



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:46 AM UTC

PDB ID : 7NAC / pdb_00007nac
EMDB ID : EMD-24269
Title : State E2 nucleolar 60S ribosomal biogenesis intermediate - Composite model
Authors : Cruz, V.E.; Sekulski, K.; Peddada, N.; Erzberger, J.P.
Deposited on : 2021-06-21
Resolution : 3.04 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:

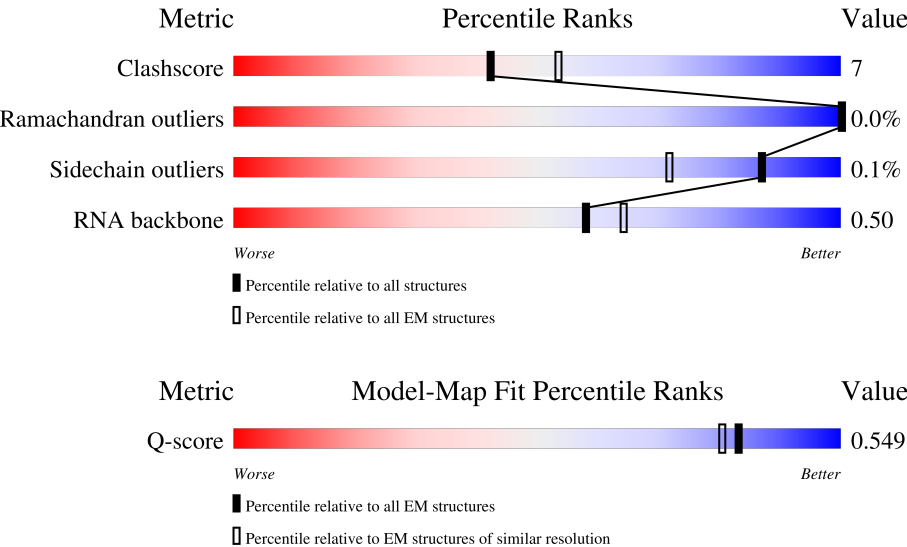
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.04 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	13952 (2.54 - 3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	13% 46% 26% 6% 22%
2	2	158	7% 65% 32% .
3	7	204	8% 54% 9% 37%

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Mol	Chain	Length	Quality of chain
4	A	291	
5	B	387	
6	C	362	
7	E	176	
8	F	244	
9	H	191	
10	J	427	
11	L	199	
12	M	138	
13	N	204	
14	O	199	
15	P	184	
16	Q	186	
17	S	172	
18	T	160	
19	W	236	
20	X	142	
21	Y	127	
22	b	647	
23	d	113	
24	e	130	
25	f	107	
26	h	120	
27	i	100	
28	j	88	

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Mol	Chain	Length	Quality of chain
29	l	181	
30	m	807	
31	q	618	
32	r	261	
33	s	520	
34	u	199	
35	v	231	
36	y	245	
37	z	106	
38	8	710	
39	I	663	
40	K	376	
41	V	137	
42	R	189	
43	G	256	
44	Z	136	
45	U	121	
46	c	105	
47	g	121	
48	k	78	
49	n	605	
50	p	460	
51	t	322	
52	6	87	
53	D	505	

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Mol	Chain	Length	Quality of chain
54	o	220	15% 49% 11% 40%
55	w	841	23% 64% 16% 20%
56	a	217	98% 72% 25% ..
57	5	235	44% 51% 9% 40%
58	x	606	77% 71% 18% • 11%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 158246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2661	Total	C	N	O	P	0	0
			56944	25427	10267	18590	2660		

- Molecule 2 is a RNA chain called 5.8S rRNA.

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

- Molecule 3 is a protein called 60S ribosomal subunit assembly/export protein LOC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	7	129	Total	C	N	O	0	0
			1048	650	204	194		

- Molecule 4 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			2174	1382	386	400	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	335	Total	C	N	O	S	0	0
			2661	1691	492	472	6		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	359	Total	C	N	O	S	0	0
			2731	1720	518	490	3		

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	164	Total	C	N	O	S	0	0
			1309	845	234	229	1		

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 10 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	145	Total	C	N	O	S	0	0
			1215	759	225	228	3		

- Molecule 11 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	121	Total	C	N	O	0	0
			991	623	208	160		

- Molecule 12 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 13 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	189	Total	C	N	O	S	0	0
			1621	1015	343	262	1		

- Molecule 14 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	52	Total	C	N	O	S	0	0
			401	244	82	74	1		

- Molecule 19 is a protein called Ribosome assembly factor MRT4.

