



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

PDB ID : 7BT6 / pdb_00007bt6
EMDB ID : EMD-30170
Title : Cryo-EM structure of pre-60S ribosome from *Saccharomyces cerevisiae* rpl4delta63-87 strain at 3.12 Angstroms resolution(state R1)
Authors : Li, Y.; Wilson, D.M.
Deposited on : 2020-03-31
Resolution : 3.12 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:

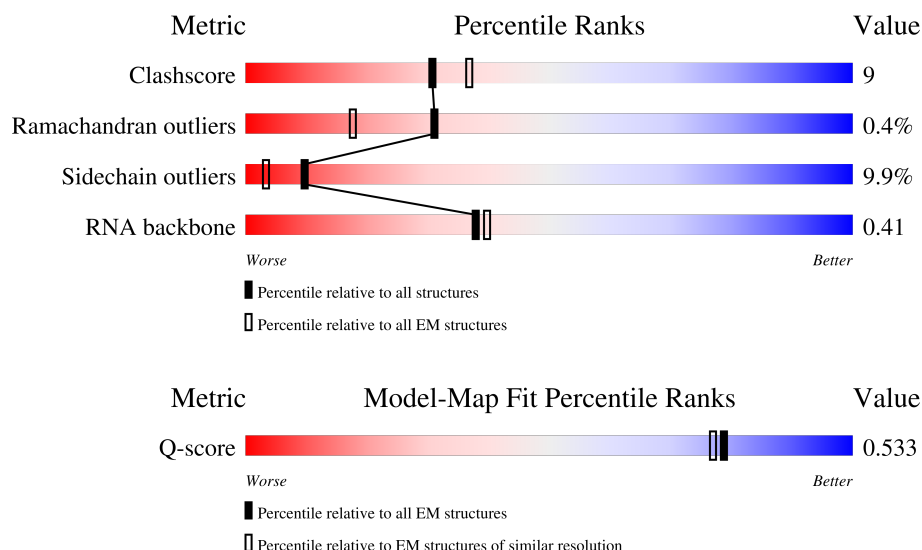
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.12 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	14478 (2.62 - 3.62)

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	A	254	
2	B	387	
3	C	362	

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	176	
6	F	244	
7	G	256	
8	H	191	
9	J	174	
10	L	199	
11	M	138	
12	N	204	
13	O	199	
14	P	184	
15	Q	186	
16	R	189	
17	S	172	
18	T	160	
19	U	121	
20	V	137	
21	W	236	
22	X	142	
23	Y	127	
24	Z	136	
25	a	149	
26	b	647	
27	c	105	
28	d	113	

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Mol	Chain	Length	Quality of chain
29	e	130	
30	f	107	
31	g	121	
32	h	120	
33	i	100	
34	j	88	
35	k	78	
36	m	486	
37	p	92	
38	r	261	
39	u	199	
40	v	344	
41	w	203	
42	x	515	
43	y	245	
44	z	106	
45	1	3396	
46	2	158	
47	3	121	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 133299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	178	Total	C	N	O	0	0
			1377	869	269	239		

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 3 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	334	Total	C	N	O	S	0	0
			2559	1619	478	459	3		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	271	Total	C	N	O	S	0	0
			2176	1376	384	414	2		

- Molecule 5 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 6 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	162	Total	C	N	O	S	0	0
			1249	801	213	233	2		

- Molecule 8 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 10 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	182	Total	C	N	O	0	0
			1459	907	300	252		

- Molecule 11 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 12 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	183	Total	C	N	O	S	0	0
			1570	984	332	253	1		

- Molecule 13 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 14 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	P	183	Total	C	N	O	0	0
			1442	896	287	259		

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 16 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	154	Total	C	N	O	0	0
			1241	772	262	207		

- Molecule 17 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 18 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	119	Total	C	N	O	S	0	0
			943	595	180	165	3		

- Molecule 19 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	102	Total	C	N	O	0	0
			812	526	134	152		

- Molecule 20 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	135	Total	C	N	O	S	0	0
			997	625	188	177	7		

- Molecule 21 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 22 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	86	Total	C	N	O	S	0	0
			687	441	114	130	2		

- Molecule 23 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 25 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 26 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	510	Total	C	N	O	S	0	0
			4146	2629	726	773	18		

- Molecule 27 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 28 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	106	Total	C	N	O	S	0	0
			865	549	164	151	1		

- Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 30 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 31 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	104	Total	C	N	O	S	0	0
			819	509	168	138	4		

- Molecule 32 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	97	Total	C	N	O	S	0	0
			750	469	149	130	2		

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	77	Total	C	N	O	S	0	0
			603	365	131	102	5		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 36 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	452	Total	C	N	O	S	0	0
			3639	2302	655	673	9		

- Molecule 37 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 39 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	144	Total	C	N	O	S	0	0
			1216	763	245	199	9		

- Molecule 40 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 41 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 42 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	x	488	Total	C	N	O	S	0	0
			3807	2398	677	711	21		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 44 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 45 is a RNA chain called RDN25-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	2962	Total	C	N	O	P	0	0
			63385	28311	11449	20663	2962		

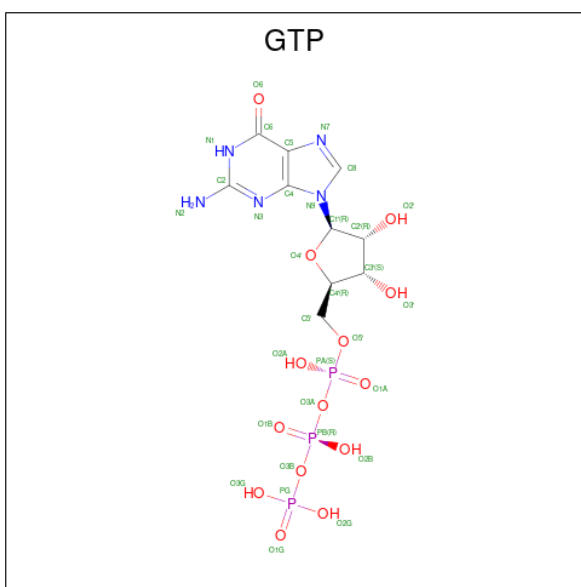
- Molecule 46 is a RNA chain called RDN5.8-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 47 is a RNA chain called RDN5-2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
48	b	1	Total 32	C 10	N 5	O 14	P 3	0
48	m	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
49	b	1	Total Mg 1 1	0
49	m	1	Total Mg 1 1	0

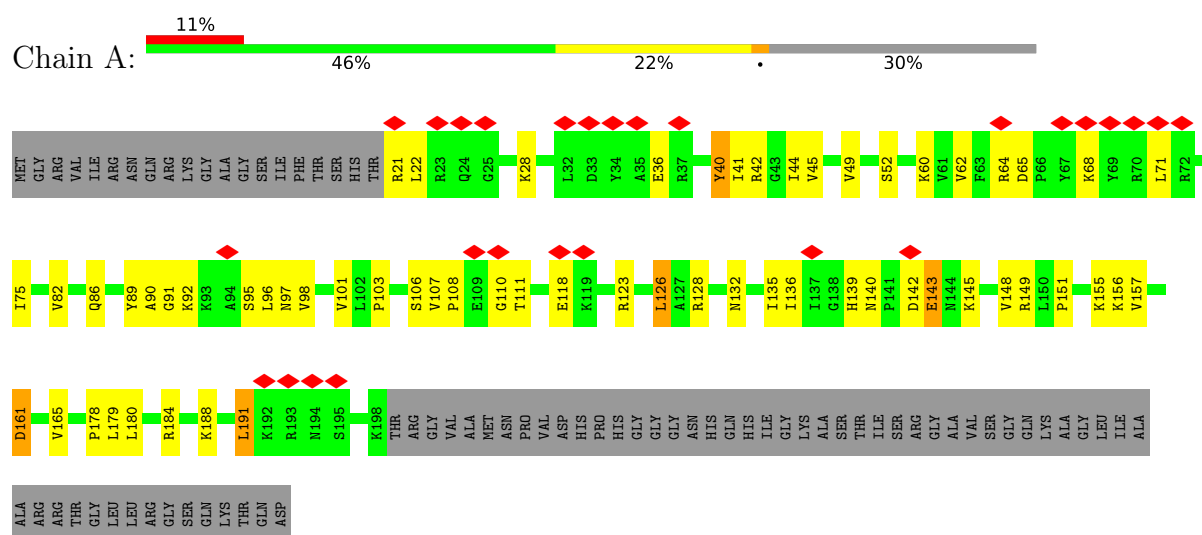
- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
50	j	1	Total Zn 1 1	0
50	p	1	Total Zn 1 1	0
50	u	1	Total Zn 1 1	0

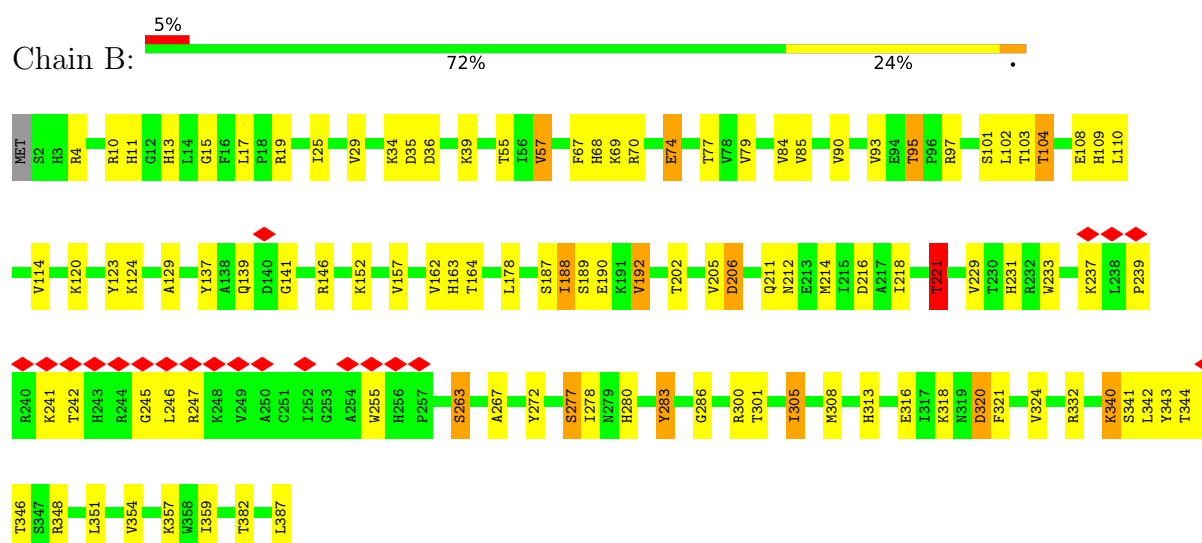
3 Residue-property plots

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

• Molecule 1: 60S ribosomal protein L2-A

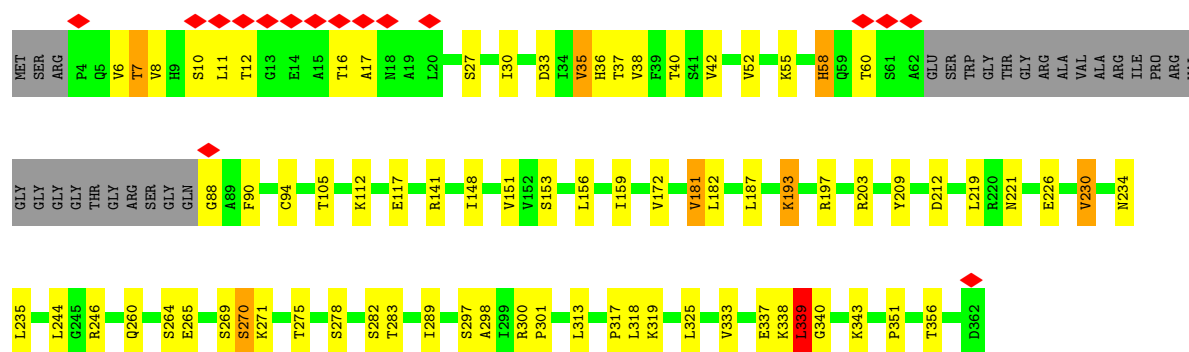


• Molecule 2: 60S ribosomal protein L3



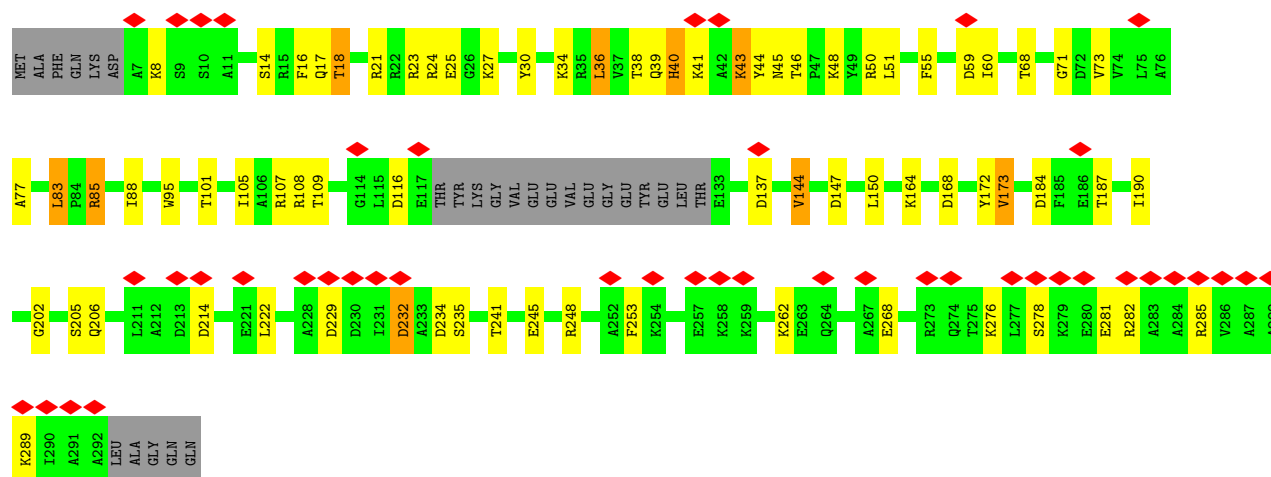
• Molecule 3: 60S ribosomal protein L4-A

Chain C:  71% 19% 8%



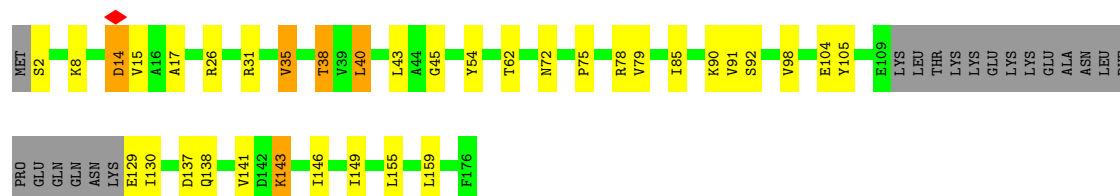
• Molecule 4: 60S ribosomal protein L5

Chain D:  15% 67% 22% 9%



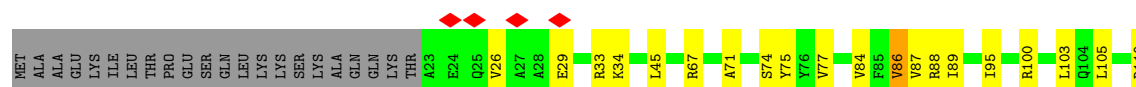
• Molecule 5: 60S ribosomal protein L6-A

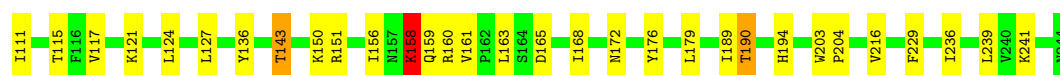
Chain E:  69% 17% 11%



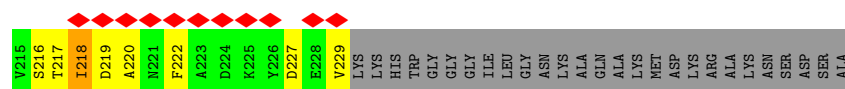
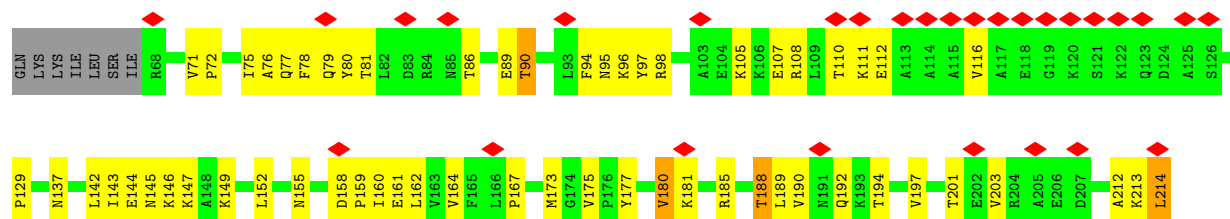
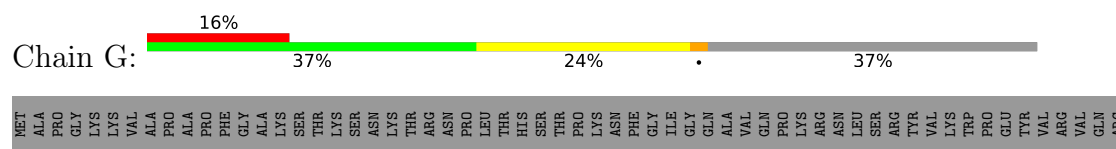
• Molecule 6: 60S ribosomal protein L7-A

Chain F:  70% 19% 9%

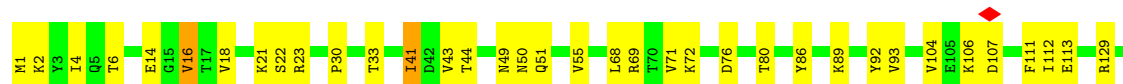




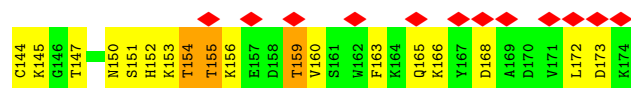
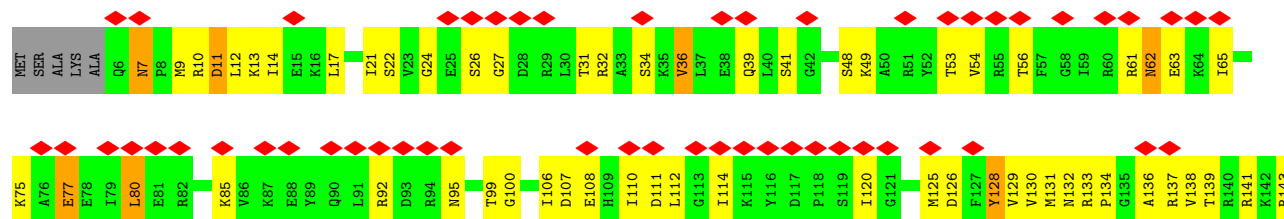
• Molecule 7: 60S ribosomal protein L8-A



• Molecule 8: 60S ribosomal protein L9-A

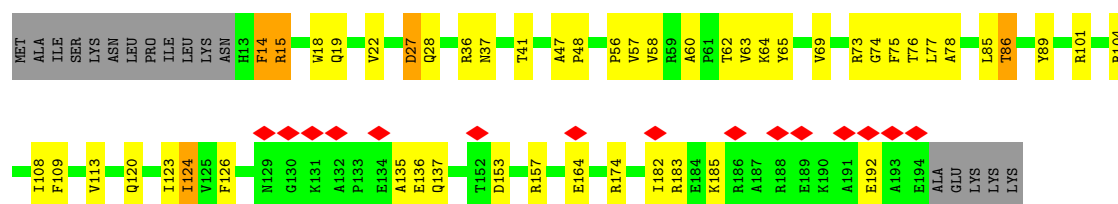


• Molecule 9: 60S ribosomal protein L11-A

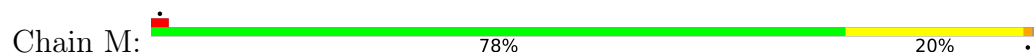


• Molecule 10: 60S ribosomal protein L13-A

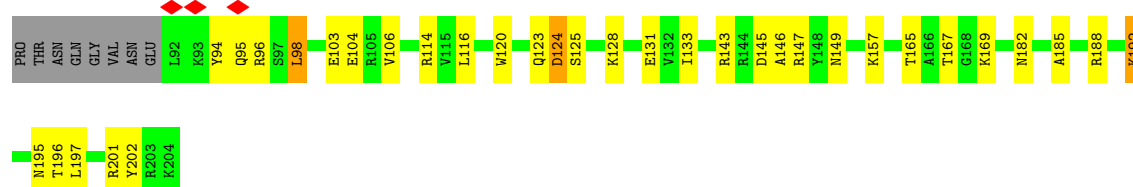




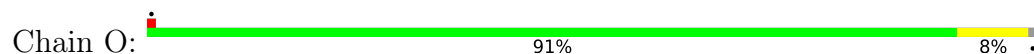
- Molecule 11: 60S ribosomal protein L14-A



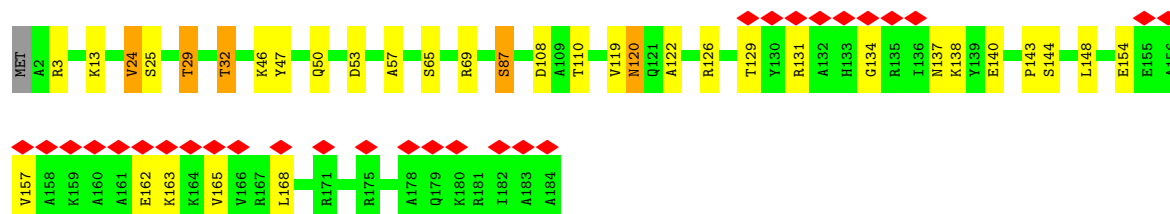
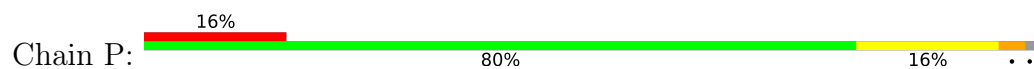
- Molecule 12: 60S ribosomal protein L15-A



- Molecule 13: 60S ribosomal protein L16-A

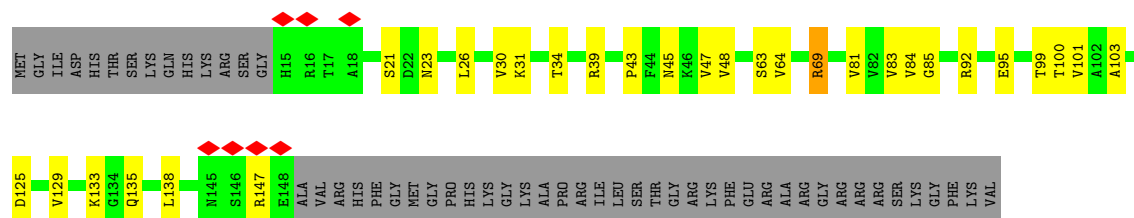


- Molecule 14: 60S ribosomal protein L17-A



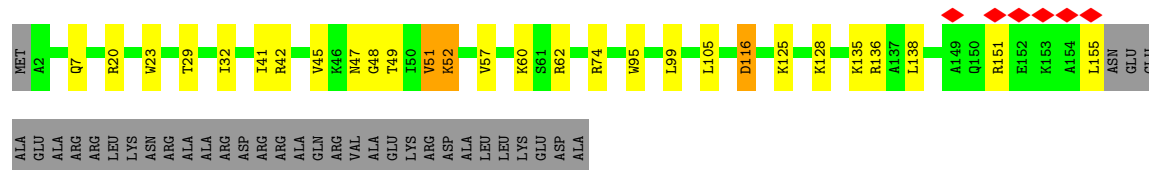
- Molecule 15: 60S ribosomal protein L18-A

Chain Q: 



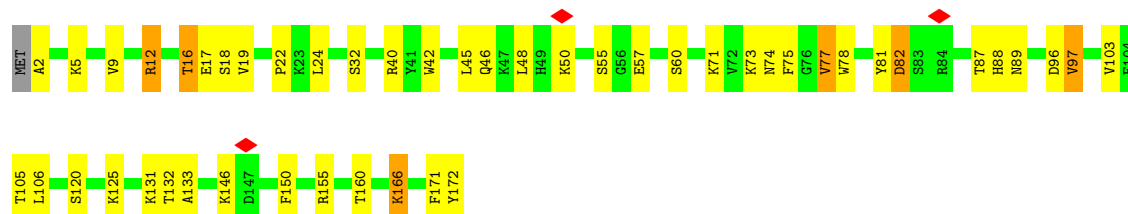
- Molecule 16: 60S ribosomal protein L19-A

Chain R: 



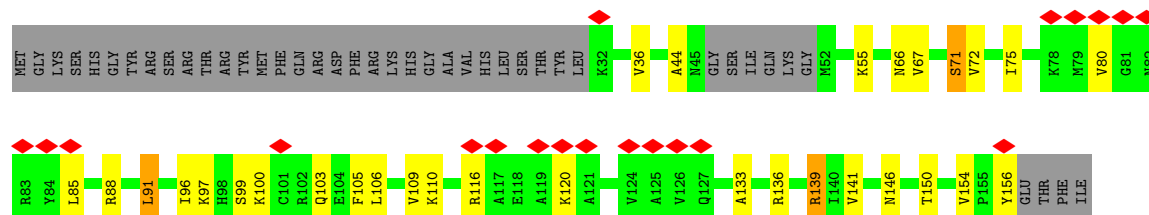
- Molecule 17: 60S ribosomal protein L20-A

Chain S: 



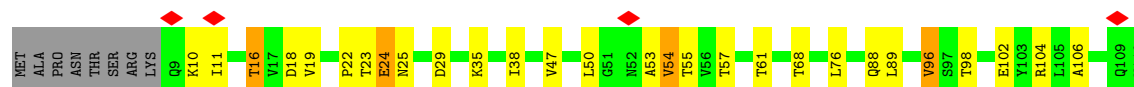
- Molecule 18: 60S ribosomal protein L21-A

Chain T: 



- Molecule 19: 60S ribosomal protein L22-A

Chain U: 



THR
PRO
GLU
GLU
ASP
GLU
GLU
ASP
GLU
GLU

• Molecule 20: 60S ribosomal protein L23-A

Chain V:  71% 25% . .

MET SER G3 L15 V19 I22 M23 N24 C25 Y35 R45 R48 L49 P50 A51 A52 S53 L54 G55 D56 M59 K63 R70 V73 M74 P75 Q81 A82 K83 S84 W85 R86 R87 R88 F92 L93 N98 V101 I102 M109 K110 G111 S112 R128

N132 V135 V136 V137

• Molecule 21: Ribosome assembly factor MRT4

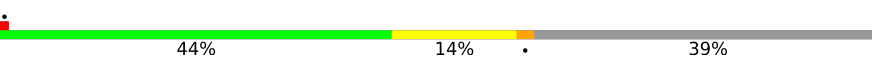
Chain W:  19% 67% 27% 5% .

M1 S4 S7 T11 T15 K18 I26 V30 D35 T36 Y37 R38 Y39 L43 H44 L45 D46 D47 V48 R49 T50 P51 V52 L53 Q54 S59 W60 A61 G62 S63 M67 R70 Q74 L77 K80 R81 E82 E83 K86 E87 N88 L89 Y90 Q91

L92 S93 K94 L95 C96 L103 F104 T105 D106 E107 D108 V109 N110 T111 S118 R126 P127 M128 T129 K130 A131 T134 I137 P138 E139 S144 R145 G146 G147 Q148 I149 P150 A151 D154 M157 I158 L161 E162 P163 T164 M165 R166 N167 K168 F169 E170 I171 P172 T173 K174 I175

K176 A177 G178 K179 I182 D183 S184 P185 V188 C189 T190 E191 G192 E193 K194 L195 D196 V197 Q199 L203 F206 G207 I208 A209 S210 S211 E212 K216 A219 Y220 Y221 D222 V228 N234 MET GLU

• Molecule 22: 60S ribosomal protein L25

Chain X:  44% 14% 39% .

MET ALA PRO SER ALA LYS ALA THR ALA ALA THR ALA ALA LYS LYS VAL VAL LYS GLY THR ASN GLY LYS LYS ALA LEU LYS VAL ARG THR SER ALA THR PHE ARG LEU PRO LYS THR LEU LYS LEU LYS ALA ARG ARG ALA PRO LYS TYR ALA SER LYS LYS ALA VAL VAL PRO HIS TYR ARG L57 I63

I67 T68 T71 A72 M73 K74 D78 V99 K100 E101 V105 T112 L113 M117 G118 T119 K120 T127 A128 D129 Y130 L133 D134 I142

• Molecule 23: 60S ribosomal protein L26-A

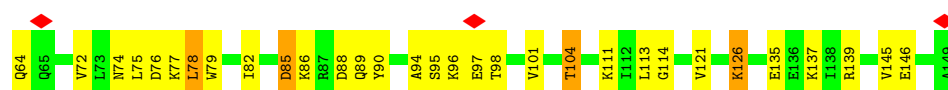
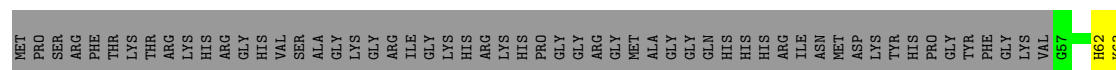
Chain Y:  77% 21% .

MET A2 K3 V8 S9 P23 S24 S25 Q26 R27 A41 I45 I50 V56 V59 R60 G61 S62 K63 K64 K69 S72 S73 Y74 Q81 V95 P96 K103 L104 V105 L109 I119 K125 L126 GLU

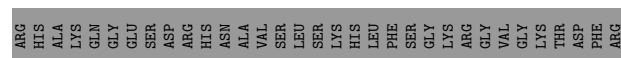
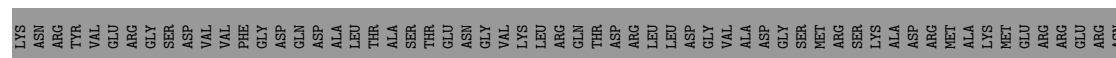
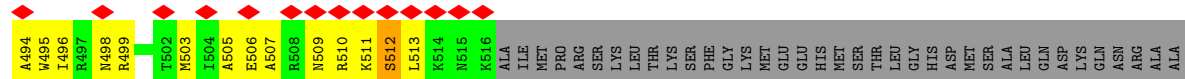
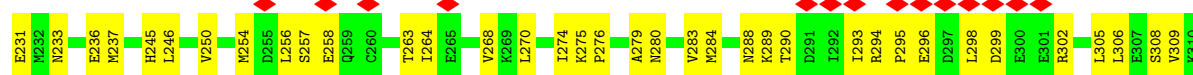
• Molecule 24: 60S ribosomal protein L27-A

Chain Z:  10% 76% 20% . . .

- Molecule 25: 60S ribosomal protein L28



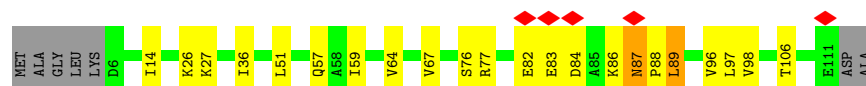
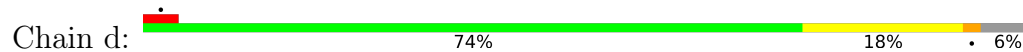
- Molecule 26: Nucleolar GTP-binding protein 1



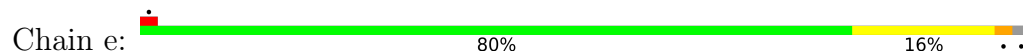
- Molecule 27: 60S ribosomal protein L30



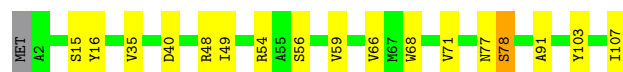
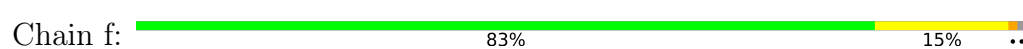
- Molecule 28: 60S ribosomal protein L31-A



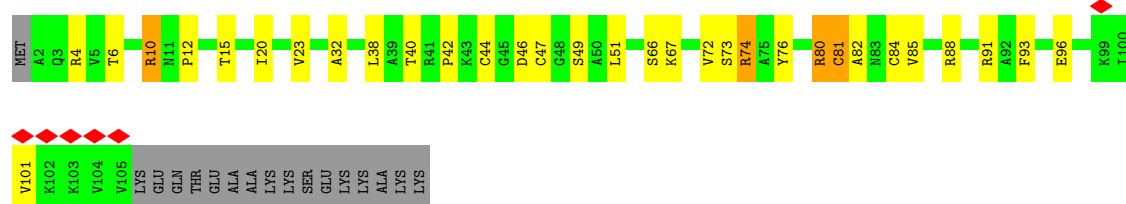
- Molecule 29: 60S ribosomal protein L32



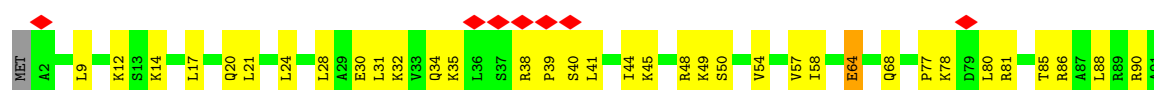
- Molecule 30: 60S ribosomal protein L33-A



- Molecule 31: 60S ribosomal protein L34-A

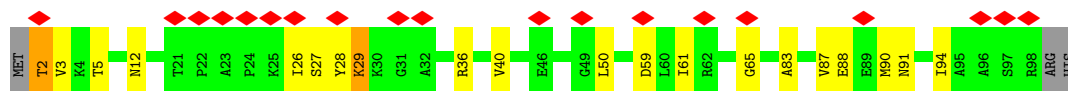
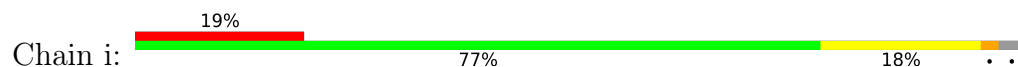


- Molecule 32: 60S ribosomal protein L35-A

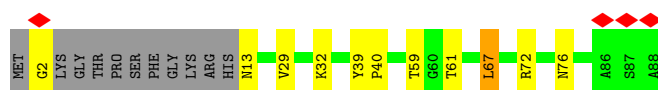
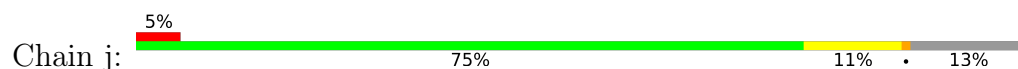




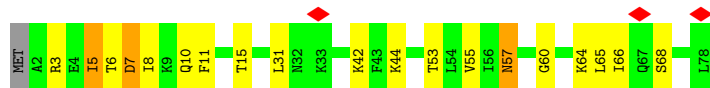
- Molecule 33: 60S ribosomal protein L36-A



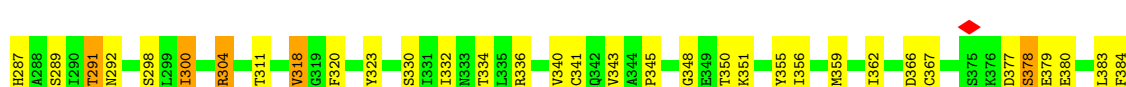
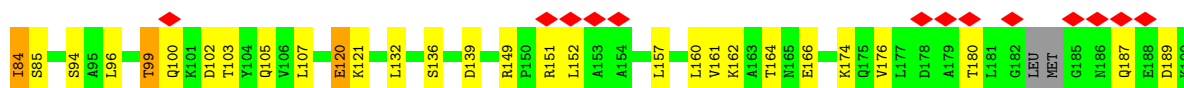
- Molecule 34: 60S ribosomal protein L37-A



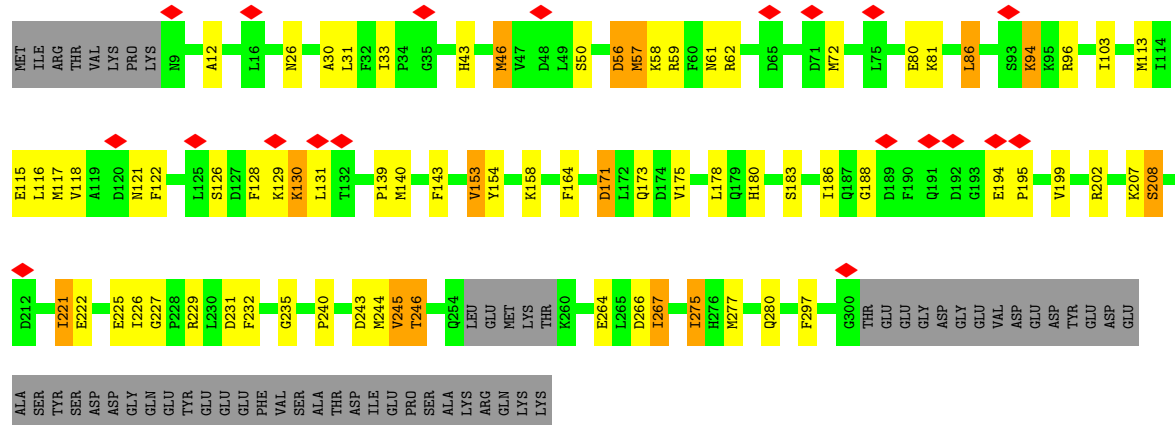
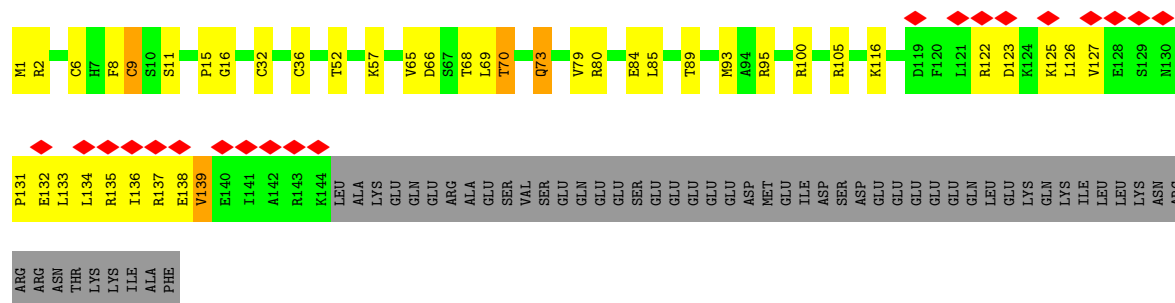
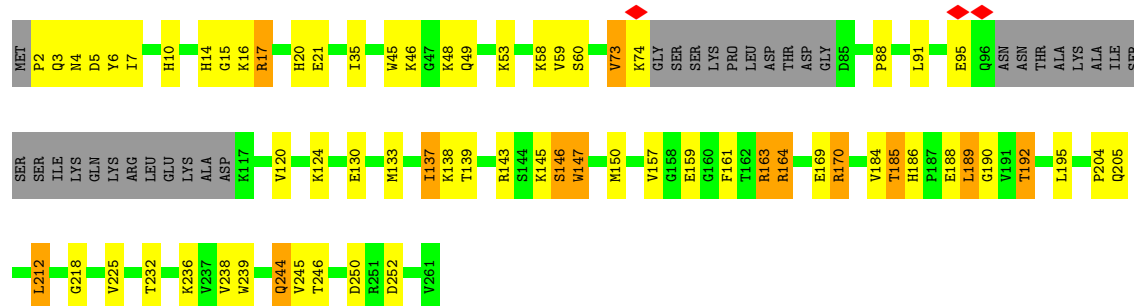
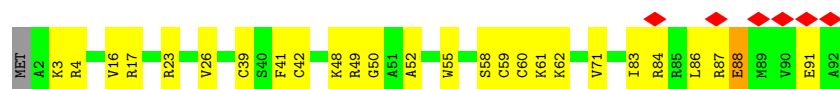
- Molecule 35: 60S ribosomal protein L38



