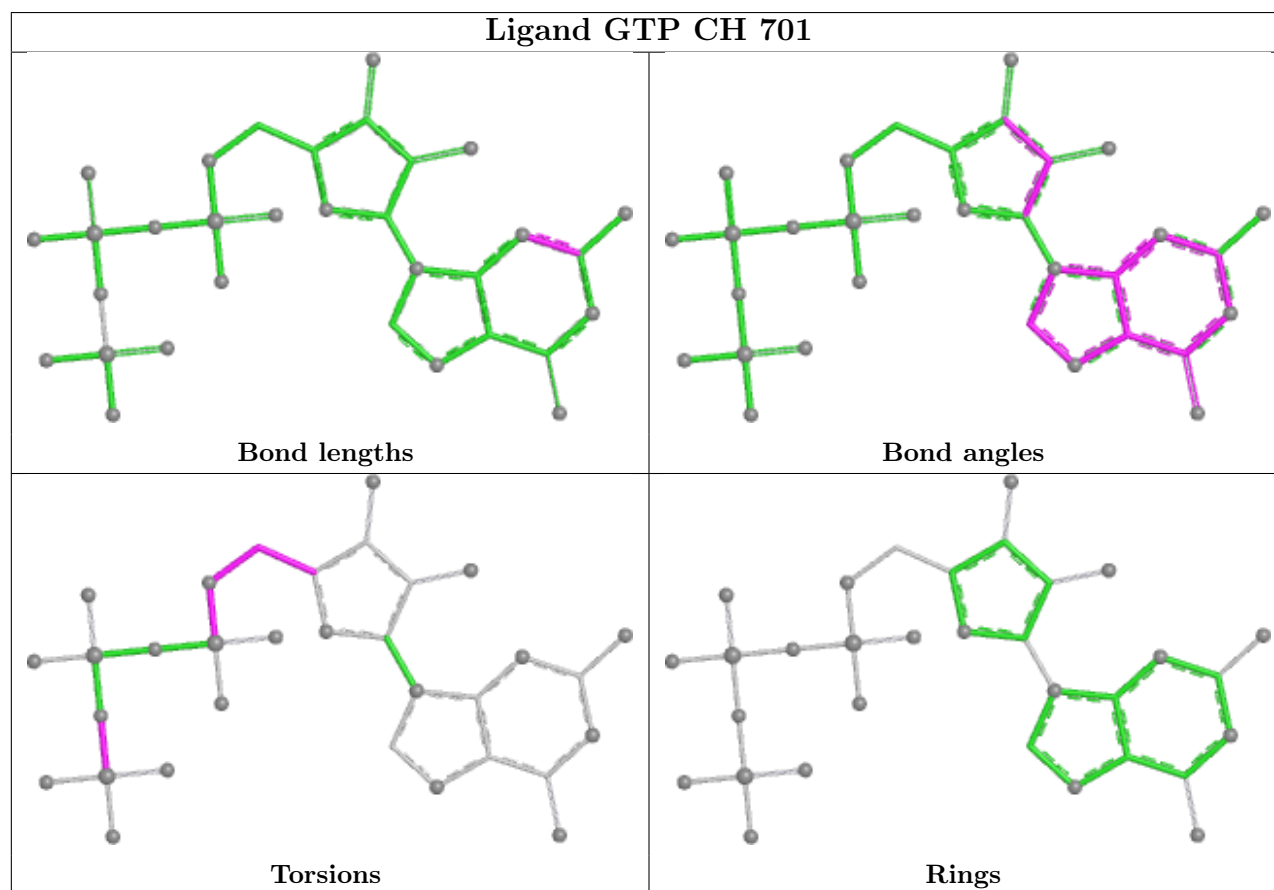
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CH	701	GTP	1	0

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.

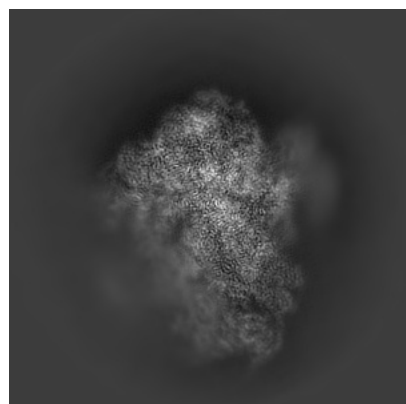
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35285. These allow visual inspection of the internal detail of the map and identification of artifacts.

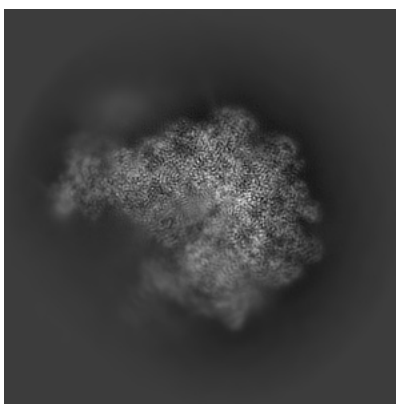
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