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

- Molecule 20 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	137	Total	C	N	O	S	0	0
			1068	682	192	192	2		

- Molecule 21 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 22 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	502	Total	C	N	O	S	0	0
			4066	2581	710	754	21		

- Molecule 23 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 24 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 25 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 27 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	79	Total	C	N	O	S	0	0
			628	388	130	108	2		

- Molecule 28 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	73	Total	C	N	O	S	0	0
			580	353	126	96	5		

- Molecule 29 is a protein called 60S ribosome subunit biogenesis protein NIP7.

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

- Molecule 30 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	666	Total	C	N	O	S	0	0
			5377	3421	936	1005	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	551	ALA	GLU	conflict	UNP Q04660

- Molecule 31 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

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

- Molecule 32 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	176	Total	C	N	O	S	0	0
			1438	906	279	248	5		

- Molecule 33 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 34 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	140	Total	C	N	O	S	0	0
			1183	742	237	195	9		

- Molecule 35 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 37 is a protein called UPF0642 protein YBL028C.

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

- Molecule 38 is a protein called NOC2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	470	Total	C	N	O	S	0	0
			3567	2269	632	655	11		

- Molecule 39 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	I	533	Total	C	N	O	S	0	0
			4247	2693	726	808	20		

- Molecule 40 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	K	284	Total	C	N	O	S	0	0
			2274	1462	375	433	4		

- Molecule 41 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 42 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	134	Total	C	N	O		0	0
			1082	679	220	183			

- Molecule 43 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	198	Total	C	N	O	S	0	0
			1549	998	271	277	3		

- Molecule 44 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O		0	0
			808	524	132	152			

- Molecule 46 is a protein called 60S ribosomal protein L30.

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

- Molecule 47 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 48 is a protein called 60S ribosomal protein L38.

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

- Molecule 49 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	n	425	Total	C	N	O	S	0	0
			3470	2241	600	615	14		

- Molecule 50 is a protein called YTM1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	337	Total	C	N	O	S	0	0
			2628	1633	470	518	7		

- Molecule 51 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	285	Total	C	N	O	S	0	0
			2293	1453	425	412	3		

- Molecule 52 is a RNA chain called 5.8S ribosomal RNA gene and internal transcribed spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	87	Total	C	N	O	P	0	0
			1838	823	309	619	87		

- Molecule 53 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D	432	Total	C	N	O	S	0	0
			3451	2227	591	621	12		

- Molecule 54 is a protein called Ribosome biogenesis protein 15.

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

- Molecule 55 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	672	Total	C	N	O	S	0	0
			5451	3430	980	1013	28		

- Molecule 56 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	a	214	Total	C	N	O	S	0	0
			1695	1083	295	308	9		

- Molecule 57 is a protein called RRP17 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	141	Total	C	N	O	S	0	0
			1208	749	226	232	1		

- Molecule 58 is a protein called ATP-dependent rRNA helicase SPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	539	Total	C	N	O	S	0	0
			4340	2781	744	795	20		

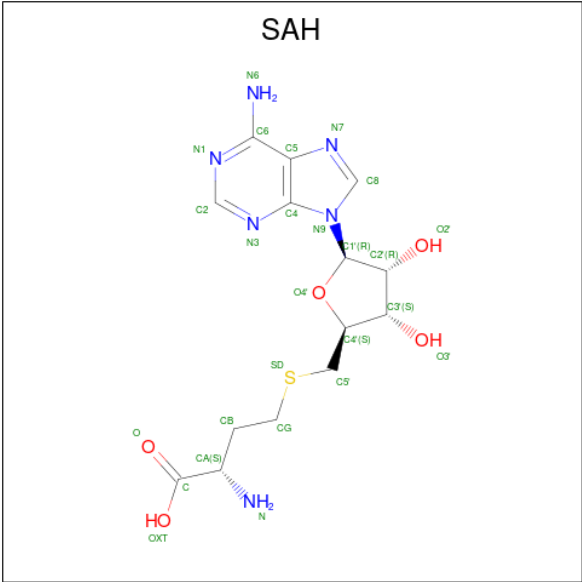
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	405	ALA	THR	conflict	UNP A7A237

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	j	1	Total	Zn	0
			1	1	
59	g	1	Total	Zn	0
			1	1	

- Molecule 60 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).