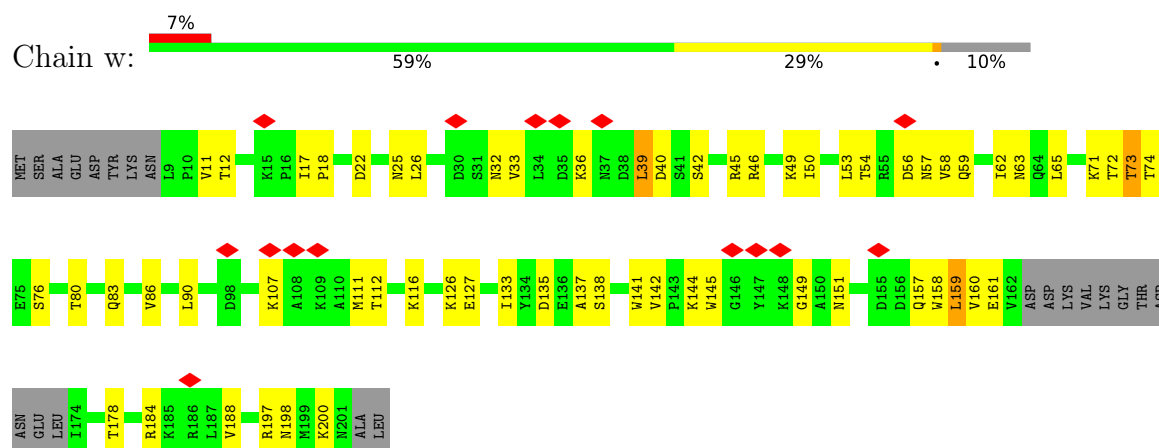
- Molecule 36: Nucleolar GTP-binding protein 2



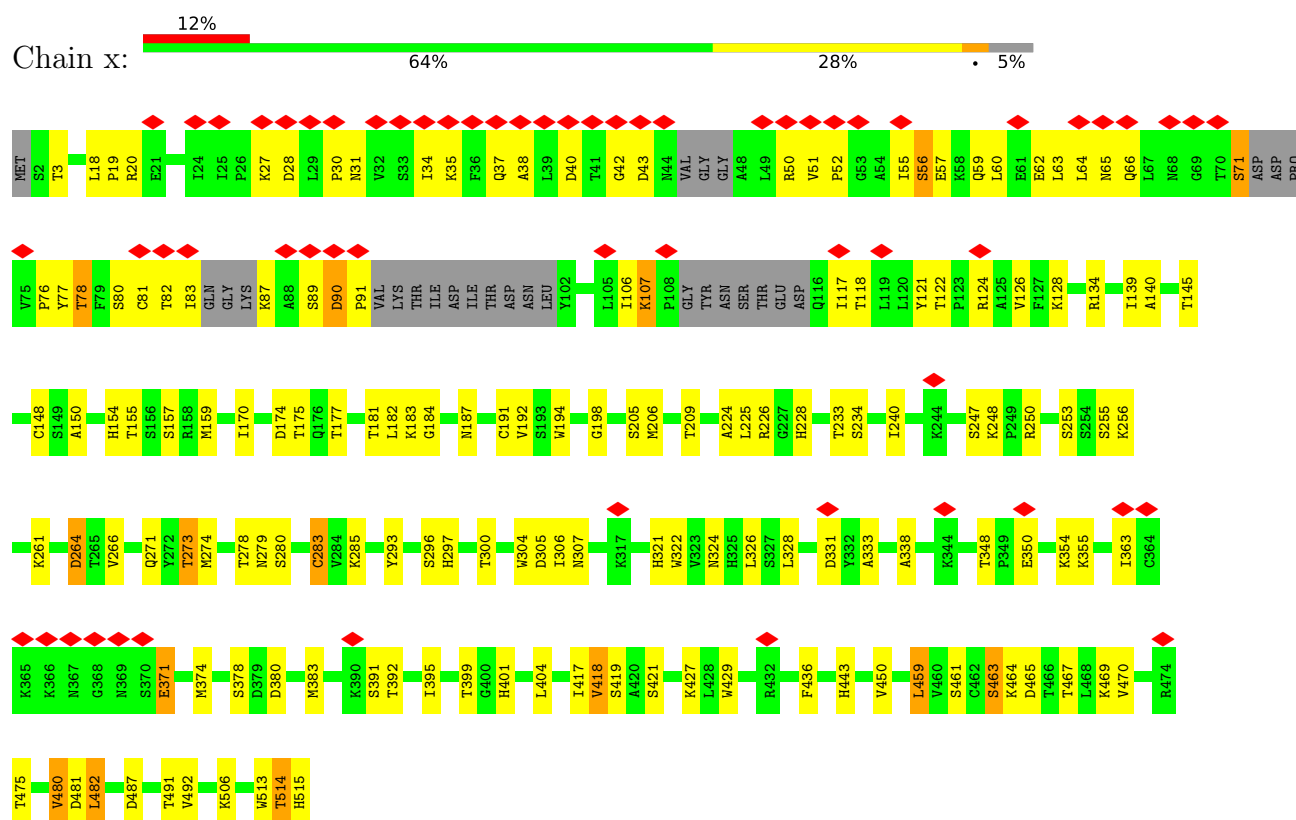
- Molecule 37: 60S ribosomal protein L43-A



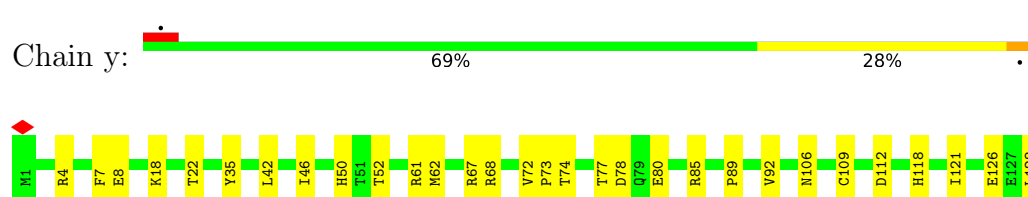
- Molecule 41: Regulator of ribosome biosynthesis



- Molecule 42: Ribosome assembly protein 4



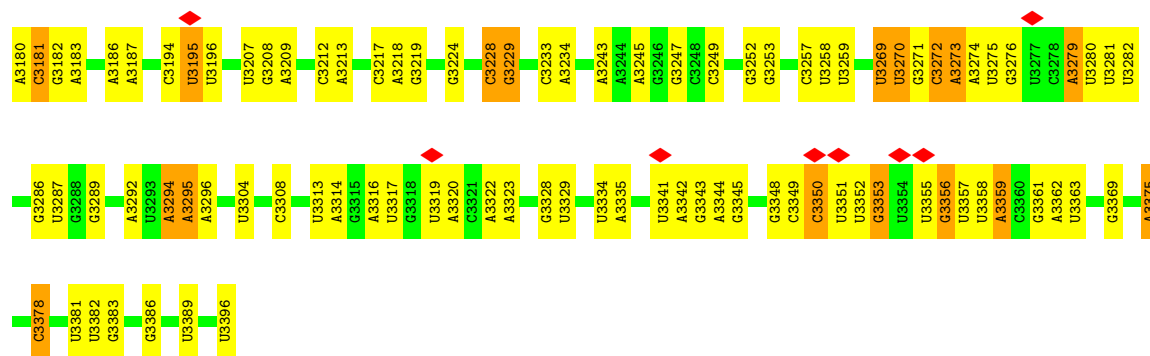
- Molecule 43: Eukaryotic translation initiation factor 6



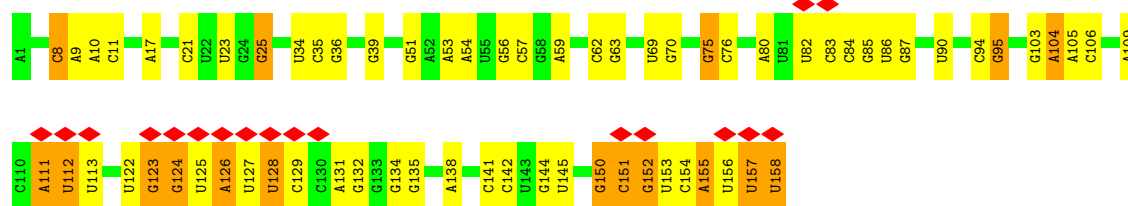




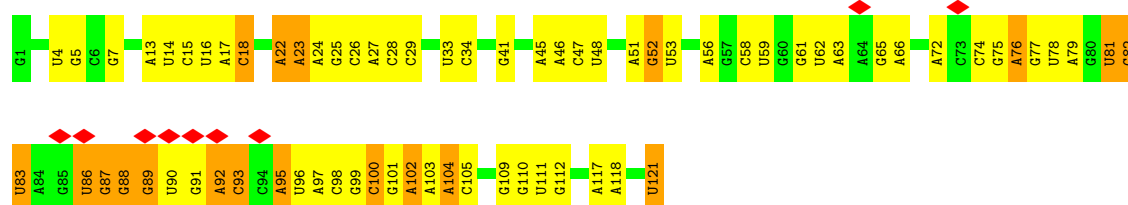




• Molecule 46: RDN5.8-1 rRNA



• Molecule 47: RDN5-2 rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103319	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 ($e^-/\text{\AA}^2$)	1.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	412.02, 412.02, 412.02	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3734, 1.3734, 1.3734	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.24	0/1403	0.47	0/1887
2	B	0.34	0/3152	0.52	0/4239
3	C	0.30	0/2607	0.50	0/3530
4	D	0.19	0/2222	0.45	0/2996
5	E	0.26	0/1260	0.43	0/1694
6	F	0.31	0/1821	0.50	0/2451
7	G	0.19	0/1268	0.49	0/1716
8	H	0.30	0/1531	0.44	0/2062
9	J	0.21	0/1374	0.49	0/1842
10	L	0.26	0/1483	0.51	0/1991
11	M	0.30	0/1074	0.44	0/1446
12	N	0.27	0/1602	0.47	0/2142
13	O	0.36	0/1585	0.50	0/2128
14	P	0.32	0/1465	0.48	0/1968
15	Q	0.26	0/1050	0.42	0/1419
16	R	0.32	0/1258	0.46	0/1679
17	S	0.28	0/1473	0.48	0/1980
18	T	0.21	0/957	0.44	0/1285
19	U	0.23	0/828	0.46	0/1121
20	V	0.34	0/1012	0.48	0/1361
21	W	0.20	0/1918	0.42	0/2586
22	X	0.25	0/695	0.42	0/937
23	Y	0.29	0/995	0.43	0/1329
24	Z	0.23	0/1118	0.48	0/1497
25	a	0.24	0/751	0.45	0/1013
26	b	0.27	0/4220	0.49	0/5687
27	c	0.23	0/751	0.39	0/1008
28	d	0.34	0/879	0.50	0/1180
29	e	0.33	0/1041	0.43	0/1394
30	f	0.35	0/868	0.48	0/1168
31	g	0.33	0/829	0.47	0/1109
32	h	0.22	0/978	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.20	0/756	0.48	1/1005 (0.1%)
34	j	0.30	0/614	0.46	0/813
35	k	0.24	0/618	0.50	0/826
36	m	0.30	0/3713	0.55	0/5006
37	p	0.30	0/701	0.51	0/934
38	r	0.33	0/1892	0.54	0/2528
39	u	0.29	0/1238	0.48	0/1646
40	v	0.21	0/2361	0.44	0/3153
41	w	0.21	0/1471	0.43	0/1980
42	x	0.23	0/3897	0.47	0/5282
43	y	0.29	0/1872	0.45	0/2548
44	z	0.20	0/445	0.39	0/585
45	1	0.31	0/70950	0.38	3/110603 (0.0%)
46	2	0.28	0/3746	0.35	0/5832
47	3	0.16	0/2883	0.33	0/4491
All	All	0.29	0/142625	0.42	4/208378 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
6	F	0	1
24	Z	0	1
26	b	0	1
31	g	0	1
36	m	0	2
38	r	0	1
39	u	0	1
41	w	0	1
42	x	0	1
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	i	28	TYR	N-CA-C	-5.60	108.23	114.62
45	1	720	A	P-O3'-C3'	5.26	128.09	120.20
45	1	160	G	C2'-C3'-O3'	5.15	117.23	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	1	646	A	N9-C1'-C2'	5.10	121.66	114.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	THR	Peptide
2	B	340	LYS	Peptide
6	F	158	LYS	Peptide
24	Z	102	GLU	Peptide
26	b	438	GLY	Peptide
31	g	80	ARG	Peptide
36	m	240	LYS	Peptide
36	m	418	ILE	Peptide
38	r	15	GLY	Peptide
39	u	79	VAL	Peptide
41	w	141	TRP	Peptide
42	x	20	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1377	0	1432	36	0
2	B	3081	0	3165	67	0
3	C	2559	0	2675	40	0
4	D	2176	0	2140	51	0
5	E	1239	0	1326	21	0
6	F	1784	0	1862	28	0
7	G	1249	0	1312	42	0
8	H	1510	0	1576	28	0
9	J	1353	0	1383	47	0
10	L	1459	0	1509	32	0
11	M	1059	0	1154	14	0
12	N	1570	0	1624	44	0
13	O	1555	0	1659	7	0
14	P	1442	0	1485	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	1035	0	1115	19	0
16	R	1241	0	1330	20	0
17	S	1437	0	1475	33	0
18	T	943	0	994	18	0
19	U	812	0	829	13	0
20	V	997	0	1043	20	0
21	W	1885	0	1921	44	0
22	X	687	0	722	7	0
23	Y	984	0	1075	13	0
24	Z	1092	0	1155	24	0
25	a	735	0	776	22	0
26	b	4146	0	4205	115	0
27	c	743	0	797	19	0
28	d	865	0	910	13	0
29	e	1020	0	1090	12	0
30	f	850	0	880	13	0
31	g	819	0	882	15	0
32	h	969	0	1078	26	0
33	i	750	0	829	11	0
34	j	603	0	602	8	0
35	k	612	0	682	11	0
36	m	3639	0	3689	90	0
37	p	694	0	734	19	0
38	r	1860	0	1965	60	0
39	u	1216	0	1264	28	0
40	v	2318	0	2398	52	0
41	w	1448	0	1510	36	0
42	x	3807	0	3790	96	0
43	y	1849	0	1836	46	0
44	z	444	0	478	6	0
45	1	63385	0	31851	830	0
46	2	3353	0	1695	37	0
47	3	2579	0	1304	62	0
48	b	32	0	12	3	0
48	m	32	0	12	2	0
49	b	1	0	0	0	0
49	m	1	0	0	0	0
50	j	1	0	0	0	0
50	p	1	0	0	0	0
50	u	1	0	0	0	0
All	All	133299	0	101230	2044	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 9.