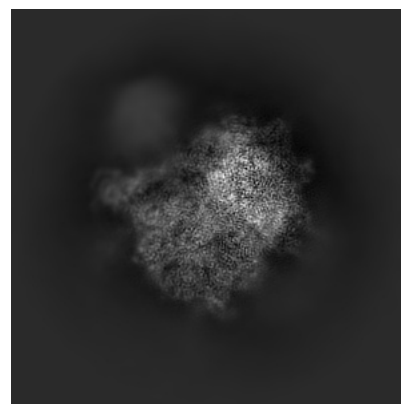
6.1.1 Primary map



X

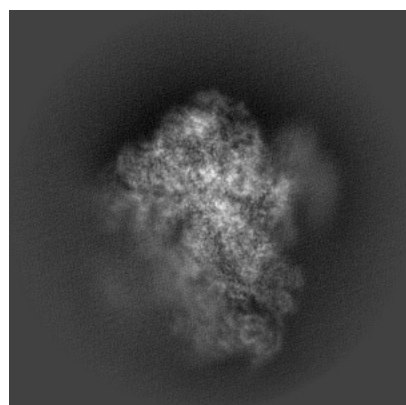


Y

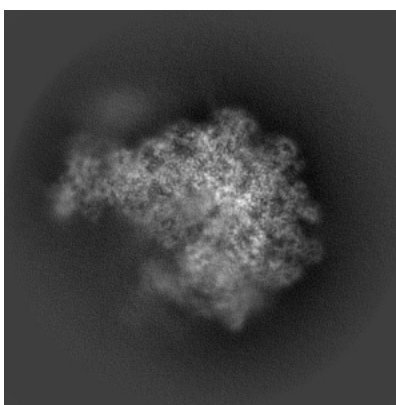


Z

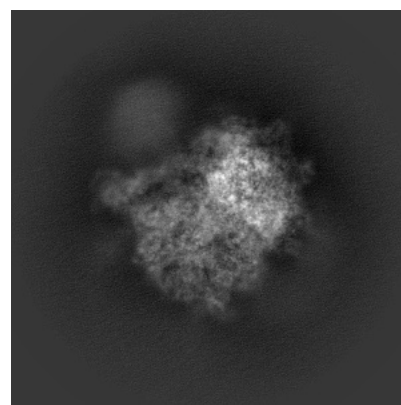
6.1.2 Raw map



X



Y

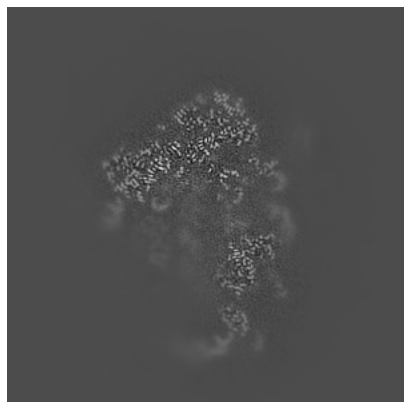


Z

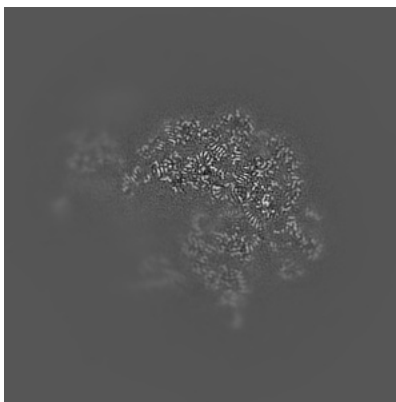
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

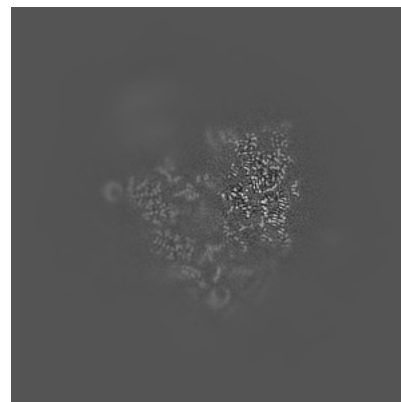
6.2.1 Primary map



X Index: 210

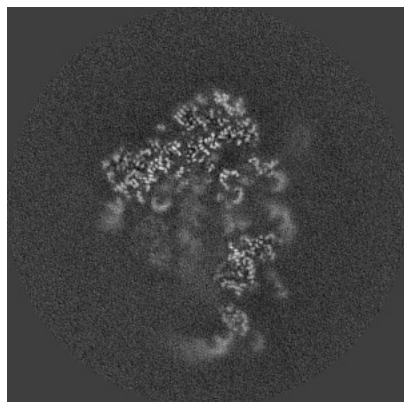


Y Index: 210

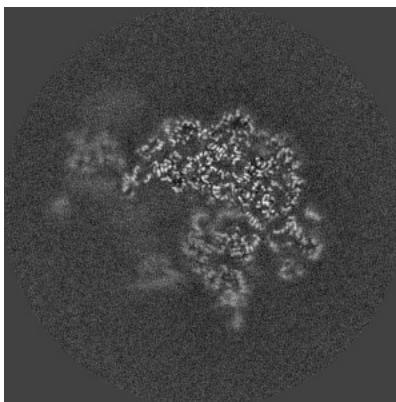


Z Index: 210

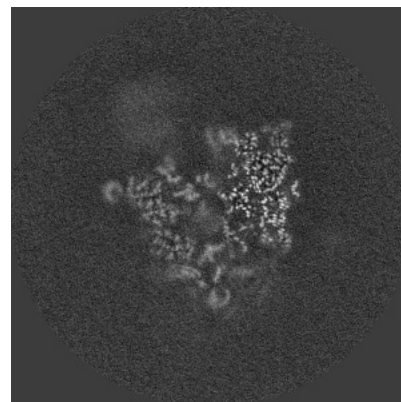
6.2.2 Raw map



X Index: 210



Y Index: 210

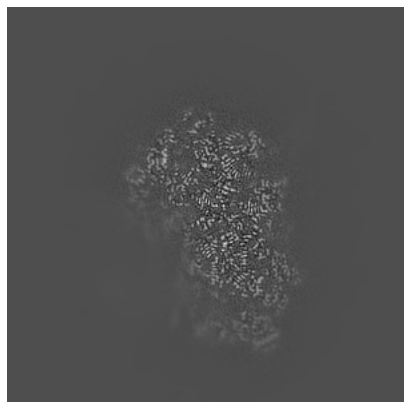


Z Index: 210

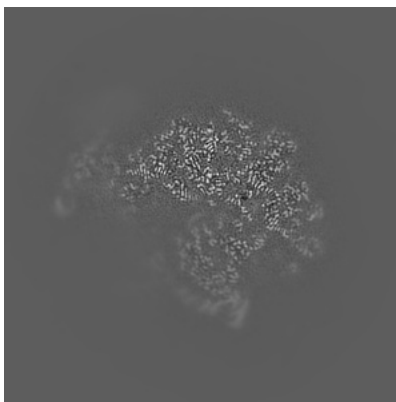
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