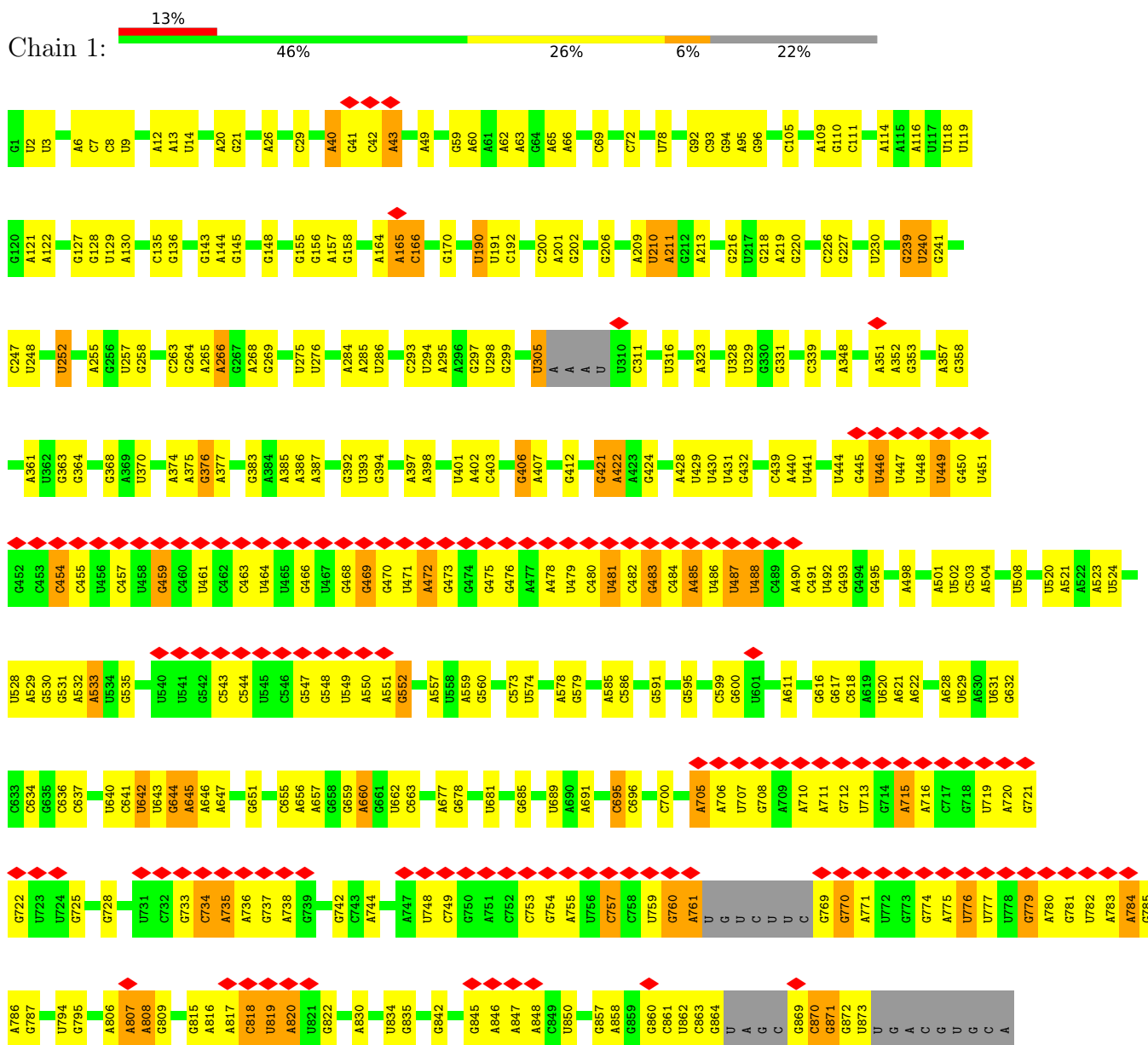


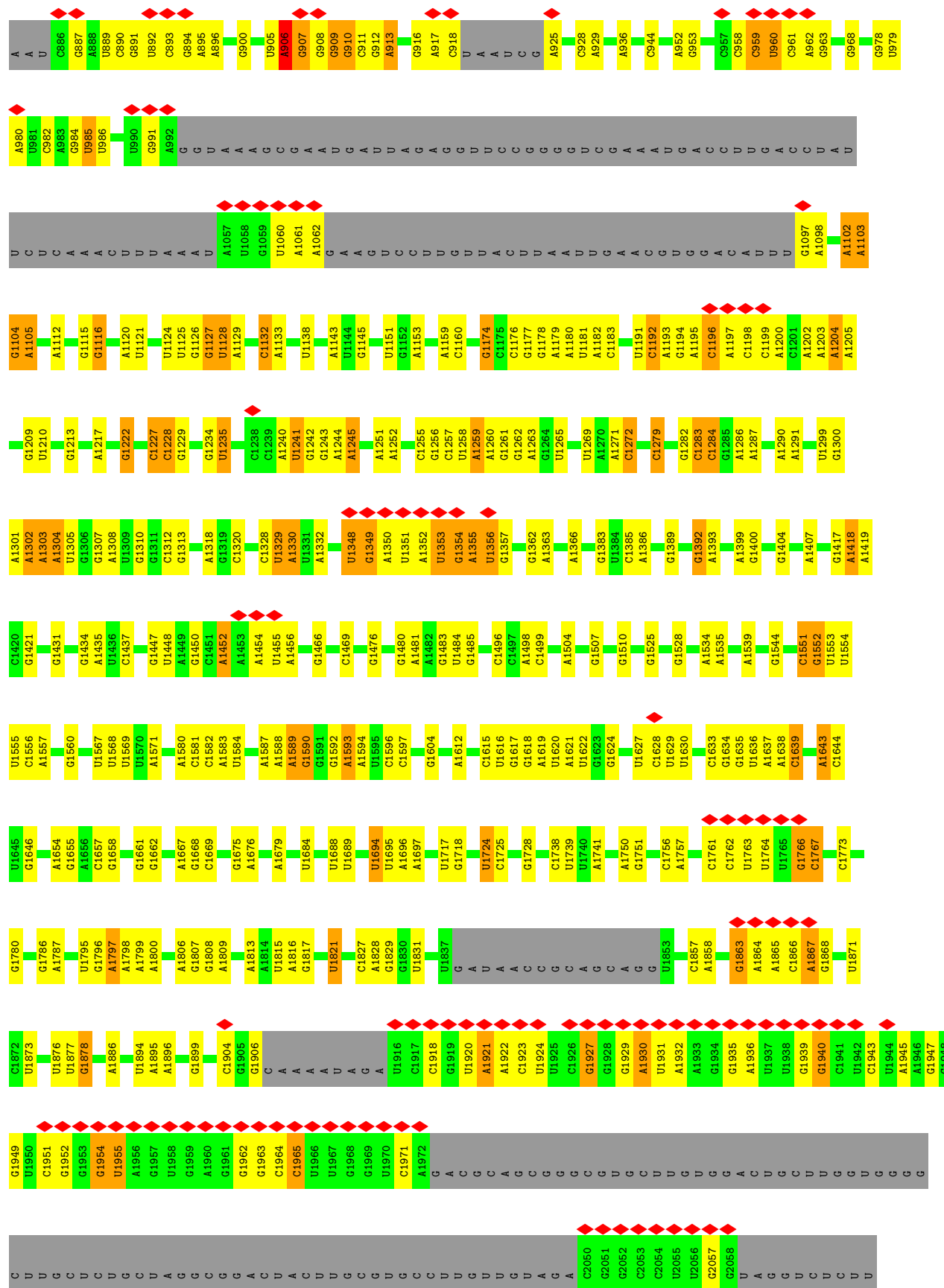
Mol	Chain	Residues	Atoms					AltConf
60	w	1	Total	C	N	O	S	0
			26	14	6	5	1	