All (2044) 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)
45:1:91:G:N3	45:1:95:A:N6	2.08	1.02
45:1:1200:A:C2	45:1:2824:G:N1	2.30	1.00
45:1:2841:G:H21	45:1:2847:A:H62	1.04	0.99
45:1:1626:U:H3	45:1:1817:G:H1	0.99	0.98
45:1:1200:A:H2	45:1:2824:G:N1	1.62	0.97
45:1:1538:G:N2	45:1:1583:A:H62	1.62	0.97
45:1:91:G:N2	45:1:95:A:H61	1.63	0.95
21:W:80:LYS:HG3	21:W:82:GLU:H	1.31	0.94
34:j:2:GLY:N	45:1:884:A:HO2'	1.67	0.92
45:1:129:U:H3	45:1:139:G:H1	1.17	0.92
45:1:3234:A:H61	45:1:3253:G:H1	0.98	0.92
45:1:1538:G:H21	45:1:1583:A:H62	0.91	0.91
45:1:1538:G:H21	45:1:1583:A:N6	1.69	0.91
10:L:76:THR:HG22	10:L:78:ALA:H	1.36	0.89
45:1:2841:G:N2	45:1:2847:A:H62	1.70	0.88
38:r:170:ARG:NH2	45:1:2727:A:OP2	2.07	0.88
45:1:170:G:H21	45:1:250:U:H1'	1.38	0.88
45:1:1539:A:H62	45:1:1553:U:H3	1.14	0.87
45:1:3234:A:N6	45:1:3253:G:H1	1.73	0.86
45:1:1233:G:H1	45:1:1255:C:H5	1.19	0.86
45:1:170:G:N2	45:1:250:U:O2	2.09	0.85
45:1:3092:C:O2'	45:1:3094:A:OP2	1.94	0.85
45:1:2210:G:N2	45:1:2235:C:O2	2.08	0.85
5:E:40:LEU:HD11	5:E:54:TYR:HB2	1.60	0.84
45:1:177:U:H3	45:1:241:G:H1	1.23	0.84
45:1:2210:G:N2	45:1:2235:C:C2	2.45	0.83
47:3:83:U:N3	47:3:97:A:N6	2.26	0.83
40:v:96:ARG:HH22	47:3:100:C:H5'	1.42	0.83
45:1:2632:G:N2	45:1:2646:C:O2	2.11	0.83
7:G:112:GLU:O	7:G:116:VAL:HB	1.77	0.82
37:p:42:CYS:SG	37:p:60:CYS:HB2	2.19	0.82
24:Z:57:HIS:HB3	24:Z:61:LYS:HG3	1.60	0.82
45:1:2723:U:O2'	45:1:2724:U:O2	1.97	0.82
45:1:2724:U:H5	45:1:2732:G:H1	1.25	0.82
36:m:240:LYS:O	36:m:242:VAL:N	2.13	0.82
45:1:1200:A:H2	45:1:2824:G:H1	0.86	0.81
45:1:255:A:H2'	45:1:256:G:H8	1.46	0.81
38:r:143:ARG:HH12	45:1:2873:U:H1'	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:x:82:THR:O	42:x:87:LYS:N	2.13	0.81
16:R:62:ARG:NH1	45:1:3068:U:OP2	2.14	0.80
36:m:416:TYR:H	36:m:417:GLU:HA	1.46	0.80
42:x:76:PRO:HB2	42:x:124:ARG:HD3	1.61	0.80
4:D:285:ARG:HH12	47:3:63:A:H5''	1.46	0.79
3:C:338:LYS:O	3:C:340:GLY:N	2.14	0.79
45:1:91:G:H21	45:1:95:A:N6	1.81	0.79
45:1:875:G:H2'	45:1:876:A:H8	1.46	0.79
45:1:177:U:O2	45:1:241:G:N2	2.14	0.79
45:1:2431:C:N3	45:1:2432:A:N6	2.31	0.79
6:F:168:ILE:O	6:F:172:ASN:ND2	2.16	0.78
45:1:91:G:H21	45:1:95:A:H61	1.29	0.78
45:1:870:G:N2	45:1:871:U:O4	2.14	0.78
45:1:2193:U:H4'	45:1:2194:G:H5''	1.64	0.78
26:b:359:ASN:OD1	43:y:170:GLN:NE2	2.17	0.78
9:J:10:ARG:HH21	9:J:133:ARG:HE	1.30	0.78
20:V:81:GLN:O	20:V:98:ASN:ND2	2.17	0.78
17:S:171:PHE:HA	17:S:172:TYR:C	2.07	0.78
45:1:437:G:H1	45:1:622:A:H61	1.30	0.77
45:1:2841:G:H21	45:1:2847:A:N6	1.83	0.77
26:b:49:LYS:NZ	45:1:2828:G:OP1	2.19	0.76
45:1:2253:G:H1	45:1:2263:C:H42	1.34	0.76
38:r:143:ARG:NH1	45:1:2873:U:O2	2.19	0.76
16:R:60:LYS:NZ	45:1:1671:C:OP1	2.18	0.76
45:1:1657:C:O2'	45:1:1797:A:OP2	2.04	0.76
45:1:2866:U:H4'	45:1:2867:C:H5''	1.65	0.76
45:1:2393:G:O2'	45:1:2982:A:N6	2.17	0.76
25:a:111:LYS:NZ	45:1:714:G:N7	2.31	0.76
9:J:95:ASN:HD22	45:1:2673:A:H5''	1.51	0.75
11:M:55:ARG:NH2	11:M:76:ALA:O	2.20	0.75
2:B:229:VAL:H	2:B:247:ARG:HH11	1.34	0.75
45:1:2687:G:H22	45:1:2690:G:H5''	1.51	0.75
42:x:187:ASN:HB3	42:x:206:MET:HB3	1.66	0.75
45:1:2630:C:N3	45:1:2649:A:N6	2.35	0.75
45:1:96:G:O2'	45:1:97:U:O5'	2.05	0.75
45:1:645:A:OP1	45:1:1153:A:N6	2.20	0.75
21:W:74:GLN:NE2	21:W:96:CYS:SG	2.60	0.74
9:J:13:LYS:HZ3	9:J:134:PRO:HG3	1.51	0.74
2:B:320:ASP:OD1	2:B:320:ASP:N	2.20	0.74
12:N:33:LYS:NZ	45:1:9:U:O2'	2.21	0.74
45:1:2721:A:H61	45:1:2735:U:H3	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:2210:G:C6	45:1:2236:G:C5	2.76	0.74
47:3:83:U:N3	47:3:97:A:C6	2.56	0.74
9:J:21:ILE:HD11	9:J:125:MET:HE2	1.69	0.73
45:1:994:G:N2	45:1:995:U:O4	2.20	0.73
45:1:1481:A:N3	45:1:1858:A:O2'	2.21	0.73
9:J:32:ARG:NH1	9:J:120:ILE:O	2.21	0.73
24:Z:87:LEU:HD11	24:Z:121:ARG:HH12	1.54	0.73
45:1:263:C:H2'	45:1:264:G:H8	1.53	0.73
45:1:2727:A:O2'	45:1:2729:U:N3	2.20	0.73
26:b:175:TYR:O	26:b:180:LYS:NZ	2.21	0.72
45:1:998:A:H2'	45:1:999:G:C8	2.24	0.72
26:b:257:SER:HA	26:b:293:ILE:HG13	1.71	0.72
45:1:172:G:O6	45:1:246:U:O2	2.06	0.72
46:2:153:U:H2'	46:2:154:C:H6	1.54	0.72
2:B:10:ARG:NH1	2:B:11:HIS:O	2.22	0.72
29:e:105:ARG:NH2	45:1:1412:G:OP1	2.23	0.72
16:R:105:LEU:HD23	16:R:138:LEU:HD23	1.72	0.72
37:p:17:ARG:NH1	45:1:860:G:OP1	2.22	0.72
39:u:16:GLY:O	45:1:3050:U:O2'	2.08	0.72
1:A:156:LYS:NZ	45:1:2158:A:OP2	2.23	0.72
43:y:121:ILE:O	43:y:139:ARG:NH2	2.23	0.72
15:Q:43:PRO:HB2	45:1:728:G:H5'	1.71	0.71
23:Y:3:LYS:HD2	23:Y:8:VAL:HG13	1.73	0.71
8:H:92:TYR:HB3	8:H:179:ILE:HG12	1.71	0.71
45:1:2628:A:N1	45:1:2651:G:N2	2.39	0.71
47:3:83:U:C2	47:3:97:A:N6	2.59	0.71
4:D:23:ARG:NH1	4:D:23:ARG:O	2.23	0.71
14:P:138:LYS:HE3	45:1:2356:A:H5'	1.72	0.71
45:1:972:A:H2'	45:1:973:A:C8	2.26	0.71
45:1:2440:G:N7	45:1:2441:A:N6	2.37	0.71
7:G:185:ARG:HD3	46:2:155:A:H5'	1.72	0.71
45:1:845:G:N2	45:1:848:A:OP2	2.24	0.70
4:D:40:HIS:HB3	4:D:41:LYS:HA	1.73	0.70
36:m:209:LYS:HG2	45:1:2869:U:H6	1.56	0.70
3:C:16:THR:HG22	3:C:17:ALA:H	1.56	0.70
45:1:1646:G:O2'	45:1:1808:G:N2	2.24	0.70
45:1:3021:A:H2	45:1:3033:A:H62	1.37	0.70
9:J:95:ASN:ND2	45:1:2673:A:OP1	2.25	0.70
45:1:2822:U:H2'	45:1:2823:G:H2'	1.72	0.70
41:w:135:ASP:HB2	41:w:142:VAL:HG11	1.73	0.70
45:1:549:U:H2'	45:1:550:A:H8	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:43:ARG:NH2	26:b:119:GLY:O	2.25	0.69
8:H:89:LYS:HG2	8:H:145:VAL:HG22	1.74	0.69
9:J:128:TYR:HE1	45:1:2672:G:H21	1.41	0.69
45:1:3233:C:H2'	45:1:3234:A:C8	2.27	0.69
45:1:2434:U:O2	45:1:2593:A:O2'	2.09	0.69
45:1:3158:G:O6	45:1:3292:A:N1	2.26	0.69
9:J:137:ARG:NH1	47:3:28:C:OP1	2.24	0.69
10:L:36:ARG:NH2	45:1:687:U:OP2	2.23	0.69
17:S:22:PRO:O	18:T:146:ASN:ND2	2.24	0.69
21:W:134:THR:HG23	21:W:191:GLU:H	1.56	0.69
2:B:36:ASP:HB3	2:B:39:LYS:HD2	1.73	0.69
26:b:92:LYS:HZ2	45:1:2863:G:H22	1.40	0.69
42:x:80:SER:HA	42:x:91:PRO:HA	1.74	0.69
9:J:92:ARG:NH2	9:J:173:ASP:OD2	2.26	0.69
36:m:304:ARG:NH1	45:1:2249:G:OP2	2.24	0.69
26:b:494:ALA:O	26:b:498:ASN:ND2	2.21	0.68
45:1:2830:G:H2'	45:1:2831:G:C8	2.28	0.68
13:O:164:SER:HG	45:1:3181:C:HO2'	1.38	0.68
12:N:68:ARG:NH2	45:1:292:U:OP2	2.27	0.68
45:1:170:G:H2'	45:1:171:G:C8	2.29	0.68
45:1:1482:A:N6	45:1:1866:C:O2	2.26	0.68
36:m:31:ARG:NH2	45:1:2966:G:O6	2.26	0.68
45:1:2929:C:O2'	45:1:2930:A:O5'	2.10	0.68
3:C:197:ARG:NH1	45:1:1381:A:OP1	2.27	0.68
27:c:97:ASP:OD1	27:c:97:ASP:N	2.27	0.68
40:v:207:LYS:NZ	40:v:208:SER:O	2.27	0.68
45:1:1200:A:N1	45:1:2824:G:O6	2.25	0.68
14:P:162:GLU:HG2	14:P:163:LYS:H	1.58	0.68
26:b:368:ALA:O	26:b:370:ASP:N	2.26	0.68
45:1:2511:A:N6	45:1:2593:A:OP2	2.26	0.68
47:3:74:C:H2'	47:3:75:G:C4	2.29	0.68
40:v:116:LEU:HD12	40:v:232:PHE:HB3	1.74	0.67
34:j:29:VAL:O	34:j:32:LYS:NZ	2.27	0.67
42:x:378:SER:OG	42:x:380:ASP:OD1	2.10	0.67
7:G:78:PHE:O	7:G:79:GLN:HG2	1.95	0.67
42:x:83:ILE:O	42:x:87:LYS:N	2.27	0.67
12:N:63:ARG:NH2	12:N:131:GLU:OE2	2.27	0.67
14:P:122:ALA:HB3	14:P:143:PRO:HB2	1.76	0.67
21:W:144:SER:HA	21:W:157:MET:HG3	1.77	0.67
45:1:1896:A:H61	45:1:2339:C:H42	1.40	0.67
45:1:2203:U:H2'	45:1:2204:C:C6	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:84:ASP:OD1	28:d:86:LYS:N	2.26	0.67
45:1:170:G:N1	45:1:249:U:N3	2.43	0.67
45:1:1187:C:H5	45:1:1319:G:H1	1.43	0.67
2:B:10:ARG:HH21	2:B:263:SER:HB2	1.59	0.67
45:1:157:A:H61	45:1:264:G:H2'	1.60	0.67
43:y:233:SER:HA	43:y:236:LEU:HB2	1.77	0.67
27:c:49:PRO:HG2	27:c:52:ARG:HG3	1.77	0.66
45:1:1778:G:O2'	45:1:1780:G:OP2	2.11	0.66
9:J:41:SER:O	9:J:75:LYS:NZ	2.26	0.66
12:N:147:ARG:NH2	45:1:113:C:OP1	2.28	0.66
37:p:4:ARG:NH1	45:1:837:A:OP2	2.28	0.66
2:B:187:SER:O	2:B:190:GLU:N	2.28	0.66
14:P:134:GLY:O	45:1:1846:C:N4	2.27	0.66
21:W:38:ARG:NE	21:W:222:ASP:OD1	2.28	0.66
44:z:14:LYS:NZ	45:1:3100:U:OP2	2.28	0.66
10:L:14:PHE:HD2	10:L:15:ARG:H	1.43	0.66
16:R:23:TRP:HB3	16:R:51:VAL:HG22	1.75	0.66
26:b:505:ALA:O	26:b:509:ASN:ND2	2.28	0.66
36:m:416:TYR:N	36:m:417:GLU:HA	2.10	0.66
45:1:1553:U:H4'	45:1:1554:U:H5'	1.77	0.66
45:1:2728:G:H21	45:1:2729:U:H3'	1.60	0.66
45:1:1493:G:OP2	45:1:1493:G:N2	2.23	0.65
42:x:27:LYS:HB2	42:x:28:ASP:HA	1.77	0.65
45:1:1347:U:O2'	45:1:1349:G:O6	2.14	0.65
39:u:131:PRO:HA	39:u:134:LEU:HD12	1.79	0.65
36:m:350:THR:OG1	48:m:501:GTP:O2G	2.14	0.65
45:1:998:A:H3'	45:1:999:G:H2'	1.77	0.65
45:1:2515:A:H61	45:1:2594:C:H5	1.44	0.65
9:J:9:MET:SD	47:3:52:G:N2	2.70	0.65
15:Q:147:ARG:HG2	45:1:786:A:H3'	1.79	0.65
31:g:4:ARG:HD3	45:1:1858:A:H1'	1.79	0.65
45:1:263:C:H2'	45:1:264:G:C8	2.32	0.65
16:R:125:LYS:NZ	45:1:1724:U:O4	2.30	0.65
31:g:74:ARG:NH2	31:g:82:ALA:HB2	2.12	0.65
36:m:239:CYS:HB2	36:m:323:TYR:HE1	1.62	0.65
45:1:937:G:N1	45:1:2411:U:OP1	2.24	0.65
45:1:1253:U:H5'	45:1:1254:C:H5'	1.78	0.65
38:r:2:PRO:HB2	45:1:3027:A:C2	2.32	0.65
8:H:151:VAL:O	8:H:155:SER:OG	2.14	0.65
11:M:20:VAL:O	11:M:66:THR:OG1	2.15	0.65
38:r:170:ARG:H	45:1:2727:A:H8	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:2400:G:O6	45:1:2402:A:N6	2.31	0.65
32:h:78:LYS:HA	32:h:81:ARG:HD2	1.78	0.64
40:v:221:ILE:HD11	41:w:59:GLN:HA	1.78	0.64
45:1:971:G:H1	45:1:1111:U:H3	1.43	0.64
45:1:91:G:N2	45:1:95:A:N6	2.38	0.64
45:1:2692:A:N6	45:1:2701:U:O4	2.30	0.64
9:J:143:ARG:NH2	47:3:5:G:OP1	2.31	0.64
21:W:165:MET:HA	21:W:169:PHE:HB2	1.79	0.64
45:1:1231:A:H5''	45:1:1232:C:H5'	1.78	0.64
24:Z:133:LYS:NZ	45:1:1807:G:OP1	2.30	0.64
36:m:162:LYS:O	36:m:166:GLU:HG2	1.98	0.64
45:1:2411:U:HO2'	45:1:2412:G:H8	1.45	0.64
12:N:185:ALA:HA	12:N:188:ARG:HG2	1.79	0.64
21:W:221:TYR:HD1	21:W:228:VAL:HG12	1.63	0.64
7:G:185:ARG:O	7:G:188:THR:OG1	2.16	0.64
41:w:198:ASN:HD22	45:1:2757:U:H5'	1.62	0.64
45:1:1:G:H1'	45:1:3:U:C4	2.33	0.64
45:1:971:G:O6	45:1:1111:U:O4	2.16	0.64
38:r:7:ILE:H	45:1:2898:G:N2	1.96	0.64
42:x:154:HIS:CD2	42:x:155:THR:HG22	2.33	0.64
1:A:108:PRO:HG2	37:p:86:LEU:HD13	1.80	0.63
2:B:29:VAL:HG22	2:B:218:ILE:HD13	1.79	0.63
3:C:203:ARG:NH1	45:1:1383:G:OP1	2.32	0.63
42:x:297:HIS:HA	42:x:322:TRP:HB2	1.80	0.63
45:1:255:A:H2'	45:1:256:G:C8	2.29	0.63
8:H:129:ARG:H	8:H:157:ASN:HD21	1.45	0.63
32:h:30:GLU:OE1	32:h:34:GLN:NE2	2.31	0.63
45:1:2222:A:N3	47:3:82:G:O2'	2.30	0.63
45:1:2878:G:O2'	45:1:2879:C:O5'	2.16	0.63
16:R:7:GLN:N	16:R:7:GLN:OE1	2.31	0.63
45:1:644:G:H2'	45:1:646:A:C5	2.33	0.63
45:1:990:U:O2'	45:1:991:G:OP1	2.17	0.63
45:1:2435:G:N2	45:1:2514:U:O4	2.31	0.63
45:1:2437:G:H2'	45:1:2438:A:H8	1.62	0.63
45:1:3020:U:H3'	45:1:3021:A:H5'	1.79	0.63
4:D:18:THR:HG1	4:D:24:ARG:HH21	1.42	0.63
21:W:38:ARG:NH1	21:W:39:TYR:OH	2.31	0.63
45:1:2716:U:OP2	45:1:2753:G:O2'	2.16	0.63
45:1:2858:U:H3'	45:1:2859:U:C5'	2.29	0.63
9:J:54:VAL:HG13	9:J:56:THR:H	1.64	0.63
16:R:62:ARG:NH2	45:1:3070:A:OP1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:h:85:THR:OG1	46:2:36:G:OP2	2.16	0.63
42:x:27:LYS:H	42:x:28:ASP:HB2	1.64	0.63
37:p:4:ARG:NH2	45:1:838:G:O6	2.32	0.63
41:w:53:LEU:O	41:w:57:ASN:ND2	2.32	0.63
45:1:1661:G:H2'	45:1:1662:G:C8	2.33	0.63
26:b:227:ARG:NE	26:b:231:GLU:O	2.29	0.63
45:1:870:G:H1	45:1:889:U:H3	1.47	0.63
45:1:1740:U:H4'	45:1:1741:A:H5''	1.79	0.63
47:3:100:C:H3'	47:3:101:G:H8	1.64	0.63
1:A:188:LYS:NZ	45:1:1793:C:O2	2.32	0.62
4:D:234:ASP:OD2	4:D:235:SER:N	2.32	0.62
29:e:125:ARG:NH1	45:1:1392:G:OP1	2.31	0.62
15:Q:39:ARG:NH1	45:1:1348:U:OP1	2.32	0.62
36:m:330:SER:OG	48:m:501:GTP:O2A	2.17	0.62
10:L:153:ASP:OD2	10:L:157:ARG:NH1	2.32	0.62
10:L:174:ARG:NH2	45:1:712:G:OP1	2.32	0.62
29:e:3:SER:OG	29:e:71:HIS:NE2	2.33	0.62
45:1:878:G:H4'	45:1:879:U:H5'	1.81	0.62
45:1:2363:A:H61	45:1:2398:A:H5''	1.63	0.62
5:E:45:GLY:HA2	45:1:3273:A:H5'	1.81	0.62
20:V:101:VAL:HG21	20:V:109:MET:HE1	1.80	0.62
45:1:708:G:N2	45:1:711:A:OP2	2.26	0.62
30:f:78:SER:O	30:f:78:SER:OG	2.18	0.62
36:m:61:PHE:O	36:m:62:GLN:NE2	2.33	0.62
45:1:2715:A:H5'	45:1:2754:G:OP2	1.98	0.62
8:H:138:THR:O	8:H:139:ASN:ND2	2.33	0.62
42:x:333:ALA:HB2	42:x:363:ILE:HG13	1.81	0.62
43:y:109:CYS:HB2	43:y:149:GLY:HA2	1.81	0.62
45:1:2201:G:H2'	45:1:2245:C:H42	1.65	0.62
47:3:27:A:H2'	47:3:28:C:C6	2.34	0.62
38:r:164:ARG:NH1	45:1:2727:A:N3	2.48	0.62
45:1:2608:G:H2'	45:1:2609:A:C8	2.35	0.62
32:h:9:LEU:HD23	32:h:12:LYS:HD2	1.82	0.62
45:1:2691:A:H62	45:1:2702:A:H61	1.47	0.62
45:1:2436:U:H3	45:1:2511:A:H2	1.48	0.62
1:A:136:ILE:HG13	1:A:148:VAL:HG12	1.81	0.61
38:r:192:THR:HG21	45:1:2856:G:H21	1.63	0.61
45:1:254:A:H2'	45:1:255:A:C8	2.35	0.61
45:1:1067:U:H2'	45:1:1068:C:C6	2.35	0.61
6:F:150:LYS:HD3	6:F:151:ARG:HG2	1.82	0.61
21:W:157:MET:HE1	21:W:165:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:2642:A:N7	45:1:2643:A:N6	2.47	0.61
26:b:288:ASN:OD1	26:b:289:LYS:N	2.32	0.61
26:b:483:ALA:O	26:b:486:VAL:N	2.30	0.61
45:1:1112:A:H2'	45:1:1113:G:C8	2.36	0.61
2:B:129:ALA:O	45:1:3149:G:O2'	2.15	0.61
7:G:146:LYS:NZ	7:G:173:MET:O	2.22	0.61
26:b:366:PRO:HB3	43:y:178:GLN:HA	1.82	0.61
7:G:152:LEU:HD11	7:G:180:VAL:HB	1.83	0.61
9:J:48:SER:O	9:J:65:ILE:N	2.32	0.61
26:b:227:ARG:O	26:b:229:THR:N	2.28	0.61
40:v:96:ARG:NH1	47:3:101:G:OP2	2.32	0.61
41:w:17:ILE:HD12	41:w:32:ASN:HA	1.82	0.61
45:1:254:A:H2'	45:1:255:A:H8	1.65	0.61
45:1:971:G:N1	45:1:1111:U:N3	2.49	0.61
6:F:67:ARG:HH21	45:1:517:G:H5'	1.64	0.61
32:h:35:LYS:HE3	32:h:40:SER:HA	1.83	0.61
6:F:86:VAL:HG13	6:F:136:TYR:HB3	1.81	0.61
35:k:8:ILE:HD11	35:k:65:LEU:HD21	1.83	0.61
38:r:88:PRO:HD2	38:r:91:LEU:HB2	1.83	0.61
45:1:1646:G:HO2'	45:1:1808:G:H22	1.48	0.61
8:H:49:ASN:O	8:H:51:GLN:N	2.33	0.61
23:Y:74:TYR:OH	46:2:75:G:OP2	2.18	0.61
36:m:300:ILE:HG23	36:m:359:MET:HE1	1.81	0.61
4:D:18:THR:OG1	4:D:24:ARG:NH2	2.27	0.61
38:r:45:TRP:HA	38:r:48:LYS:HG3	1.81	0.61
12:N:49:ARG:NH2	45:1:149:U:OP1	2.30	0.61
43:y:163:PRO:HA	43:y:183:ALA:HB1	1.81	0.61
23:Y:59:VAL:O	23:Y:64:LYS:NZ	2.33	0.60
45:1:1544:G:O6	45:1:1549:U:O4	2.18	0.60
13:O:49:ARG:NH1	45:1:1191:U:OP2	2.29	0.60
45:1:1088:U:H2'	45:1:1089:G:C8	2.36	0.60
7:G:212:ALA:O	7:G:216:SER:OG	2.19	0.60
10:L:124:ILE:HD11	10:L:126:PHE:HE1	1.66	0.60
26:b:478:TYR:OH	39:u:116:LYS:O	2.20	0.60
45:1:1088:U:N3	45:1:1089:G:O6	2.34	0.60
1:A:60:LYS:HD3	1:A:75:ILE:HG12	1.83	0.60
26:b:290:THR:HG21	26:b:319:THR:HG23	1.82	0.60
45:1:2137:U:OP2	45:1:2142:A:N6	2.31	0.60
47:3:28:C:H2'	47:3:29:C:O4'	2.02	0.60
17:S:89:ASN:HD21	18:T:156:TYR:H	1.47	0.60
4:D:45:ASN:ND2	40:v:173:GLN:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:77:LYS:O	25:a:79:TRP:N	2.33	0.60
29:e:23:ASP:OD2	29:e:24:ARG:NH1	2.33	0.60
45:1:2653:C:O2'	45:1:2656:A:OP2	2.19	0.60
45:1:3159:C:H2'	45:1:3160:U:C6	2.36	0.60
12:N:169:LYS:NZ	45:1:64:G:OP2	2.33	0.60
45:1:876:A:N1	45:1:881:C:N4	2.49	0.60
5:E:17:ALA:O	45:1:591:G:O2'	2.17	0.60
26:b:92:LYS:HZ2	45:1:2863:G:N2	1.99	0.60
45:1:1087:G:H2'	45:1:1088:U:O4'	2.02	0.60
45:1:3344:A:H2	45:1:3361:G:H21	1.49	0.60
47:3:103:A:O2'	47:3:104:A:O5'	2.17	0.60
1:A:36:GLU:HB3	1:A:91:GLY:HA2	1.84	0.60
45:1:2726:C:H1'	45:1:2728:G:OP1	2.02	0.60
45:1:2818:U:H4'	45:1:2819:A:H4'	1.84	0.60
12:N:201:ARG:NH2	45:1:692:A:OP1	2.34	0.60
17:S:46:GLN:O	17:S:46:GLN:NE2	2.35	0.60
21:W:95:LEU:HD13	21:W:219:ALA:HB2	1.84	0.60
26:b:488:ASP:HA	26:b:491:GLU:HG2	1.84	0.60
42:x:463:SER:OG	42:x:465:ASP:OD1	2.19	0.60
8:H:69:ARG:NH1	45:1:3114:A:OP1	2.35	0.59
45:1:2820:A:O2'	45:1:2821:C:OP1	2.20	0.59
3:C:193:LYS:NZ	46:2:21:C:OP1	2.29	0.59
16:R:20:ARG:NH1	45:1:1874:A:N7	2.49	0.59
36:m:224:VAL:HG13	36:m:318:VAL:HB	1.82	0.59
7:G:149:LYS:NZ	7:G:201:THR:O	2.34	0.59
17:S:82:ASP:HA	17:S:87:THR:HG22	1.85	0.59
30:f:49:ILE:HD11	30:f:71:VAL:HG22	1.82	0.59
45:1:5:G:C2	46:2:155:A:H1'	2.37	0.59
45:1:2267:C:H1'	45:1:2268:U:H3	1.67	0.59
31:g:81:CYS:HB2	31:g:84:CYS:HB2	1.84	0.59
43:y:67:ARG:NE	43:y:112:ASP:OD2	2.34	0.59
45:1:1:G:H1'	45:1:3:U:N3	2.17	0.59
45:1:160:G:H2'	45:1:161:G:C8	2.36	0.59
46:2:69:U:H2'	46:2:70:G:O4'	2.01	0.59
14:P:13:LYS:NZ	14:P:154:GLU:OE2	2.35	0.59
20:V:54:LEU:H	20:V:81:GLN:HE21	1.50	0.59
42:x:482:LEU:HD12	42:x:513:TRP:CE3	2.37	0.59
45:1:2148:U:H2'	45:1:2149:A:C8	2.37	0.59
3:C:337:GLU:HB2	3:C:339:LEU:HG	1.85	0.59
29:e:100:ILE:O	29:e:105:ARG:NH1	2.36	0.59
38:r:185:THR:HB	38:r:192:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:97:U:H2'	45:1:98:G:C8	2.37	0.59
45:1:646:A:H1'	45:1:647:A:C8	2.38	0.59
45:1:2678:A:H2'	45:1:2679:A:C4	2.37	0.59
2:B:341:SER:O	2:B:343:TYR:N	2.36	0.59
6:F:156:ILE:C	6:F:158:LYS:H	2.10	0.59
42:x:321:HIS:CD2	42:x:322:TRP:H	2.21	0.59
1:A:140:ASN:ND2	1:A:142:ASP:O	2.35	0.59
42:x:209:THR:HB	42:x:224:ALA:HB1	1.84	0.59
45:1:2635:A:N6	45:1:2642:A:OP2	2.36	0.59
45:1:2216:G:N2	45:1:2230:C:C2	2.70	0.59
45:1:2646:C:H42	45:1:2647:A:H62	1.50	0.59
10:L:37:ASN:O	10:L:41:THR:HG23	2.03	0.59
26:b:492:LYS:O	26:b:496:ILE:HG13	2.03	0.59
36:m:345:PRO:HB3	36:m:459:ARG:HD3	1.83	0.59
45:1:1112:A:H2'	45:1:1113:G:H8	1.67	0.59
35:k:5:ILE:HD11	35:k:11:PHE:HD2	1.68	0.58
45:1:417:A:H2'	45:1:418:A:C8	2.38	0.58
45:1:966:U:H2'	45:1:967:A:C8	2.37	0.58
45:1:1542:G:O2'	45:1:2169:G:N1	2.32	0.58
45:1:1814:A:H5''	45:1:1816:A:N3	2.18	0.58
5:E:72:ASN:ND2	5:E:159:LEU:O	2.34	0.58
13:O:164:SER:OG	45:1:3181:C:O2'	2.11	0.58
7:G:145:ASN:N	7:G:146:LYS:HA	2.17	0.58
12:N:192:LYS:O	12:N:196:THR:OG1	2.17	0.58
45:1:2758:A:O2'	45:1:2759:U:OP1	2.20	0.58
3:C:317:PRO:C	3:C:319:LYS:H	2.11	0.58
18:T:75:ILE:HG22	18:T:88:ARG:HG2	1.84	0.58
25:a:96:LYS:O	25:a:97:GLU:HG3	2.03	0.58
45:1:1057:A:H4'	45:1:1058:U:OP1	2.01	0.58
45:1:2276:G:H2'	45:1:2277:C:C6	2.37	0.58
45:1:2768:U:H2'	45:1:2769:A:H8	1.68	0.58
40:v:139:PRO:HB3	40:v:180:HIS:NE2	2.19	0.58
45:1:2221:G:O2'	45:1:2223:A:N6	2.35	0.58
45:1:3166:C:H2'	45:1:3167:A:H8	1.69	0.58
39:u:85:LEU:O	39:u:89:THR:HG23	2.03	0.58
40:v:171:ASP:OD2	40:v:171:ASP:N	2.33	0.58
42:x:487:ASP:HB3	42:x:506:LYS:HB3	1.85	0.58
45:1:41:G:OP2	45:1:42:C:N4	2.31	0.58
45:1:1200:A:O2'	45:1:1201:C:O2	2.21	0.58
45:1:2788:C:O2'	45:1:2789:U:O4'	2.21	0.58
14:P:47:TYR:OH	14:P:57:ALA:O	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:57:GLU:OE1	18:T:139:ARG:NH1	2.37	0.58
26:b:167:THR:OG1	26:b:168:ARG:N	2.36	0.58
26:b:421:LEU:O	39:u:80:ARG:NH1	2.32	0.58
38:r:2:PRO:HB2	45:1:3027:A:H2	1.68	0.58
45:1:2436:U:N3	45:1:2437:G:N7	2.51	0.58
4:D:50:ARG:NH1	4:D:147:ASP:OD2	2.37	0.58
11:M:124:ARG:NH2	45:1:3212:C:OP2	2.37	0.58
45:1:972:A:H2'	45:1:973:A:H8	1.68	0.58
45:1:1102:A:O2'	45:1:1103:A:O5'	2.19	0.58
5:E:26:ARG:NH1	45:1:502:U:O2'	2.37	0.58
6:F:143:THR:HG22	6:F:241:LYS:HE2	1.85	0.58
8:H:76:ASP:O	8:H:80:THR:HG23	2.03	0.58
39:u:6:CYS:SG	39:u:9:CYS:N	2.75	0.58
40:v:96:ARG:NH2	47:3:100:C:OP2	2.37	0.58
47:3:17:A:H2'	47:3:18:C:C6	2.38	0.58
32:h:50:SER:O	32:h:54:VAL:HG23	2.03	0.57
36:m:48:ILE:HD11	36:m:57:ARG:HB3	1.86	0.57
42:x:31:ASN:HB3	42:x:51:VAL:HG12	1.86	0.57
3:C:36:HIS:O	3:C:40:THR:HG23	2.04	0.57
4:D:172:TYR:CD2	42:x:134:ARG:HD3	2.39	0.57
40:v:56:ASP:OD2	40:v:56:ASP:N	2.25	0.57
12:N:3:ALA:HB1	12:N:7:LEU:HD13	1.86	0.57
26:b:419:LYS:NZ	43:y:35:TYR:OH	2.36	0.57
47:3:109:G:H2'	47:3:110:G:H8	1.68	0.57
2:B:237:LYS:NZ	45:1:2340:U:OP2	2.27	0.57
4:D:108:ARG:NE	4:D:253:PHE:HB2	2.19	0.57
7:G:161:GLU:HA	7:G:164:VAL:HG22	1.84	0.57
45:1:2724:U:O2'	45:1:2725:U:H5''	2.04	0.57
46:2:150:G:N2	46:2:152:G:O6	2.37	0.57
1:A:118:GLU:OE1	1:A:156:LYS:NZ	2.37	0.57
19:U:11:ILE:H	19:U:11:ILE:HD12	1.69	0.57
19:U:19:VAL:O	19:U:23:THR:OG1	2.17	0.57
10:L:27:ASP:OD1	10:L:27:ASP:N	2.32	0.57
23:Y:23:PRO:HG2	23:Y:26:GLN:HG3	1.87	0.57
26:b:488:ASP:OD2	26:b:489:ILE:N	2.37	0.57
40:v:86:LEU:HD22	40:v:164:PHE:HD2	1.69	0.57
10:L:73:ARG:NH2	45:1:77:A:OP2	2.37	0.57
26:b:195:GLN:HB2	26:b:197:TYR:CE2	2.39	0.57
26:b:457:GLU:OE2	39:u:95:ARG:NE	2.35	0.57
37:p:49:ARG:NH2	37:p:52:ALA:HB2	2.18	0.57
42:x:205:SER:OG	42:x:206:MET:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:29:LYS:O	45:1:266:A:N6	2.37	0.57
23:Y:59:VAL:HG23	23:Y:60:ARG:HG2	1.87	0.57
45:1:2210:G:H2'	45:1:2211:U:O4'	2.04	0.57
45:1:2410:U:O2'	45:1:2411:U:O4'	2.21	0.57
2:B:214:MET:HB2	2:B:345:ASN:HD21	1.70	0.57
2:B:255:TRP:H	2:B:255:TRP:CD1	2.21	0.57
3:C:270:SER:O	3:C:270:SER:OG	2.19	0.57
15:Q:92:ARG:HG2	25:a:76:ASP:HB3	1.87	0.57
19:U:16:THR:OG1	19:U:102:GLU:OE1	2.22	0.57
38:r:139:THR:OG1	45:1:2971:A:OP2	2.17	0.57
45:1:1200:A:N1	45:1:2824:G:C6	2.72	0.57
47:3:87:G:N3	47:3:95:A:N6	2.42	0.57
2:B:229:VAL:HG12	2:B:247:ARG:HD2	1.86	0.56
2:B:387:LEU:HD22	39:u:105:ARG:HE	1.70	0.56
14:P:126:ARG:HA	14:P:140:GLU:HG2	1.85	0.56
37:p:39:CYS:HB3	37:p:42:CYS:HB2	1.86	0.56
45:1:2603:G:H2'	45:1:2604:U:C6	2.39	0.56
9:J:26:SER:OG	9:J:63:GLU:O	2.23	0.56
26:b:25:THR:O	26:b:29:THR:OG1	2.23	0.56
32:h:14:LYS:HA	32:h:17:LEU:HD12	1.86	0.56
43:y:68:ARG:NH1	43:y:112:ASP:O	2.38	0.56
21:W:177:ALA:O	21:W:179:LYS:N	2.38	0.56
26:b:258:GLU:HG2	26:b:293:ILE:HD11	1.87	0.56
45:1:436:A:H2'	45:1:437:G:C8	2.41	0.56
45:1:1082:U:H2'	45:1:1083:G:C8	2.40	0.56
45:1:2210:G:C6	45:1:2236:G:C6	2.94	0.56
45:1:2411:U:O2'	45:1:2412:G:H8	1.88	0.56
3:C:35:VAL:HG21	3:C:244:LEU:HD21	1.87	0.56
5:E:35:VAL:O	5:E:38:THR:OG1	2.21	0.56
24:Z:57:HIS:HA	24:Z:61:LYS:HE2	1.88	0.56
42:x:331:ASP:OD2	42:x:331:ASP:N	2.36	0.56
45:1:2425:G:H2'	45:1:2426:U:O4'	2.06	0.56
45:1:2646:C:N4	45:1:2647:A:H62	2.03	0.56
45:1:2728:G:N2	45:1:2729:U:H3'	2.20	0.56
2:B:13:HIS:CD2	2:B:15:GLY:H	2.24	0.56
45:1:158:G:O6	45:1:159:A:N6	2.38	0.56
47:3:76:A:H62	47:3:103:A:H62	1.52	0.56
3:C:187:LEU:HD22	3:C:193:LYS:HD3	1.88	0.56
43:y:118:HIS:CD2	43:y:146:ILE:HG23	2.41	0.56
45:1:435:C:H2'	45:1:436:A:C8	2.41	0.56
45:1:2212:C:H1'	45:1:2233:A:H61	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:GLN:O	45:1:2688:U:N3	2.37	0.56
9:J:10:ARG:HH21	9:J:133:ARG:NE	1.99	0.56
34:j:13:ASN:HD21	46:2:111:A:H61	1.54	0.56
36:m:208:SER:O	36:m:208:SER:OG	2.21	0.56
37:p:49:ARG:HH21	37:p:52:ALA:HB2	1.71	0.56
38:r:170:ARG:HB3	45:1:2727:A:H5'	1.88	0.56
42:x:250:ARG:NH1	42:x:271:GLN:OE1	2.39	0.56
45:1:1696:A:H2'	45:1:1697:A:C8	2.41	0.56
2:B:300:ARG:HD2	26:b:433:PRO:HB3	1.87	0.56
15:Q:45:ASN:HA	15:Q:48:VAL:HG22	1.87	0.56
32:h:77:PRO:HD2	32:h:80:LEU:HD12	1.88	0.56
36:m:187:GLN:O	36:m:191:GLU:HG3	2.06	0.56
45:1:2979:U:H6	45:1:2980:U:H5	1.53	0.56
46:2:8:C:H2'	46:2:9:A:C8	2.40	0.56
47:3:81:U:H2'	47:3:82:G:C8	2.40	0.56
18:T:66:ASN:OD1	18:T:67:VAL:N	2.39	0.55
26:b:506:GLU:HA	28:d:97:LEU:HD21	1.88	0.55
45:1:2816:G:O2'	45:1:2817:A:H5'	2.07	0.55
45:1:2917:G:H1	45:1:2929:C:H5	1.54	0.55
10:L:62:THR:O	10:L:64:LYS:N	2.40	0.55
27:c:14:LEU:HD21	27:c:43:ILE:HD13	1.88	0.55
38:r:16:LYS:O	38:r:17:ARG:HB2	2.05	0.55
39:u:70:THR:O	39:u:73:GLN:NE2	2.33	0.55
7:G:105:LYS:HZ2	45:1:121:A:H8	1.52	0.55
21:W:70:ARG:O	21:W:74:GLN:HG2	2.06	0.55
26:b:434:GLU:HA	26:b:441:VAL:HB	1.88	0.55
26:b:470:ASN:N	26:b:470:ASN:OD1	2.39	0.55
36:m:291:THR:OG1	36:m:292:ASN:OD1	2.25	0.55
45:1:2831:G:H1	45:1:2857:C:H42	1.53	0.55
3:C:33:ASP:O	3:C:37:THR:HG23	2.07	0.55
24:Z:51:LEU:HB2	24:Z:65:ARG:HB3	1.86	0.55
27:c:30:THR:HG22	27:c:91:SER:HB3	1.88	0.55
42:x:34:ILE:HG22	42:x:117:ILE:HG23	1.89	0.55
7:G:158:ASP:HB3	7:G:159:PRO:HD3	1.88	0.55
31:g:74:ARG:NH2	45:1:1639:C:OP2	2.40	0.55
36:m:202:ILE:HG13	36:m:388:VAL:HG13	1.88	0.55
45:1:40:A:H4'	45:1:41:G:OP1	2.05	0.55
45:1:1064:A:H4'	45:1:1065:A:O5'	2.06	0.55
45:1:1067:U:H2'	45:1:1068:C:H6	1.72	0.55
45:1:2874:G:O2'	45:1:2875:U:O4'	2.16	0.55
46:2:152:G:H2'	46:2:153:U:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:131:LEU:H	40:v:226:ILE:HD13	1.72	0.55
45:1:1362:G:H2'	45:1:1363:A:C8	2.42	0.55
45:1:1626:U:O4	45:1:1817:G:O6	2.25	0.55
4:D:232:ASP:OD1	4:D:232:ASP:N	2.33	0.55
12:N:114:ARG:NH2	12:N:157:LYS:HG2	2.22	0.55
15:Q:83:VAL:HG12	15:Q:85:GLY:H	1.72	0.55
42:x:228:HIS:CE1	42:x:255:SER:HG	2.21	0.55
45:1:291:C:H2'	45:1:292:U:O2	2.07	0.55
47:3:14:U:H2'	47:3:15:C:H6	1.72	0.55
1:A:161:ASP:N	1:A:161:ASP:OD1	2.39	0.55
7:G:81:THR:HG21	7:G:181:LYS:HB2	1.88	0.55
26:b:439:LYS:HD3	26:b:439:LYS:N	2.21	0.55
42:x:55:ILE:HD12	42:x:59:GLN:HB3	1.87	0.55
45:1:971:G:C6	45:1:972:A:C6	2.95	0.55
45:1:2210:G:N1	45:1:2235:C:N3	2.55	0.55
45:1:3165:A:H2'	45:1:3166:C:H6	1.72	0.55
8:H:22:SER:OG	8:H:23:ARG:N	2.39	0.55
9:J:53:THR:HG23	9:J:61:ARG:HB2	1.88	0.55
40:v:80:GLU:OE1	40:v:81:LYS:NZ	2.39	0.55
42:x:514:THR:OG1	42:x:515:HIS:N	2.40	0.55
45:1:644:G:H2'	45:1:646:A:C6	2.42	0.55
45:1:2503:G:H1'	45:1:2504:U:H5	1.71	0.55
2:B:108:GLU:HB2	2:B:137:TYR:CE2	2.42	0.55
2:B:214:MET:CB	2:B:345:ASN:HD21	2.20	0.55
7:G:105:LYS:HZ2	45:1:121:A:H2'	1.71	0.55
10:L:75:PHE:O	10:L:101:ARG:NH1	2.40	0.55
35:k:11:PHE:O	35:k:15:THR:HG23	2.07	0.55
39:u:1:MET:HE3	39:u:15:PRO:HG2	1.88	0.55
45:1:2228:A:H2'	45:1:2229:A:H8	1.71	0.55
45:1:2836:C:H5	45:1:2852:C:H42	1.55	0.55
45:1:3042:U:OP2	45:1:3092:C:N4	2.26	0.55
45:1:358:G:N2	45:1:361:A:OP2	2.34	0.54
45:1:966:U:H2'	45:1:967:A:H8	1.72	0.54
45:1:1201:C:H2'	45:1:1202:A:N3	2.21	0.54
7:G:160:ILE:O	7:G:164:VAL:HG13	2.06	0.54
9:J:141:ARG:HH21	9:J:144:CYS:HB2	1.72	0.54
26:b:193:ASP:OD2	26:b:195:GLN:NE2	2.32	0.54
45:1:975:C:H42	45:1:1107:C:H41	1.55	0.54
38:r:6:TYR:N	45:1:2898:G:H22	2.05	0.54
40:v:240:PRO:HB2	40:v:245:VAL:HG23	1.89	0.54
42:x:250:ARG:HG2	42:x:264:ASP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:537:A:H61	45:1:554:A:H1'	1.73	0.54
47:3:16:U:H2'	47:3:17:A:H8	1.72	0.54
8:H:106:LYS:HE2	8:H:111:PHE:CE1	2.43	0.54
12:N:46:ASP:N	12:N:46:ASP:OD1	2.39	0.54
21:W:4:SER:HA	45:1:1208:U:H1'	1.88	0.54
25:a:77:LYS:C	25:a:79:TRP:H	2.13	0.54
38:r:164:ARG:CZ	45:1:2727:A:H1'	2.37	0.54
45:1:2788:C:O2'	45:1:2789:U:O5'	2.23	0.54
2:B:241:LYS:HG2	45:1:874:U:H2'	1.89	0.54
15:Q:99:THR:OG1	15:Q:100:THR:N	2.41	0.54
19:U:24:GLU:OE1	19:U:25:ASN:ND2	2.41	0.54
31:g:20:ILE:HD12	31:g:32:ALA:HB1	1.90	0.54
45:1:2685:C:H2'	45:1:2686:A:H8	1.73	0.54
4:D:184:ASP:OD1	4:D:187:THR:OG1	2.23	0.54
26:b:74:VAL:HG23	26:b:75:HIS:H	1.71	0.54
34:j:76:ASN:ND2	46:2:95:G:OP1	2.39	0.54
45:1:1277:C:HO2'	45:1:1278:A:H8	1.56	0.54
45:1:2955:U:O4	45:1:2977:G:O2'	2.25	0.54
2:B:57:VAL:HG22	2:B:357:LYS:HB2	1.90	0.54
9:J:77:GLU:HA	9:J:80:LEU:HB3	1.90	0.54
38:r:7:ILE:H	45:1:2898:G:H22	1.54	0.54
40:v:103:ILE:HG23	40:v:113:MET:HG2	1.89	0.54
42:x:37:GLN:HA	42:x:43:ASP:HA	1.89	0.54
45:1:1351:U:O2'	45:1:1352:A:N3	2.38	0.54
45:1:2752:U:H2'	45:1:2753:G:C8	2.43	0.54
40:v:243:ASP:OD2	40:v:244:MET:N	2.41	0.54
41:w:54:THR:O	41:w:58:VAL:HG23	2.08	0.54
43:y:240:LEU:HD22	43:y:244:TYR:HE2	1.73	0.54
45:1:407:A:C2	46:2:17:A:H1'	2.43	0.54
45:1:2690:G:H2'	45:1:2690:G:N3	2.22	0.54
46:2:109:A:O2'	46:2:112:U:O4	2.20	0.54
47:3:77:G:H1'	47:3:78:U:C5	2.43	0.54
3:C:10:SER:HA	3:C:153:SER:HB3	1.89	0.53
7:G:190:VAL:O	7:G:192:GLN:NE2	2.36	0.53
26:b:323:GLN:OE1	48:b:701:GTP:N1	2.37	0.53
42:x:38:ALA:N	42:x:42:GLY:O	2.32	0.53
42:x:57:GLU:HA	42:x:60:LEU:HD13	1.89	0.53
45:1:1539:A:N6	45:1:1553:U:H3	1.95	0.53
47:3:14:U:H2'	47:3:15:C:C6	2.43	0.53
6:F:95:ILE:O	6:F:100:ARG:NH2	2.42	0.53
9:J:32:ARG:HD2	9:J:120:ILE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:121:ARG:HH21	24:Z:126:LYS:HB2	1.72	0.53
31:g:93:PHE:O	31:g:96:GLU:HG3	2.09	0.53
35:k:44:LYS:HG2	35:k:53:THR:HG23	1.89	0.53
36:m:423:ASP:O	36:m:425:THR:N	2.41	0.53
41:w:157:GLN:NE2	41:w:159:LEU:O	2.40	0.53
46:2:8:C:H2'	46:2:9:A:H8	1.73	0.53
47:3:23:A:H2'	47:3:24:A:C8	2.42	0.53
17:S:77:VAL:HG11	17:S:106:LEU:HD22	1.91	0.53
40:v:128:PHE:O	40:v:130:LYS:NZ	2.29	0.53
45:1:1239:C:H2'	45:1:1240:A:O4'	2.07	0.53
45:1:2240:G:H2'	45:1:2241:U:C6	2.44	0.53
8:H:72:LYS:NZ	8:H:76:ASP:OD2	2.37	0.53
45:1:146:U:H5''	45:1:148:G:H5'	1.91	0.53
45:1:675:C:O2'	45:1:679:U:OP1	2.25	0.53
45:1:720:A:O2'	45:1:721:G:OP2	2.22	0.53
45:1:2865:U:H1'	45:1:2866:U:H5'	1.88	0.53
45:1:3020:U:H3'	45:1:3021:A:C5'	2.37	0.53
10:L:157:ARG:NH2	25:a:146:GLU:OE2	2.42	0.53
13:O:160:ARG:NH2	45:1:3182:G:OP1	2.42	0.53
26:b:379:PRO:HG2	26:b:382:VAL:HG23	1.89	0.53
32:h:20:GLN:O	32:h:24:LEU:HG	2.08	0.53
42:x:467:THR:OG1	42:x:469:LYS:NZ	2.42	0.53
43:y:42:LEU:HD13	43:y:46:ILE:HD11	1.89	0.53
45:1:3166:C:H2'	45:1:3167:A:C8	2.44	0.53
6:F:34:LYS:NZ	45:1:596:C:OP2	2.38	0.53
37:p:49:ARG:HB2	37:p:55:TRP:CZ3	2.43	0.53
45:1:41:G:N2	45:1:42:C:O4'	2.42	0.53
45:1:3160:U:H2'	45:1:3161:C:H6	1.73	0.53
1:A:28:LYS:HB3	1:A:123:ARG:HB3	1.91	0.53
14:P:24:VAL:HG12	14:P:25:SER:H	1.73	0.53
15:Q:147:ARG:NH1	15:Q:147:ARG:O	2.42	0.53
24:Z:102:GLU:OE1	24:Z:102:GLU:N	2.41	0.53
43:y:222:PHE:HB2	43:y:224:LEU:HD22	1.91	0.53
45:1:2831:G:H1	45:1:2857:C:N4	2.07	0.53
46:2:123:G:H2'	46:2:124:G:C8	2.44	0.53
1:A:179:LEU:O	1:A:184:ARG:HD2	2.09	0.53
9:J:36:VAL:O	9:J:39:GLN:NE2	2.41	0.53
26:b:256:LEU:HD23	26:b:295:PRO:HB3	1.89	0.53
45:1:1351:U:O2'	45:1:1352:A:H5'	2.09	0.53
45:1:2437:G:H2'	45:1:2438:A:C8	2.42	0.53
45:1:2830:G:H2'	45:1:2831:G:H8	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:87:U:H2'	45:1:88:A:H8	1.73	0.53
45:1:1940:G:H21	45:1:3362:A:H8	1.57	0.53
23:Y:41:ALA:O	23:Y:125:LYS:NZ	2.35	0.53
25:a:75:LEU:HG	25:a:114:GLY:HA2	1.91	0.53
26:b:181:SER:OG	48:b:701:GTP:O1A	2.18	0.53
43:y:225:GLN:HB3	43:y:228:GLN:HE22	1.74	0.53
45:1:2198:A:H61	45:1:2247:G:H1	1.57	0.53
45:1:2267:C:H1'	45:1:2268:U:N3	2.24	0.53
45:1:2614:G:O2'	45:1:2615:G:OP2	2.26	0.53
26:b:359:ASN:ND2	43:y:165:THR:O	2.37	0.52
38:r:45:TRP:HH2	45:1:2828:G:C6	2.27	0.52
43:y:237:ARG:O	43:y:241:ILE:HG13	2.08	0.52
3:C:300:ARG:O	15:Q:39:ARG:NH2	2.30	0.52
10:L:135:ALA:C	10:L:136:GLU:HG3	2.35	0.52
45:1:2210:G:C2	45:1:2235:C:C2	2.97	0.52
45:1:2621:G:H2'	45:1:2622:C:H5'	1.91	0.52
1:A:44:ILE:HD12	1:A:86:GLN:O	2.08	0.52
3:C:181:VAL:O	3:C:182:LEU:HG	2.10	0.52
27:c:51:LEU:O	27:c:55:GLU:HG2	2.09	0.52
45:1:314:U:H2'	45:1:315:C:C6	2.45	0.52
20:V:112:SER:O	20:V:132:ASN:ND2	2.35	0.52
32:h:44:ILE:O	32:h:48:ARG:HG3	2.09	0.52
34:j:13:ASN:ND2	46:2:111:A:H61	2.07	0.52
42:x:224:ALA:O	42:x:226:ARG:NH1	2.42	0.52
45:1:2400:G:H2'	45:1:2401:A:H5''	1.91	0.52
4:D:202:GLY:O	4:D:206:GLN:HG2	2.10	0.52
10:L:109:PHE:O	10:L:113:VAL:HG23	2.10	0.52
18:T:116:ARG:NH1	45:1:1093:A:OP1	2.42	0.52
26:b:104:LEU:HB3	26:b:139:ILE:HD13	1.91	0.52
28:d:82:GLU:O	28:d:83:GLU:HG2	2.09	0.52
35:k:42:LYS:HG2	35:k:55:VAL:HG22	1.91	0.52
1:A:41:ILE:HG23	1:A:90:ALA:HB3	1.92	0.52
16:R:7:GLN:HG2	16:R:32:ILE:HG22	1.91	0.52
36:m:224:VAL:O	36:m:318:VAL:HA	2.10	0.52
45:1:97:U:O2'	45:1:98:G:O5'	2.28	0.52
4:D:83:LEU:HD13	4:D:88:ILE:HD12	1.91	0.52
4:D:276:LYS:HD3	47:3:61:G:H5''	1.91	0.52
6:F:67:ARG:NH2	45:1:517:G:H5'	2.24	0.52
36:m:120:GLU:O	36:m:120:GLU:HG2	2.09	0.52
39:u:89:THR:O	39:u:93:MET:HG3	2.09	0.52
42:x:247:SER:OG	42:x:248:LYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:974:G:N2	45:1:1108:U:H5	2.08	0.52
45:1:2108:C:H1'	45:1:3344:A:C8	2.45	0.52
45:1:3164:C:O2'	45:1:3165:A:O5'	2.28	0.52
2:B:74:GLU:OE2	2:B:283:TYR:OH	2.26	0.52
4:D:25:GLU:O	4:D:27:LYS:N	2.42	0.52
10:L:86:THR:HG23	10:L:89:TYR:HB3	1.91	0.52
32:h:90:ARG:NH2	45:1:20:A:OP2	2.43	0.52
45:1:44:U:H2'	45:1:45:A:C8	2.45	0.52
45:1:2877:G:H1'	45:1:2878:G:H5'	1.92	0.52
1:A:40:TYR:HA	1:A:90:ALA:O	2.10	0.52
3:C:264:SER:OG	3:C:265:GLU:N	2.43	0.52
7:G:219:ASP:OD2	7:G:220:ALA:N	2.43	0.52
9:J:133:ARG:NH1	9:J:153:LYS:O	2.43	0.52
17:S:2:ALA:HA	45:1:1324:U:H5'	1.91	0.52
17:S:171:PHE:HA	17:S:172:TYR:O	2.09	0.52
45:1:160:G:H2'	45:1:161:G:H8	1.75	0.52
45:1:1760:A:N1	45:1:1766:G:N1	2.58	0.52
45:1:2397:A:O2'	45:1:2399:A:OP1	2.27	0.52
5:E:105:TYR:OH	5:E:137:ASP:OD2	2.26	0.52
8:H:49:ASN:C	8:H:51:GLN:H	2.18	0.52
26:b:361:ILE:O	43:y:237:ARG:NH1	2.43	0.52
45:1:974:G:H22	45:1:1108:U:H5	1.57	0.52
45:1:1127:G:N1	45:1:1128:U:O4	2.43	0.52
45:1:1539:A:N7	45:1:1553:U:O4	2.43	0.52
45:1:2838:A:H2'	45:1:2839:G:O4'	2.10	0.52
45:1:3164:C:O2'	45:1:3165:A:H8	1.93	0.52
2:B:139:GLN:C	2:B:141:GLY:H	2.18	0.51
7:G:72:PRO:HG3	12:N:18:VAL:HA	1.92	0.51
7:G:75:ILE:HG13	7:G:76:ALA:H	1.75	0.51
24:Z:33:SER:OG	24:Z:34:LYS:N	2.42	0.51
25:a:75:LEU:HD22	25:a:78:LEU:HD22	1.92	0.51
30:f:35:VAL:HG13	30:f:40:ASP:HB3	1.92	0.51
43:y:7:PHE:CD1	43:y:8:GLU:HG2	2.44	0.51
45:1:96:G:HO2'	45:1:97:U:P	2.31	0.51
45:1:172:G:C6	45:1:246:U:O2	2.63	0.51
45:1:1759:C:N3	45:1:1760:A:N6	2.59	0.51
45:1:2511:A:H2'	45:1:2512:C:C6	2.45	0.51
6:F:88:ARG:HD2	6:F:103:LEU:HD22	1.93	0.51
21:W:46:ASP:OD1	21:W:47:ASP:N	2.41	0.51
21:W:108:ASP:OD1	21:W:111:THR:OG1	2.23	0.51
36:m:85:SER:HB3	38:r:236:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:r:138:LYS:HA	38:r:146:SER:HA	1.91	0.51
40:v:280:GLN:O	45:1:2271:A:N6	2.42	0.51
41:w:149:GLY:HA3	45:1:2656:A:H62	1.75	0.51
42:x:280:SER:O	42:x:296:SER:OG	2.19	0.51
45:1:42:C:O2'	45:1:43:A:H5'	2.10	0.51
2:B:286:GLY:HA3	2:B:321:PHE:CE2	2.46	0.51
3:C:260:GLN:O	3:C:270:SER:HB3	2.10	0.51
7:G:108:ARG:HA	7:G:111:LYS:HZ3	1.75	0.51
7:G:213:LYS:O	7:G:217:THR:HG23	2.10	0.51
25:a:104:THR:OG1	25:a:126:LYS:O	2.27	0.51
38:r:138:LYS:HG2	38:r:146:SER:HB3	1.93	0.51
40:v:12:ALA:HB3	45:1:2694:A:C8	2.45	0.51
45:1:2357:A:H2'	45:1:2358:A:C8	2.45	0.51
26:b:483:ALA:O	26:b:485:GLU:N	2.43	0.51
45:1:139:G:H2'	45:1:140:C:C6	2.44	0.51
45:1:972:A:C6	45:1:973:A:C6	2.98	0.51
45:1:1055:A:O2'	45:1:1056:U:H2'	2.10	0.51
45:1:2865:U:O2'	45:1:2866:U:OP2	2.26	0.51
45:1:2945:G:H4'	45:1:2946:A:H5'	1.93	0.51
1:A:28:LYS:HE2	1:A:123:ARG:HB2	1.92	0.51
4:D:108:ARG:HE	4:D:253:PHE:HB2	1.75	0.51
10:L:18:TRP:HE1	12:N:195:ASN:ND2	2.09	0.51
45:1:130:A:H2'	45:1:131:C:H6	1.75	0.51
45:1:239:G:H2'	45:1:240:U:C6	2.46	0.51
4:D:55:PHE:HE2	4:D:60:ILE:HG23	1.75	0.51
31:g:42:PRO:HB2	31:g:51:LEU:HD12	1.92	0.51
42:x:326:LEU:HD11	42:x:374:MET:SD	2.51	0.51
45:1:2980:U:O2'	45:1:2981:U:H5'	2.11	0.51
26:b:92:LYS:NZ	45:1:2863:G:H22	2.07	0.51
27:c:22:LYS:HB2	27:c:94:GLU:HB3	1.93	0.51
36:m:31:ARG:NH2	45:1:2964:G:O2'	2.43	0.51
45:1:2199:G:H22	45:1:2236:G:H5''	1.75	0.51
47:3:104:A:H2'	47:3:105:C:C6	2.46	0.51
2:B:242:THR:OG1	2:B:245:GLY:O	2.25	0.51
4:D:40:HIS:CB	4:D:41:LYS:HA	2.40	0.51
4:D:248:ARG:NH2	42:x:174:ASP:OD1	2.43	0.51
9:J:155:THR:OG1	9:J:156:LYS:N	2.43	0.51
21:W:43:LEU:HD11	21:W:103:LEU:HB2	1.93	0.51
26:b:298:LEU:HG	26:b:302:ARG:HB2	1.93	0.51
27:c:23:TYR:OH	27:c:83:LYS:NZ	2.43	0.51
36:m:52:LYS:H	36:m:53:GLY:HA2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:13:A:H5'	45:1:14:U:OP2	2.11	0.51
45:1:567:G:H2'	45:1:568:G:C8	2.46	0.51
45:1:2951:G:H2'	45:1:2951:G:N3	2.25	0.51
15:Q:69:ARG:NH1	45:1:720:A:H5'	2.26	0.51
21:W:39:TYR:HB2	21:W:105:THR:HG22	1.93	0.51
23:Y:72:SER:OG	23:Y:81:GLN:OE1	2.29	0.51
43:y:85:ARG:NH1	43:y:89:PRO:O	2.44	0.51
45:1:507:U:H2'	45:1:508:U:C6	2.46	0.51
4:D:36:LEU:HD22	4:D:50:ARG:HD3	1.93	0.51
26:b:512:SER:O	26:b:512:SER:OG	2.29	0.51
33:i:88:GLU:HA	33:i:91:ASN:HD22	1.76	0.51
45:1:737:G:H2'	45:1:738:A:C8	2.46	0.51
45:1:800:G:H2'	45:1:801:A:N7	2.26	0.51
45:1:3349:C:H2'	45:1:3350:C:C6	2.45	0.51
2:B:68:HIS:O	2:B:70:ARG:NH1	2.44	0.50
20:V:63:LYS:O	20:V:70:ARG:NH1	2.44	0.50
36:m:69:ALA:HB2	38:r:205:GLN:HB3	1.93	0.50
43:y:106:ASN:HB3	43:y:147:LEU:HD22	1.93	0.50
45:1:159:A:O2'	45:1:160:G:H5'	2.11	0.50
45:1:643:U:H3	45:1:953:G:N2	2.08	0.50
45:1:1624:G:H2'	45:1:1625:A:H8	1.75	0.50
46:2:153:U:H2'	46:2:154:C:C6	2.40	0.50
26:b:245:HIS:NE2	36:m:164:THR:OG1	2.44	0.50
45:1:3279:A:H2'	45:1:3279:A:N3	2.27	0.50
1:A:107:VAL:HB	1:A:111:THR:HG21	1.93	0.50
2:B:387:LEU:HD21	39:u:105:ARG:HH11	1.77	0.50
8:H:112:ILE:HD11	8:H:134:ILE:HD13	1.93	0.50
11:M:24:LYS:NZ	11:M:25:LYS:HE3	2.25	0.50
26:b:58:VAL:HG21	26:b:106:GLU:HG3	1.93	0.50
45:1:2421:U:H2'	45:1:2422:C:C6	2.46	0.50
45:1:2627:C:H2'	45:1:2628:A:C8	2.47	0.50
45:1:3047:U:O2'	45:1:3048:A:H5'	2.11	0.50
45:1:3358:U:H2'	45:1:3359:A:H8	1.76	0.50
46:2:9:A:H2'	46:2:10:A:C8	2.46	0.50
29:e:42:VAL:O	29:e:52:GLN:NE2	2.45	0.50
32:h:38:ARG:HB3	32:h:41:LEU:HD21	1.92	0.50
36:m:281:ARG:NH1	36:m:281:ARG:HG2	2.26	0.50
41:w:26:LEU:HD22	41:w:65:LEU:HD11	1.91	0.50
45:1:89:A:O2'	45:1:90:C:O5'	2.27	0.50
45:1:130:A:H2'	45:1:131:C:C6	2.47	0.50
45:1:2859:U:H4'	45:1:2860:U:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:83:U:C4	47:3:97:A:N6	2.79	0.50
11:M:19:ARG:HG2	11:M:65:LEU:HD22	1.93	0.50
31:g:66:SER:OG	31:g:67:LYS:N	2.45	0.50
36:m:189:ASP:OD1	36:m:194:TRP:NE1	2.39	0.50
42:x:145:THR:OG1	42:x:506:LYS:HA	2.11	0.50
45:1:1117:G:H1	45:1:1142:G:N2	2.10	0.50
45:1:2095:G:H2'	45:1:2096:A:C8	2.46	0.50
45:1:2624:G:N2	45:1:2754:G:H22	2.09	0.50
45:1:2657:A:O2'	45:1:2658:G:O4'	2.24	0.50
6:F:74:SER:OG	6:F:75:TYR:N	2.44	0.50
9:J:49:LYS:HB2	9:J:62:ASN:HA	1.92	0.50
12:N:4:TYR:OH	33:i:36:ARG:NE	2.44	0.50
14:P:32:THR:HG21	14:P:87:SER:HB2	1.94	0.50
39:u:80:ARG:H	43:y:85:ARG:HG2	1.77	0.50
42:x:338:ALA:HB1	42:x:355:LYS:HE2	1.93	0.50
43:y:234:GLY:HA2	43:y:237:ARG:HE	1.77	0.50
45:1:1128:U:O2'	45:1:1129:A:O5'	2.29	0.50
45:1:2376:G:H2'	45:1:2377:G:C8	2.46	0.50
45:1:2769:A:H2'	45:1:2770:G:C8	2.47	0.50
1:A:64:ARG:HA	1:A:71:LEU:HD23	1.92	0.50
9:J:107:ASP:OD1	9:J:108:GLU:N	2.43	0.50
12:N:36:ILE:HG12	12:N:64:VAL:HG23	1.92	0.50
26:b:264:ILE:O	26:b:268:VAL:HG22	2.12	0.50
26:b:434:GLU:OE2	39:u:1:MET:HB2	2.12	0.50
31:g:72:VAL:HG12	31:g:73:SER:H	1.77	0.50
41:w:111:MET:HB3	41:w:116:LYS:HG3	1.93	0.50
45:1:643:U:H6	45:1:644:G:N2	2.09	0.50
45:1:655:C:H2'	45:1:656:A:C8	2.47	0.50
45:1:1050:U:O2'	45:1:1052:U:O4	2.17	0.50
45:1:1750:A:H4'	45:1:1751:G:H5'	1.94	0.50
10:L:28:GLN:NE2	45:1:683:U:OP2	2.45	0.50
22:X:119:THR:OG1	22:X:120:LYS:N	2.44	0.50
36:m:400:ILE:HG13	36:m:428:ILE:HD11	1.94	0.50
38:r:10:HIS:CD2	38:r:14:HIS:HD2	2.29	0.50
42:x:76:PRO:HG3	42:x:126:VAL:HG23	1.93	0.50
45:1:1349:G:H2'	45:1:1349:G:N3	2.27	0.50
45:1:1646:G:HO2'	45:1:1808:G:N2	2.07	0.50
45:1:2890:A:O2'	45:1:2933:A:N3	2.43	0.50
17:S:146:LYS:NZ	45:1:535:G:OP1	2.45	0.50
26:b:80:ASP:O	26:b:84:THR:HG23	2.12	0.50
35:k:68:SER:O	35:k:68:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:153:U:O2'	45:1:158:G:O2'	2.29	0.50
45:1:1082:U:H2'	45:1:1083:G:H8	1.76	0.50
45:1:2278:C:O2'	45:1:2279:A:O4'	2.30	0.50
45:1:2423:U:H3	45:1:2607:G:H1	1.58	0.50
47:3:110:G:H2'	47:3:111:U:C6	2.47	0.50
1:A:52:SER:HB3	1:A:191:LEU:HD12	1.93	0.49
20:V:59:MET:HE1	20:V:75:PRO:HG3	1.93	0.49
41:w:142:VAL:O	41:w:142:VAL:HG13	2.12	0.49
4:D:17:GLN:OE1	4:D:17:GLN:N	2.45	0.49
7:G:89:GLU:HG3	7:G:214:LEU:HD22	1.94	0.49
13:O:131:PRO:HB3	17:S:155:ARG:HH11	1.76	0.49
16:R:136:ARG:NH1	45:1:1947:G:OP1	2.45	0.49
26:b:511:LYS:HD3	45:1:1681:U:H5''	1.94	0.49
31:g:76:TYR:HB3	31:g:80:ARG:HB2	1.94	0.49
36:m:139:ASP:OD2	36:m:139:ASP:N	2.44	0.49
42:x:305:ASP:OD2	42:x:306:ILE:N	2.45	0.49
45:1:170:G:C2	45:1:249:U:C2	3.00	0.49
45:1:2731:U:H1'	45:1:2732:G:C8	2.47	0.49
2:B:163:HIS:ND1	2:B:164:THR:O	2.45	0.49
9:J:27:GLY:O	9:J:31:THR:HG23	2.12	0.49
26:b:305:LEU:O	26:b:308:SER:OG	2.15	0.49
45:1:437:G:H1	45:1:622:A:N6	2.03	0.49
45:1:1544:G:H2'	45:1:1545:A:O4'	2.12	0.49
45:1:2357:A:H2'	45:1:2358:A:H8	1.77	0.49
26:b:298:LEU:HD12	26:b:299:ASP:H	1.76	0.49
45:1:163:C:H42	45:1:259:C:H42	1.60	0.49
45:1:2420:C:H2'	45:1:2421:U:O2	2.11	0.49
45:1:2653:C:O2'	45:1:2655:U:O5'	2.27	0.49
4:D:172:TYR:CG	42:x:134:ARG:HD3	2.48	0.49
10:L:75:PHE:O	10:L:76:THR:OG1	2.23	0.49
12:N:120:TRP:HZ2	12:N:123:GLN:HG2	1.78	0.49
20:V:45:ARG:HG2	20:V:48:ARG:HH11	1.77	0.49
21:W:196:ASP:N	21:W:199:GLN:OE1	2.45	0.49
36:m:336:ARG:HG2	36:m:340:VAL:HG21	1.93	0.49
45:1:3016:A:HO2'	45:1:3017:A:H8	1.59	0.49
45:1:3343:G:H21	45:1:3362:A:H2	1.60	0.49
4:D:164:LYS:NZ	4:D:168:ASP:OD2	2.45	0.49
7:G:218:ILE:O	7:G:222:PHE:HB2	2.13	0.49
20:V:102:ILE:HD11	20:V:110:LYS:HD3	1.94	0.49
33:i:36:ARG:O	33:i:40:VAL:HG23	2.12	0.49
38:r:3:GLN:O	38:r:4:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:x:150:ALA:O	42:x:159:MET:HG2	2.12	0.49
43:y:118:HIS:HD2	43:y:146:ILE:HG23	1.78	0.49
16:R:47:ASN:OD1	16:R:48:GLY:N	2.46	0.49
42:x:480:VAL:HG13	42:x:482:LEU:HD22	1.94	0.49
45:1:1811:G:H2'	45:1:1812:G:C8	2.47	0.49
45:1:2243:A:O5'	45:1:2243:A:H8	1.94	0.49
45:1:2669:G:H2'	45:1:2670:G:H8	1.77	0.49
17:S:16:THR:HG23	17:S:19:VAL:HB	1.95	0.49
38:r:137:ILE:HD11	38:r:150:MET:HE3	1.95	0.49
38:r:164:ARG:HE	45:1:2728:G:C5'	2.25	0.49
45:1:239:G:O2'	45:1:240:U:OP1	2.31	0.49
2:B:277:SER:OG	2:B:280:HIS:NE2	2.34	0.49
37:p:16:VAL:HG12	45:1:2320:A:H2	1.77	0.49
45:1:737:G:H2'	45:1:738:A:H8	1.76	0.49
45:1:996:A:H1'	45:1:997:A:H3'	1.94	0.49
45:1:2437:G:O6	45:1:2510:U:O2	2.31	0.49
6:F:29:GLU:OE1	6:F:33:ARG:NH2	2.41	0.49
26:b:270:LEU:O	26:b:274:ILE:HG12	2.13	0.49
26:b:294:ARG:O	26:b:296:GLU:N	2.46	0.49
26:b:511:LYS:HE2	26:b:513:LEU:HD12	1.95	0.49
38:r:164:ARG:CZ	45:1:2728:G:H4'	2.43	0.49
38:r:164:ARG:NH2	45:1:2728:G:H4'	2.28	0.49
38:r:169:GLU:HG3	45:1:2727:A:C8	2.47	0.49
41:w:45:ARG:HB3	41:w:49:LYS:HE3	1.94	0.49
42:x:321:HIS:HD2	42:x:322:TRP:H	1.58	0.49
45:1:196:G:N2	45:1:198:A:H3'	2.28	0.49
45:1:1545:A:H4'	45:1:2167:A:C2	2.48	0.49
45:1:2399:A:H2'	45:1:2400:G:O4'	2.12	0.49
45:1:2697:A:H2'	45:1:2698:G:N7	2.28	0.49
2:B:10:ARG:NH2	2:B:263:SER:O	2.46	0.48
3:C:234:ASN:OD1	3:C:235:LEU:N	2.46	0.48
21:W:163:PRO:O	21:W:167:ASN:ND2	2.46	0.48
38:r:204:PRO:O	38:r:205:GLN:HG2	2.13	0.48
40:v:50:SER:OG	40:v:59:ARG:NH2	2.46	0.48
42:x:274:MET:HB3	42:x:304:TRP:CZ3	2.48	0.48
43:y:126:GLU:OE1	43:y:139:ARG:NH1	2.31	0.48
45:1:2364:G:H1	45:1:2396:G:H21	1.60	0.48
45:1:2624:G:H1'	45:1:2625:C:OP1	2.13	0.48
47:3:75:G:H2'	47:3:76:A:C5	2.48	0.48
40:v:115:GLU:HB2	40:v:235:GLY:HA3	1.96	0.48
40:v:194:GLU:HG2	40:v:195:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:170:G:N1	45:1:249:U:C2	2.81	0.48
45:1:758:C:H2'	45:1:759:U:O4'	2.13	0.48
45:1:2768:U:H2'	45:1:2769:A:C8	2.48	0.48
1:A:21:ARG:HG2	1:A:22:LEU:HG	1.95	0.48
7:G:129:PRO:HG2	45:1:121:A:N1	2.28	0.48
10:L:18:TRP:CD1	10:L:19:GLN:H	2.32	0.48
26:b:57:PHE:CE1	26:b:140:VAL:HG21	2.48	0.48
45:1:1194:G:H2'	45:1:1195:A:C8	2.48	0.48
45:1:2203:U:C4	45:1:2240:G:N2	2.82	0.48
45:1:2655:U:H5''	45:1:2657:A:H62	1.77	0.48
45:1:2761:G:O2'	45:1:2762:A:OP1	2.24	0.48
47:3:91:G:H3'	47:3:92:A:H5''	1.94	0.48
36:m:281:ARG:HG2	36:m:281:ARG:HH11	1.78	0.48
38:r:2:PRO:HD2	45:1:3026:G:H4'	1.95	0.48
42:x:183:LYS:HG2	42:x:184:GLY:N	2.28	0.48
45:1:2228:A:H2'	45:1:2229:A:C8	2.48	0.48
45:1:2621:G:C2'	45:1:2622:C:H5'	2.44	0.48
1:A:135:ILE:HG23	1:A:149:ARG:HB3	1.95	0.48
2:B:343:TYR:CE2	2:B:345:ASN:HA	2.48	0.48
3:C:156:LEU:HD23	3:C:159:ILE:HD12	1.96	0.48
4:D:68:THR:HG23	4:D:71:GLY:H	1.78	0.48
7:G:142:LEU:O	7:G:145:ASN:HB2	2.14	0.48
7:G:144:GLU:HA	7:G:173:MET:HE2	1.94	0.48
27:c:34:LEU:HD23	27:c:59:TYR:HB3	1.95	0.48
27:c:87:VAL:HG23	45:1:1728:G:O2'	2.14	0.48
45:1:1200:A:H2	45:1:2824:G:C2	2.29	0.48
45:1:2137:U:O2	45:1:2137:U:H2'	2.14	0.48
45:1:3165:A:H2'	45:1:3166:C:C6	2.48	0.48
2:B:4:ARG:HG3	45:1:2881:C:N4	2.28	0.48
9:J:12:LEU:HD22	9:J:133:ARG:HG2	1.94	0.48
26:b:279:ALA:O	26:b:280:ASN:ND2	2.46	0.48
31:g:6:THR:HG22	45:1:1486:G:H21	1.77	0.48
45:1:435:C:H2'	45:1:436:A:H8	1.79	0.48
45:1:2797:C:O2'	45:1:2798:C:H5'	2.13	0.48
2:B:120:LYS:HE2	45:1:3000:A:H5''	1.95	0.48
6:F:176:TYR:HB3	6:F:194:HIS:CD2	2.49	0.48
14:P:25:SER:O	14:P:29:THR:OG1	2.28	0.48
24:Z:115:LYS:NZ	24:Z:119:GLU:OE2	2.37	0.48
38:r:169:GLU:HG3	45:1:2727:A:N7	2.29	0.48
41:w:184:ARG:O	41:w:188:VAL:HG23	2.13	0.48
26:b:354:ILE:HA	26:b:357:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:355:TYR:O	36:m:356:ILE:HG13	2.13	0.48
45:1:649:A:H2'	45:1:650:C:H6	1.79	0.48
45:1:2817:A:H1'	45:1:2818:U:H5'	1.95	0.48
2:B:34:LYS:O	2:B:35:ASP:HB2	2.14	0.48
8:H:4:ILE:HD11	17:S:150:PHE:CD1	2.48	0.48
12:N:4:TYR:CG	12:N:5:LYS:N	2.82	0.48
18:T:100:LYS:HB3	18:T:103:GLN:HG3	1.95	0.48
26:b:496:ILE:HG23	39:u:133:LEU:HD12	1.96	0.48
27:c:75:ASN:O	27:c:79:THR:HG23	2.14	0.48
32:h:85:THR:HG23	32:h:88:LEU:H	1.77	0.48
36:m:419:SER:HB2	36:m:430:ILE:HG21	1.95	0.48
42:x:470:VAL:HB	42:x:480:VAL:HG12	1.96	0.48
45:1:735:A:OP2	45:1:735:A:H8	1.96	0.48
2:B:123:TYR:CE1	2:B:124:LYS:HG3	2.49	0.48
2:B:188:ILE:O	2:B:192:VAL:HG13	2.13	0.48
7:G:75:ILE:HG13	7:G:76:ALA:N	2.28	0.48
26:b:13:PRO:HG2	26:b:16:ASP:OD2	2.14	0.48
36:m:151:ARG:HB3	36:m:152:LEU:HG	1.96	0.48
43:y:199:VAL:HG23	43:y:204:ALA:HB2	1.96	0.48
45:1:137:G:H2'	45:1:138:U:C6	2.48	0.48
45:1:2398:A:H2'	45:1:2399:A:O4'	2.13	0.48
45:1:2650:U:H2'	45:1:2651:G:C4	2.48	0.48
1:A:128:ARG:NH2	45:1:2176:U:OP1	2.46	0.47
8:H:16:VAL:HG12	8:H:30:PRO:HD3	1.97	0.47
11:M:24:LYS:HZ3	11:M:25:LYS:HE3	1.78	0.47
38:r:164:ARG:NE	45:1:2728:G:H4'	2.29	0.47
41:w:149:GLY:HA3	45:1:2656:A:N6	2.28	0.47
45:1:242:C:O2'	45:1:243:G:H8	1.97	0.47
45:1:261:U:O2'	45:1:262:U:O5'	2.24	0.47
45:1:3294:A:H2'	45:1:3295:A:O4'	2.14	0.47
47:3:58:C:H2'	47:3:59:U:C6	2.49	0.47
3:C:58:HIS:O	3:C:60:THR:N	2.46	0.47
10:L:47:ALA:O	10:L:137:GLN:NE2	2.47	0.47
36:m:54:ASN:OD1	36:m:54:ASN:N	2.39	0.47
36:m:330:SER:O	36:m:334:THR:HG22	2.14	0.47
41:w:145:TRP:HA	45:1:2656:A:N6	2.28	0.47
43:y:143:SER:O	43:y:143:SER:OG	2.23	0.47
45:1:345:G:O2'	46:2:25:G:N3	2.44	0.47
45:1:954:U:O4	45:1:1115:G:H1'	2.14	0.47
45:1:2710:C:H2'	45:1:2711:C:C6	2.49	0.47
45:1:2747:A:H2'	45:1:2748:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:PHE:CZ	20:V:88:ARG:HG3	2.49	0.47
9:J:132:ASN:ND2	9:J:136:ALA:HB2	2.30	0.47
18:T:106:LEU:O	18:T:110:LYS:HG2	2.13	0.47
21:W:45:LEU:HB2	21:W:48:VAL:HG21	1.95	0.47
26:b:306:LEU:O	26:b:309:VAL:HG22	2.14	0.47
28:d:77:ARG:HD2	28:d:89:LEU:HD23	1.96	0.47
35:k:57:ASN:N	35:k:57:ASN:OD1	2.46	0.47
37:p:59:CYS:C	37:p:61:LYS:H	2.22	0.47
42:x:194:TRP:HE1	42:x:198:GLY:HA2	1.78	0.47
42:x:228:HIS:NE2	42:x:261:LYS:HD2	2.30	0.47
42:x:443:HIS:CE1	42:x:469:LYS:HG3	2.49	0.47
43:y:226:ASP:HA	43:y:227:ALA:HA	1.50	0.47
45:1:293:C:H2'	45:1:294:U:O4'	2.14	0.47
45:1:2213:A:H3'	45:1:2214:A:H8	1.78	0.47
45:1:2436:U:N3	45:1:2511:A:H2	2.12	0.47
45:1:3358:U:H2'	45:1:3359:A:C8	2.49	0.47
47:3:22:A:H2'	47:3:22:A:N3	2.28	0.47
4:D:276:LYS:HB2	4:D:276:LYS:HE2	1.73	0.47
12:N:19:LEU:O	12:N:23:GLN:HG2	2.14	0.47
42:x:305:ASP:OD2	42:x:307:ASN:N	2.48	0.47
42:x:450:VAL:HG12	42:x:461:SER:HB2	1.96	0.47
2:B:108:GLU:HB2	2:B:137:TYR:CZ	2.49	0.47
5:E:8:LYS:NZ	45:1:1354:G:H1'	2.29	0.47
7:G:107:GLU:O	7:G:111:LYS:HG3	2.15	0.47
45:1:2249:G:O2'	45:1:2250:G:H8	1.97	0.47
22:X:117:ASN:OD1	22:X:118:GLY:N	2.48	0.47
36:m:50:ASN:HB3	36:m:56:ILE:HD11	1.96	0.47
36:m:151:ARG:HA	36:m:152:LEU:HA	1.48	0.47