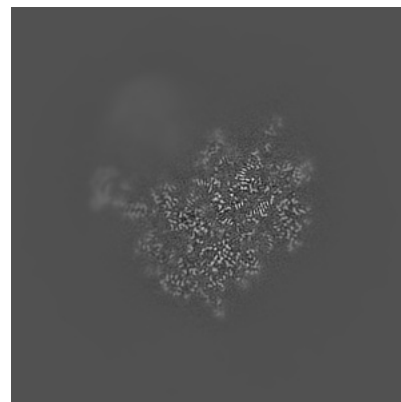
6.3.1 Primary map



X Index: 247

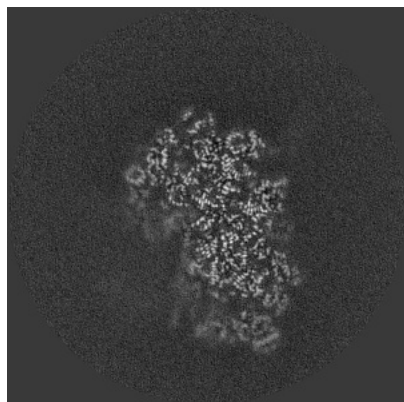


Y Index: 217

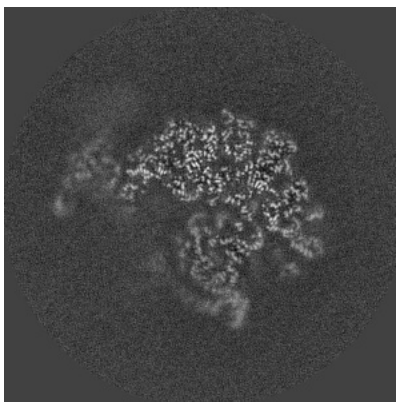


Z Index: 247

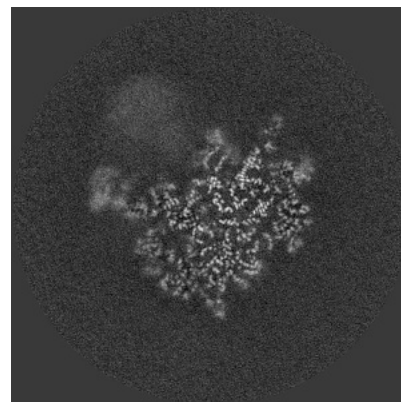
6.3.2 Raw map



X Index: 247



Y Index: 216

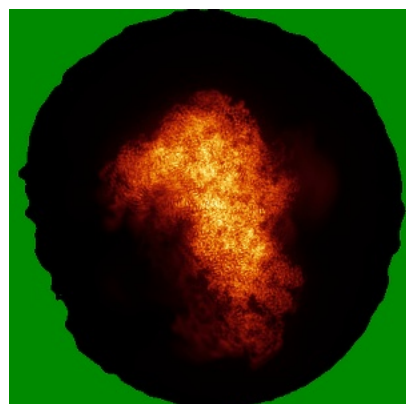


Z Index: 246

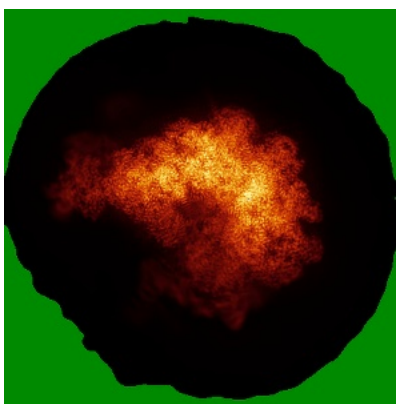
The images above show the largest variance slices of the map in three orthogonal directions.