3 Residue-property plots

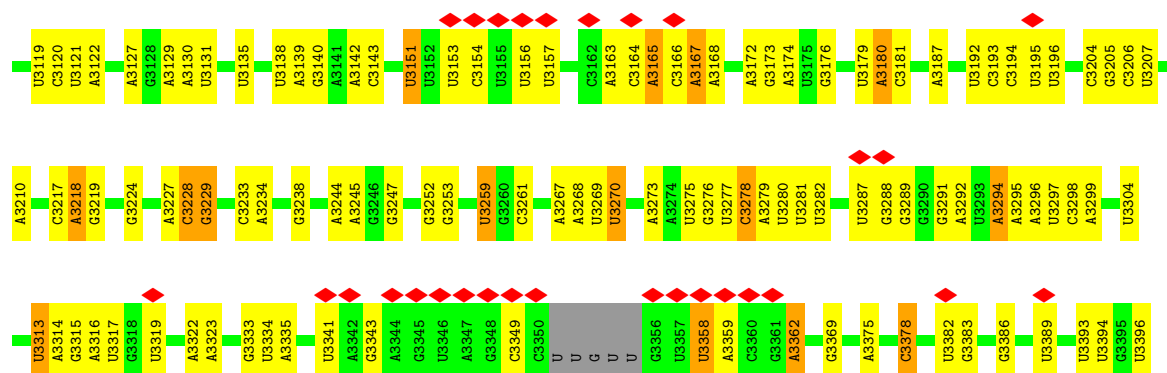
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