42:x:350:GLU:O	42:x:354:LYS:HG2	2.14	0.47
45:1:10:C:H5''	45:1:11:A:OP2	2.13	0.47
45:1:539:C:H2'	45:1:540:U:C6	2.50	0.47
45:1:970:A:N1	45:1:971:G:C6	2.83	0.47
45:1:1348:U:H5''	45:1:1349:G:C5	2.50	0.47
45:1:1699:A:H2'	45:1:1700:G:C8	2.49	0.47
45:1:2201:G:H2'	45:1:2245:C:N4	2.29	0.47
45:1:2687:G:N2	45:1:2690:G:H5''	2.26	0.47
4:D:268:GLU:HG2	47:3:121:U:O2	2.15	0.47
6:F:216:VAL:HG23	6:F:216:VAL:O	2.15	0.47
9:J:139:THR:O	9:J:145:LYS:NZ	2.34	0.47
21:W:158:ILE:HG13	21:W:161:LEU:HD22	1.97	0.47
22:X:105:VAL:HG12	22:X:130:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:369:ARG:HB3	43:y:178:GLN:OE1	2.15	0.47
26:b:463:LEU:HB3	26:b:468:PHE:HB2	1.96	0.47
36:m:384:PHE:HE2	36:m:403:VAL:HG22	1.79	0.47
36:m:414:ARG:HG2	40:v:297:PHE:O	2.14	0.47
36:m:449:VAL:HA	36:m:452:GLN:HE21	1.78	0.47
38:r:5:ASP:N	38:r:5:ASP:OD1	2.46	0.47
39:u:1:MET:HE2	39:u:1:MET:HB3	1.71	0.47
41:w:71:LYS:HD3	41:w:83:GLN:HE22	1.80	0.47
45:1:86:G:O2'	45:1:98:G:O6	2.24	0.47
45:1:647:A:H8	45:1:647:A:O5'	1.98	0.47
45:1:1151:U:H3'	45:1:1152:G:N2	2.29	0.47
45:1:1816:A:O2'	45:1:1817:G:OP1	2.32	0.47
45:1:2630:C:H2'	45:1:2631:U:C6	2.50	0.47
45:1:2781:U:H2'	45:1:2782:U:C6	2.50	0.47
45:1:2876:C:H1'	45:1:2877:G:H5'	1.97	0.47
45:1:3194:C:H2'	45:1:3195:U:H5''	1.97	0.47
45:1:3269:U:H4'	45:1:3270:U:O5'	2.14	0.47
45:1:3348:G:H2'	45:1:3349:C:C6	2.49	0.47
47:3:17:A:H2'	47:3:18:C:H6	1.80	0.47
16:R:52:LYS:O	16:R:52:LYS:HG2	2.15	0.47
20:V:19:VAL:HG23	20:V:50:PRO:O	2.15	0.47
20:V:136:VAL:HG12	20:V:137:VAL:HG23	1.97	0.47
21:W:90:TYR:O	21:W:94:LYS:HG2	2.15	0.47
24:Z:105:SER:HB2	24:Z:108:GLU:HB3	1.96	0.47
26:b:370:ASP:OD1	26:b:371:ASP:N	2.45	0.47
45:1:1544:G:H1	45:1:1549:U:H3	1.61	0.47
45:1:1550:C:H1'	45:1:2168:A:N1	2.30	0.47
47:3:47:C:H2'	47:3:48:U:H6	1.80	0.47
47:3:72:A:C6	47:3:74:C:C4	3.02	0.47
4:D:241:THR:O	4:D:245:GLU:HG2	2.14	0.47
9:J:166:LYS:C	9:J:168:ASP:H	2.22	0.47
16:R:128:LYS:NZ	45:1:1724:U:OP1	2.47	0.47
26:b:418:ASP:HA	26:b:428:LYS:HD3	1.95	0.47
26:b:507:ALA:HA	26:b:510:ARG:HG2	1.97	0.47
35:k:8:ILE:CD1	35:k:65:LEU:HD21	2.44	0.47
41:w:59:GLN:NE2	41:w:63:ASN:OD1	2.47	0.47
45:1:124:U:H1'	45:1:149:U:O2	2.15	0.47
45:1:243:G:C2	45:1:244:G:C4	3.03	0.47
45:1:849:C:O2'	45:1:850:U:OP1	2.29	0.47
45:1:1202:A:H2'	45:1:1203:A:C2	2.50	0.47
45:1:2439:A:OP2	45:1:2439:A:H8	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HG23	1:A:62:VAL:HG12	1.97	0.47
8:H:86:TYR:CE2	8:H:151:VAL:HG13	2.49	0.47
24:Z:121:ARG:NH2	24:Z:126:LYS:HB2	2.29	0.47
36:m:262:CYS:HB2	36:m:286:PHE:O	2.15	0.47
40:v:46:MET:SD	40:v:59:ARG:HD3	2.54	0.47
45:1:2410:U:H5	45:1:2811:A:N1	2.13	0.47
45:1:2769:A:H2'	45:1:2770:G:H8	1.80	0.47
45:1:3252:G:H2'	45:1:3253:G:C8	2.49	0.47
47:3:26:C:H2'	47:3:27:A:O4'	2.15	0.47
7:G:108:ARG:HA	7:G:111:LYS:NZ	2.30	0.46
7:G:147:LYS:O	7:G:201:THR:OG1	2.20	0.46
9:J:100:GLY:HA3	9:J:159:THR:HG21	1.97	0.46
23:Y:81:GLN:HG2	23:Y:96:PRO:HB2	1.97	0.46
32:h:28:LEU:HG	32:h:32:LYS:HE3	1.97	0.46
43:y:182:VAL:HG22	43:y:221:ILE:HG12	1.97	0.46
45:1:95:A:H2'	45:1:96:G:O4'	2.15	0.46
45:1:122:A:N1	45:1:145:G:O2'	2.42	0.46
45:1:747:A:H2'	45:1:748:U:C6	2.50	0.46
6:F:84:VAL:HG21	6:F:127:LEU:HD11	1.96	0.46
7:G:86:THR:O	7:G:90:THR:OG1	2.31	0.46
10:L:123:ILE:HG22	32:h:118:ILE:HG12	1.97	0.46
12:N:94:TYR:OH	12:N:96:ARG:NH1	2.48	0.46
18:T:71:SER:HB2	18:T:91:LEU:O	2.15	0.46
33:i:26:ILE:HG22	33:i:29:LYS:HE2	1.97	0.46
33:i:83:ALA:O	33:i:87:VAL:HG22	2.15	0.46
40:v:186:ILE:H	40:v:186:ILE:HD12	1.80	0.46
42:x:40:ASP:OD2	42:x:40:ASP:N	2.47	0.46
42:x:90:ASP:OD1	42:x:90:ASP:N	2.47	0.46
45:1:2222:A:H2'	45:1:2223:A:C4	2.50	0.46
45:1:2615:G:N2	45:1:2619:G:OP2	2.48	0.46
1:A:110:GLY:HA2	1:A:135:ILE:HD11	1.97	0.46
2:B:316:GLU:O	2:B:318:LYS:HG3	2.16	0.46
4:D:282:ARG:NH2	47:3:63:A:OP2	2.43	0.46
10:L:56:PRO:HB3	10:L:75:PHE:CD2	2.50	0.46
15:Q:92:ARG:NH1	45:1:784:A:O2'	2.48	0.46
21:W:67:MET:HE2	21:W:67:MET:HB3	1.88	0.46
26:b:416:LEU:HD23	26:b:416:LEU:HA	1.79	0.46
26:b:503:MET:HE3	26:b:503:MET:HB2	1.80	0.46
42:x:383:MET:HE3	42:x:383:MET:HB2	1.84	0.46
45:1:2421:U:H2'	45:1:2422:C:H6	1.79	0.46
45:1:2658:G:C4	45:1:2659:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:2728:G:N2	45:1:2730:G:OP2	2.44	0.46
1:A:95:SER:OG	1:A:96:LEU:N	2.47	0.46
2:B:17:LEU:HD11	2:B:233:TRP:HH2	1.80	0.46
9:J:49:LYS:HE3	9:J:62:ASN:HB3	1.96	0.46
21:W:87:GLU:OE2	21:W:88:ASN:ND2	2.48	0.46
25:a:85:ASP:O	25:a:89:GLN:NE2	2.48	0.46
25:a:96:LYS:C	25:a:98:THR:H	2.24	0.46
45:1:275:U:H2'	45:1:276:U:C6	2.51	0.46
45:1:2100:A:O2'	45:1:2101:C:H5'	2.15	0.46
45:1:2842:U:H2'	45:1:2843:U:C6	2.50	0.46
47:3:86:U:O2'	47:3:88:G:OP1	2.34	0.46
6:F:121:LYS:HB3	18:T:133:ALA:HB3	1.96	0.46
12:N:98:LEU:HD13	12:N:128:LYS:HD2	1.98	0.46
15:Q:147:ARG:HH11	15:Q:147:ARG:C	2.22	0.46
17:S:166:LYS:HE2	17:S:166:LYS:HB3	1.68	0.46
18:T:55:LYS:HE3	18:T:55:LYS:HB2	1.75	0.46
26:b:180:LYS:NZ	48:b:701:GTP:O2B	2.46	0.46
26:b:397:LYS:HA	26:b:397:LYS:HD2	1.68	0.46
28:d:57:GLN:NE2	45:1:1474:A:O2'	2.49	0.46
42:x:427:LYS:HG2	42:x:436:PHE:HE1	1.81	0.46
45:1:2981:U:O2'	45:1:2982:A:H5'	2.15	0.46
45:1:3234:A:N1	45:1:3253:G:N2	2.46	0.46
14:P:69:ARG:HD2	45:1:3308:C:O2	2.16	0.46
42:x:175:THR:O	42:x:177:THR:HG23	2.16	0.46
45:1:13:A:H61	46:2:145:U:H3	1.64	0.46
45:1:115:A:H2'	45:1:265:A:N3	2.31	0.46
45:1:1597:C:H5'	45:1:1696:A:H1'	1.98	0.46
45:1:2929:C:HO2'	45:1:2930:A:P	2.38	0.46
45:1:3174:A:H2'	45:1:3175:U:H5'	1.97	0.46
45:1:3257:C:H2'	45:1:3258:U:O4'	2.15	0.46
1:A:180:LEU:HD11	37:p:26:VAL:HG11	1.98	0.46
20:V:109:MET:HG2	20:V:128:ARG:HG2	1.97	0.46
26:b:92:LYS:CE	45:1:2863:G:H22	2.28	0.46
30:f:68:TRP:HZ2	45:1:3275:U:H5'	1.81	0.46
40:v:199:VAL:HG23	40:v:232:PHE:HB2	1.97	0.46
41:w:54:THR:HA	41:w:57:ASN:HD22	1.80	0.46
42:x:128:LYS:HA	42:x:128:LYS:HD2	1.73	0.46
45:1:734:C:H2'	45:1:735:A:C8	2.51	0.46
45:1:915:A:C4	45:1:917:A:H1'	2.50	0.46
45:1:2270:A:H2'	45:1:2270:A:N3	2.31	0.46
45:1:2883:U:H2'	45:1:2884:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:TYR:O	3:C:230:VAL:HG22	2.16	0.46
10:L:56:PRO:HG3	10:L:74:GLY:O	2.16	0.46
25:a:79:TRP:CE3	25:a:82:ILE:HD12	2.51	0.46
36:m:220:ASP:HB3	38:r:163:ARG:HD3	1.97	0.46
36:m:227:HIS:NE2	36:m:238:ARG:O	2.49	0.46
36:m:257:TYR:HB2	36:m:283:THR:HA	1.97	0.46
36:m:289:SER:HB3	36:m:292:ASN:O	2.14	0.46
42:x:62:GLU:HA	42:x:65:ASN:ND2	2.30	0.46
45:1:306:A:H3'	45:1:307:A:H5''	1.98	0.46
45:1:2251:G:H22	45:1:2266:U:H1'	1.81	0.46
45:1:3163:A:O2'	45:1:3164:C:H5'	2.15	0.46
45:1:3357:U:H2'	45:1:3358:U:C6	2.51	0.46
47:3:4:U:H2'	47:3:5:G:H8	1.80	0.46
7:G:167:PRO:HB3	7:G:177:TYR:CE2	2.51	0.46
28:d:82:GLU:HG3	28:d:83:GLU:N	2.31	0.46
38:r:17:ARG:HB3	38:r:20:HIS:HB2	1.98	0.46
45:1:63:A:N3	45:1:78:U:O2'	2.45	0.46
45:1:162:G:C6	45:1:163:C:C4	3.03	0.46
45:1:304:G:N3	45:1:304:G:H2'	2.30	0.46
45:1:527:A:H2'	45:1:528:U:C6	2.50	0.46
45:1:1350:A:H2'	45:1:1351:U:H6	1.81	0.46
45:1:2197:C:H4'	45:1:2198:A:OP2	2.16	0.46
45:1:2909:U:H2'	45:1:2910:A:O4'	2.15	0.46
47:3:83:U:O2	47:3:83:U:H2'	2.15	0.46
4:D:144:VAL:HG23	4:D:173:VAL:HG13	1.98	0.46
6:F:159:GLN:O	45:1:1362:G:H4'	2.15	0.46
6:F:159:GLN:O	6:F:160:ARG:C	2.59	0.46
10:L:183:ARG:NE	45:1:765:C:O2'	2.41	0.46
26:b:284:MET:HE3	26:b:284:MET:HB2	1.77	0.46
27:c:83:LYS:HB3	27:c:85:PHE:CE2	2.51	0.46
33:i:5:THR:HG22	33:i:12:ASN:O	2.16	0.46
36:m:46:LYS:HD3	36:m:46:LYS:HA	1.67	0.46
38:r:58:LYS:NZ	45:1:1206:G:OP2	2.44	0.46
40:v:30:ALA:HA	40:v:86:LEU:HB2	1.97	0.46
44:z:4:SER:OG	44:z:5:LEU:N	2.49	0.46
45:1:959:C:N3	45:1:960:U:H5	2.14	0.46
45:1:1799:A:H2'	45:1:1800:A:C8	2.50	0.46
45:1:1896:A:H61	45:1:2339:C:N4	2.12	0.46
45:1:2211:U:H2'	45:1:2212:C:O4'	2.16	0.46
45:1:3159:C:H2'	45:1:3160:U:H6	1.78	0.46
46:2:9:A:H2'	46:2:10:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HB2	1:A:155:LYS:HE2	1.73	0.45
1:A:178:PRO:HD2	37:p:26:VAL:HG12	1.98	0.45
4:D:36:LEU:O	4:D:36:LEU:HD23	2.16	0.45
12:N:4:TYR:HD1	12:N:4:TYR:H	1.63	0.45
12:N:114:ARG:HH21	12:N:157:LYS:HG2	1.80	0.45
16:R:116:ASP:OD1	16:R:116:ASP:N	2.35	0.45
21:W:134:THR:HG23	21:W:191:GLU:N	2.28	0.45
32:h:86:ARG:HH11	46:2:36:G:H2'	1.81	0.45
34:j:39:TYR:CD1	34:j:40:PRO:HA	2.51	0.45
45:1:19:U:H2'	45:1:20:A:C8	2.51	0.45
45:1:961:C:H2'	45:1:962:A:O4'	2.17	0.45
45:1:1124:U:H2'	45:1:1125:U:C6	2.51	0.45
45:1:2799:A:H2'	45:1:2800:G:C8	2.50	0.45
45:1:2923:U:H2'	45:1:2923:U:O2	2.17	0.45
15:Q:83:VAL:O	15:Q:103:ALA:HA	2.16	0.45
26:b:16:ASP:O	26:b:20:ILE:HG13	2.16	0.45
26:b:161:PRO:HB3	38:r:3:GLN:HB2	1.98	0.45
32:h:38:ARG:HD2	32:h:39:PRO:HD2	1.98	0.45
40:v:139:PRO:HB3	40:v:180:HIS:CE1	2.51	0.45
42:x:18:LEU:HG	42:x:19:PRO:O	2.16	0.45
45:1:434:U:H2'	45:1:435:C:C6	2.51	0.45
45:1:1277:C:O2'	45:1:1278:A:O5'	2.35	0.45
45:1:2396:G:H2'	45:1:2398:A:H5'	1.97	0.45
45:1:2766:U:H2'	45:1:2767:U:C6	2.51	0.45
45:1:2953:U:H5'	45:1:2954:U:H5''	1.99	0.45
47:3:75:G:H2'	47:3:76:A:N7	2.31	0.45
2:B:313:HIS:CD2	2:B:332:ARG:HH21	2.33	0.45
3:C:226:GLU:OE2	3:C:246:ARG:NH2	2.44	0.45
6:F:105:LEU:O	45:1:1100:U:O2'	2.33	0.45
7:G:137:ASN:HA	12:N:2:GLY:HA2	1.99	0.45
16:R:151:ARG:HB3	16:R:151:ARG:HH11	1.81	0.45
19:U:104:ARG:NH1	19:U:106:ALA:HB2	2.32	0.45
24:Z:83:THR:HG22	24:Z:85:TYR:H	1.81	0.45
26:b:224:ILE:HA	26:b:236:GLU:HG3	1.98	0.45
26:b:488:ASP:C	26:b:492:LYS:HZ3	2.24	0.45
33:i:2:THR:O	33:i:2:THR:OG1	2.27	0.45
37:p:88:GLU:HA	37:p:91:GLU:OE1	2.17	0.45
43:y:221:ILE:HD12	43:y:230:GLU:HG2	1.99	0.45
45:1:722:G:H2'	45:1:723:U:H6	1.81	0.45
45:1:3228:C:H4'	45:1:3229:G:O5'	2.15	0.45
4:D:172:TYR:HD2	4:D:172:TYR:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:81:TYR:OH	17:S:88:HIS:NE2	2.45	0.45
28:d:36:ILE:HD12	28:d:59:ILE:HD11	1.98	0.45
42:x:34:ILE:HG12	42:x:52:PRO:HD2	1.98	0.45
45:1:1047:A:H1'	45:1:1048:A:N7	2.32	0.45
45:1:1117:G:H1	45:1:1142:G:H21	1.63	0.45
46:2:155:A:C2	46:2:156:U:H1'	2.52	0.45
3:C:7:THR:HG22	3:C:8:VAL:H	1.81	0.45
4:D:214:ASP:OD1	4:D:214:ASP:N	2.48	0.45
8:H:187:ILE:O	8:H:189:GLU:HB3	2.16	0.45
12:N:40:ALA:HB2	45:1:9:U:OP1	2.16	0.45
21:W:49:ARG:HD3	21:W:126:ARG:NH2	2.32	0.45
35:k:7:ASP:OD2	35:k:10:GLN:HB2	2.17	0.45
36:m:82:ARG:O	38:r:239:TRP:CD1	2.70	0.45
36:m:84:ILE:HG13	42:x:3:THR:HB	1.98	0.45
40:v:117:MET:HE2	40:v:117:MET:HB2	1.89	0.45
41:w:39:LEU:O	41:w:46:ARG:NE	2.43	0.45
42:x:50:ARG:CZ	42:x:51:VAL:H	2.30	0.45
45:1:707:U:H2'	45:1:708:G:C8	2.51	0.45
45:1:900:G:H1'	45:1:1589:A:N6	2.32	0.45
45:1:1001:G:H1	45:1:1050:U:H3	1.65	0.45
45:1:1329:U:O2'	45:1:1330:A:OP1	2.27	0.45
45:1:1641:U:O2'	45:1:1642:A:H3'	2.16	0.45
45:1:3000:A:H2'	45:1:3001:C:C6	2.52	0.45
45:1:3160:U:H2'	45:1:3161:C:C6	2.51	0.45
18:T:105:PHE:O	18:T:109:VAL:HG23	2.17	0.45
40:v:225:GLU:OE2	40:v:227:GLY:N	2.49	0.45
43:y:180:PRO:HG2	43:y:230:GLU:OE2	2.15	0.45
45:1:1688:U:H2'	45:1:1689:U:C6	2.52	0.45
45:1:2761:G:OP2	45:1:2762:A:N6	2.49	0.45
47:3:16:U:H2'	47:3:17:A:C8	2.50	0.45
2:B:123:TYR:CZ	2:B:124:LYS:HG3	2.52	0.45
2:B:202:THR:O	44:z:44:GLN:NE2	2.44	0.45
5:E:91:VAL:HG12	5:E:92:SER:N	2.31	0.45
9:J:7:ASN:OD1	9:J:7:ASN:N	2.49	0.45
16:R:95:TRP:CZ2	16:R:99:LEU:HD22	2.51	0.45
26:b:4:SER:O	26:b:4:SER:OG	2.27	0.45
38:r:2:PRO:O	38:r:3:GLN:HG2	2.17	0.45
42:x:71:SER:O	42:x:71:SER:OG	2.27	0.45
45:1:978:G:H1'	45:1:979:U:H5	1.82	0.45
45:1:2227:C:H2'	45:1:2228:A:H8	1.82	0.45
6:F:203:TRP:CD1	6:F:204:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:213:LYS:O	7:G:213:LYS:HD3	2.17	0.45
14:P:131:ARG:HH12	14:P:137:ASN:HB2	1.82	0.45
20:V:86:ARG:HB2	20:V:92:PHE:CE2	2.52	0.45
21:W:50:THR:O	21:W:54:GLN:HG3	2.17	0.45
26:b:355:ASN:HA	26:b:358:LEU:HD12	1.99	0.45
38:r:95:GLU:N	38:r:95:GLU:OE2	2.49	0.45
42:x:64:LEU:HD22	42:x:77:TYR:CZ	2.52	0.45
42:x:148:CYS:SG	42:x:192:VAL:HG22	2.56	0.45
45:1:1699:A:H2'	45:1:1700:G:H8	1.82	0.45
45:1:2728:G:C1'	45:1:2729:U:H5''	2.47	0.45
47:3:24:A:H2'	47:3:25:G:O4'	2.17	0.45
5:E:75:PRO:HA	5:E:138:GLN:HE21	1.80	0.45
21:W:179:LYS:HE2	21:W:179:LYS:HB2	1.85	0.45
26:b:343:ARG:HD2	26:b:343:ARG:HA	1.87	0.45
29:e:94:ALA:O	29:e:120:THR:HG23	2.16	0.45
30:f:66:VAL:HG21	45:1:3275:U:O4'	2.16	0.45
37:p:23:ARG:HA	37:p:26:VAL:HG22	1.99	0.45
40:v:202:ARG:NE	40:v:229:ARG:HE	2.15	0.45
45:1:297:G:OP2	45:1:297:G:N2	2.50	0.45
45:1:995:U:H2'	45:1:997:A:N6	2.32	0.45
45:1:1126:G:H2'	45:1:1127:G:O4'	2.17	0.45
45:1:2198:A:N6	45:1:2247:G:H1	2.14	0.45
45:1:2661:G:H2'	45:1:2662:G:C8	2.52	0.45
2:B:308:MET:HE2	2:B:308:MET:HB3	1.86	0.45
3:C:112:LYS:HE2	12:N:202:TYR:HB3	1.99	0.45
7:G:80:TYR:HE2	7:G:229:VAL:HG21	1.82	0.45
19:U:53:ALA:O	19:U:68:THR:HG22	2.17	0.45
20:V:22:ILE:HG12	20:V:35:TYR:HD1	1.80	0.45
24:Z:50:PRO:HD3	24:Z:68:ILE:HG12	1.99	0.45
26:b:51:LYS:O	26:b:55:GLU:HG3	2.16	0.45
26:b:366:PRO:C	26:b:368:ALA:H	2.25	0.45
26:b:406:ASN:N	26:b:407:GLY:HA3	2.32	0.45
45:1:307:A:H2'	45:1:308:A:C8	2.52	0.45
45:1:971:G:H2'	45:1:972:A:C8	2.52	0.45
45:1:2136:C:H3'	45:1:2142:A:N6	2.32	0.45
45:1:2209:U:C5	45:1:2209:U:OP2	2.70	0.45
45:1:3027:A:H2'	45:1:3028:G:O4'	2.16	0.45
45:1:3353:G:C6	45:1:3356:G:C6	3.05	0.45
47:3:78:U:OP2	47:3:101:G:N1	2.46	0.45
2:B:69:LYS:HE3	26:b:416:LEU:HG	1.99	0.44
15:Q:23:ASN:HB3	15:Q:26:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:125:ASP:OD1	15:Q:125:ASP:N	2.50	0.44
17:S:12:ARG:HB2	17:S:24:LEU:HD23	1.99	0.44
21:W:18:LYS:HD3	21:W:18:LYS:HA	1.73	0.44
21:W:145:ARG:NH1	21:W:206:PHE:O	2.50	0.44
25:a:77:LYS:C	25:a:79:TRP:N	2.75	0.44
31:g:44:CYS:N	31:g:49:SER:O	2.41	0.44
36:m:77:TRP:O	36:m:78:PHE:CD2	2.70	0.44
38:r:73:VAL:HG22	38:r:74:LYS:HD2	1.99	0.44
45:1:187:A:N3	45:1:208:C:O2'	2.49	0.44
45:1:970:A:N1	45:1:1112:A:C6	2.85	0.44
45:1:1716:U:O2'	45:1:1717:U:O5'	2.33	0.44
45:1:2430:A:H2'	45:1:2431:C:O4'	2.17	0.44
45:1:2435:G:H21	45:1:2436:U:H1'	1.82	0.44
45:1:2647:A:O2'	45:1:2648:G:O4'	2.31	0.44
4:D:116:ASP:OD1	4:D:116:ASP:N	2.49	0.44
10:L:15:ARG:HA	45:1:97:U:OP2	2.17	0.44
17:S:73:LYS:HE2	17:S:75:PHE:CZ	2.52	0.44
25:a:94:ALA:HB2	25:a:121:VAL:HG22	2.00	0.44
41:w:22:ASP:OD1	41:w:25:ASN:ND2	2.45	0.44
42:x:56:SER:OG	42:x:59:GLN:HB2	2.17	0.44
43:y:180:PRO:HG2	43:y:230:GLU:CD	2.42	0.44
45:1:250:U:H2'	45:1:251:G:C8	2.52	0.44
45:1:377:A:H1'	45:1:392:G:N2	2.33	0.44
45:1:665:A:H2'	45:1:666:A:C8	2.53	0.44
45:1:806:A:H1'	45:1:2812:C:O2'	2.17	0.44
45:1:847:A:H2'	45:1:848:A:C8	2.52	0.44
45:1:1111:U:O2'	45:1:1112:A:OP2	2.28	0.44
45:1:1745:C:H2'	45:1:1746:U:C6	2.52	0.44
45:1:1798:A:H2'	45:1:1799:A:C8	2.53	0.44
45:1:2969:A:H2'	45:1:2970:C:O4'	2.18	0.44
1:A:132:ASN:HD22	1:A:151:PRO:HB3	1.82	0.44
2:B:152:LYS:HD3	2:B:189:SER:HA	1.99	0.44
3:C:209:TYR:CE2	3:C:212:ASP:HB2	2.52	0.44
4:D:107:ARG:HA	4:D:107:ARG:HD3	1.72	0.44
5:E:155:LEU:HD12	5:E:155:LEU:HA	1.84	0.44
8:H:55:VAL:HG23	8:H:68:LEU:HD11	1.98	0.44
10:L:101:ARG:HG3	45:1:76:G:N7	2.32	0.44
12:N:37:HIS:CE1	12:N:63:ARG:HD2	2.52	0.44
12:N:66:VAL:HG21	12:N:98:LEU:HB3	1.99	0.44
19:U:35:LYS:O	19:U:38:ILE:HG22	2.18	0.44
26:b:436:LEU:HA	26:b:436:LEU:HD12	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:88:PRO:HD2	28:d:89:LEU:HD13	1.99	0.44
38:r:161:PHE:HZ	45:1:2727:A:N1	2.15	0.44
42:x:418:VAL:HG11	42:x:459:LEU:HD11	1.99	0.44
45:1:428:A:H2'	45:1:429:U:C6	2.53	0.44
45:1:2266:U:H2'	45:1:2267:C:C6	2.53	0.44
47:3:34:C:H42	47:3:46:A:H1'	1.81	0.44
47:3:117:A:H2'	47:3:118:A:C8	2.53	0.44
2:B:348:ARG:HD3	45:1:3037:U:H5'	1.99	0.44
17:S:50:LYS:N	17:S:50:LYS:HD2	2.31	0.44
18:T:116:ARG:HH12	45:1:1096:U:H5	1.64	0.44
20:V:87:ARG:HG3	20:V:93:LEU:HD21	2.00	0.44
24:Z:87:LEU:HD12	24:Z:87:LEU:HA	1.90	0.44
26:b:256:LEU:HD21	26:b:298:LEU:HD22	1.99	0.44
26:b:417:LYS:O	26:b:418:ASP:HB2	2.17	0.44
27:c:11:ASN:N	27:c:11:ASN:OD1	2.51	0.44
42:x:463:SER:OG	42:x:464:LYS:N	2.50	0.44
45:1:97:U:H2'	45:1:98:G:H8	1.78	0.44
45:1:2243:A:O5'	45:1:2243:A:C8	2.70	0.44
45:1:2251:G:N2	45:1:2266:U:O2'	2.50	0.44
45:1:2650:U:H2'	45:1:2651:G:C5	2.53	0.44
45:1:2691:A:H62	45:1:2702:A:N6	2.13	0.44
45:1:2951:G:H5''	45:1:2952:G:N7	2.33	0.44
46:2:134:G:H2'	46:2:135:G:O4'	2.18	0.44
5:E:78:ARG:NH2	45:1:3272:C:OP2	2.43	0.44
8:H:44:THR:OG1	45:1:3186:A:N3	2.50	0.44
12:N:103:GLU:HA	12:N:106:VAL:HG12	1.99	0.44
14:P:53:ASP:OD1	14:P:53:ASP:N	2.50	0.44
26:b:283:VAL:HB	26:b:315:VAL:HG22	1.99	0.44
26:b:440:ASN:HD21	39:u:2:ARG:HA	1.82	0.44
28:d:86:LYS:HA	28:d:86:LYS:HD3	1.77	0.44
32:h:85:THR:HG22	32:h:88:LEU:HD12	1.99	0.44
36:m:377:ASP:O	36:m:378:SER:OG	2.33	0.44
36:m:440:LYS:HD3	36:m:440:LYS:HA	1.83	0.44
37:p:84:ARG:HD3	37:p:87:ARG:HH21	1.83	0.44
45:1:1621:A:H2'	45:1:1622:U:H6	1.82	0.44
2:B:67:PHE:CE1	20:V:88:ARG:HG3	2.53	0.44
5:E:143:LYS:HE3	5:E:143:LYS:HB3	1.68	0.44
8:H:21:LYS:HA	8:H:21:LYS:HD2	1.84	0.44
14:P:120:ASN:N	14:P:120:ASN:OD1	2.51	0.44
28:d:84:ASP:CG	28:d:86:LYS:H	2.24	0.44
30:f:54:ARG:HE	45:1:3279:A:H62	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:284:LEU:HD11	36:m:298:SER:HB3	1.99	0.44
42:x:50:ARG:NH1	42:x:51:VAL:H	2.16	0.44
43:y:61:ARG:HD3	43:y:106:ASN:HD21	1.83	0.44
45:1:85:A:H61	45:1:99:A:H5''	1.82	0.44
45:1:880:G:N3	45:1:882:A:N6	2.66	0.44
45:1:1276:U:O2'	45:1:1277:C:H5'	2.18	0.44
45:1:1281:G:C2	45:1:1282:G:C8	3.06	0.44
45:1:1620:U:H2'	45:1:1621:A:C8	2.52	0.44
45:1:2246:G:O2'	45:1:2247:G:H8	2.00	0.44
45:1:2602:G:H2'	45:1:2603:G:C8	2.52	0.44
45:1:2615:G:H22	45:1:2619:G:P	2.41	0.44
45:1:2840:C:H2'	45:1:2841:G:C8	2.53	0.44
4:D:278:SER:OG	4:D:281:GLU:HG2	2.18	0.44
9:J:110:ILE:HA	9:J:114:ILE:HG23	2.00	0.44
12:N:22:LEU:HA	12:N:25:VAL:HG12	1.99	0.44
13:O:115:LYS:HG2	45:1:3178:A:C2	2.53	0.44
15:Q:69:ARG:NH2	45:1:784:A:OP2	2.50	0.44
36:m:250:THR:HB	36:m:253:LYS:HG3	1.98	0.44
36:m:304:ARG:NH1	45:1:2248:C:H3'	2.33	0.44
42:x:482:LEU:HD23	42:x:482:LEU:H	1.82	0.44
43:y:7:PHE:O	43:y:8:GLU:C	2.60	0.44
45:1:242:C:C2	45:1:243:G:C8	3.05	0.44
45:1:643:U:H3'	45:1:644:G:N2	2.32	0.44
45:1:1540:U:H2'	45:1:1541:G:H5'	2.00	0.44
2:B:39:LYS:HD3	44:z:30:GLU:OE2	2.17	0.44
5:E:129:GLU:HB3	5:E:130:ILE:H	1.60	0.44
29:e:17:PHE:CD1	29:e:53:PRO:HD3	2.52	0.44
36:m:218:VAL:HG21	36:m:367:CYS:HB3	1.99	0.44
38:r:145:LYS:HD3	38:r:145:LYS:HA	1.72	0.44
40:v:140:MET:HE2	40:v:178:LEU:HB3	2.00	0.44
41:w:56:ASP:OD1	41:w:57:ASN:N	2.51	0.44
45:1:41:G:H5'	45:1:42:C:H5	1.82	0.44
45:1:161:G:C6	45:1:162:G:C6	3.06	0.44
45:1:717:C:OP1	45:1:751:A:O2'	2.36	0.44
45:1:874:U:H3'	45:1:875:G:C5'	2.48	0.44
45:1:916:G:H4'	45:1:917:A:H8	1.83	0.44
45:1:1786:G:H2'	45:1:1787:A:C8	2.53	0.44
45:1:2838:A:N6	45:1:2850:G:O2'	2.44	0.44
47:3:41:G:N2	47:3:45:A:C4	2.86	0.44
47:3:102:A:C6	47:3:103:A:N6	2.86	0.44
6:F:189:ILE:HG23	6:F:190:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:105:LYS:NZ	45:1:121:A:H2'	2.33	0.44
11:M:3:THR:O	11:M:3:THR:HG22	2.18	0.44
27:c:24:THR:HG22	27:c:91:SER:HB3	2.00	0.44
35:k:60:GLY:O	35:k:64:LYS:HG2	2.18	0.44
36:m:149:ARG:NH2	36:m:149:ARG:HB3	2.32	0.44
36:m:157:LEU:O	36:m:161:VAL:HG23	2.17	0.44
45:1:43:A:H5''	45:1:2611:U:H4'	1.99	0.44
45:1:90:C:H3'	45:1:91:G:C8	2.52	0.44
45:1:172:G:C2	45:1:173:G:C8	3.06	0.44
45:1:2210:G:C2	45:1:2235:C:O2	2.69	0.44
45:1:2219:A:H2'	45:1:2220:A:C8	2.53	0.44
45:1:2267:C:O2	45:1:2268:U:N3	2.48	0.44
45:1:2632:G:H2'	45:1:2633:U:C6	2.53	0.44
45:1:2758:A:HO2'	45:1:2759:U:P	2.40	0.44
45:1:2863:G:H5'	45:1:2863:G:N3	2.31	0.44
47:3:100:C:H3'	47:3:101:G:C8	2.50	0.44
1:A:143:GLU:O	1:A:145:LYS:HG2	2.17	0.43
7:G:96:LYS:HG3	7:G:97:TYR:CD1	2.53	0.43
14:P:108:ASP:OD2	14:P:110:THR:OG1	2.33	0.43
25:a:114:GLY:O	25:a:137:LYS:NZ	2.50	0.43
26:b:208:HIS:CD2	45:1:3027:A:H8	2.36	0.43
26:b:344:ILE:HD13	26:b:344:ILE:HA	1.83	0.43
38:r:218:GLY:O	38:r:244:GLN:NE2	2.51	0.43
39:u:135:ARG:HH11	39:u:138:GLU:HB3	1.83	0.43
40:v:143:PHE:CE1	40:v:158:LYS:HG3	2.52	0.43
40:v:266:ASP:OD1	40:v:267:ILE:N	2.50	0.43
42:x:34:ILE:C	42:x:35:LYS:HD3	2.43	0.43
45:1:96:G:O2'	45:1:97:U:P	2.76	0.43
45:1:2210:G:C2	45:1:2236:G:C8	3.06	0.43
45:1:2698:G:C2	45:1:2699:G:H1'	2.53	0.43
46:2:157:U:O2'	46:2:158:U:H3'	2.17	0.43
2:B:109:HIS:O	2:B:110:LEU:HD23	2.18	0.43
2:B:344:THR:O	2:B:346:THR:N	2.52	0.43
4:D:43:LYS:HG3	4:D:44:TYR:H	1.83	0.43
26:b:71:ILE:HD13	26:b:88:LYS:HG3	1.99	0.43
30:f:77:ASN:HB2	45:1:1180:A:H5''	2.00	0.43
37:p:60:CYS:SG	37:p:62:LYS:HG3	2.58	0.43
45:1:2108:C:H1'	45:1:3344:A:H8	1.81	0.43
45:1:2199:G:H2'	45:1:2199:G:N3	2.33	0.43
45:1:3357:U:H2'	45:1:3358:U:H6	1.84	0.43
12:N:182:ASN:ND2	45:1:279:U:O2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:402:ILE:HA	26:b:405:GLU:HG2	2.00	0.43
36:m:248:LYS:HB3	36:m:248:LYS:HE2	1.78	0.43
36:m:348:GLY:O	36:m:351:LYS:NZ	2.51	0.43
41:w:135:ASP:OD2	41:w:138:SER:N	2.47	0.43
42:x:139:ILE:HG22	42:x:140:ALA:O	2.17	0.43
45:1:738:A:H2'	45:1:739:G:H8	1.84	0.43
45:1:1124:U:H5	45:1:1134:G:H1	1.65	0.43
1:A:101:VAL:HB	1:A:165:VAL:HG12	2.01	0.43
17:S:131:LYS:HE3	17:S:131:LYS:HB3	1.65	0.43
26:b:100:ARG:NH2	45:1:2860:U:OP2	2.37	0.43
30:f:54:ARG:NE	45:1:3279:A:H62	2.16	0.43
32:h:54:VAL:O	32:h:58:ILE:HG13	2.19	0.43
40:v:275:ILE:HD12	40:v:275:ILE:HA	1.77	0.43
41:w:112:THR:O	41:w:198:ASN:ND2	2.51	0.43
41:w:126:LYS:HE2	41:w:126:LYS:HB3	1.77	0.43
45:1:87:U:H2'	45:1:88:A:C8	2.53	0.43
45:1:88:A:H2'	45:1:89:A:H5'	2.00	0.43
47:3:82:G:C2	47:3:99:G:N1	2.86	0.43
4:D:105:ILE:O	4:D:109:THR:HG22	2.19	0.43
7:G:143:ILE:HG23	7:G:175:VAL:HG21	2.01	0.43
9:J:163:PHE:C	9:J:165:GLN:H	2.26	0.43
25:a:63:LYS:O	25:a:64:GLN:HG2	2.19	0.43
26:b:149:TYR:O	26:b:153:VAL:HG23	2.17	0.43
30:f:16:TYR:OH	30:f:91:ALA:HB2	2.18	0.43
36:m:99:THR:HG23	36:m:100:GLN:H	1.83	0.43
39:u:93:MET:HE2	39:u:93:MET:HB3	1.83	0.43
42:x:64:LEU:HD22	42:x:77:TYR:CE2	2.53	0.43
42:x:273:THR:OG1	42:x:274:MET:N	2.51	0.43
45:1:501:A:H2'	45:1:502:U:C6	2.54	0.43
45:1:664:U:H2'	45:1:665:A:C8	2.53	0.43
45:1:997:A:H5''	45:1:998:A:OP1	2.18	0.43
3:C:298:ALA:HB1	15:Q:133:LYS:HE2	2.00	0.43
9:J:10:ARG:NH2	9:J:133:ARG:HE	2.08	0.43
23:Y:23:PRO:O	23:Y:27:ARG:HG3	2.18	0.43
27:c:33:SER:OG	27:c:39:SER:OG	2.19	0.43
32:h:35:LYS:HZ2	32:h:41:LEU:HG	1.84	0.43
40:v:130:LYS:HE2	40:v:130:LYS:HB2	1.78	0.43
43:y:215:LEU:HD12	43:y:215:LEU:HA	1.84	0.43
45:1:542:G:O6	45:1:550:A:N6	2.51	0.43
45:1:547:G:H1'	45:1:548:G:N7	2.34	0.43
45:1:1110:U:C2	45:1:1111:U:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1:1355:A:H4'	45:1:1356:U:O5'	2.18	0.43
45:1:2703:A:H2'	45:1:2703:A:N3	2.34	0.43
47:3:41:G:N2	47:3:45:A:N3	2.67	0.43
2:B:305:ILE:HD12	2:B:321:PHE:CE1	2.53	0.43
2:B:351:LEU:HD11	44:z:22:PHE:CE2	2.53	0.43
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.82	0.43
5:E:31:ARG:NH2	30:f:107:ILE:O	2.52	0.43
8:H:41:ILE:HG21	8:H:71:VAL:HG21	2.01	0.43
9:J:150:ASN:HA	9:J:153:LYS:HG3	2.00	0.43
12:N:145:ASP:C	12:N:147:ARG:H	2.27	0.43
13:O:37:ARG:HH22	45:1:3183:A:P	2.42	0.43
17:S:71:LYS:NZ	45:1:563:U:OP1	2.44	0.43
18:T:136:ARG:HD2	18:T:139:ARG:HH22	1.83	0.43
23:Y:69:LYS:HB2	23:Y:69:LYS:HE2	1.78	0.43
26:b:126:LYS:O	26:b:130:ARG:HG3	2.19	0.43
36:m:102:ASP:HB3	36:m:105:GLN:HG3	2.00	0.43
36:m:410:LYS:HB3	36:m:410:LYS:HE3	1.77	0.43
39:u:8:PHE:HB3	39:u:36:CYS:HB3	2.00	0.43
45:1:250:U:H5'	45:1:251:G:OP2	2.18	0.43
45:1:2926:A:H2'	45:1:2927:C:C6	2.53	0.43
7:G:95:ASN:HD22	7:G:98:ARG:HD2	1.84	0.43
9:J:132:ASN:ND2	9:J:133:ARG:O	2.51	0.43
18:T:44:ALA:HB2	41:w:158:TRP:CZ3	2.53	0.43
25:a:62:HIS:HD1	45:1:2777:G:N2	2.16	0.43
28:d:26:LYS:HA	28:d:26:LYS:HD3	1.77	0.43
31:g:10:ARG:O	31:g:12:PRO:HD3	2.19	0.43
32:h:31:LEU:HA	32:h:31:LEU:HD23	1.80	0.43
36:m:239:CYS:HB2	36:m:323:TYR:CE1	2.48	0.43
38:r:21:GLU:CD	38:r:21:GLU:H	2.27	0.43
42:x:50:ARG:HD2	42:x:50:ARG:HA	1.92	0.43
45:1:1621:A:H2'	45:1:1622:U:C6	2.54	0.43
45:1:2209:U:H3'	45:1:2209:U:H6	1.84	0.43
45:1:2210:G:C2	45:1:2236:G:N9	2.86	0.43
45:1:2257:C:H2'	45:1:2258:U:C6	2.53	0.43
45:1:2266:U:H2'	45:1:2267:C:C5	2.54	0.43
45:1:3000:A:H2'	45:1:3001:C:H6	1.84	0.43
46:2:103:G:OP2	46:2:105:A:O2'	2.35	0.43
2:B:4:ARG:HG3	45:1:2881:C:H41	1.84	0.43
3:C:338:LYS:C	3:C:340:GLY:H	2.25	0.43
6:F:124:LEU:HD23	6:F:124:LEU:HA	1.91	0.43
36:m:229:LEU:HB2	36:m:259:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:50:SER:HB2	40:v:57:MET:SD	2.59	0.43
43:y:155:SER:OG	43:y:156:ASN:N	2.52	0.43
45:1:41:G:H3'	45:1:41:G:N3	2.34	0.43
45:1:159:A:H2'	45:1:160:G:C8	2.54	0.43
45:1:874:U:H3'	45:1:875:G:H5''	2.00	0.43
45:1:1733:G:H2'	45:1:1734:G:H8	1.84	0.43
45:1:2220:A:H3'	45:1:2221:G:C8	2.54	0.43
45:1:2635:A:H4'	45:1:2636:A:C6	2.54	0.43
5:E:43:LEU:HD11	5:E:85:ILE:HG13	2.01	0.43
12:N:124:ASP:CG	12:N:125:SER:N	2.77	0.43
19:U:89:LEU:HD23	19:U:89:LEU:HA	1.77	0.43
19:U:96:VAL:HG23	19:U:104:ARG:HG3	2.00	0.43
22:X:74:LYS:HG2	22:X:78:ASP:OD2	2.19	0.43
26:b:18:LEU:HD12	26:b:18:LEU:HA	1.87	0.43
26:b:28:LYS:HE2	26:b:28:LYS:HB3	1.80	0.43
32:h:45:LYS:O	32:h:49:LYS:HG2	2.19	0.43
36:m:244:GLU:HG3	36:m:245:TYR:N	2.34	0.43
36:m:282:PRO:HB3	40:v:277:MET:CE	2.49	0.43
45:1:100:A:H2'	45:1:101:G:N3	2.34	0.43
45:1:971:G:O6	45:1:1111:U:C4	2.71	0.43
45:1:1299:U:H2'	45:1:1300:G:O4'	2.19	0.43
45:1:2693:C:H3'	45:1:2695:A:OP2	2.19	0.43
45:1:2842:U:H2'	45:1:2843:U:H6	1.84	0.43
4:D:85:ARG:O	4:D:85:ARG:HG3	2.18	0.42
6:F:159:GLN:HA	45:1:1362:G:O2'	2.19	0.42
6:F:229:PHE:CD2	6:F:229:PHE:C	2.97	0.42
9:J:11:ASP:OD1	9:J:11:ASP:N	2.51	0.42
16:R:135:LYS:HB3	16:R:135:LYS:HE3	1.74	0.42
19:U:10:LYS:HB3	19:U:68:THR:OG1	2.19	0.42
20:V:74:MET:HE2	20:V:74:MET:HB3	1.85	0.42
22:X:68:THR:HB	22:X:73:MET:HE3	2.01	0.42
28:d:87:ASN:N	28:d:87:ASN:OD1	2.52	0.42
29:e:104:ASN:O	29:e:108:ILE:HG13	2.19	0.42
36:m:226:ILE:HD13	36:m:320:PHE:CE2	2.53	0.42
39:u:6:CYS:HB2	39:u:32:CYS:HB3	2.01	0.42
40:v:183:SER:OG	40:v:202:ARG:HB2	2.19	0.42
45:1:738:A:H2'	45:1:739:G:C8	2.53	0.42
45:1:992:A:H2	45:1:1057:A:N1	2.17	0.42
45:1:1130:A:H2'	45:1:1131:G:O4'	2.19	0.42
47:3:81:U:O2'	47:3:82:G:O4'	2.32	0.42
5:E:137:ASP:O	5:E:141:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:78:TRP:CD1	17:S:125:LYS:HB3	2.54	0.42
18:T:91:LEU:HD22	41:w:159:LEU:HB2	2.01	0.42
23:Y:60:ARG:HH21	45:1:190:U:H2'	1.83	0.42
24:Z:61:LYS:H	24:Z:61:LYS:HG2	1.61	0.42
26:b:71:ILE:HG13	26:b:82:MET:HE2	2.00	0.42
26:b:131:ALA:O	26:b:135:ARG:HG3	2.18	0.42
36:m:471:LYS:HE2	36:m:471:LYS:HB3	1.67	0.42
38:r:184:VAL:HB	38:r:195:LEU:HD12	2.01	0.42
40:v:62:ARG:HH22	45:1:2699:G:P	2.42	0.42
42:x:371:GLU:H	42:x:371:GLU:CD	2.28	0.42
43:y:163:PRO:HD3	43:y:184:GLY:O	2.18	0.42
45:1:209:A:O2'	45:1:211:A:OP2	2.32	0.42
45:1:296:A:H2'	45:1:297:G:C4	2.54	0.42
45:1:665:A:H2'	45:1:666:A:H8	1.84	0.42
45:1:834:U:H2'	45:1:835:G:O4'	2.19	0.42
45:1:1814:A:H4'	45:1:1815:U:O4'	2.19	0.42
45:1:2731:U:H4'	45:1:2732:G:OP1	2.17	0.42
45:1:2731:U:O2'	45:1:2733:A:OP2	2.25	0.42
47:3:47:C:H2'	47:3:48:U:C6	2.54	0.42
47:3:74:C:H2'	47:3:75:G:N9	2.33	0.42
1:A:126:LEU:HD22	45:1:2157:G:N2	2.34	0.42
5:E:90:LYS:HE2	5:E:90:LYS:HB3	1.76	0.42
20:V:53:SER:O	20:V:56:ASP:HB2	2.20	0.42
26:b:338:LYS:HD3	26:b:338:LYS:HA	1.80	0.42
27:c:22:LYS:HB3	27:c:22:LYS:HE2	1.79	0.42
36:m:72:GLN:O	36:m:77:TRP:HZ3	2.01	0.42
40:v:62:ARG:NH2	45:1:2699:G:O5'	2.51	0.42
42:x:401:HIS:HE1	42:x:419:SER:OG	2.02	0.42
43:y:62:MET:O	43:y:73:PRO:HD3	2.19	0.42
45:1:127:G:H2'	45:1:128:G:C8	2.54	0.42
45:1:370:U:H4'	45:1:404:G:H5'	2.00	0.42
45:1:1624:G:H2'	45:1:1625:A:C8	2.52	0.42
45:1:1628:C:O2	45:1:1814:A:O2'	2.37	0.42
2:B:346:THR:O	2:B:346:THR:HG23	2.20	0.42
4:D:172:TYR:CE2	42:x:134:ARG:HD3	2.54	0.42
4:D:262:LYS:HE3	4:D:262:LYS:HB3	1.90	0.42
5:E:75:PRO:HA	5:E:138:GLN:NE2	2.35	0.42
9:J:108:GLU:HG3	9:J:111:ASP:OD2	2.19	0.42
11:M:116:GLU:O	11:M:120:VAL:HG23	2.20	0.42
15:Q:26:LEU:O	15:Q:30:VAL:HG23	2.19	0.42
21:W:4:SER:HA	45:1:1208:U:C1'	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:35:ASP:OD1	21:W:35:ASP:N	2.42	0.42
21:W:39:TYR:HB3	21:W:220:TYR:CE1	2.55	0.42
25:a:98:THR:HG23	25:a:98:THR:O	2.19	0.42
33:i:88:GLU:HA	33:i:91:ASN:ND2	2.33	0.42
36:m:208:SER:O	36:m:210:ARG:N	2.52	0.42
42:x:240:ILE:HD13	42:x:240:ILE:HA	1.88	0.42
43:y:162:HIS:O	43:y:165:THR:OG1	2.31	0.42
45:1:8:C:C2	45:1:9:U:C5	3.08	0.42
45:1:572:A:H2'	45:1:573:C:C6	2.55	0.42
45:1:1838:G:H4'	45:1:1839:A:N3	2.33	0.42
45:1:2669:G:H2'	45:1:2670:G:C8	2.54	0.42
46:2:10:A:H2'	46:2:11:C:C6	2.54	0.42
1:A:42:ARG:HG3	1:A:89:TYR:CE1	2.54	0.42
2:B:221:THR:O	2:B:221:THR:OG1	2.26	0.42
3:C:38:VAL:O	3:C:42:VAL:HG23	2.20	0.42
36:m:332:ILE:CD1	36:m:366:ASP:HB3	2.49	0.42
42:x:56:SER:OG	42:x:59:GLN:N	2.53	0.42
45:1:2196:C:C2	45:1:2198:A:C6	3.07	0.42
45:1:2728:G:H1'	45:1:2729:U:H5''	2.01	0.42
45:1:2849:C:H3'	45:1:2850:G:H8	1.84	0.42
45:1:2954:U:O2'	45:1:2955:U:OP2	2.32	0.42
2:B:104:THR:HG22	45:1:3147:G:O2'	2.19	0.42
2:B:206:ASP:OD1	2:B:206:ASP:N	2.34	0.42
2:B:211:GLN:HG2	2:B:212:ASN:OD1	2.19	0.42
9:J:14:ILE:HG22	9:J:131:MET:SD	2.60	0.42
12:N:44:ARG:NH2	45:1:269:G:OP2	2.47	0.42
36:m:413:GLU:HG2	36:m:418:ILE:HG21	2.01	0.42
42:x:107:LYS:HE3	42:x:107:LYS:HB3	1.74	0.42
45:1:494:G:O2'	45:1:495:G:H8	2.03	0.42
45:1:2216:G:H22	45:1:2229:A:H2	1.68	0.42
45:1:2951:G:H4'	45:1:2951:G:OP1	2.18	0.42
2:B:25:ILE:HD12	2:B:272:TYR:OH	2.20	0.42
5:E:91:VAL:HG12	5:E:92:SER:H	1.85	0.42
9:J:24:GLY:HA3	45:1:2680:A:H2	1.85	0.42
9:J:85:LYS:HE2	9:J:85:LYS:HB2	1.82	0.42
16:R:105:LEU:HD22	16:R:135:LYS:HG2	2.01	0.42
17:S:78:TRP:CD1	17:S:78:TRP:N	2.88	0.42
17:S:132:THR:HG22	17:S:133:ALA:H	1.85	0.42
19:U:19:VAL:O	19:U:22:PRO:HD2	2.19	0.42
21:W:26:ILE:O	21:W:30:VAL:HG12	2.19	0.42
36:m:422:LYS:O	36:m:426:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:449:VAL:O	36:m:453:ILE:HG13	2.19	0.42
38:r:159:GLU:HG2	45:1:2730:G:C2	2.55	0.42
40:v:153:VAL:HG23	40:v:154:TYR:HD2	1.84	0.42
42:x:80:SER:OG	42:x:81:CYS:N	2.52	0.42
45:1:2216:G:C2	45:1:2230:C:C2	3.08	0.42
45:1:2224:A:H3'	45:1:2225:U:H6	1.85	0.42
45:1:2730:G:O2'	45:1:2731:U:OP2	2.34	0.42
1:A:92:LYS:HD3	1:A:103:PRO:HG2	2.00	0.42
2:B:187:SER:HB3	2:B:190:GLU:HB2	2.02	0.42
9:J:131:MET:HE3	9:J:131:MET:HB3	1.88	0.42
11:M:25:LYS:HE2	11:M:25:LYS:HB3	1.56	0.42
11:M:45:LEU:HD12	11:M:56:GLN:O	2.20	0.42
12:N:32:GLN:N	12:N:32:GLN:OE1	2.53	0.42
19:U:50:LEU:HD22	19:U:54:VAL:HG22	2.02	0.42
21:W:11:THR:HG21	45:1:1278:A:H5''	2.01	0.42
21:W:203:LEU:HD22	21:W:208:ILE:HD11	2.02	0.42
23:Y:103:LYS:HE2	45:1:217:U:O2'	2.19	0.42
26:b:491:GLU:HG3	26:b:492:LYS:N	2.35	0.42
26:b:495:TRP:HZ3	39:u:133:LEU:HB3	1.85	0.42
28:d:97:LEU:HD12	28:d:97:LEU:HA	1.72	0.42
37:p:48:LYS:HD3	37:p:48:LYS:HA	1.81	0.42
40:v:31:LEU:HD12	40:v:58:LYS:O	2.20	0.42
41:w:197:ARG:NH2	45:1:2796:G:O4'	2.53	0.42
42:x:285:LYS:HD3	42:x:285:LYS:HA	1.87	0.42
45:1:953:G:H5''	45:1:954:U:C6	2.55	0.42
45:1:1348:U:H4'	45:1:1349:G:H5''	2.02	0.42
45:1:1715:A:O3'	45:1:1716:U:H3'	2.19	0.42
45:1:2647:A:H2'	45:1:2648:G:C8	2.54	0.42
45:1:2726:C:H1'	45:1:2728:G:P	2.60	0.42
6:F:236:ILE:HD12	6:F:236:ILE:HA	1.79	0.42
11:M:12:TRP:CH2	17:S:172:TYR:HE1	2.38	0.42
11:M:120:VAL:O	11:M:124:ARG:HG3	2.20	0.42
12:N:71:ARG:HD2	12:N:94:TYR:HB2	2.02	0.42
16:R:74:ARG:NH2	45:1:1942:U:OP2	2.49	0.42
17:S:171:PHE:HD1	17:S:172:TYR:C	2.26	0.42
21:W:86:LYS:H	21:W:89:LEU:HD11	1.84	0.42
21:W:131:ALA:HB2	21:W:195:LEU:HD21	2.01	0.42
22:X:63:ILE:HD11	22:X:99:VAL:HG23	2.02	0.42
24:Z:53:VAL:HG23	24:Z:57:HIS:HD2	1.84	0.42
26:b:246:LEU:HD23	26:b:246:LEU:HA	1.77	0.42
26:b:324:LEU:HD23	26:b:324:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:85:VAL:HA	31:g:88:ARG:HG2	2.00	0.42
36:m:69:ALA:O	38:r:124:LYS:HA	2.20	0.42
38:r:49:GLN:O	38:r:53:LYS:HG3	2.20	0.42
38:r:145:LYS:HG3	45:1:2970:C:H5'	2.02	0.42
42:x:28:ASP:OD2	42:x:30:PRO:HD2	2.19	0.42
43:y:42:LEU:HD22	43:y:46:ILE:HG12	2.02	0.42
43:y:235:ASN:OD1	43:y:235:ASN:N	2.53	0.42
45:1:2438:A:H3'	45:1:2439:A:C8	2.54	0.42
12:N:143:ARG:NE	32:h:92:LEU:HD23	2.35	0.42
18:T:80:VAL:HG21	18:T:85:LEU:HD23	2.02	0.42
24:Z:106:GLN:O	24:Z:109:GLU:HG3	2.20	0.42
26:b:495:TRP:CG	39:u:137:ARG:HD2	2.55	0.42
27:c:53:LYS:HB2	27:c:53:LYS:HE3	1.79	0.42
36:m:41:MET:HE3	38:r:147:TRP:CZ3	2.55	0.42
38:r:10:HIS:CD2	38:r:14:HIS:CD2	3.07	0.42
41:w:137:ALA:N	41:w:138:SER:O	2.52	0.42
42:x:256:LYS:HA	42:x:280:SER:OG	2.20	0.42
43:y:4:ARG:HA	43:y:206:THR:O	2.19	0.42
45:1:88:A:C2'	45:1:89:A:H5'	2.50	0.42
45:1:174:C:H2'	45:1:175:C:C6	2.55	0.42
45:1:174:C:H2'	45:1:175:C:H6	1.85	0.42
45:1:2202:C:OP1	45:1:2245:C:N4	2.53	0.42
1:A:65:ASP:H	1:A:71:LEU:HA	1.85	0.41
2:B:247:ARG:HH12	2:B:267:ALA:HB2	1.84	0.41
3:C:317:PRO:C	3:C:319:LYS:N	2.77	0.41
3:C:338:LYS:C	3:C:340:GLY:N	2.78	0.41
4:D:30:TYR:O	4:D:34:LYS:HG2	2.20	0.41
10:L:77:LEU:HD11	45:1:156:G:H1'	2.02	0.41
17:S:5:LYS:NZ	17:S:32:SER:O	2.53	0.41
17:S:73:LYS:HE2	17:S:75:PHE:HZ	1.84	0.41
30:f:15:SER:OG	30:f:16:TYR:N	2.53	0.41
32:h:77:PRO:O	32:h:81:ARG:HG3	2.20	0.41
33:i:91:ASN:O	33:i:94:ILE:HG22	2.20	0.41
35:k:44:LYS:NZ	45:1:1750:A:OP1	2.40	0.41
36:m:22:LEU:H	36:m:22:LEU:HG	1.70	0.41
40:v:81:LYS:HA	40:v:81:LYS:HD3	1.77	0.41
40:v:86:LEU:HD22	40:v:164:PHE:CD2	2.52	0.41
40:v:207:LYS:O	40:v:222:GLU:N	2.52	0.41
41:w:200:LYS:HD2	41:w:200:LYS:HA	1.82	0.41
42:x:56:SER:O	42:x:59:GLN:N	2.50	0.41
45:1:114:A:H2'	45:1:115:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HD3	1:A:145:LYS:HA	1.88	0.41
2:B:19:ARG:NH2	45:1:3045:G:OP1	2.52	0.41
3:C:55:LYS:HE3	3:C:55:LYS:HB3	1.72	0.41
8:H:21:LYS:HG3	8:H:22:SER:H	1.84	0.41
10:L:60:ALA:HB3	10:L:65:TYR:O	2.20	0.41
12:N:149:ASN:OD1	12:N:149:ASN:N	2.43	0.41
21:W:145:ARG:O	21:W:206:PHE:HB3	2.20	0.41
25:a:86:LYS:HB3	25:a:90:TYR:CE2	2.55	0.41
26:b:164:ASP:HA	26:b:165:PRO:HD3	1.89	0.41
26:b:233:ASN:O	26:b:237:MET:HG2	2.19	0.41
36:m:241:SER:HB2	45:1:2867:C:N4	2.35	0.41
39:u:68:THR:HG21	39:u:100:ARG:HB2	2.02	0.41
39:u:136:ILE:O	39:u:139:VAL:HG12	2.20	0.41
40:v:94:LYS:HD2	47:3:77:G:N7	2.34	0.41
45:1:2:U:H5''	45:1:3:U:H5	1.84	0.41
45:1:731:U:H2'	45:1:732:C:C6	2.56	0.41
45:1:3161:C:H2'	45:1:3162:C:C6	2.56	0.41
47:3:29:C:H2'	47:3:51:A:H61	1.85	0.41
2:B:93:VAL:HG23	2:B:102:LEU:HB2	2.01	0.41
2:B:95:THR:C	2:B:97:ARG:H	2.27	0.41
2:B:162:VAL:O	2:B:178:LEU:HD12	2.20	0.41
3:C:88:GLY:HA3	3:C:94:CYS:HB3	2.02	0.41
3:C:343:LYS:HE2	3:C:343:LYS:HB3	1.92	0.41
4:D:39:GLN:H	4:D:39:GLN:HG3	1.64	0.41
4:D:71:GLY:O	47:3:7:G:O2'	2.35	0.41
7:G:77:GLN:HE22	7:G:167:PRO:HB2	1.85	0.41
26:b:254:MET:HE2	26:b:254:MET:HB3	1.94	0.41
27:c:77:LEU:O	27:c:81:VAL:HG22	2.20	0.41
34:j:67:LEU:HD23	34:j:67:LEU:HA	1.82	0.41
41:w:73:THR:OG1	41:w:74:THR:N	2.53	0.41
42:x:418:VAL:HG13	42:x:450:VAL:HG21	2.02	0.41
43:y:206:THR:OG1	43:y:207:GLY:N	2.53	0.41
45:1:1053:A:C5	45:1:1054:A:C5	3.09	0.41
45:1:2216:G:N2	45:1:2229:A:H2	2.17	0.41
45:1:2682:C:H2'	45:1:2683:U:H6	1.85	0.41
45:1:2958:A:H2'	45:1:2959:C:C6	2.55	0.41
9:J:133:ARG:NH1	9:J:154:THR:HG22	2.35	0.41
10:L:74:GLY:O	10:L:101:ARG:NH1	2.53	0.41
17:S:73:LYS:NZ	17:S:97:VAL:O	2.52	0.41
21:W:53:LEU:HD11	21:W:67:MET:SD	2.59	0.41
24:Z:121:ARG:CZ	24:Z:121:ARG:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:511:LYS:HD2	26:b:511:LYS:HA	1.98	0.41
30:f:54:ARG:HE	45:1:3279:A:N6	2.19	0.41
45:1:161:G:H2'	45:1:162:G:N9	2.35	0.41
45:1:1068:C:H2'	45:1:1069:C:H6	1.85	0.41
45:1:1151:U:H3'	45:1:1152:G:H21	1.85	0.41
45:1:2593:A:H4'	45:1:2594:C:H6	1.86	0.41
1:A:65:ASP:OD2	1:A:68:LYS:HB3	2.20	0.41
4:D:83:LEU:HB3	4:D:88:ILE:HB	2.01	0.41
8:H:2:LYS:HE3	8:H:2:LYS:HB3	1.88	0.41
8:H:150:SER:OG	8:H:152:GLU:OE1	2.39	0.41
21:W:37:TYR:HB3	21:W:105:THR:O	2.21	0.41
21:W:44:HIS:HB2	21:W:216:LYS:CG	2.50	0.41
27:c:18:ILE:HG13	27:c:81:VAL:O	2.20	0.41
29:e:101:SER:OG	29:e:104:ASN:ND2	2.44	0.41
32:h:64:GLU:O	32:h:68:GLN:HG2	2.20	0.41
41:w:197:ARG:NH1	45:1:2796:G:OP1	2.53	0.41
45:1:1896:A:N6	45:1:2339:C:H42	2.11	0.41
45:1:2667:A:N6	45:1:2668:U:O2	2.53	0.41
45:1:3164:C:C2	45:1:3165:A:C8	3.08	0.41
46:2:126:A:O2'	46:2:128:U:OP2	2.38	0.41
3:C:351:PRO:HA	6:F:71:ALA:HA	2.02	0.41
4:D:289:LYS:HB2	4:D:289:LYS:HE3	1.74	0.41
10:L:85:LEU:HD13	10:L:120:GLN:NE2	2.35	0.41
11:M:60:LEU:HA	11:M:60:LEU:HD23	1.85	0.41
17:S:42:TRP:HA	17:S:42:TRP:CE3	2.56	0.41
20:V:15:LEU:HD13	20:V:51:ALA:HB3	2.00	0.41
21:W:139:GLU:N	21:W:139:GLU:OE1	2.54	0.41
24:Z:87:LEU:HG	24:Z:88:ASP:H	1.86	0.41
26:b:92:LYS:HG2	45:1:2863:G:H22	1.85	0.41
38:r:6:TYR:H	45:1:2898:G:H22	1.67	0.41
45:1:664:U:H2'	45:1:665:A:H8	1.84	0.41
45:1:1233:G:N1	45:1:1255:C:H5	2.01	0.41
45:1:1667:A:H2'	45:1:1668:G:C8	2.55	0.41
45:1:2141:U:O2'	45:1:2976:A:O2'	2.38	0.41
45:1:2623:G:O2'	45:1:2624:G:H5'	2.20	0.41
45:1:2667:A:C6	45:1:2687:G:C8	3.09	0.41
3:C:221:ASN:HD21	45:1:212:G:H2'	1.86	0.41
12:N:4:TYR:CD1	12:N:4:TYR:N	2.89	0.41
12:N:145:ASP:O	12:N:147:ARG:N	2.54	0.41
20:V:84:SER:HA	20:V:93:LEU:O	2.21	0.41
26:b:264:ILE:HG12	26:b:302:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:r:45:TRP:CH2	45:1:2828:G:C5	3.09	0.41
40:v:225:GLU:HG2	40:v:229:ARG:NH1	2.36	0.41
43:y:197:MET:HE3	43:y:197:MET:HB2	1.95	0.41
44:z:49:LEU:HD12	44:z:49:LEU:HA	1.93	0.41
45:1:993:G:N1	45:1:1056:U:N3	2.69	0.41
45:1:1154:A:H5'	45:1:1155:C:H5	1.85	0.41
45:1:1538:G:H2'	45:1:1539:A:C8	2.56	0.41
45:1:2401:A:OP2	45:1:2402:A:H2'	2.20	0.41
45:1:2674:A:H2'	45:1:2675:C:C6	2.56	0.41
46:2:122:U:H2'	46:2:123:G:C8	2.56	0.41
46:2:151:C:O2'	46:2:153:U:OP2	2.39	0.41
47:3:61:G:H2'	47:3:62:U:O4'	2.20	0.41
8:H:188:THR:O	8:H:188:THR:OG1	2.30	0.41
14:P:46:LYS:O	14:P:50:GLN:HG3	2.21	0.41
17:S:96:ASP:CG	17:S:97:VAL:H	2.28	0.41
22:X:127:THR:HG22	22:X:128:ALA:H	1.86	0.41
26:b:144:ARG:CZ	26:b:144:ARG:HB3	2.50	0.41
27:c:19:LYS:HE3	27:c:19:LYS:HB2	1.77	0.41
29:e:101:SER:HB3	45:1:1389:G:H5''	2.03	0.41
34:j:72:ARG:NH1	46:2:95:G:OP2	2.53	0.41
36:m:199:LYS:HE2	36:m:379:GLU:HG3	2.02	0.41
38:r:186:HIS:HB3	38:r:188:GLU:O	2.21	0.41
42:x:293:TYR:CE2	42:x:328:LEU:HD21	2.56	0.41
45:1:155:G:N1	45:1:265:A:OP2	2.54	0.41
45:1:735:A:H2'	45:1:736:A:O4'	2.21	0.41
45:1:972:A:O2'	45:1:973:A:H5'	2.21	0.41
45:1:1643:A:H2'	45:1:1644:C:C2	2.55	0.41
45:1:2278:C:H5	45:1:2315:G:H1	1.69	0.41
45:1:2401:A:H5'	45:1:2402:A:C8	2.56	0.41
45:1:2601:A:H2'	45:1:2602:G:C8	2.56	0.41
45:1:2954:U:H1'	45:1:2955:U:O4'	2.21	0.41
45:1:3322:A:H2'	45:1:3323:A:C8	2.55	0.41
46:2:56:G:H2'	46:2:57:C:O4'	2.21	0.41
2:B:308:MET:HE3	45:1:3329:U:H5''	2.02	0.41
3:C:300:ARG:HB2	3:C:301:PRO:HD2	2.03	0.41
4:D:21:ARG:O	4:D:25:GLU:HG2	2.20	0.41
4:D:38:THR:O	4:D:38:THR:HG22	2.21	0.41
6:F:163:LEU:O	6:F:165:ASP:N	2.54	0.41
7:G:214:LEU:HD12	7:G:214:LEU:HA	1.84	0.41
10:L:47:ALA:HB3	10:L:48:PRO:HD3	2.03	0.41
12:N:197:LEU:HD12	12:N:197:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:78:TRP:HD1	17:S:125:LYS:O	2.04	0.41
19:U:18:ASP:OD1	19:U:19:VAL:N	2.54	0.41
25:a:74:ASN:ND2	25:a:113:LEU:HB2	2.35	0.41
25:a:135:GLU:OE2	25:a:139:ARG:HD3	2.20	0.41
31:g:38:LEU:HD23	31:g:38:LEU:HA	1.88	0.41
36:m:74:ASP:OD2	36:m:75:ARG:N	2.54	0.41
36:m:194:TRP:CD1	36:m:194:TRP:C	2.99	0.41
36:m:291:THR:OG1	36:m:292:ASN:N	2.52	0.41
38:r:212:LEU:HD12	38:r:212:LEU:HA	1.86	0.41
39:u:66:ASP:H	39:u:69:LEU:HD12	1.85	0.41
42:x:63:LEU:O	42:x:66:GLN:HG3	2.21	0.41
43:y:156:ASN:HB2	43:y:201:ASP:OD1	2.21	0.41
45:1:993:G:N7	45:1:995:U:H5	2.18	0.41
45:1:1544:G:N1	45:1:1549:U:N3	2.65	0.41
45:1:2199:G:H22	45:1:2236:G:C5'	2.33	0.41
45:1:2246:G:HO2'	45:1:2247:G:C5'	2.34	0.41
45:1:2669:G:O6	45:1:2686:A:N6	2.54	0.41
45:1:2883:U:H2'	45:1:2884:C:C6	2.55	0.41
45:1:3295:A:H2'	45:1:3296:A:C8	2.56	0.41
9:J:92:ARG:HA	9:J:172:LEU:HB3	2.02	0.41
10:L:164:GLU:H	10:L:164:GLU:CD	2.28	0.41
24:Z:97:SER:N	24:Z:100:THR:OG1	2.52	0.41
24:Z:110:ALA:O	24:Z:114:VAL:HG23	2.20	0.41
40:v:243:ASP:O	40:v:246:THR:HG22	2.20	0.41
41:w:133:ILE:HG23	41:w:144:LYS:HB2	2.03	0.41
43:y:18:LYS:HE2	43:y:18:LYS:HB2	1.68	0.41
45:1:8:C:H2'	45:1:9:U:C6	2.55	0.41
45:1:109:A:H4'	45:1:110:G:OP1	2.20	0.41
45:1:733:G:N2	45:1:735:A:OP2	2.54	0.41
45:1:1109:U:C4	45:1:1110:U:C4	3.08	0.41
45:1:1176:C:H2'	45:1:1177:G:N2	2.36	0.41
45:1:2779:A:H2'	45:1:2780:A:H8	1.85	0.41
45:1:3015:G:O2'	45:1:3016:A:H5'	2.21	0.41
45:1:3252:G:H2'	45:1:3253:G:H8	1.86	0.41
46:2:131:A:H2'	46:2:132:G:H8	1.86	0.41
2:B:146:ARG:HA	2:B:146:ARG:HD2	1.70	0.40
5:E:14:ASP:OD1	5:E:14:ASP:N	2.54	0.40
6:F:156:ILE:HD12	6:F:161:VAL:HB	2.03	0.40
7:G:78:PHE:C	7:G:80:TYR:H	2.29	0.40
15:Q:95:GLU:H	15:Q:95:GLU:HG3	1.65	0.40
26:b:275:LYS:N	26:b:276:PRO:HD2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:48:ARG:HD3	30:f:103:TYR:HE2	1.87	0.40
36:m:377:ASP:OD1	36:m:377:ASP:C	2.64	0.40
38:r:188:GLU:C	38:r:190:GLY:H	2.28	0.40
40:v:231:ASP:OD1	40:v:231:ASP:N	2.54	0.40
41:w:11:VAL:O	41:w:59:GLN:NE2	2.54	0.40
42:x:78:THR:O	42:x:121:TYR:HA	2.21	0.40
45:1:379:C:H2'	45:1:380:U:H6	1.85	0.40
45:1:649:A:O2'	45:1:650:C:OP1	2.36	0.40
45:1:2209:U:C3'	45:1:2209:U:C6	3.03	0.40
45:1:2224:A:H3'	45:1:2225:U:C6	2.56	0.40
45:1:2661:G:H2'	45:1:2662:G:H8	1.86	0.40
45:1:2868:U:H4'	45:1:2869:U:H2'	2.02	0.40
45:1:3375:A:O2'	45:1:3378:C:OP2	2.37	0.40
3:C:269:SER:OG	3:C:271:LYS:HB2	2.21	0.40
8:H:138:THR:C	8:H:140:VAL:H	2.29	0.40
9:J:131:MET:HG3	9:J:159:THR:HG22	2.03	0.40
16:R:41:ILE:O	16:R:45:VAL:HG23	2.22	0.40
17:S:40:ARG:HA	17:S:40:ARG:HD2	1.79	0.40
23:Y:95:VAL:HA	23:Y:96:PRO:HD3	1.97	0.40
24:Z:128:GLN:H	24:Z:128:GLN:HG2	1.73	0.40
26:b:120:GLN:HE21	26:b:120:GLN:HB3	1.73	0.40
36:m:52:LYS:HB2	36:m:52:LYS:HE2	1.84	0.40
42:x:87:LYS:C	42:x:89:SER:H	2.29	0.40
42:x:274:MET:HB3	42:x:304:TRP:CH2	2.56	0.40
42:x:487:ASP:CB	42:x:506:LYS:HB3	2.51	0.40
45:1:170:G:N2	45:1:249:U:C2	2.89	0.40
45:1:304:G:OP2	45:1:2777:G:O2'	2.36	0.40
45:1:309:U:H2'	45:1:310:U:C6	2.57	0.40
45:1:907:G:OP1	45:1:909:G:O2'	2.36	0.40
45:1:1201:C:H2'	45:1:1202:A:C4	2.57	0.40
45:1:1340:G:H2'	45:1:1341:U:C6	2.56	0.40
45:1:2224:A:H8	45:1:2225:U:C6	2.40	0.40
45:1:2592:G:HO2'	45:1:2593:A:P	2.43	0.40
47:3:89:G:H2'	47:3:93:C:H42	1.85	0.40
3:C:282:SER:OG	3:C:283:THR:N	2.54	0.40
4:D:77:ALA:O	4:D:108:ARG:NH1	2.55	0.40
12:N:3:ALA:O	12:N:7:LEU:HB2	2.21	0.40
12:N:96:ARG:NE	12:N:104:GLU:OE2	2.54	0.40
18:T:97:LYS:HD2	18:T:97:LYS:HA	1.89	0.40
24:Z:49:TYR:CE2	24:Z:133:LYS:HA	2.55	0.40
25:a:95:SER:OG	25:a:96:LYS:O	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:47:ARG:NH1	45:1:634:C:H4'	2.36	0.40
33:i:61:ILE:HA	33:i:65:GLY:O	2.22	0.40
39:u:123:ASP:HA	39:u:126:LEU:HB3	2.04	0.40
40:v:188:GLY:HA3	41:w:36:LYS:HA	2.03	0.40
42:x:417:ILE:HG22	42:x:429:TRP:HD1	1.87	0.40
45:1:747:A:H2'	45:1:748:U:H6	1.86	0.40
45:1:1290:A:H2'	45:1:1291:A:C8	2.56	0.40
45:1:2198:A:C6	45:1:2247:G:N2	2.90	0.40
46:2:39:G:H1'	46:2:104:A:N6	2.36	0.40
46:2:141:C:H2'	46:2:142:C:H6	1.86	0.40
3:C:141:ARG:HH22	45:1:1386:A:H5''	1.86	0.40
8:H:1:MET:HE3	8:H:1:MET:HB2	1.94	0.40
12:N:17:ASP:HA	12:N:20:ARG:HG2	2.04	0.40
36:m:32:ASP:O	36:m:36:VAL:HG23	2.20	0.40
37:p:49:ARG:HG2	37:p:50:GLY:N	2.37	0.40
38:r:189:LEU:HD23	38:r:189:LEU:HA	1.85	0.40
39:u:122:ARG:O	39:u:125:LYS:HG2	2.21	0.40
41:w:17:ILE:HA	41:w:18:PRO:HD3	1.93	0.40
45:1:97:U:O2'	45:1:98:G:O4'	2.39	0.40
45:1:150:A:C5	45:1:151:A:N7	2.90	0.40
45:1:1799:A:H2'	45:1:1800:A:H8	1.85	0.40
45:1:2203:U:H3	45:1:2239:G:H1	1.68	0.40
4:D:48:LYS:HD3	4:D:48:LYS:HA	1.76	0.40
8:H:41:ILE:HG23	8:H:43:VAL:HG13	2.04	0.40
11:M:135:LEU:HD12	11:M:135:LEU:HA	1.83	0.40
17:S:17:GLU:O	17:S:18:SER:OG	2.35	0.40
21:W:44:HIS:HB2	21:W:216:LYS:HG3	2.03	0.40
24:Z:97:SER:OG	24:Z:98:THR:N	2.54	0.40
32:h:21:LEU:HD11	32:h:58:ILE:HD12	2.02	0.40
36:m:157:LEU:HA	36:m:160:LEU:HB3	2.04	0.40
36:m:300:ILE:HG21	45:1:2195:C:H1'	2.04	0.40
40:v:129:LYS:HD3	40:v:129:LYS:C	2.46	0.40
41:w:50:ILE:HD13	41:w:50:ILE:HA	1.86	0.40
42:x:234:SER:OG	42:x:283:CYS:HA	2.21	0.40
45:1:199:A:C4	45:1:201:A:C8	3.09	0.40
45:1:1050:U:O2'	45:1:1051:U:H5''	2.22	0.40
45:1:1816:A:H2'	45:1:1817:G:O4'	2.21	0.40
46:2:94:C:HO2'	46:2:95:G:H8	1.70	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	
1	A	176/254 (69%)	164 (93%)	12 (7%)	0	100	100
2	B	384/387 (99%)	332 (86%)	49 (13%)	3 (1%)	16	45
3	C	330/362 (91%)	292 (88%)	37 (11%)	1 (0%)	36	65
4	D	267/297 (90%)	240 (90%)	27 (10%)	0	100	100
5	E	152/176 (86%)	141 (93%)	11 (7%)	0	100	100
6	F	220/244 (90%)	201 (91%)	18 (8%)	1 (0%)	24	55
7	G	160/256 (62%)	140 (88%)	20 (12%)	0	100	100
8	H	188/191 (98%)	167 (89%)	20 (11%)	1 (0%)	24	55
9	J	167/174 (96%)	136 (81%)	31 (19%)	0	100	100
10	L	180/199 (90%)	157 (87%)	22 (12%)	1 (1%)	21	50
11	M	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
12	N	179/204 (88%)	165 (92%)	12 (7%)	2 (1%)	11	36
13	O	195/199 (98%)	187 (96%)	8 (4%)	0	100	100
14	P	181/184 (98%)	166 (92%)	15 (8%)	0	100	100
15	Q	132/186 (71%)	126 (96%)	6 (4%)	0	100	100
16	R	152/189 (80%)	145 (95%)	7 (5%)	0	100	100
17	S	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
18	T	115/160 (72%)	101 (88%)	14 (12%)	0	100	100
19	U	100/121 (83%)	87 (87%)	13 (13%)	0	100	100
20	V	133/137 (97%)	125 (94%)	8 (6%)	0	100	100
21	W	232/236 (98%)	209 (90%)	22 (10%)	1 (0%)	30	60
22	X	84/142 (59%)	78 (93%)	6 (7%)	0	100	100
23	Y	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
24	Z	133/136 (98%)	115 (86%)	17 (13%)	1 (1%)	16	45
25	a	91/149 (61%)	80 (88%)	10 (11%)	1 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	b	506/647 (78%)	437 (86%)	64 (13%)	5 (1%)	12	39
27	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
28	d	104/113 (92%)	98 (94%)	6 (6%)	0	100	100
29	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
30	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
31	g	102/121 (84%)	95 (93%)	7 (7%)	0	100	100
32	h	117/120 (98%)	101 (86%)	15 (13%)	1 (1%)	14	42
33	i	95/100 (95%)	86 (90%)	9 (10%)	0	100	100
34	j	74/88 (84%)	69 (93%)	5 (7%)	0	100	100
35	k	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
36	m	448/486 (92%)	384 (86%)	56 (12%)	8 (2%)	6	26
37	p	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
38	r	224/261 (86%)	186 (83%)	34 (15%)	4 (2%)	6	26
39	u	142/199 (71%)	135 (95%)	7 (5%)	0	100	100
40	v	283/344 (82%)	264 (93%)	19 (7%)	0	100	100
41	w	178/203 (88%)	155 (87%)	23 (13%)	0	100	100
42	x	476/515 (92%)	429 (90%)	47 (10%)	0	100	100
43	y	242/245 (99%)	223 (92%)	19 (8%)	0	100	100
44	z	53/106 (50%)	51 (96%)	2 (4%)	0	100	100
All	All	7910/9080 (87%)	7130 (90%)	750 (10%)	30 (0%)	31	60