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

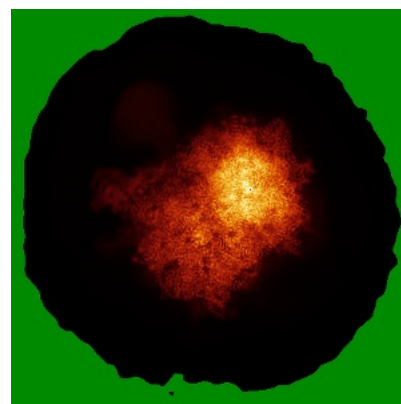
6.4.1 Primary map



X

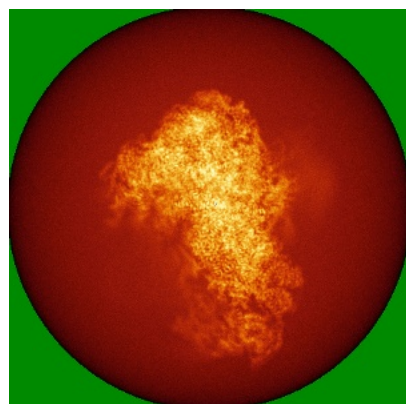


Y

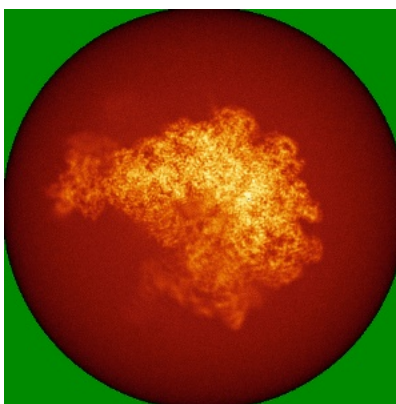


Z

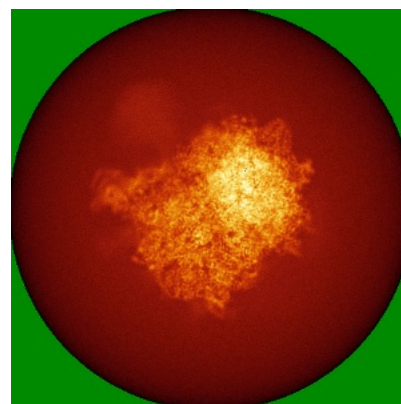
6.4.2 Raw map



X



Y

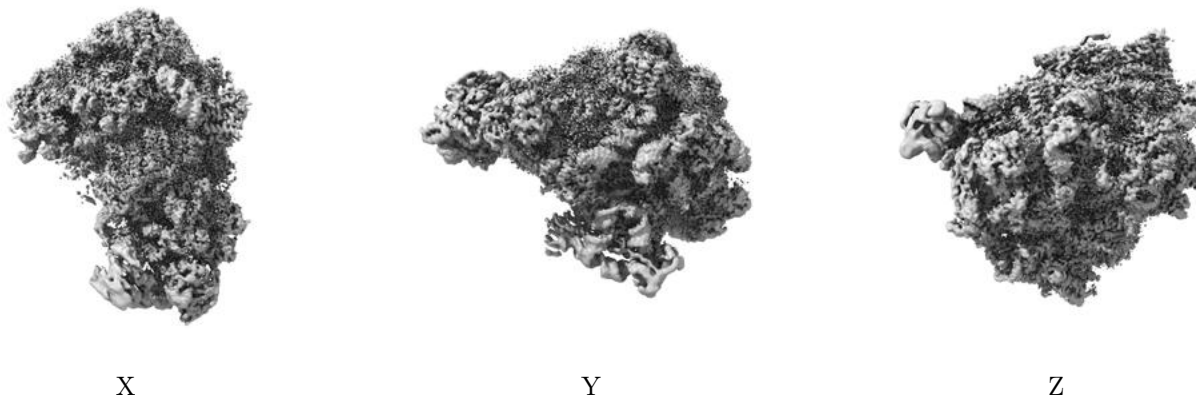


Z

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

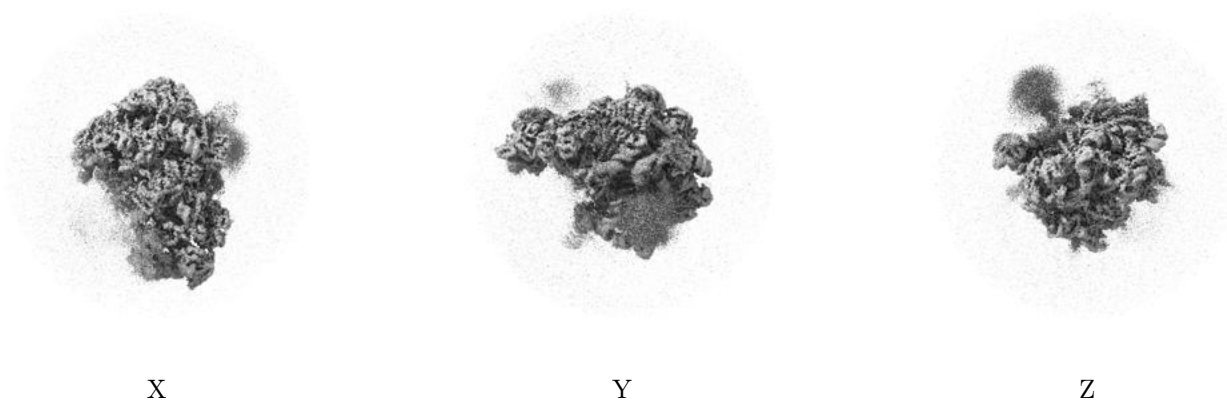
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

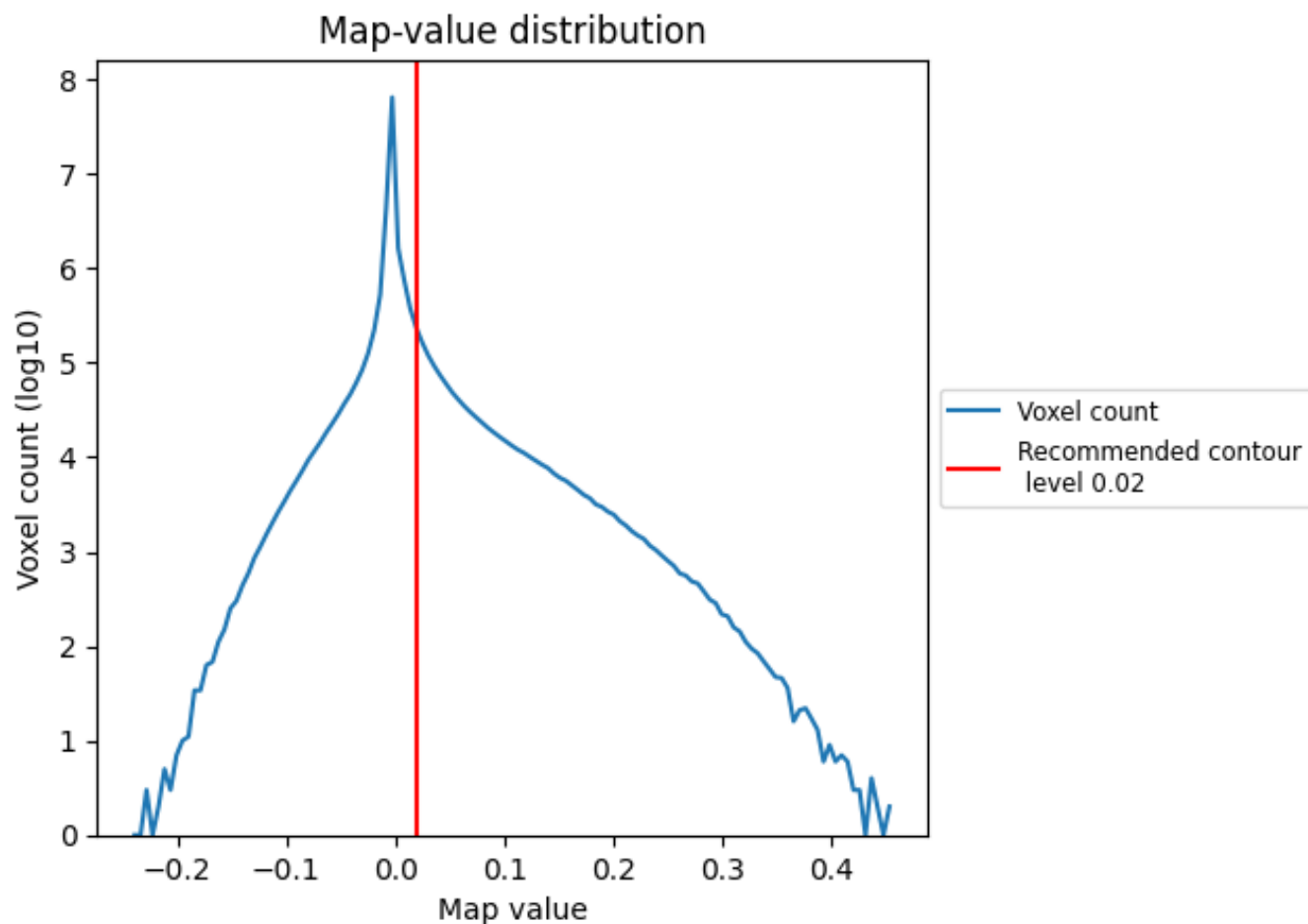
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