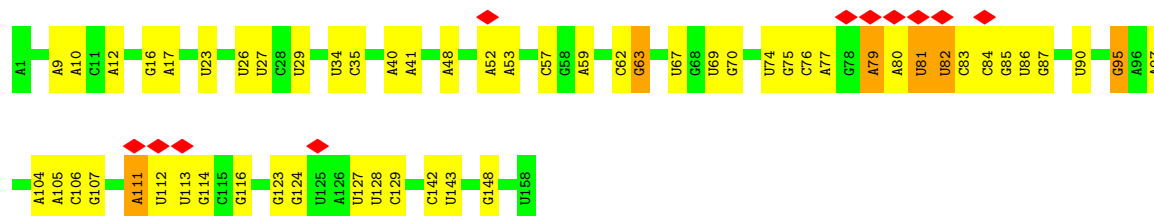




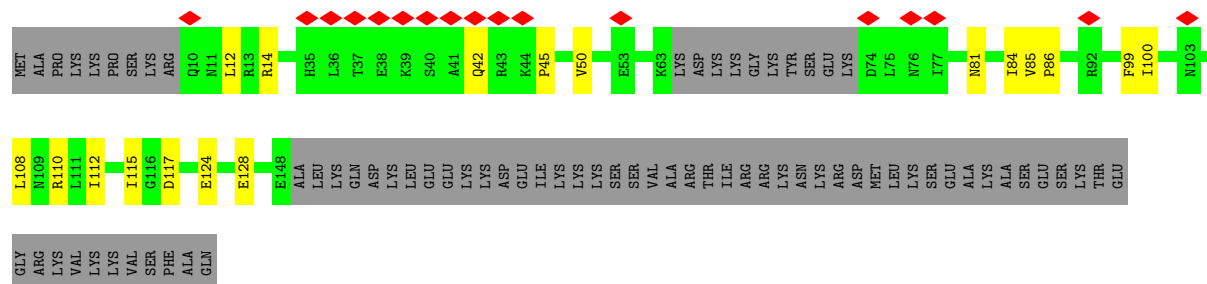




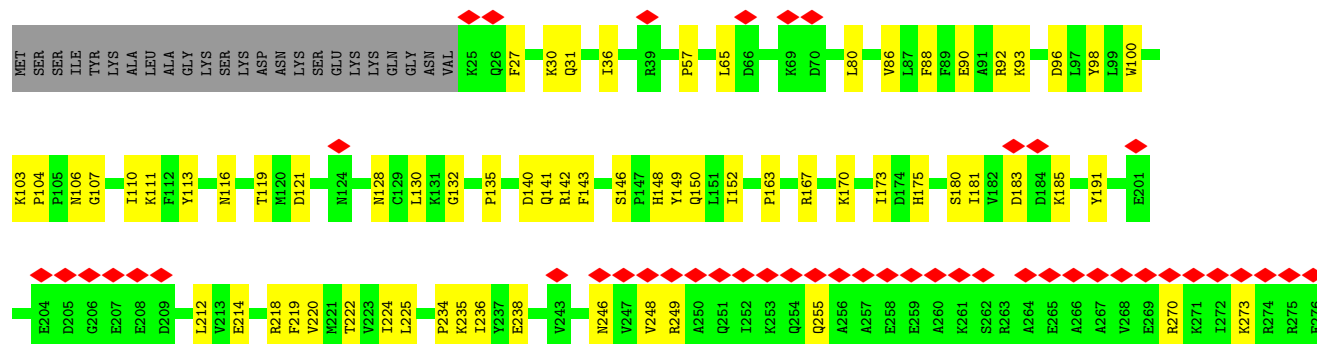
- Molecule 2: 5.8S rRNA

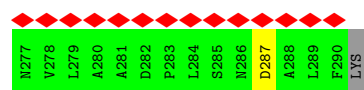


- Molecule 3: 60S ribosomal subunit assembly/export protein LOC1



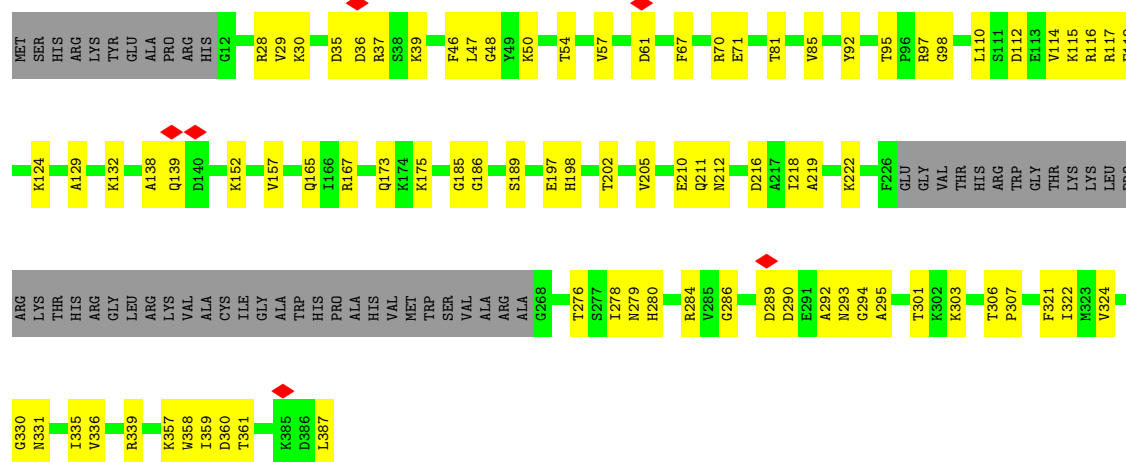
- Molecule 4: Ribosome biogenesis protein BRX1





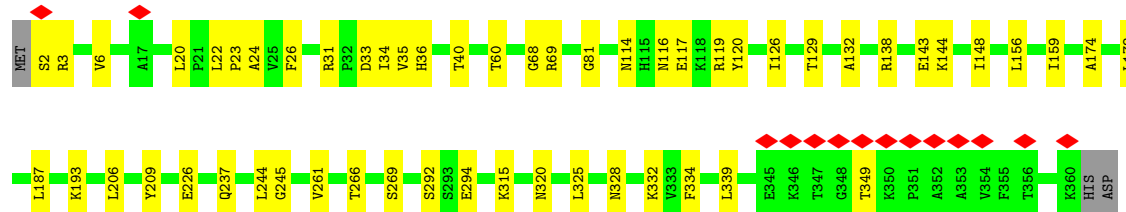
• Molecule 5: 60S ribosomal protein L3

Chain B: 65% 22% 13%



• Molecule 6: 60S ribosomal protein L4-A

Chain C: 84% 15%



• Molecule 7: 60S ribosomal protein L6-A

Chain E: 9% 81% 12% 7%

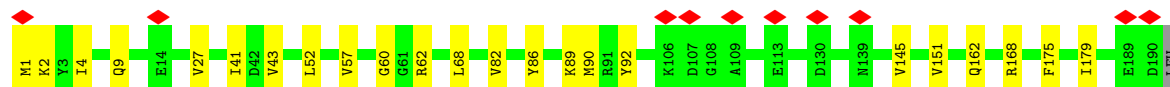
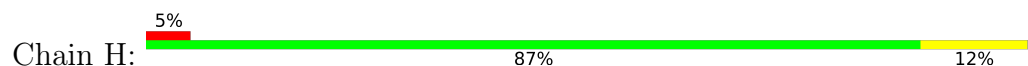