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	339	LEU
36	m	209	LYS
36	m	241	SER
10	L	63	VAL
12	N	146	ALA
24	Z	102	GLU
25	a	78	LEU
26	b	369	ARG
26	b	484	SER
36	m	78	PHE
36	m	424	ALA

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Mol	Chain	Res	Type
6	F	158	LYS
8	H	50	ASN
21	W	178	GLY
26	b	399	ALA
36	m	240	LYS
38	r	17	ARG
38	r	147	TRP
2	B	342	LEU
26	b	483	ALA
36	m	136	SER
36	m	378	SER
38	r	163	ARG
12	N	95	GLN
32	h	92	LEU
38	r	146	SER
36	m	77	TRP
2	B	188	ILE
2	B	239	PRO
26	b	9	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	
1	A	140/196 (71%)	127 (91%)	13 (9%)	8	29
2	B	322/323 (100%)	289 (90%)	33 (10%)	7	26
3	C	271/289 (94%)	242 (89%)	29 (11%)	6	24
4	D	224/245 (91%)	200 (89%)	24 (11%)	6	24
5	E	134/153 (88%)	121 (90%)	13 (10%)	8	28
6	F	186/205 (91%)	171 (92%)	15 (8%)	11	34
7	G	131/208 (63%)	116 (88%)	15 (12%)	5	21
8	H	170/171 (99%)	151 (89%)	19 (11%)	6	22
9	J	147/150 (98%)	123 (84%)	24 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	144/159 (91%)	130 (90%)	14 (10%)	8	28
11	M	108/109 (99%)	93 (86%)	15 (14%)	3	14
12	N	159/176 (90%)	146 (92%)	13 (8%)	10	34
13	O	160/162 (99%)	150 (94%)	10 (6%)	16	43
14	P	145/146 (99%)	131 (90%)	14 (10%)	8	28
15	Q	110/151 (73%)	97 (88%)	13 (12%)	5	20
16	R	127/154 (82%)	119 (94%)	8 (6%)	16	43
17	S	155/156 (99%)	139 (90%)	16 (10%)	7	26
18	T	102/137 (74%)	91 (89%)	11 (11%)	6	23
19	U	89/107 (83%)	77 (86%)	12 (14%)	4	15
20	V	103/105 (98%)	94 (91%)	9 (9%)	9	32
21	W	211/213 (99%)	188 (89%)	23 (11%)	6	23
22	X	76/118 (64%)	64 (84%)	12 (16%)	2	11
23	Y	108/110 (98%)	98 (91%)	10 (9%)	8	29
24	Z	115/116 (99%)	109 (95%)	6 (5%)	21	49
25	a	76/119 (64%)	69 (91%)	7 (9%)	8	30
26	b	458/573 (80%)	415 (91%)	43 (9%)	8	29
27	c	81/88 (92%)	73 (90%)	8 (10%)	7	27
28	d	93/97 (96%)	82 (88%)	11 (12%)	5	20
29	e	109/111 (98%)	101 (93%)	8 (7%)	13	38
30	f	90/91 (99%)	87 (97%)	3 (3%)	33	61
31	g	89/103 (86%)	79 (89%)	10 (11%)	6	22
32	h	104/105 (99%)	99 (95%)	5 (5%)	23	52
33	i	79/82 (96%)	72 (91%)	7 (9%)	9	31
34	j	62/71 (87%)	59 (95%)	3 (5%)	23	52
35	k	68/69 (99%)	61 (90%)	7 (10%)	7	26
36	m	399/428 (93%)	356 (89%)	43 (11%)	6	23
37	p	71/72 (99%)	65 (92%)	6 (8%)	10	33
38	r	203/229 (89%)	179 (88%)	24 (12%)	5	20
39	u	128/180 (71%)	117 (91%)	11 (9%)	10	32
40	v	258/309 (84%)	233 (90%)	25 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	w	161/179 (90%)	142 (88%)	19 (12%)	5	20
42	x	428/451 (95%)	386 (90%)	42 (10%)	7	28
43	y	210/211 (100%)	187 (89%)	23 (11%)	6	23
44	z	48/95 (50%)	46 (96%)	2 (4%)	26	56
All	All	6852/7722 (89%)	6174 (90%)	678 (10%)	10	27