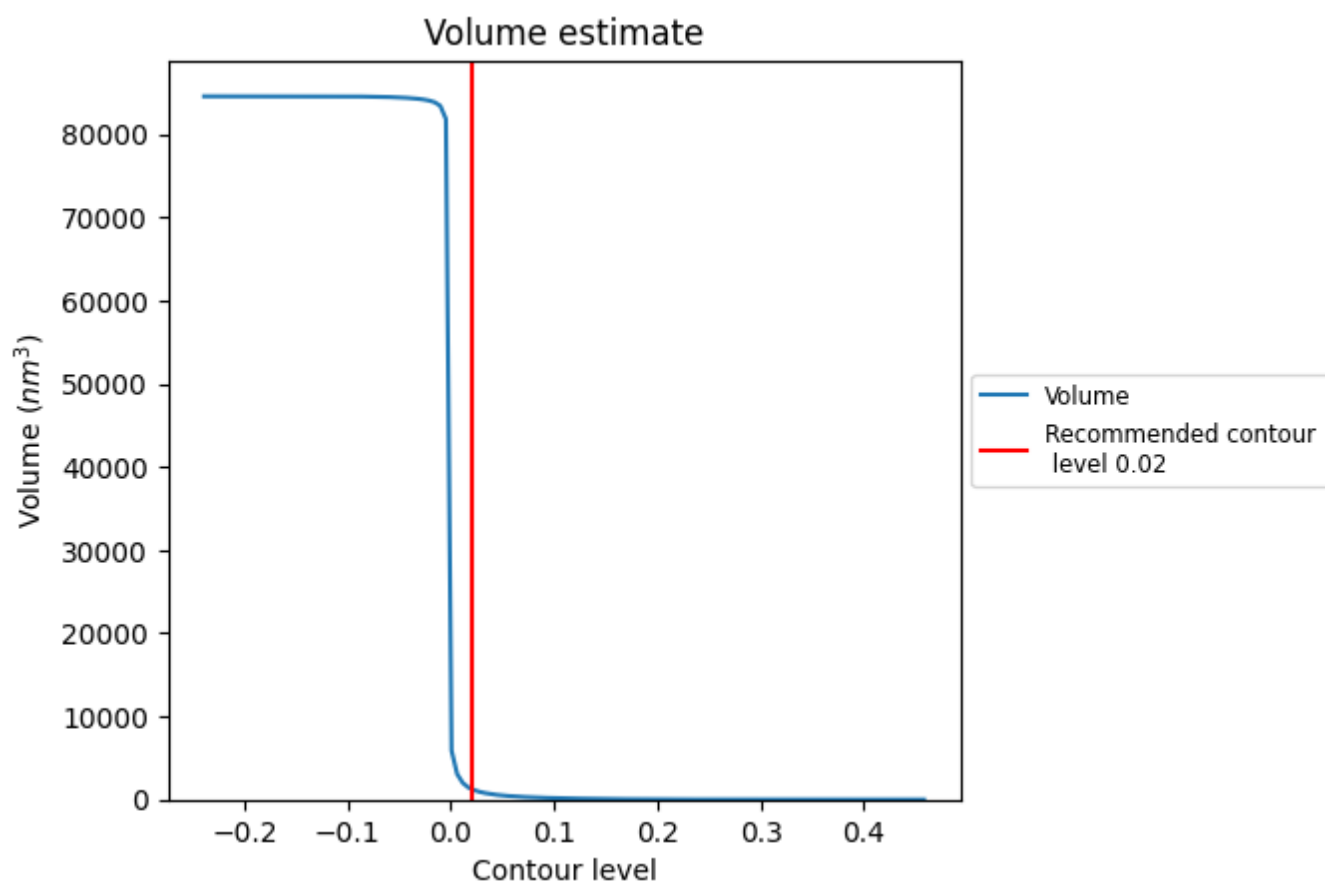
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