• Molecule 8: 60S ribosomal protein L7-A

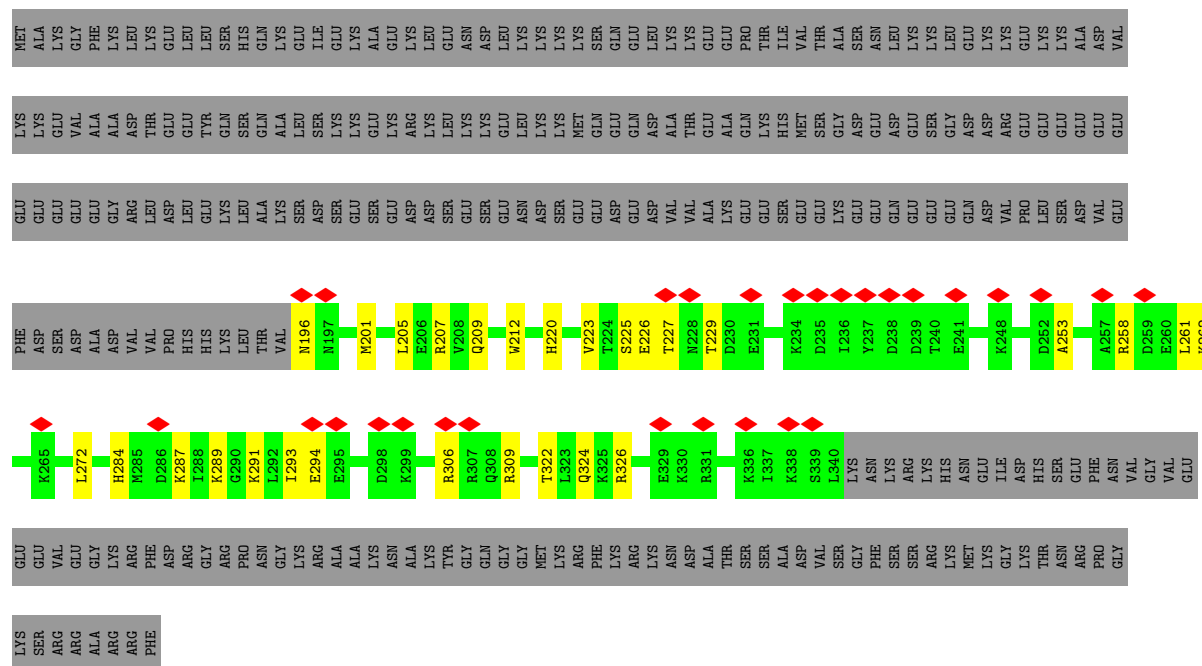
Chain F: 77% 14% 9%



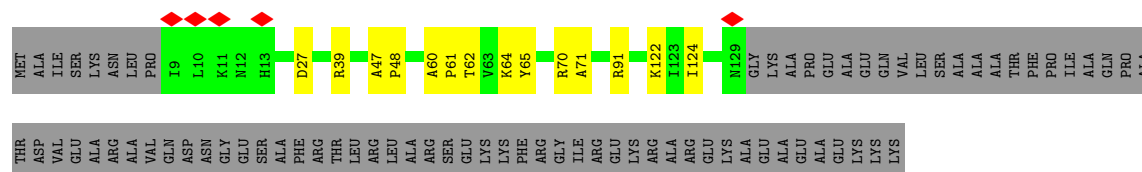
- Molecule 9: 60S ribosomal protein L9-A



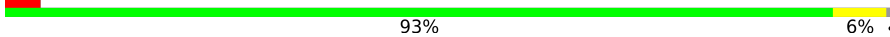
- Molecule 10: rRNA-processing protein EBP2



- Molecule 11: 60S ribosomal protein L13-A



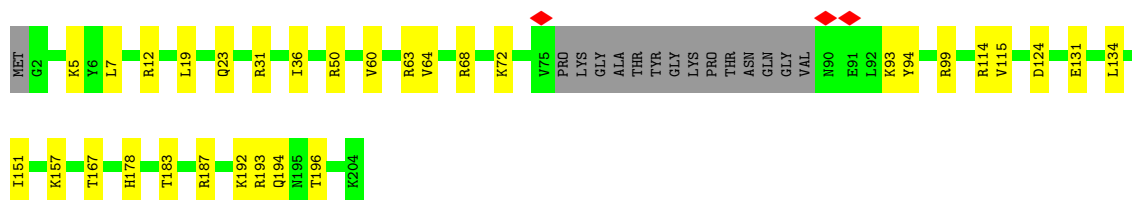
- Molecule 12: 60S ribosomal protein L14-A