All (678) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TYR
1	A	45	VAL
1	A	49	VAL
1	A	82	VAL
1	A	97	ASN
1	A	98	VAL
1	A	106	SER
1	A	126	LEU
1	A	139	HIS
1	A	143	GLU
1	A	157	VAL
1	A	161	ASP
1	A	191	LEU
2	B	55	THR
2	B	57	VAL
2	B	74	GLU
2	B	77	THR
2	B	79	VAL
2	B	84	VAL
2	B	85	VAL
2	B	90	VAL
2	B	95	THR
2	B	101	SER
2	B	103	THR
2	B	104	THR
2	B	114	VAL
2	B	157	VAL
2	B	192	VAL
2	B	205	VAL
2	B	206	ASP
2	B	216	ASP
2	B	221	THR

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Mol	Chain	Res	Type
2	B	231	HIS
2	B	246	LEU
2	B	263	SER
2	B	277	SER
2	B	278	ILE
2	B	283	TYR
2	B	301	THR
2	B	305	ILE
2	B	320	ASP
2	B	324	VAL
2	B	340	LYS
2	B	354	VAL
2	B	359	ILE
2	B	382	THR
3	C	6	VAL
3	C	7	THR
3	C	11	LEU
3	C	12	THR
3	C	27	SER
3	C	30	ILE
3	C	35	VAL
3	C	52	VAL
3	C	58	HIS
3	C	90	PHE
3	C	105	THR
3	C	117	GLU
3	C	148	ILE
3	C	151	VAL
3	C	172	VAL
3	C	181	VAL
3	C	193	LYS
3	C	230	VAL
3	C	270	SER
3	C	275	THR
3	C	278	SER
3	C	289	ILE
3	C	297	SER
3	C	313	LEU
3	C	318	LEU
3	C	325	LEU
3	C	333	VAL
3	C	339	LEU

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Mol	Chain	Res	Type
3	C	356	THR
4	D	8	LYS
4	D	14	SER
4	D	16	PHE
4	D	18	THR
4	D	36	LEU
4	D	40	HIS
4	D	43	LYS
4	D	46	THR
4	D	51	LEU
4	D	59	ASP
4	D	73	VAL
4	D	83	LEU
4	D	85	ARG
4	D	95	TRP
4	D	101	THR
4	D	137	ASP
4	D	144	VAL
4	D	150	LEU
4	D	173	VAL
4	D	190	ILE
4	D	205	SER
4	D	222	LEU
4	D	229	ASP
4	D	232	ASP
5	E	2	SER
5	E	14	ASP
5	E	15	VAL
5	E	35	VAL
5	E	38	THR
5	E	40	LEU
5	E	62	THR
5	E	79	VAL
5	E	98	VAL
5	E	104	GLU
5	E	143	LYS
5	E	146	ILE
5	E	149	ILE
6	F	26	VAL
6	F	45	LEU
6	F	77	VAL
6	F	86	VAL

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Mol	Chain	Res	Type
6	F	87	VAL
6	F	89	ILE
6	F	110	ARG
6	F	111	ILE
6	F	115	THR
6	F	117	VAL
6	F	143	THR
6	F	158	LYS
6	F	179	LEU
6	F	190	THR
6	F	239	LEU
7	G	71	VAL
7	G	90	THR
7	G	94	PHE
7	G	110	THR
7	G	155	ASN
7	G	162	LEU
7	G	180	VAL
7	G	188	THR
7	G	189	LEU
7	G	194	THR
7	G	197	VAL
7	G	203	VAL
7	G	214	LEU
7	G	218	ILE
7	G	227	ASP
8	H	6	THR
8	H	14	GLU
8	H	16	VAL
8	H	18	VAL
8	H	33	THR
8	H	41	ILE
8	H	93	VAL
8	H	104	VAL
8	H	107	ASP
8	H	113	GLU
8	H	132	VAL
8	H	133	THR
8	H	139	ASN
8	H	144	ILE
8	H	151	VAL
8	H	155	SER