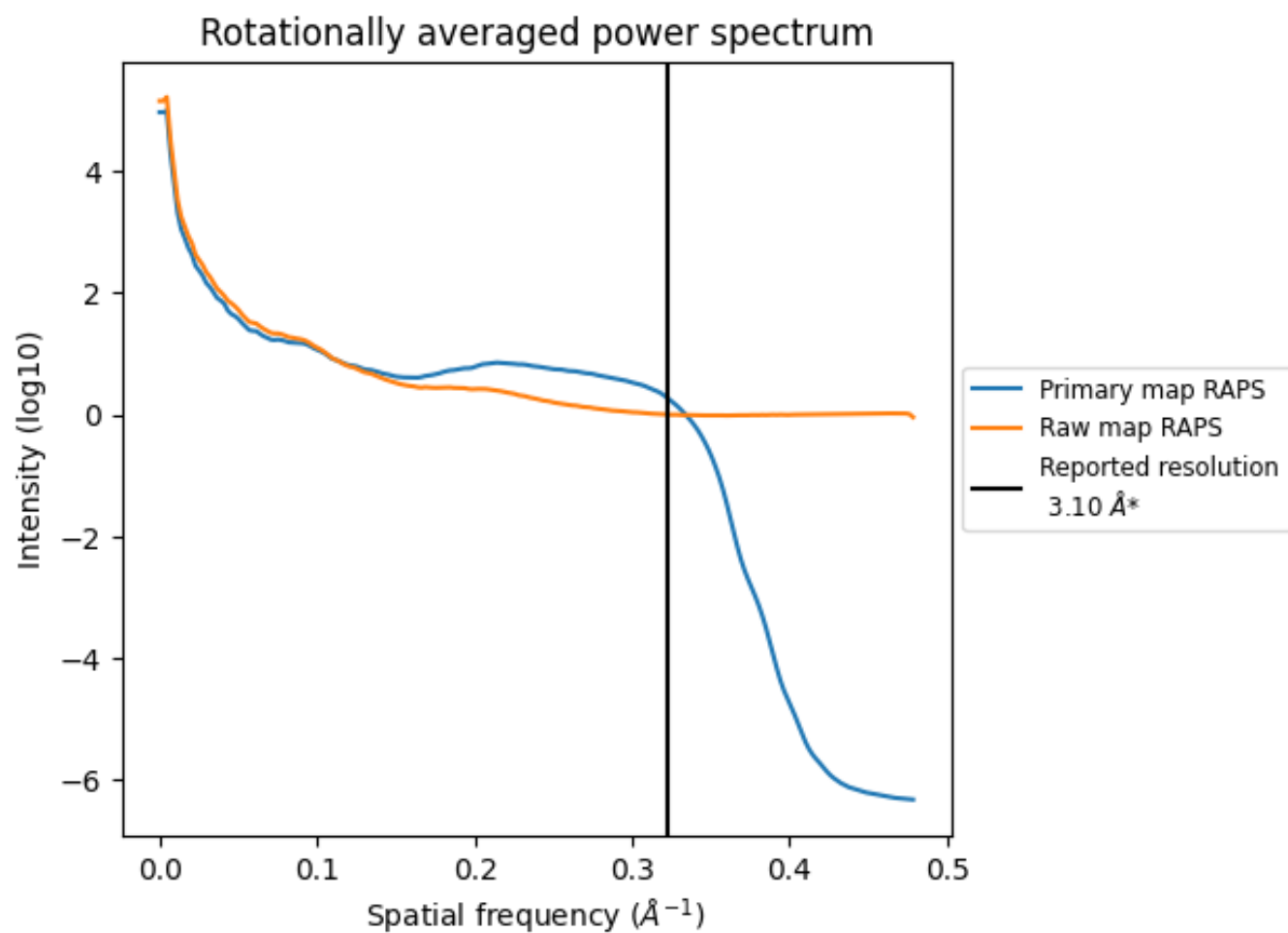
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1277 nm^3 ; this corresponds to an approximate mass of 1154 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 ⓘ