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Mol	Chain	Res	Type
8	H	161	LEU
8	H	164	ILE
8	H	189	GLU
9	J	7	ASN
9	J	11	ASP
9	J	17	LEU
9	J	22	SER
9	J	34	SER
9	J	36	VAL
9	J	62	ASN
9	J	77	GLU
9	J	80	LEU
9	J	99	THR
9	J	106	ILE
9	J	112	LEU
9	J	126	ASP
9	J	128	TYR
9	J	129	VAL
9	J	130	VAL
9	J	138	VAL
9	J	147	THR
9	J	151	SER
9	J	152	HIS
9	J	154	THR
9	J	155	THR
9	J	159	THR
9	J	160	VAL
10	L	14	PHE
10	L	15	ARG
10	L	22	VAL
10	L	27	ASP
10	L	57	VAL
10	L	58	VAL
10	L	69	VAL
10	L	86	THR
10	L	104	ARG
10	L	108	ILE
10	L	124	ILE
10	L	182	ILE
10	L	185	LYS
10	L	192	GLU
11	M	6	ILE

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Mol	Chain	Res	Type
11	M	8	LYS
11	M	15	VAL
11	M	20	VAL
11	M	22	LEU
11	M	36	VAL
11	M	38	ILE
11	M	44	VAL
11	M	63	VAL
11	M	64	VAL
11	M	90	VAL
11	M	91	CYS
11	M	121	MET
11	M	133	LYS
11	M	135	LEU
12	N	13	LYS
12	N	18	VAL
12	N	38	ARG
12	N	51	LEU
12	N	61	ILE
12	N	66	VAL
12	N	98	LEU
12	N	116	LEU
12	N	124	ASP
12	N	133	ILE
12	N	165	THR
12	N	167	THR
12	N	192	LYS
13	O	22	VAL
13	O	34	VAL
13	O	56	ASP
13	O	84	LEU
13	O	92	THR
13	O	106	GLU
13	O	119	VAL
13	O	143	THR
13	O	178	VAL
13	O	184	THR
14	P	3	ARG
14	P	24	VAL
14	P	29	THR
14	P	32	THR
14	P	65	SER

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Mol	Chain	Res	Type
14	P	87	SER
14	P	119	VAL
14	P	120	ASN
14	P	129	THR
14	P	144	SER
14	P	148	LEU
14	P	157	VAL
14	P	165	VAL
14	P	168	LEU
15	Q	21	SER
15	Q	31	LYS
15	Q	34	THR
15	Q	47	VAL
15	Q	63	SER
15	Q	64	VAL
15	Q	69	ARG
15	Q	81	VAL
15	Q	84	VAL
15	Q	101	VAL
15	Q	129	VAL
15	Q	135	GLN
15	Q	138	LEU
16	R	29	THR
16	R	42	ARG
16	R	49	THR
16	R	51	VAL
16	R	52	LYS
16	R	57	VAL
16	R	116	ASP
16	R	155	LEU
17	S	9	VAL
17	S	12	ARG
17	S	16	THR
17	S	45	LEU
17	S	48	LEU
17	S	55	SER
17	S	60	SER
17	S	74	ASN
17	S	77	VAL
17	S	82	ASP
17	S	97	VAL
17	S	103	VAL

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Mol	Chain	Res	Type
17	S	105	THR
17	S	120	SER
17	S	160	THR
17	S	166	LYS
18	T	36	VAL
18	T	71	SER
18	T	72	VAL
18	T	91	LEU
18	T	96	ILE
18	T	99	SER
18	T	120	LYS
18	T	139	ARG
18	T	141	VAL
18	T	150	THR
18	T	154	VAL
19	U	16	THR
19	U	24	GLU
19	U	29	ASP
19	U	47	VAL
19	U	54	VAL
19	U	55	THR
19	U	57	THR
19	U	61	THR
19	U	76	LEU
19	U	88	GLN
19	U	96	VAL
19	U	98	THR
20	V	22	ILE
20	V	24	ASN
20	V	25	CYS
20	V	73	VAL
20	V	83	LYS
20	V	84	SER
20	V	112	SER
20	V	135	VAL
20	V	137	VAL
21	W	7	SER
21	W	11	THR
21	W	15	THR
21	W	35	ASP
21	W	43	LEU
21	W	45	LEU

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Mol	Chain	Res	Type
21	W	52	VAL
21	W	59	SER
21	W	63	SER
21	W	77	LEU
21	W	92	LEU
21	W	105	THR
21	W	107	GLU
21	W	108	ASP
21	W	109	VAL
21	W	111	THR
21	W	134	THR
21	W	137	ILE
21	W	158	ILE
21	W	196	ASP
21	W	198	ARG
21	W	208	ILE
21	W	228	VAL
22	X	57	LEU
22	X	67	ILE
22	X	71	THR
22	X	101	GLU
22	X	105	VAL
22	X	112	THR
22	X	113	LEU
22	X	119	THR
22	X	127	THR
22	X	129	ASP
22	X	133	LEU
22	X	134	ASP
23	Y	9	SER
23	Y	24	SER
23	Y	45	ILE
23	Y	50	ILE
23	Y	56	VAL
23	Y	62	SER
23	Y	104	LEU
23	Y	105	VAL
23	Y	109	LEU
23	Y	119	ILE
24	Z	53	VAL
24	Z	81	LEU
24	Z	88	ASP

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Mol	Chain	Res	Type
24	Z	100	THR
24	Z	105	SER
24	Z	134	LEU
25	a	72	VAL
25	a	85	ASP
25	a	88	ASP
25	a	101	VAL
25	a	104	THR
25	a	126	LYS
25	a	145	VAL
26	b	5	TRP
26	b	18	LEU
26	b	31	THR
26	b	39	ILE
26	b	93	ILE
26	b	94	SER
26	b	116	LEU
26	b	170	LEU
26	b	175	TYR
26	b	178	VAL
26	b	188	THR
26	b	212	LYS
26	b	250	VAL
26	b	263	THR
26	b	311	GLU
26	b	315	VAL
26	b	319	THR
26	b	321	SER
26	b	324	LEU
26	b	326	GLU
26	b	332	ARG
26	b	338	LYS
26	b	339	LEU
26	b	342	SER
26	b	362	HIS
26	b	363	VAL
26	b	391	GLU
26	b	398	LEU
26	b	411	VAL
26	b	414	VAL
26	b	420	TYR
26	b	421	LEU

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Mol	Chain	Res	Type
26	b	428	LYS
26	b	430	ASP
26	b	434	GLU
26	b	435	ILE
26	b	439	LYS
26	b	445	LEU
26	b	470	ASN
26	b	477	ILE
26	b	484	SER
26	b	499	ARG
26	b	512	SER
27	c	10	ILE
27	c	16	LEU
27	c	41	LEU
27	c	48	THR
27	c	61	MET
27	c	91	SER
27	c	97	ASP
27	c	99	ASP
28	d	14	ILE
28	d	27	LYS
28	d	51	LEU
28	d	64	VAL
28	d	67	VAL
28	d	76	SER
28	d	87	ASN
28	d	89	LEU
28	d	96	VAL
28	d	98	VAL
28	d	106	THR
29	e	23	ASP
29	e	42	VAL
29	e	51	SER
29	e	54	LYS
29	e	55	ILE
29	e	79	VAL
29	e	91	THR
29	e	126	LEU
30	f	56	SER
30	f	59	VAL
30	f	78	SER
31	g	10	ARG

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Mol	Chain	Res	Type
31	g	15	THR
31	g	23	VAL
31	g	40	THR
31	g	46	ASP
31	g	47	CYS
31	g	74	ARG
31	g	81	CYS
31	g	91	ARG
31	g	101	VAL
32	h	57	VAL
32	h	64	GLU
32	h	92	LEU
32	h	101	THR
32	h	109	ILE
33	i	2	THR
33	i	3	VAL
33	i	27	SER
33	i	29	LYS
33	i	50	LEU
33	i	59	ASP
33	i	90	MET
34	j	59	THR
34	j	61	THR
34	j	67	LEU
35	k	3	ARG
35	k	5	ILE
35	k	6	THR
35	k	7	ASP
35	k	31	LEU
35	k	57	ASN
35	k	66	ILE
36	m	22	LEU
36	m	24	VAL
36	m	30	TYR
36	m	32	ASP
36	m	54	ASN
36	m	84	ILE
36	m	94	SER
36	m	96	LEU
36	m	99	THR
36	m	103	THR
36	m	107	LEU

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Mol	Chain	Res	Type
36	m	120	GLU
36	m	121	LYS
36	m	132	LEU
36	m	174	LYS
36	m	176	VAL
36	m	180	THR
36	m	205	LYS
36	m	211	ILE
36	m	224	VAL
36	m	226	ILE
36	m	233	ASP
36	m	235	LEU
36	m	278	SER
36	m	280	GLU
36	m	287	HIS
36	m	291	THR
36	m	300	ILE
36	m	304	ARG
36	m	311	THR
36	m	318	VAL
36	m	341	CYS
36	m	343	VAL
36	m	362	ILE
36	m	380	GLU
36	m	383	LEU
36	m	390	VAL
36	m	391	GLU
36	m	404	LEU
36	m	409	VAL
36	m	418	ILE
36	m	425	THR
36	m	471	LYS
37	p	3	LYS
37	p	41	PHE
37	p	58	SER
37	p	71	VAL
37	p	83	ILE
37	p	88	GLU
38	r	35	ILE
38	r	46	LYS
38	r	59	VAL
38	r	60	SER

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Mol	Chain	Res	Type
38	r	73	VAL
38	r	120	VAL
38	r	130	GLU
38	r	133	MET
38	r	137	ILE
38	r	157	VAL
38	r	164	ARG
38	r	170	ARG
38	r	185	THR
38	r	189	LEU
38	r	192	THR
38	r	212	LEU
38	r	225	VAL
38	r	232	THR
38	r	238	VAL
38	r	244	GLN
38	r	245	VAL
38	r	246	THR
38	r	250	ASP
38	r	252	ASP
39	u	9	CYS
39	u	11	SER
39	u	52	THR
39	u	57	LYS
39	u	65	VAL
39	u	70	THR
39	u	73	GLN
39	u	84	GLU
39	u	127	VAL
39	u	132	GLU
39	u	139	VAL
40	v	26	ASN
40	v	33	ILE
40	v	43	HIS
40	v	46	MET
40	v	56	ASP
40	v	57	MET
40	v	61	ASN
40	v	72	MET
40	v	86	LEU
40	v	94	LYS
40	v	118	VAL

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Mol	Chain	Res	Type
40	v	121	ASN
40	v	122	PHE
40	v	126	SER
40	v	130	LYS
40	v	153	VAL
40	v	171	ASP
40	v	175	VAL
40	v	208	SER
40	v	221	ILE
40	v	245	VAL
40	v	246	THR
40	v	264	GLU
40	v	267	ILE
40	v	275	ILE
41	w	12	THR
41	w	33	VAL
41	w	39	LEU
41	w	40	ASP
41	w	42	SER
41	w	62	ILE
41	w	72	THR
41	w	73	THR
41	w	76	SER
41	w	80	THR
41	w	86	VAL
41	w	90	LEU
41	w	107	LYS
41	w	127	GLU
41	w	151	ASN
41	w	159	LEU
41	w	160	VAL
41	w	161	GLU
41	w	178	THR
42	x	56	SER
42	x	71	SER
42	x	78	THR
42	x	90	ASP
42	x	106	ILE
42	x	107	LYS
42	x	118	THR
42	x	122	THR
42	x	157	SER

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Mol	Chain	Res	Type
42	x	170	ILE
42	x	181	THR
42	x	182	LEU
42	x	191	CYS
42	x	225	LEU
42	x	233	THR
42	x	253	SER
42	x	264	ASP
42	x	266	VAL
42	x	273	THR
42	x	278	THR
42	x	279	ASN
42	x	283	CYS
42	x	300	THR
42	x	324	ASN
42	x	348	THR
42	x	371	GLU
42	x	391	SER
42	x	392	THR
42	x	395	ILE
42	x	399	THR
42	x	404	LEU
42	x	418	VAL
42	x	421	SER
42	x	459	LEU
42	x	463	SER
42	x	475	THR
42	x	480	VAL
42	x	481	ASP
42	x	482	LEU
42	x	491	THR
42	x	492	VAL
42	x	514	THR
43	y	22	THR
43	y	50	HIS
43	y	52	THR
43	y	72	VAL
43	y	74	THR
43	y	77	THR
43	y	78	ASP
43	y	80	GLU
43	y	92	VAL

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Mol	Chain	Res	Type
43	y	128	LEU
43	y	141	THR
43	y	143	SER
43	y	146	ILE
43	y	165	THR
43	y	166	SER
43	y	175	SER
43	y	182	VAL
43	y	198	VAL
43	y	205	VAL
43	y	206	THR
43	y	224	LEU
43	y	235	ASN
43	y	239	THR
44	z	9	SER
44	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	139	HIS
2	B	13	HIS
2	B	165	GLN
2	B	211	GLN
2	B	224	HIS
2	B	231	HIS
2	B	243	HIS
2	B	256	HIS
2	B	259	HIS
2	B	345	ASN
3	C	116	ASN
3	C	221	ASN
3	C	307	GLN
4	D	45	ASN
4	D	90	HIS
4	D	264	GLN
5	E	138	GLN
5	E	167	ASN
6	F	81	HIS
6	F	172	ASN
6	F	194	HIS

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Mol	Chain	Res	Type
6	F	209	ASN
7	G	77	GLN
7	G	79	GLN
7	G	95	ASN
8	H	125	ASN
8	H	157	ASN
8	H	183	HIS
9	J	6	GLN
9	J	95	ASN
9	J	132	ASN
9	J	152	HIS
10	L	17	HIS
10	L	28	GLN
11	M	59	ASN
11	M	126	GLN
13	O	50	ASN
13	O	90	HIS
13	O	182	ASN
14	P	55	GLN
15	Q	23	ASN
15	Q	45	ASN
15	Q	73	GLN
15	Q	136	ASN
15	Q	145	ASN
16	R	34	GLN
16	R	75	HIS
17	S	89	ASN
17	S	122	HIS
17	S	138	GLN
17	S	157	GLN
18	T	54	HIS
19	U	25	ASN
19	U	101	ASN
19	U	109	GLN
21	W	14	GLN
21	W	74	GLN
21	W	88	ASN
21	W	110	ASN
21	W	148	GLN
22	X	94	GLN
22	X	137	ASN
23	Y	4	GLN

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Mol	Chain	Res	Type
23	Y	26	GLN
23	Y	91	ASN
23	Y	98	ASN
24	Z	36	HIS
24	Z	57	HIS
25	a	74	ASN
26	b	89	ASN
26	b	120	GLN
26	b	124	GLN
26	b	280	ASN
26	b	415	ASN
26	b	440	ASN
27	c	47	ASN
28	d	56	ASN
29	e	13	HIS
29	e	49	ASN
29	e	88	HIS
31	g	52	GLN
31	g	61	GLN
32	h	68	GLN
33	i	91	ASN
34	j	13	ASN
34	j	76	ASN
35	k	10	GLN
35	k	67	GLN
36	m	100	GLN
36	m	111	ASN
36	m	392	HIS
36	m	452	GLN
38	r	4	ASN
38	r	10	HIS
38	r	14	HIS
38	r	68	HIS
38	r	205	GLN
38	r	211	GLN
39	u	37	HIS
40	v	29	GLN
40	v	36	GLN
40	v	64	ASN
40	v	82	ASN
40	v	151	HIS
40	v	173	GLN

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Mol	Chain	Res	Type
40	v	213	GLN
40	v	249	HIS
41	w	37	ASN
41	w	57	ASN
41	w	59	GLN
41	w	83	GLN
41	w	157	GLN
41	w	194	GLN
41	w	195	GLN
41	w	198	ASN
42	x	31	ASN
42	x	116	GLN
42	x	166	ASN
42	x	208	ASN
42	x	241	HIS
42	x	321	HIS
42	x	401	HIS
42	x	515	HIS
43	y	11	ASN
43	y	33	ASN
43	y	83	HIS
43	y	106	ASN
43	y	140	GLN
43	y	162	HIS
43	y	168	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	1	2950/3396 (86%)	795 (26%)	58 (1%)
46	2	157/158 (99%)	41 (26%)	2 (1%)
47	3	120/121 (99%)	29 (24%)	1 (0%)
All	All	3227/3675 (87%)	865 (26%)	61 (1%)

All (865) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	1	2	U
45	1	5	G
45	1	7	C
45	1	10	C

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Mol	Chain	Res	Type
45	1	11	A
45	1	13	A
45	1	14	U
45	1	15	C
45	1	18	G
45	1	26	A
45	1	40	A
45	1	41	G
45	1	42	C
45	1	43	A
45	1	49	A
45	1	51	A
45	1	59	G
45	1	60	A
45	1	65	A
45	1	66	A
45	1	70	A
45	1	75	G
45	1	76	G
45	1	83	U
45	1	90	C
45	1	91	G
45	1	92	G
45	1	93	C
45	1	94	G
45	1	96	G
45	1	97	U
45	1	98	G
45	1	100	A
45	1	102	C
45	1	103	G
45	1	110	G
45	1	111	C
45	1	116	A
45	1	117	U
45	1	120	G
45	1	121	A
45	1	122	A
45	1	135	C
45	1	136	G
45	1	146	U
45	1	148	G

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Mol	Chain	Res	Type
45	1	154	U
45	1	156	G
45	1	157	A
45	1	158	G
45	1	160	G
45	1	161	G
45	1	165	A
45	1	168	U
45	1	170	G
45	1	172	G
45	1	173	G
45	1	187	A
45	1	190	U
45	1	191	U
45	1	206	G
45	1	210	U
45	1	211	A
45	1	213	A
45	1	218	G
45	1	219	A
45	1	239	G
45	1	240	U
45	1	241	G
45	1	243	G
45	1	245	U
45	1	248	U
45	1	249	U
45	1	251	G
45	1	252	U
45	1	254	A
45	1	258	G
45	1	260	C
45	1	261	U
45	1	262	U
45	1	263	C
45	1	269	G
45	1	282	G
45	1	284	A
45	1	295	A
45	1	305	U
45	1	306	A
45	1	307	A

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Mol	Chain	Res	Type
45	1	323	A
45	1	329	U
45	1	349	A
45	1	352	A
45	1	368	G
45	1	376	G
45	1	395	A
45	1	398	A
45	1	399	A
45	1	401	U
45	1	402	A
45	1	403	C
45	1	421	G
45	1	422	A
45	1	439	C
45	1	440	A
45	1	495	G
45	1	496	C
45	1	498	A
45	1	516	A
45	1	518	G
45	1	521	A
45	1	535	G
45	1	544	C
45	1	545	U
45	1	547	G
45	1	548	G
45	1	549	U
45	1	550	A
45	1	551	A
45	1	553	U
45	1	555	U
45	1	557	A
45	1	558	U
45	1	559	A
45	1	568	G
45	1	578	A
45	1	579	G
45	1	582	G
45	1	592	A
45	1	603	A
45	1	604	G

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Mol	Chain	Res	Type
45	1	611	A
45	1	620	U
45	1	621	A
45	1	643	U
45	1	644	G
45	1	645	A
45	1	646	A
45	1	647	A
45	1	650	C
45	1	660	A
45	1	665	A
45	1	677	A
45	1	681	U
45	1	684	G
45	1	689	U
45	1	690	A
45	1	691	A
45	1	695	C
45	1	705	A
45	1	708	G
45	1	712	G
45	1	715	A
45	1	720	A
45	1	721	G
45	1	722	G
45	1	733	G
45	1	735	A
45	1	736	A
45	1	738	A
45	1	762	U
45	1	765	C
45	1	766	U
45	1	767	U
45	1	777	U
45	1	779	G
45	1	780	A
45	1	781	G
45	1	784	A
45	1	785	G
45	1	806	A
45	1	809	G
45	1	817	A

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Mol	Chain	Res	Type
45	1	830	A
45	1	837	A
45	1	849	C
45	1	850	U
45	1	861	C
45	1	870	G
45	1	871	U
45	1	872	U
45	1	874	U
45	1	875	G
45	1	879	U
45	1	884	A
45	1	885	U
45	1	886	C
45	1	896	A
45	1	897	U
45	1	907	G
45	1	908	G
45	1	909	G
45	1	914	A
45	1	916	G
45	1	917	A
45	1	918	C
45	1	921	A
45	1	922	U
45	1	924	G
45	1	925	A
45	1	926	A
45	1	936	A
45	1	937	G
45	1	944	C
45	1	956	U
45	1	958	C
45	1	960	U
45	1	971	G
45	1	974	G
45	1	975	C
45	1	977	C
45	1	978	G
45	1	980	A
45	1	991	G
45	1	993	G

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Mol	Chain	Res	Type
45	1	994	G
45	1	995	U
45	1	997	A
45	1	999	G
45	1	1000	C
45	1	1002	A
45	1	1003	A
45	1	1048	A
45	1	1049	C
45	1	1052	U
45	1	1053	A
45	1	1054	A
45	1	1057	A
45	1	1058	U
45	1	1059	G
45	1	1064	A
45	1	1065	A
45	1	1066	G
45	1	1074	U
45	1	1085	A
45	1	1086	C
45	1	1088	U
45	1	1089	G
45	1	1090	G
45	1	1093	A
45	1	1094	U
45	1	1095	U
45	1	1096	U
45	1	1097	G
45	1	1098	A
45	1	1103	A
45	1	1104	G
45	1	1105	A
45	1	1111	U
45	1	1112	A
45	1	1117	G
45	1	1118	C
45	1	1127	G
45	1	1129	A
45	1	1132	C
45	1	1145	G
45	1	1155	C

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Mol	Chain	Res	Type
45	1	1159	A
45	1	1160	C
45	1	1173	U
45	1	1174	G
45	1	1180	A
45	1	1181	U
45	1	1186	G
45	1	1189	C
45	1	1192	C
45	1	1196	C
45	1	1197	A
45	1	1198	C
45	1	1199	C
45	1	1200	A
45	1	1201	C
45	1	1203	A
45	1	1204	A
45	1	1206	G
45	1	1209	G
45	1	1212	A
45	1	1220	U
45	1	1222	G
45	1	1227	C
45	1	1237	G
45	1	1241	U
45	1	1242	G
45	1	1244	A
45	1	1245	A
45	1	1262	G
45	1	1263	A
45	1	1264	G
45	1	1271	A
45	1	1272	C
45	1	1278	A
45	1	1280	C
45	1	1286	A
45	1	1287	A
45	1	1301	A
45	1	1302	A
45	1	1303	A
45	1	1304	A
45	1	1305	U

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Mol	Chain	Res	Type
45	1	1307	G
45	1	1309	U
45	1	1313	G
45	1	1330	A
45	1	1332	A
45	1	1348	U
45	1	1349	G
45	1	1350	A
45	1	1351	U
45	1	1352	A
45	1	1353	U
45	1	1354	G
45	1	1355	A
45	1	1356	U
45	1	1357	G
45	1	1364	C
45	1	1380	G
45	1	1386	A
45	1	1399	A
45	1	1400	G
45	1	1418	A
45	1	1419	A
45	1	1431	G
45	1	1434	G
45	1	1437	C
45	1	1446	A
45	1	1450	G
45	1	1455	U
45	1	1475	A
45	1	1481	A
45	1	1482	A
45	1	1508	C
45	1	1523	U
45	1	1533	U
45	1	1542	G
45	1	1544	G
45	1	1547	G
45	1	1549	U
45	1	1550	C
45	1	1555	U
45	1	1556	C
45	1	1583	A

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Mol	Chain	Res	Type
45	1	1587	A
45	1	1589	A
45	1	1593	A
45	1	1607	U
45	1	1619	A
45	1	1623	G
45	1	1629	U
45	1	1639	C
45	1	1641	U
45	1	1643	A
45	1	1657	C
45	1	1716	U
45	1	1717	U
45	1	1718	G
45	1	1724	U
45	1	1725	C
45	1	1736	G
45	1	1741	A
45	1	1742	U
45	1	1743	G
45	1	1750	A
45	1	1751	G
45	1	1752	A
45	1	1760	A
45	1	1762	C
45	1	1763	U
45	1	1765	U
45	1	1770	G
45	1	1780	G
45	1	1796	G
45	1	1797	A
45	1	1813	A
45	1	1814	A
45	1	1815	U
45	1	1816	A
45	1	1817	G
45	1	1820	U
45	1	1821	U
45	1	1839	A
45	1	1841	A
45	1	1842	A
45	1	1847	A

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Mol	Chain	Res	Type
45	1	1849	C
45	1	1851	G
45	1	1866	C
45	1	1867	A
45	1	1872	C
45	1	1874	A
45	1	1878	G
45	1	1880	U
45	1	1881	A
45	1	1886	A
45	1	1906	G
45	1	1907	C
45	1	1909	A
45	1	1926	C
45	1	1953	G
45	1	2094	C
45	1	2101	C
45	1	2102	U
45	1	2112	U
45	1	2113	A
45	1	2116	G
45	1	2121	G
45	1	2122	G
45	1	2131	A
45	1	2136	C
45	1	2137	U
45	1	2138	A
45	1	2139	A
45	1	2140	U
45	1	2143	A
45	1	2144	A
45	1	2145	A
45	1	2158	A
45	1	2163	C
45	1	2169	G
45	1	2170	U
45	1	2174	G
45	1	2185	G
45	1	2194	G
45	1	2195	C
45	1	2196	C
45	1	2197	C

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Mol	Chain	Res	Type
45	1	2198	A
45	1	2199	G
45	1	2200	U
45	1	2201	G
45	1	2202	C
45	1	2205	U
45	1	2206	G
45	1	2207	A
45	1	2208	A
45	1	2209	U
45	1	2210	G
45	1	2218	G
45	1	2222	A
45	1	2237	C
45	1	2242	A
45	1	2243	A
45	1	2245	C
45	1	2247	G
45	1	2249	G
45	1	2254	U
45	1	2255	A
45	1	2256	A
45	1	2257	C
45	1	2259	A
45	1	2260	U
45	1	2261	G
45	1	2262	A
45	1	2263	C
45	1	2265	C
45	1	2266	U
45	1	2267	C
45	1	2268	U
45	1	2269	U
45	1	2270	A
45	1	2271	A
45	1	2277	C
45	1	2278	C
45	1	2279	A
45	1	2280	A
45	1	2316	G
45	1	2317	A
45	1	2318	U

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Mol	Chain	Res	Type
45	1	2334	U
45	1	2336	U
45	1	2370	G
45	1	2371	G
45	1	2381	G
45	1	2385	G
45	1	2393	G
45	1	2395	G
45	1	2397	A
45	1	2398	A
45	1	2399	A
45	1	2401	A
45	1	2402	A
45	1	2411	U
45	1	2415	C
45	1	2418	G
45	1	2419	A
45	1	2423	U
45	1	2424	A
45	1	2426	U
45	1	2428	U
45	1	2430	A
45	1	2432	A
45	1	2434	U
45	1	2435	G
45	1	2439	A
45	1	2440	G
45	1	2441	A
45	1	2443	A
45	1	2444	C
45	1	2445	A
45	1	2502	A
45	1	2503	G
45	1	2507	C
45	1	2508	U
45	1	2509	U
45	1	2512	C
45	1	2514	U
45	1	2515	A
45	1	2518	C
45	1	2519	A
45	1	2593	A

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Mol	Chain	Res	Type
45	1	2594	C
45	1	2599	U
45	1	2600	C
45	1	2601	A
45	1	2602	G
45	1	2606	G
45	1	2607	G
45	1	2613	U
45	1	2614	G
45	1	2615	G
45	1	2621	G
45	1	2622	C
45	1	2623	G
45	1	2625	C
45	1	2626	A
45	1	2632	G
45	1	2635	A
45	1	2637	A
45	1	2639	G
45	1	2641	U
45	1	2643	A
45	1	2644	C
45	1	2645	G
45	1	2648	G
45	1	2649	A
45	1	2651	G
45	1	2652	U
45	1	2653	C
45	1	2654	C
45	1	2655	U
45	1	2656	A
45	1	2657	A
45	1	2659	G
45	1	2668	U
45	1	2669	G
45	1	2672	G
45	1	2674	A
45	1	2676	A
45	1	2677	G
45	1	2685	C
45	1	2686	A
45	1	2687	G

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Mol	Chain	Res	Type
45	1	2688	U
45	1	2689	A
45	1	2690	G
45	1	2692	A
45	1	2693	C
45	1	2694	A
45	1	2695	A
45	1	2696	A
45	1	2698	G
45	1	2700	G
45	1	2701	U
45	1	2702	A
45	1	2704	A
45	1	2706	G
45	1	2713	U
45	1	2717	U
45	1	2718	U
45	1	2719	U
45	1	2720	G
45	1	2721	A
45	1	2722	U
45	1	2724	U
45	1	2725	U
45	1	2726	C
45	1	2727	A
45	1	2728	G
45	1	2729	U
45	1	2730	G
45	1	2731	U
45	1	2732	G
45	1	2740	A
45	1	2741	C
45	1	2749	G
45	1	2752	U
45	1	2754	G
45	1	2758	A
45	1	2759	U
45	1	2762	A
45	1	2764	C
45	1	2765	C
45	1	2766	U
45	1	2767	U

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Mol	Chain	Res	Type
45	1	2768	U
45	1	2770	G
45	1	2771	U
45	1	2772	C
45	1	2773	C
45	1	2777	G
45	1	2788	C
45	1	2789	U
45	1	2793	G
45	1	2795	U
45	1	2796	G
45	1	2797	C
45	1	2798	C
45	1	2800	G
45	1	2801	A
45	1	2802	A
45	1	2806	U
45	1	2807	U
45	1	2809	C
45	1	2810	C
45	1	2811	A
45	1	2817	A
45	1	2818	U
45	1	2819	A
45	1	2820	A
45	1	2821	C
45	1	2822	U
45	1	2823	G
45	1	2824	G
45	1	2825	C
45	1	2826	U
45	1	2834	G
45	1	2837	A
45	1	2838	A
45	1	2842	U
45	1	2845	A
45	1	2846	U
45	1	2847	A
45	1	2849	C
45	1	2853	A
45	1	2857	C
45	1	2858	U

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Mol	Chain	Res	Type
45	1	2859	U
45	1	2861	U
45	1	2863	G
45	1	2864	A
45	1	2866	U
45	1	2867	C
45	1	2868	U
45	1	2869	U
45	1	2870	C
45	1	2872	A
45	1	2874	G
45	1	2875	U
45	1	2876	C
45	1	2877	G
45	1	2878	G
45	1	2879	C
45	1	2880	U
45	1	2887	A
45	1	2889	C
45	1	2894	C
45	1	2898	G
45	1	2899	C
45	1	2920	U
45	1	2923	U
45	1	2925	C
45	1	2926	A
45	1	2929	C
45	1	2930	A
45	1	2933	A
45	1	2935	U
45	1	2936	A
45	1	2944	U
45	1	2945	G
45	1	2947	G
45	1	2950	G
45	1	2951	G
45	1	2952	G
45	1	2953	U
45	1	2954	U
45	1	2955	U
45	1	2956	A
45	1	2957	G

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Mol	Chain	Res	Type
45	1	2968	G
45	1	2970	C
45	1	2971	A
45	1	2977	G
45	1	2978	U
45	1	2980	U
45	1	2981	U
45	1	2982	A
45	1	2983	C
45	1	2986	U
45	1	2993	G
45	1	2996	U
45	1	2997	G
45	1	3012	A
45	1	3017	A
45	1	3021	A
45	1	3022	G
45	1	3023	U
45	1	3032	A
45	1	3034	C
45	1	3037	U
45	1	3042	U
45	1	3049	A
45	1	3056	U
45	1	3058	U
45	1	3059	G
45	1	3078	U
45	1	3079	U
45	1	3080	G
45	1	3086	A
45	1	3092	C
45	1	3093	C
45	1	3100	U
45	1	3127	A
45	1	3129	A
45	1	3130	A
45	1	3131	U
45	1	3142	A
45	1	3143	C
45	1	3150	A
45	1	3153	U
45	1	3154	C

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Mol	Chain	Res	Type
45	1	3155	U
45	1	3156	U
45	1	3157	U
45	1	3158	G
45	1	3165	A
45	1	3167	A
45	1	3168	A
45	1	3172	A
45	1	3173	G
45	1	3174	A
45	1	3176	G
45	1	3179	U
45	1	3180	A
45	1	3181	C
45	1	3187	A
45	1	3195	U
45	1	3196	U
45	1	3207	U
45	1	3208	G
45	1	3209	A
45	1	3213	A
45	1	3217	C
45	1	3218	A
45	1	3219	G
45	1	3224	G
45	1	3228	C
45	1	3229	G
45	1	3243	A
45	1	3245	A
45	1	3247	G
45	1	3249	C
45	1	3259	U
45	1	3270	U
45	1	3271	G
45	1	3272	C
45	1	3273	A
45	1	3274	A
45	1	3276	G
45	1	3279	A
45	1	3280	U
45	1	3281	U
45	1	3282	U

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Mol	Chain	Res	Type
45	1	3286	G
45	1	3287	U
45	1	3289	G
45	1	3294	A
45	1	3295	A
45	1	3304	U
45	1	3313	U
45	1	3314	A
45	1	3316	A
45	1	3317	U
45	1	3319	U
45	1	3320	A
45	1	3328	G
45	1	3334	U
45	1	3335	A
45	1	3341	U
45	1	3342	A
45	1	3345	G
45	1	3350	C
45	1	3351	U
45	1	3352	U
45	1	3353	G
45	1	3355	U
45	1	3356	G
45	1	3359	A
45	1	3363	U
45	1	3369	G
45	1	3375	A
45	1	3378	C
45	1	3381	U
45	1	3382	U
45	1	3383	G
45	1	3386	G
45	1	3389	U
45	1	3396	U
46	2	8	C
46	2	23	U
46	2	25	G
46	2	34	U
46	2	35	C
46	2	51	G
46	2	53	A

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Mol	Chain	Res	Type
46	2	54	A
46	2	59	A
46	2	62	C
46	2	63	G
46	2	75	G
46	2	76	C
46	2	80	A
46	2	82	U
46	2	83	C
46	2	84	C
46	2	85	G
46	2	86	U
46	2	87	G
46	2	90	U
46	2	95	G
46	2	104	A
46	2	106	C
46	2	111	A
46	2	112	U
46	2	113	U
46	2	124	G
46	2	125	U
46	2	126	A
46	2	127	U
46	2	128	U
46	2	129	C
46	2	138	A
46	2	144	G
46	2	150	G
46	2	151	C
46	2	152	G
46	2	155	A
46	2	157	U
46	2	158	U
47	3	13	A
47	3	18	C
47	3	22	A
47	3	23	A
47	3	33	U
47	3	53	U
47	3	56	A
47	3	65	G

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Mol	Chain	Res	Type
47	3	66	A
47	3	76	A
47	3	79	A
47	3	81	U
47	3	82	G
47	3	83	U
47	3	86	U
47	3	87	G
47	3	88	G
47	3	89	G
47	3	90	U
47	3	92	A
47	3	93	C
47	3	95	A
47	3	96	U
47	3	98	C
47	3	100	C
47	3	102	A
47	3	104	A
47	3	112	G
47	3	121	U

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	1	40	A
45	1	90	C
45	1	96	G
45	1	97	U
45	1	160	G
45	1	169	U
45	1	239	G
45	1	649	A
45	1	720	A
45	1	761	A
45	1	784	A
45	1	849	C
45	1	990	U
45	1	1057	A
45	1	1064	A
45	1	1097	G
45	1	1102	A

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Mol	Chain	Res	Type
45	1	1103	A
45	1	1128	U
45	1	1159	A
45	1	1205	A
45	1	1221	A
45	1	1241	U
45	1	1302	A
45	1	1329	U
45	1	1355	A
45	1	1716	U
45	1	1816	A
45	1	2101	C
45	1	2197	C
45	1	2217	U
45	1	2254	U
45	1	2269	U
45	1	2277	C
45	1	2317	A
45	1	2593	A
45	1	2624	G
45	1	2625	C
45	1	2651	G
45	1	2652	U
45	1	2658	G
45	1	2728	G
45	1	2731	U
45	1	2753	G
45	1	2758	A
45	1	2761	G
45	1	2817	A
45	1	2822	U
45	1	2857	C
45	1	2866	U
45	1	2875	U
45	1	2946	A
45	1	3021	A
45	1	3078	U
45	1	3228	C
45	1	3269	U
45	1	3341	U
45	1	3350	C
46	2	123	G

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Mol	Chain	Res	Type
46	2	127	U
47	3	52	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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	GTP	b	701	-	33,34,34	0.90	0	50,54,54	1.68	9 (18%)
48	GTP	m	501	49	33,34,34	0.93	2 (6%)	50,54,54	1.65	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
48	GTP	b	701	-	-	3/22/38/38	0/3/3/3
48	GTP	m	501	49	-	3/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	m	501	GTP	O4'-C4'	-2.01	1.40	1.45
48	m	501	GTP	C5-N7	-2.00	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	b	701	GTP	C5-C4-N3	-5.41	119.78	128.39
48	b	701	GTP	C2-N3-C4	5.19	121.23	112.30
48	m	501	GTP	C5-C4-N3	-4.92	120.56	128.39
48	m	501	GTP	C2-N3-C4	4.49	120.04	112.30
48	b	701	GTP	N9-C4-N3	3.48	132.91	125.95
48	m	501	GTP	C2-N1-C6	-3.07	119.55	125.11
48	m	501	GTP	N9-C4-N3	2.90	131.75	125.95
48	b	701	GTP	C2-N1-C6	-2.90	119.85	125.11
48	m	501	GTP	N9-C8-N7	-2.78	108.25	113.40
48	m	501	GTP	C8-N7-C5	2.61	108.92	104.26
48	b	701	GTP	C5-C6-N1	2.61	119.89	113.25
48	b	701	GTP	C8-N7-C5	2.59	108.88	104.26
48	b	701	GTP	N9-C8-N7	-2.56	108.65	113.40
48	m	501	GTP	C5-C6-N1	2.52	119.67	113.25
48	b	701	GTP	O6-C6-C5	-2.32	120.41	126.53
48	m	501	GTP	O6-C6-C5	-2.22	120.68	126.53
48	b	701	GTP	C3'-C2'-C1'	2.14	105.51	101.46
48	m	501	GTP	O2B-PB-O3B	2.11	112.98	107.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

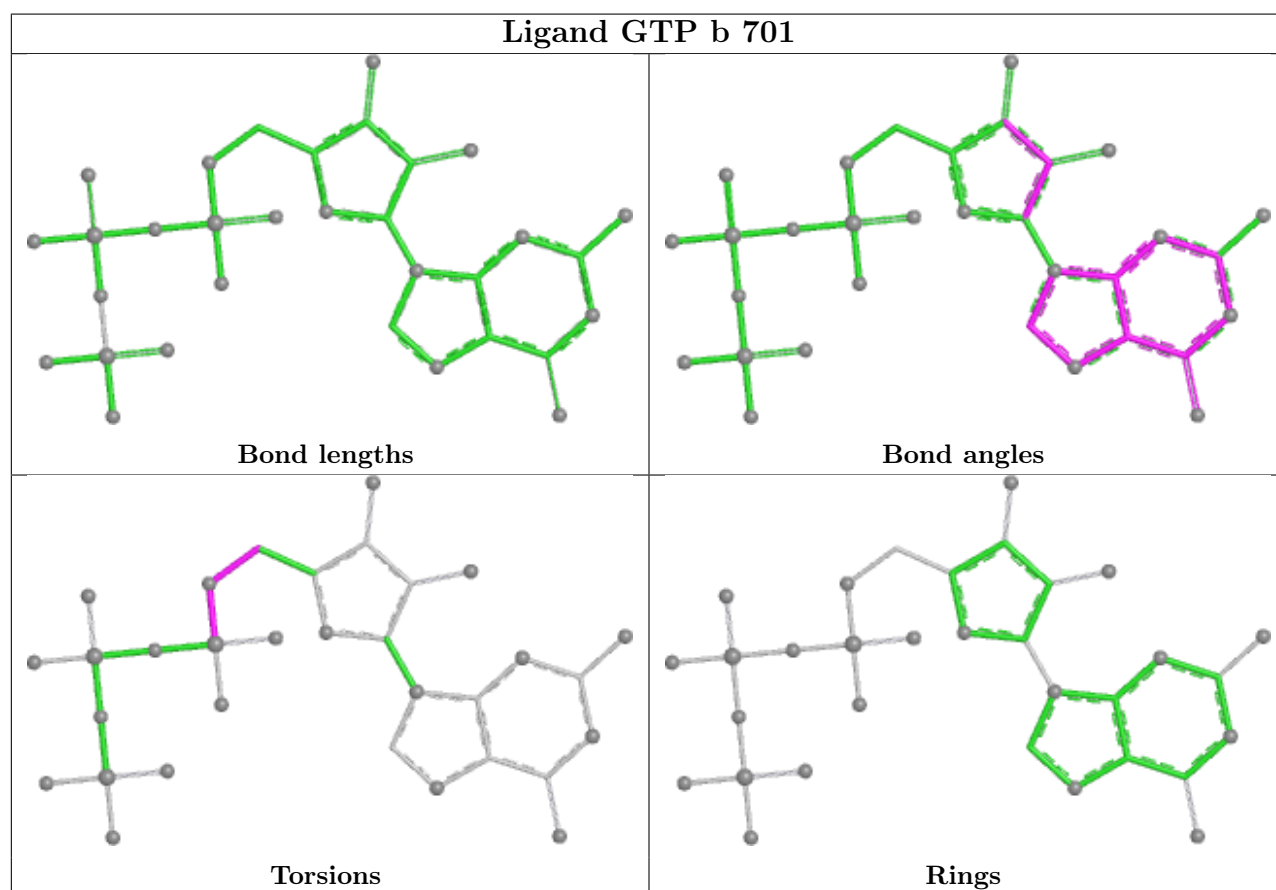
Mol	Chain	Res	Type	Atoms
48	b	701	GTP	C5'-O5'-PA-O3A
48	b	701	GTP	C5'-O5'-PA-O1A
48	m	501	GTP	PB-O3B-PG-O2G
48	b	701	GTP	C4'-C5'-O5'-PA
48	m	501	GTP	PB-O3A-PA-O1A
48	m	501	GTP	O4'-C4'-C5'-O5'

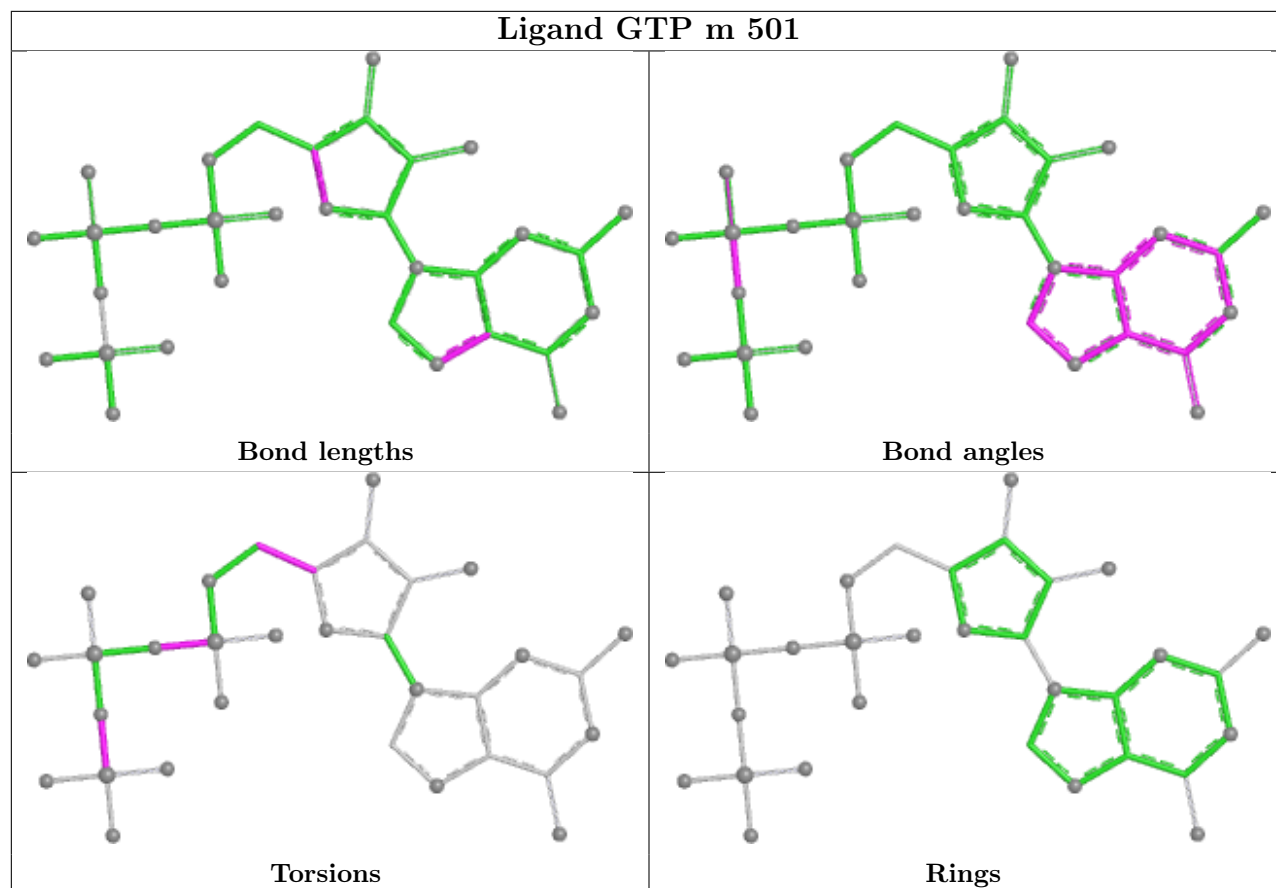
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	b	701	GTP	3	0
48	m	501	GTP	2	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.

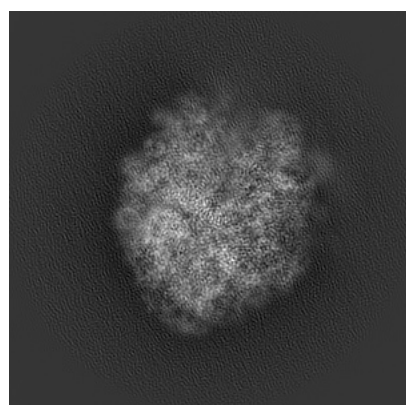
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30170. These allow visual inspection of the internal detail of the map and identification of artifacts.

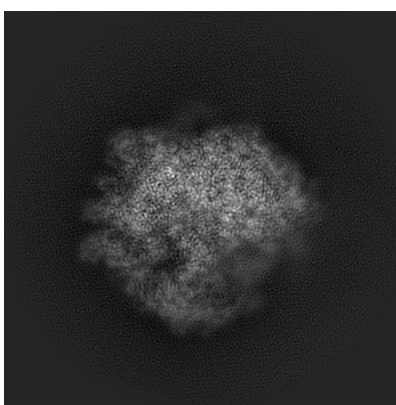
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

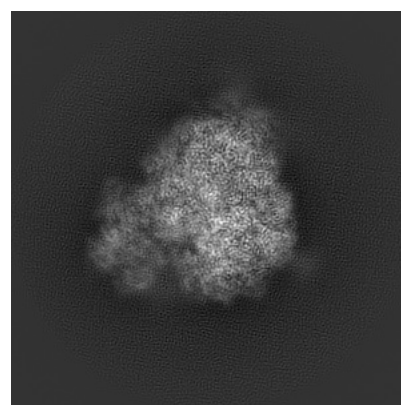
6.1.1 Primary map



X



Y

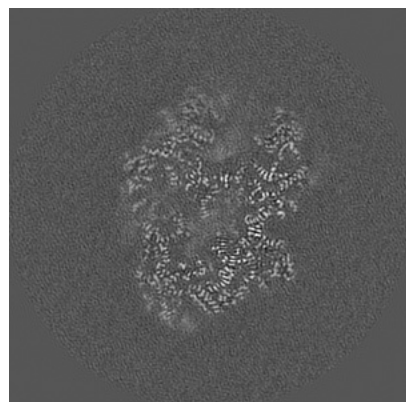


Z

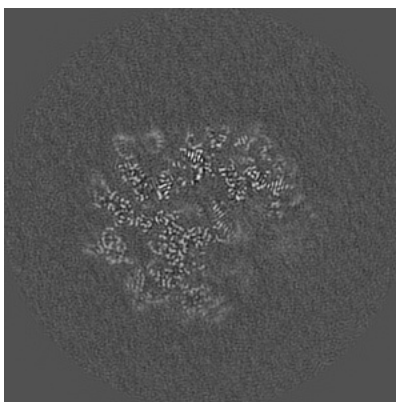
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

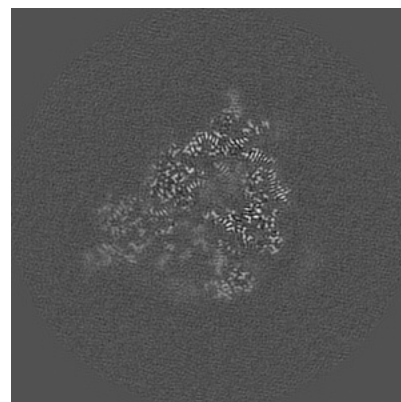
6.2.1 Primary map



X Index: 150



Y Index: 150

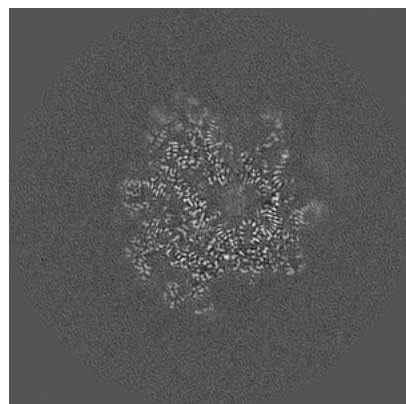


Z Index: 150

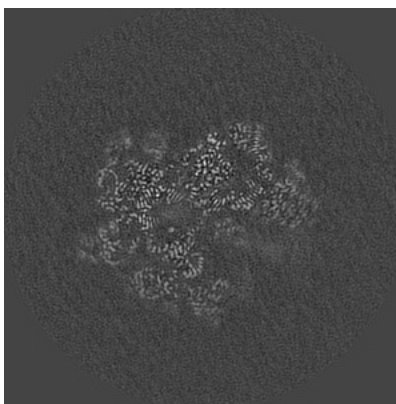
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

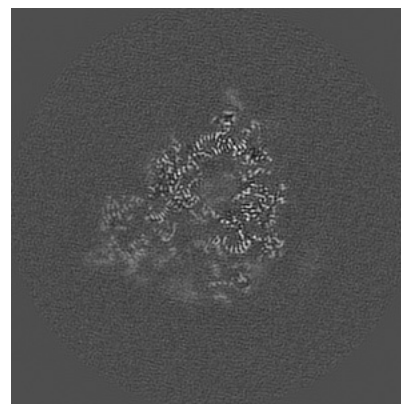
6.3.1 Primary map



X Index: 167



Y Index: 143

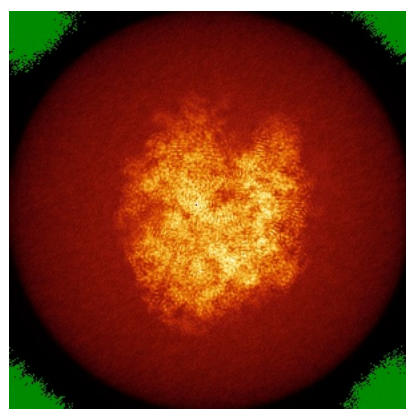


Z Index: 147

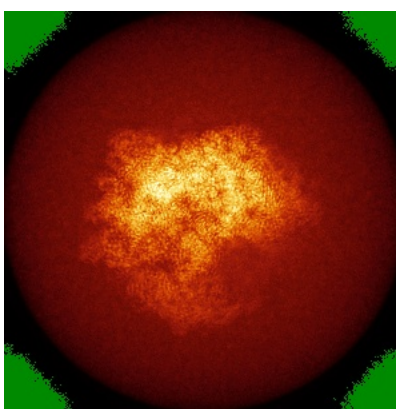
The images above show the largest variance slices of the map in three orthogonal directions.

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

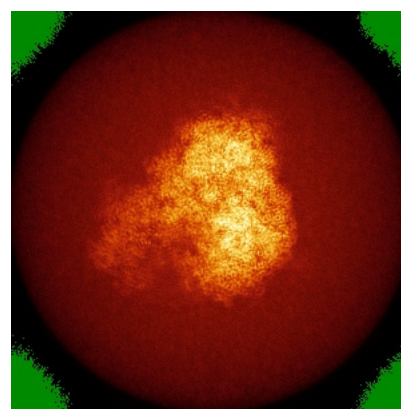
6.4.1 Primary map



X



Y

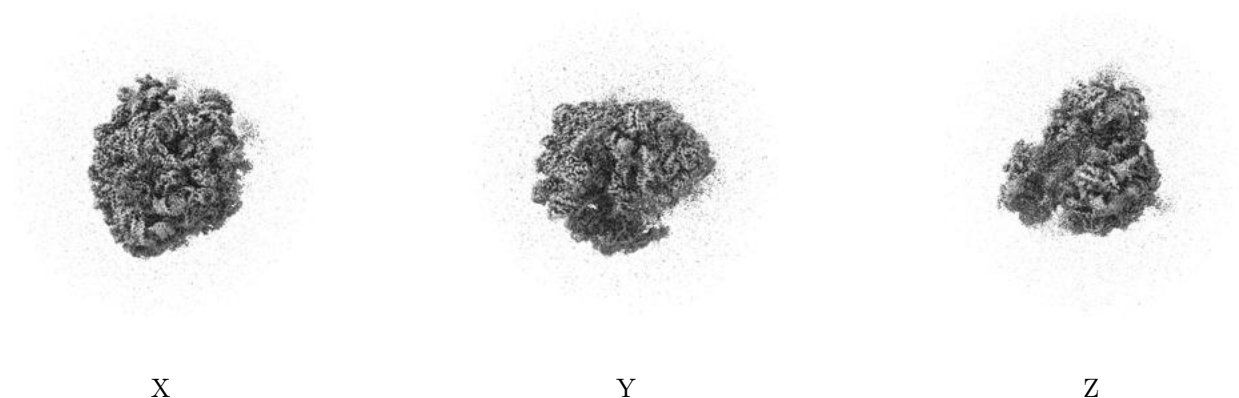


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

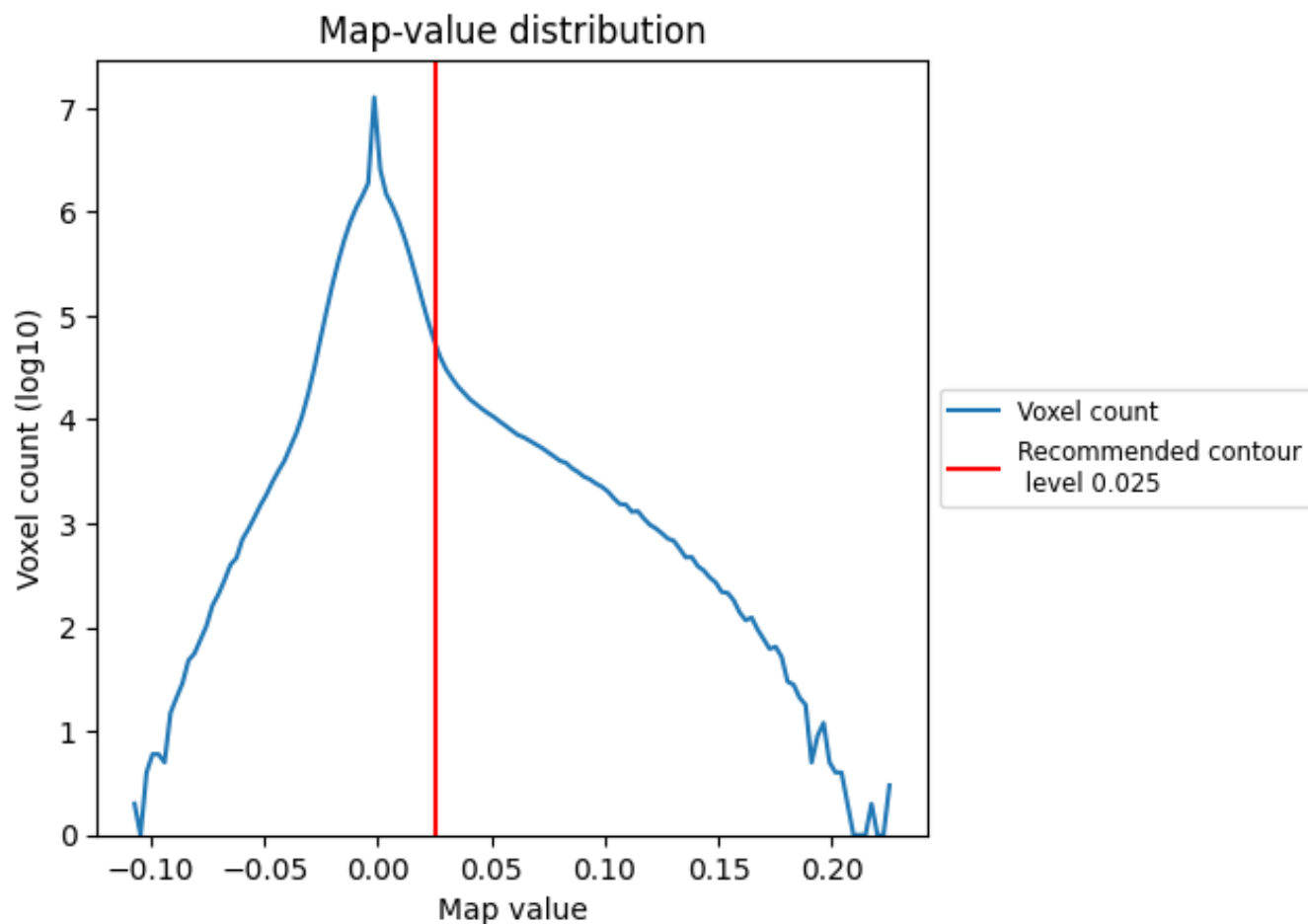
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

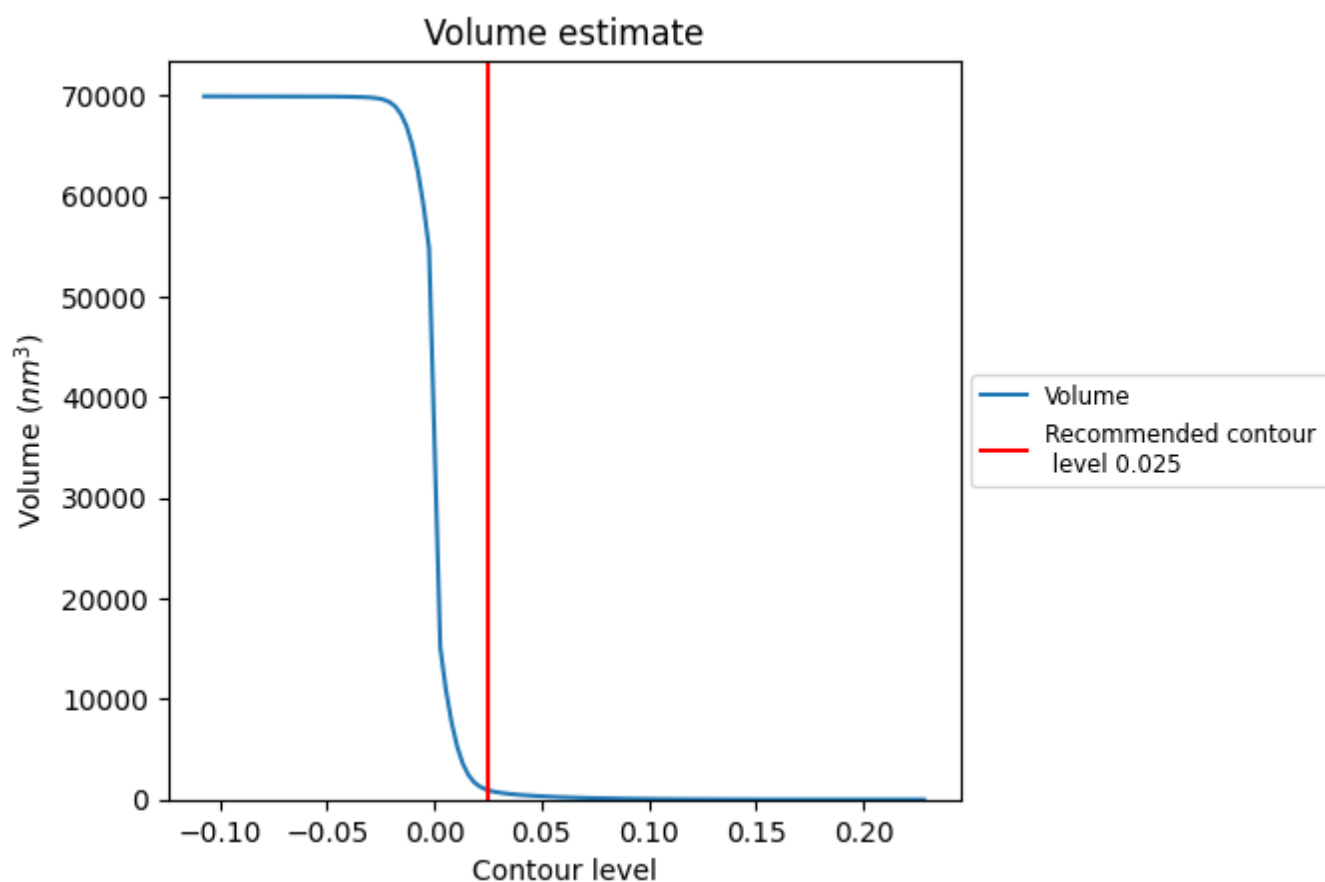
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

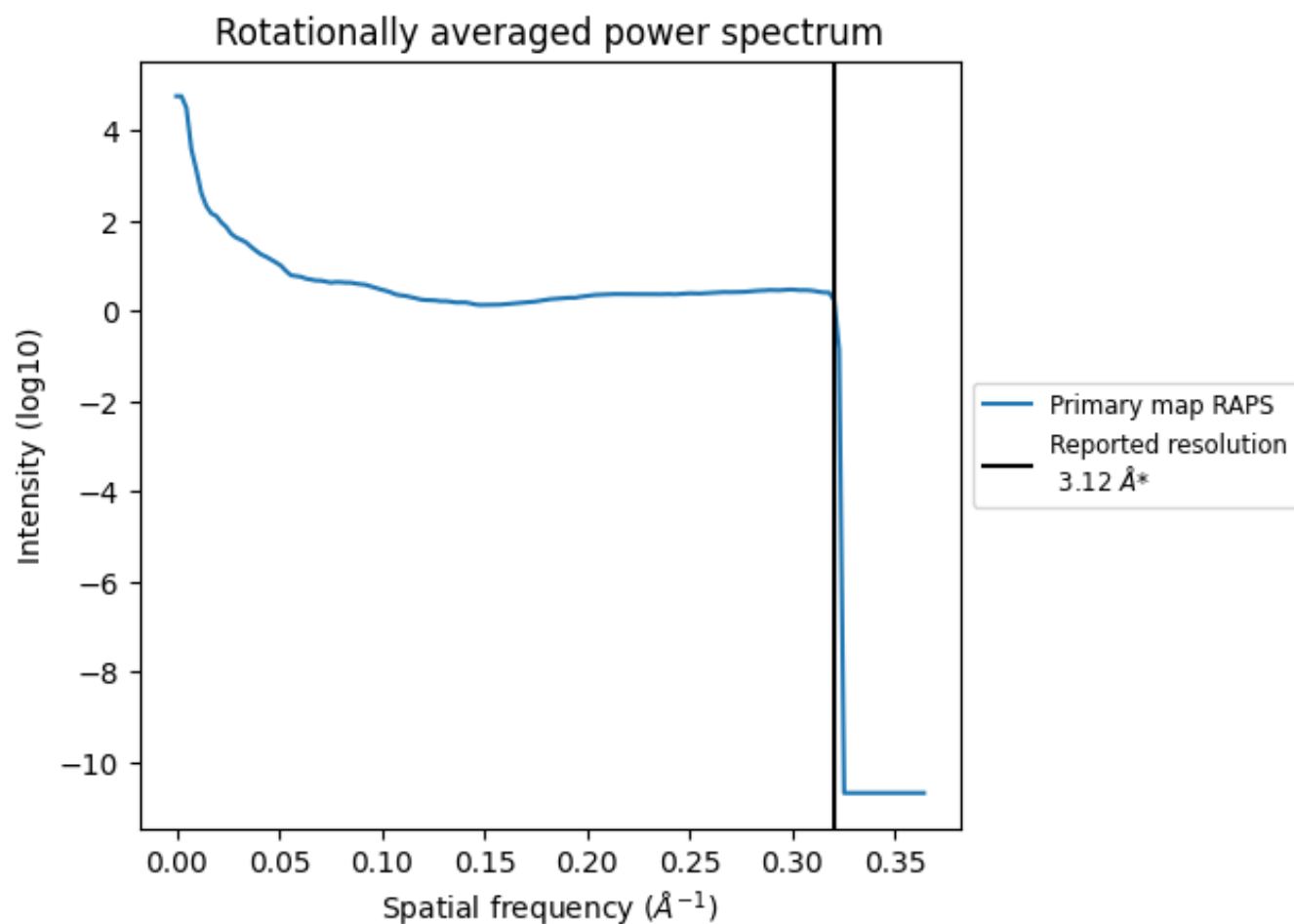
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm³; this corresponds to an approximate mass of 854 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 0.321 Å⁻¹

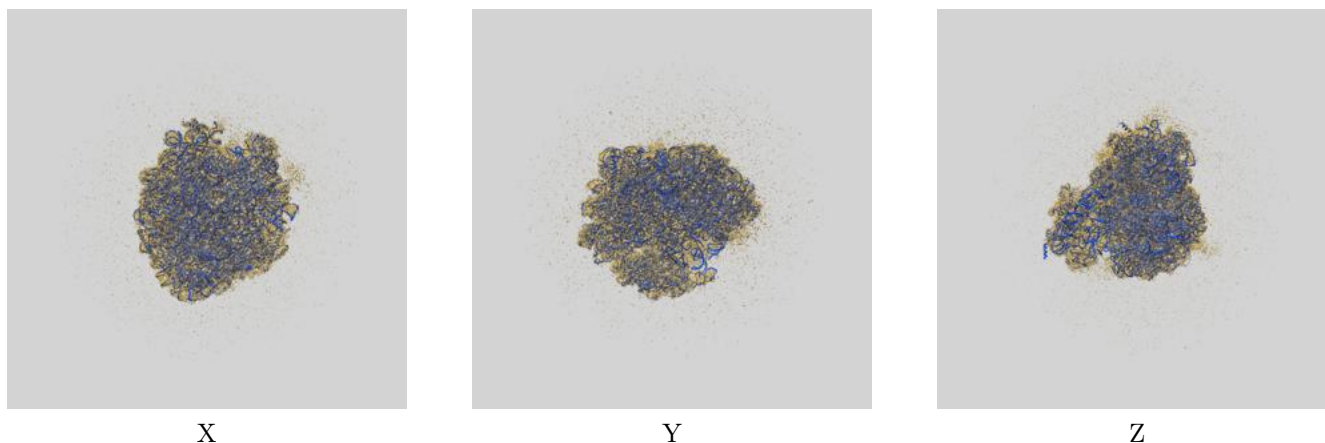
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

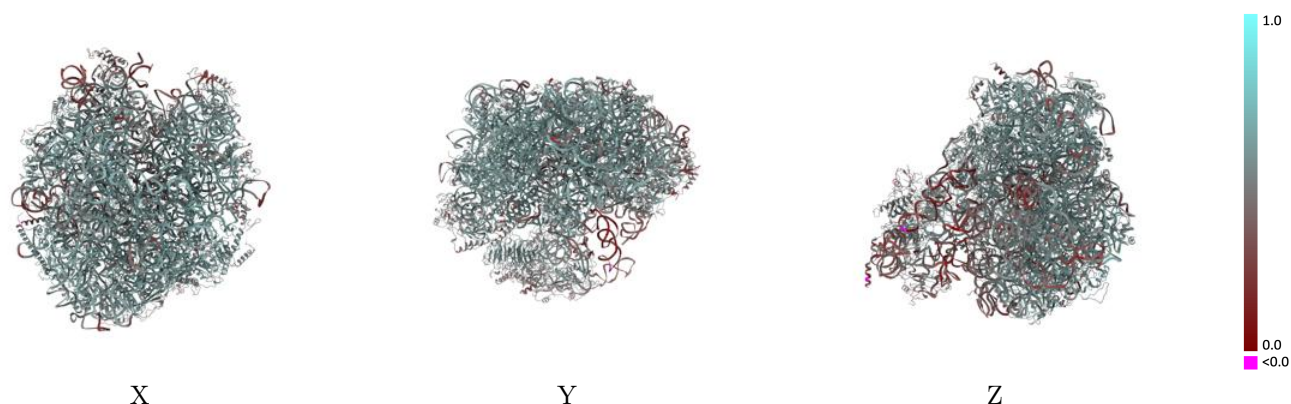
This section contains information regarding the fit between EMDB map EMD-30170 and PDB model 7BT6. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



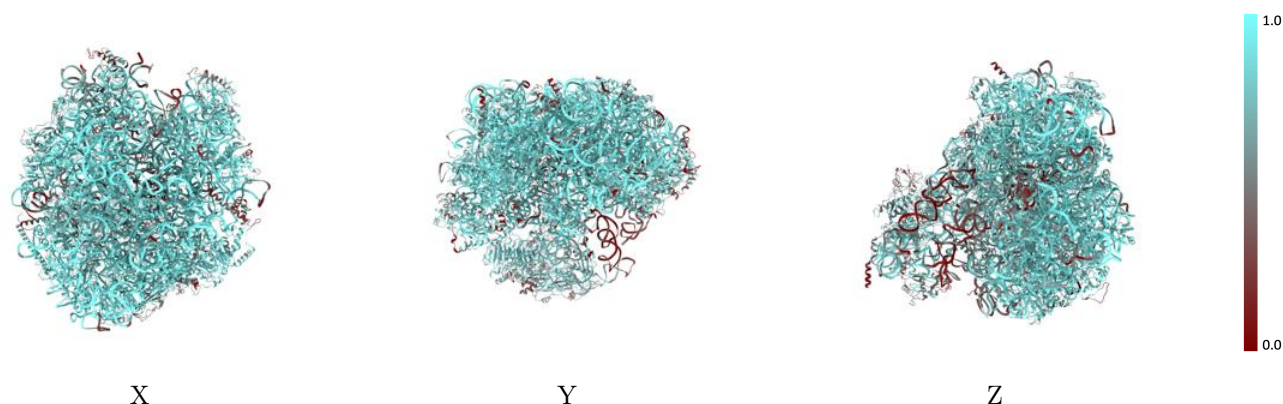
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



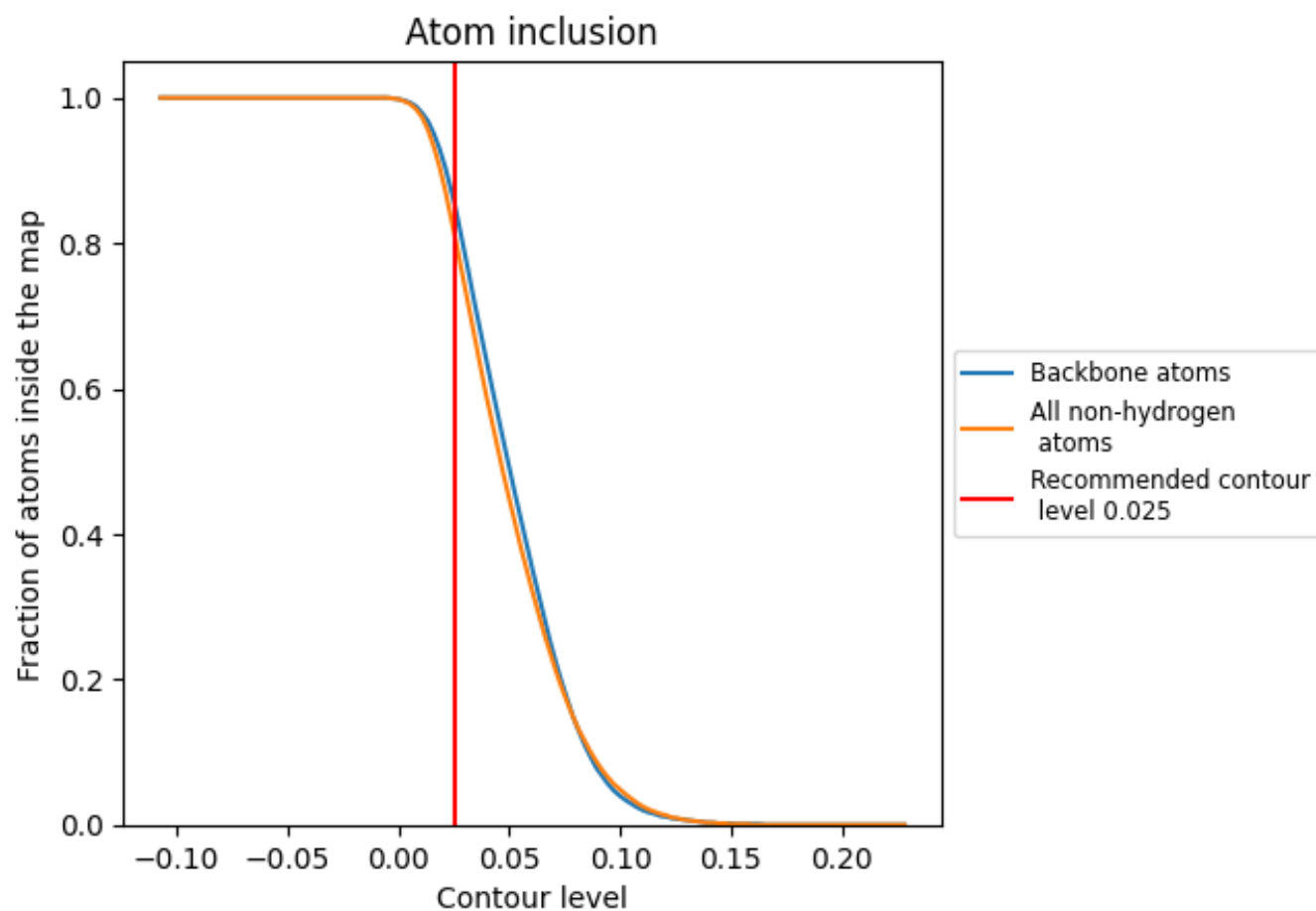
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.5330
1	 0.8470	 0.5240
2	 0.8080	 0.5180
3	 0.7550	 0.3910
A	 0.6920	 0.5150
B	 0.8870	 0.5870
C	 0.8570	 0.5820
D	 0.6580	 0.4750
E	 0.8520	 0.5720
F	 0.8960	 0.5880
G	 0.5730	 0.4510
H	 0.8810	 0.5850
J	 0.4790	 0.4120
L	 0.7850	 0.5430
M	 0.8890	 0.5840
N	 0.8360	 0.5600
O	 0.9270	 0.6060
P	 0.7990	 0.5690
Q	 0.8230	 0.5640
R	 0.8690	 0.5890
S	 0.8500	 0.5680
T	 0.6460	 0.5110
U	 0.7880	 0.5340
V	 0.9130	 0.6060
W	 0.6240	 0.4820
X	 0.8180	 0.5580
Y	 0.8800	 0.5870
Z	 0.7180	 0.5060
a	 0.7820	 0.5450
b	 0.7470	 0.5360
c	 0.7560	 0.5280
d	 0.8870	 0.5940
e	 0.8960	 0.6060
f	 0.9340	 0.6170
g	 0.8570	 0.5820



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Chain	Atom inclusion	Q-score
h	 0.7470	 0.5120
i	 0.6310	 0.4790
j	 0.8980	 0.5950
k	 0.7410	 0.5380
m	 0.8290	 0.5650
p	 0.8370	 0.5690
r	 0.8700	 0.5860
u	 0.7940	 0.5660
v	 0.7220	 0.5300
w	 0.6900	 0.5140
x	 0.7230	 0.5150
y	 0.8470	 0.5740
z	 0.5020	 0.5310