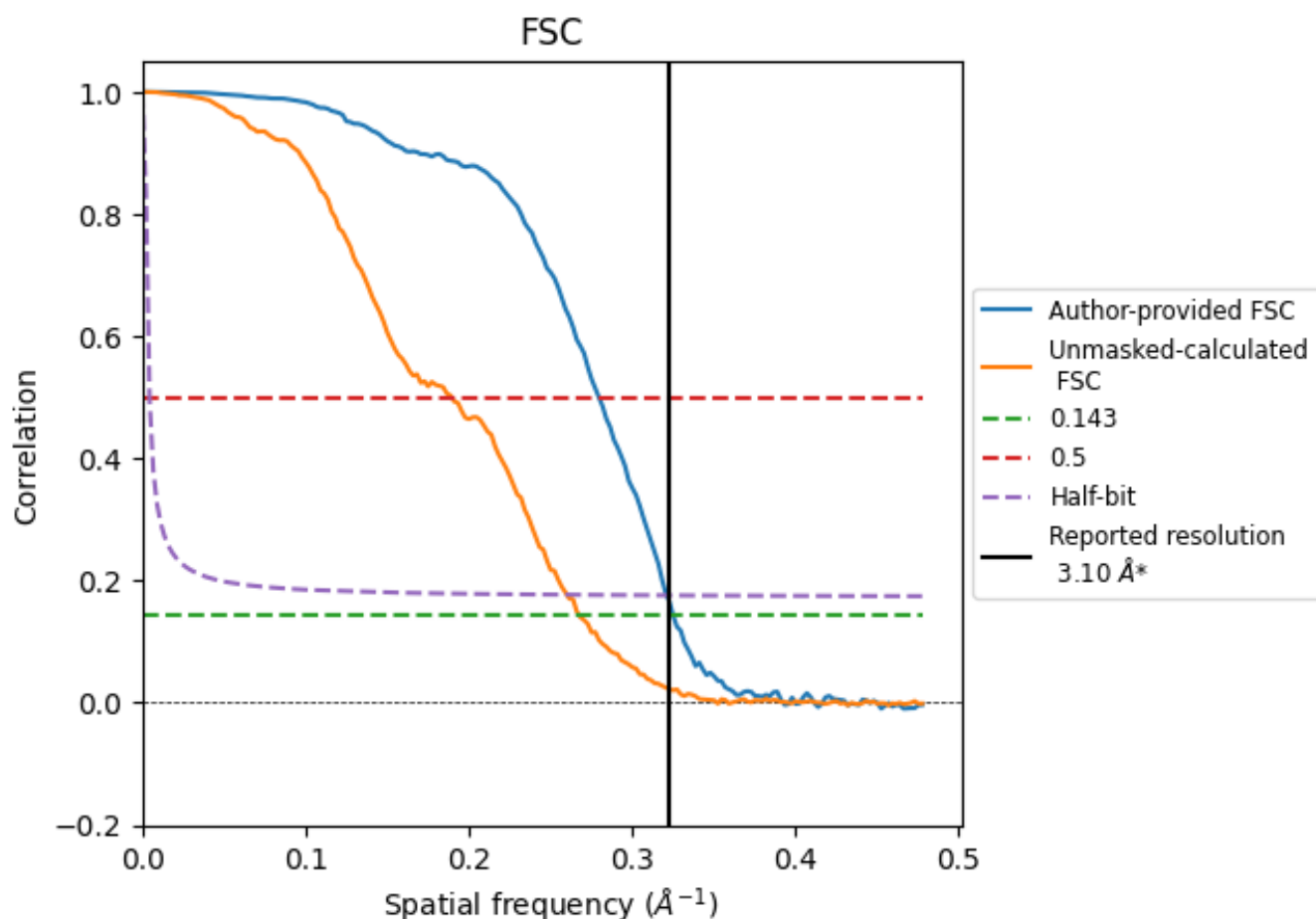


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

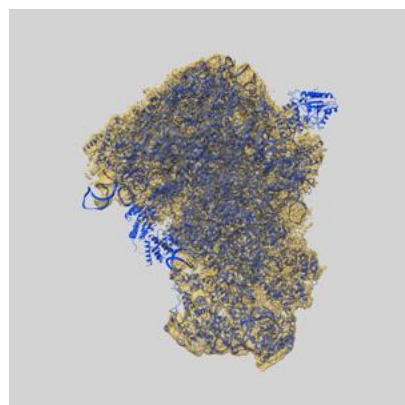
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.57	3.11
Unmasked-calculated*	3.73	5.27	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.1 by more than 10 %

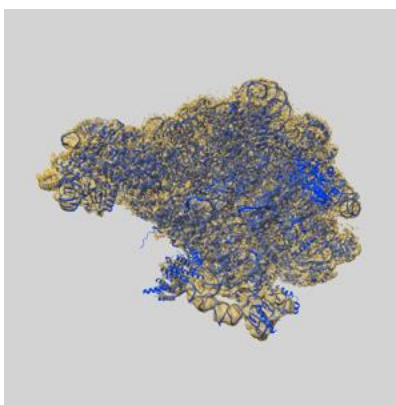
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35285 and PDB model 8I9V. Per-residue inclusion information can be found in section 3 on page 17.

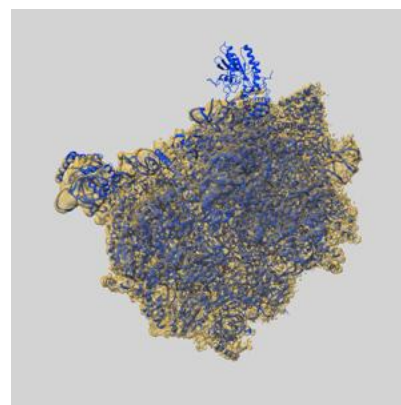
9.1 Map-model overlay [i](#)



X



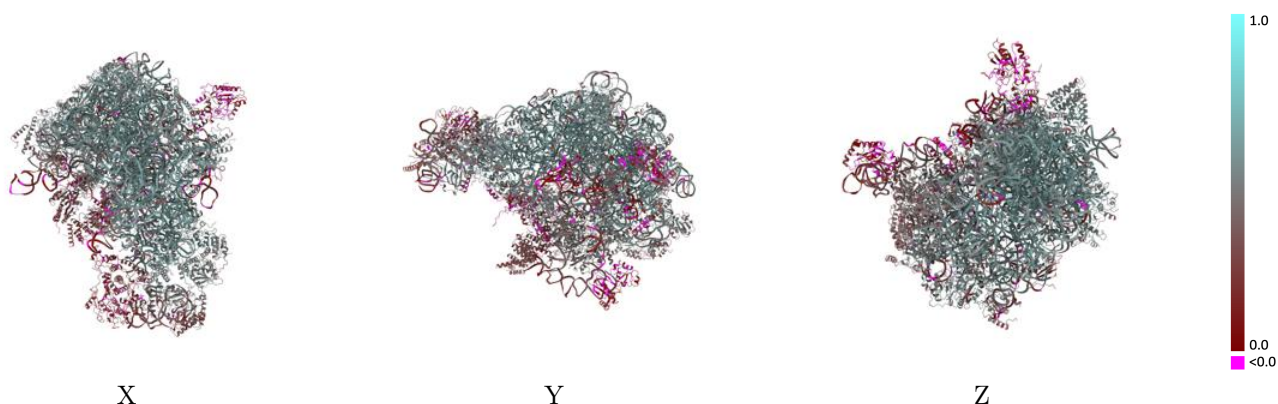
Y



Z

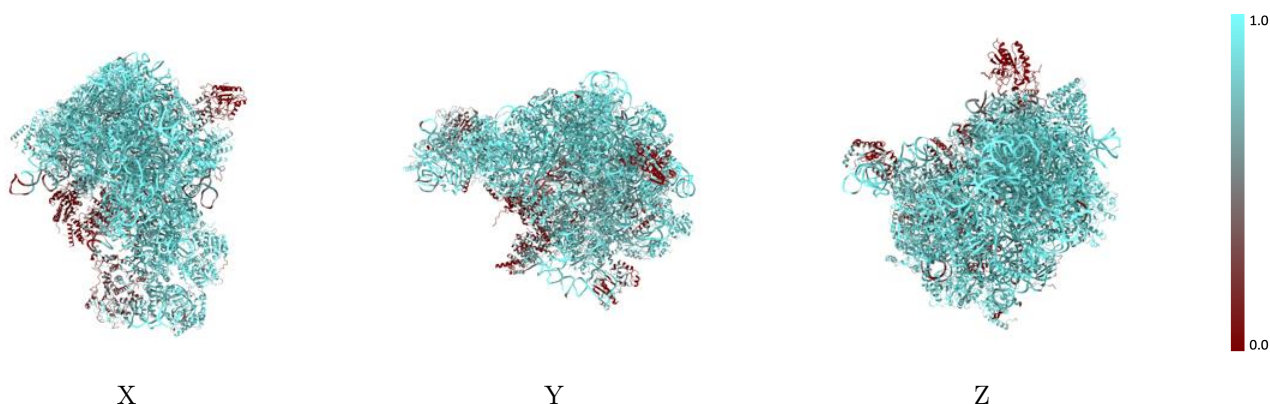
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



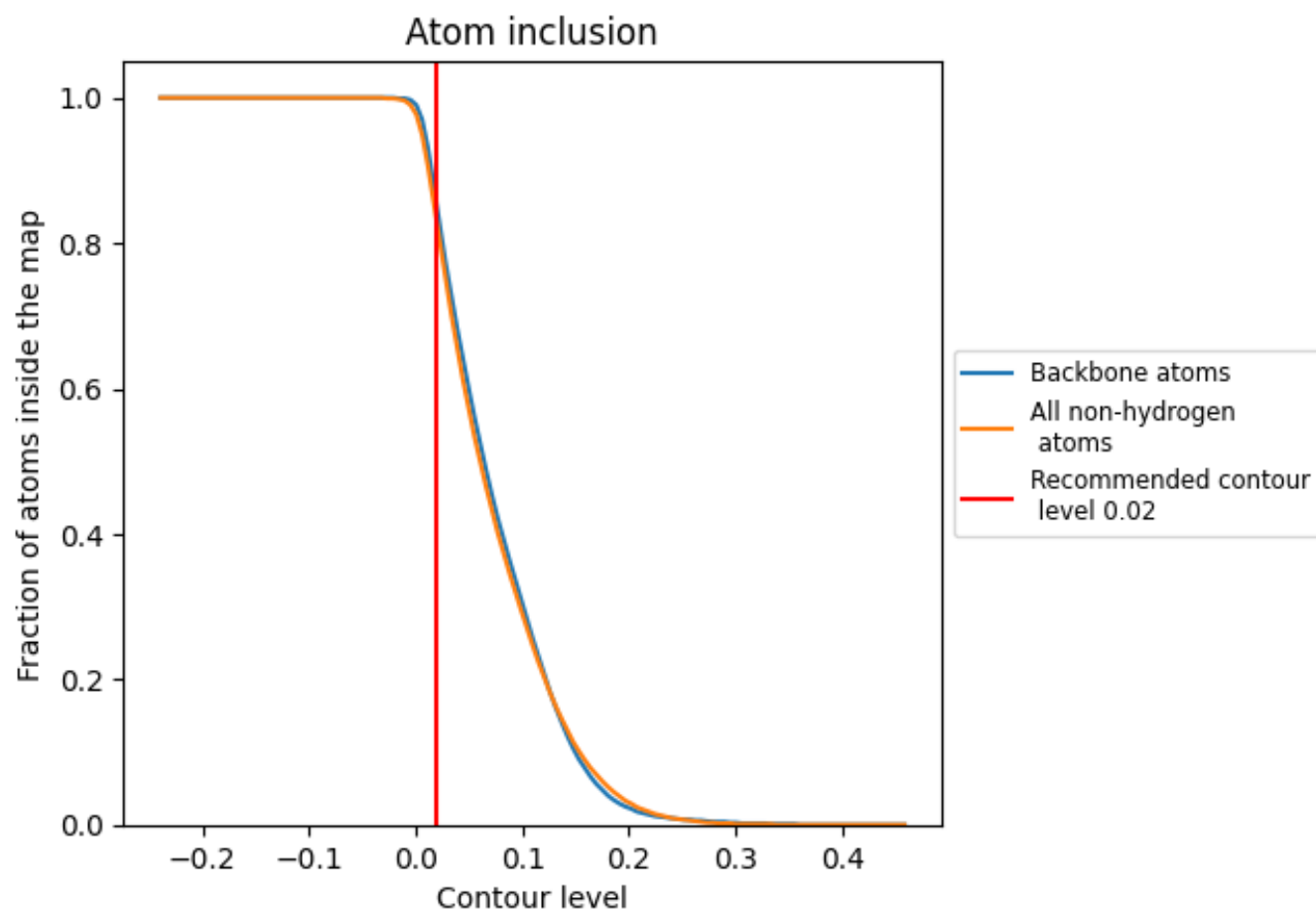
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.4600
C1	 0.9160	 0.4920
C2	 0.8890	 0.4890
C3	 0.8700	 0.3460
CA	 0.9100	 0.5190
CB	 0.7890	 0.3810
CC	 0.5130	 0.2890
CE	 0.8820	 0.4970
CF	 0.8700	 0.4630
CG	 0.7850	 0.4060
CH	 0.8810	 0.4950
CI	 0.8400	 0.4180
CJ	 0.4520	 0.1900
CK	 0.8500	 0.4840
CL	 0.3040	 0.1920
CM	 0.6100	 0.2570
CN	 0.8960	 0.5130
CO	 0.9340	 0.5560
CP	 0.8240	 0.4390
CQ	 0.9170	 0.5070
CR	 0.9130	 0.5330
CS	 0.0980	 0.2140
CT	 0.2590	 0.2500
CU	 0.8290	 0.4480
CX	 0.3990	 0.1990
CY	 0.4070	 0.2780
Cb	 0.7750	 0.4150
Cc	 0.8570	 0.5040
Cd	 0.9220	 0.5390
Ce	 0.9420	 0.5730
Cf	 0.6860	 0.3770
Cz	 0.6190	 0.3280
LB	 0.9320	 0.5570
LC	 0.9480	 0.5860
LE	 0.9180	 0.5360



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Chain	Atom inclusion	Q-score
LF	 0.9230	 0.5600
LG	 0.8410	 0.5040
LH	 0.9300	 0.5580
LK	 0.8110	 0.3740
LL	 0.9530	 0.5840
LM	 0.9440	 0.5590
LN	 0.9430	 0.5890
LO	 0.9520	 0.5830
LP	 0.9240	 0.5510
LQ	 0.9390	 0.5720
LS	 0.9310	 0.5570
LT	 0.7100	 0.3300
LV	 0.8870	 0.5150
LX	 0.3240	 0.2180
LY	 0.9190	 0.5550
Ld	 0.6000	 0.2850
Le	 0.9510	 0.5970
Lf	 0.9530	 0.5990
Lh	 0.8630	 0.4980
Li	 0.8880	 0.5080
Lj	 0.9590	 0.5960
Lq	 0.3400	 0.0810