Chain M:  93% 6%

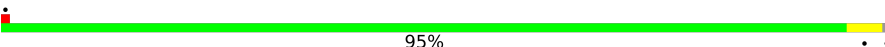


- Molecule 13: 60S ribosomal protein L15-A

Chain N:  77% 15% 7%



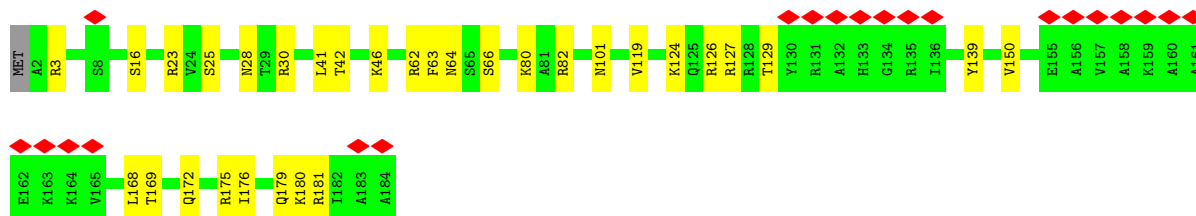
- Molecule 14: 60S ribosomal protein L16-A

Chain O:  95% ..



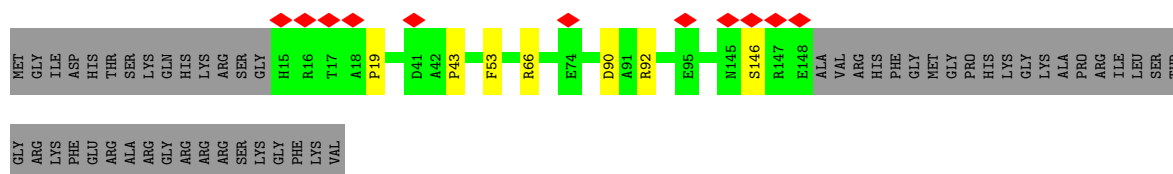
- Molecule 15: 60S ribosomal protein L17-A

Chain P:  11% 83% 17%



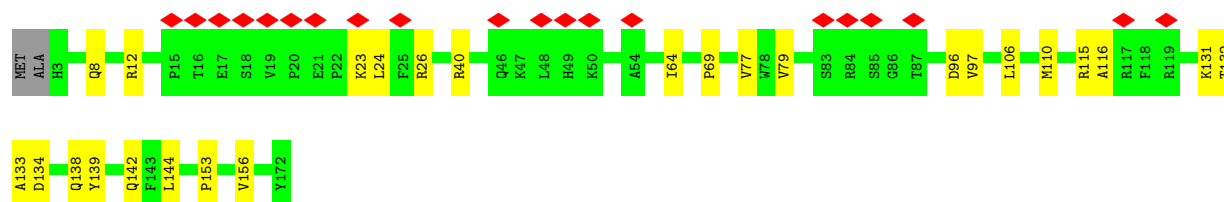
- Molecule 16: 60S ribosomal protein L18-A

Chain Q:  6% 68% 28%

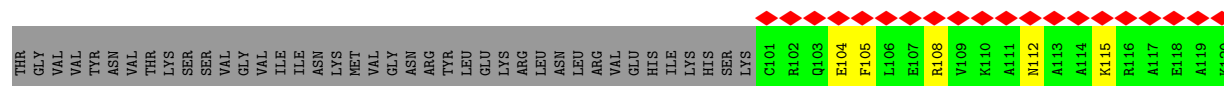
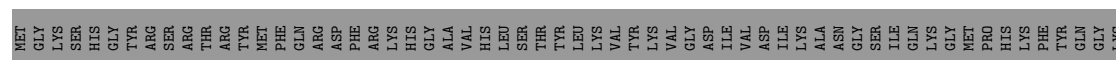


- Molecule 17: 60S ribosomal protein L20-A

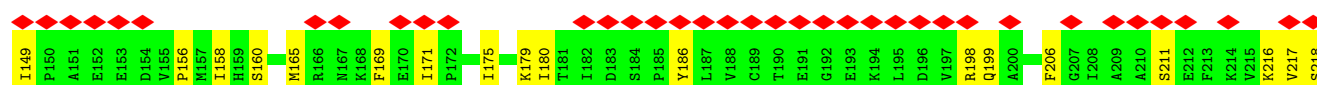
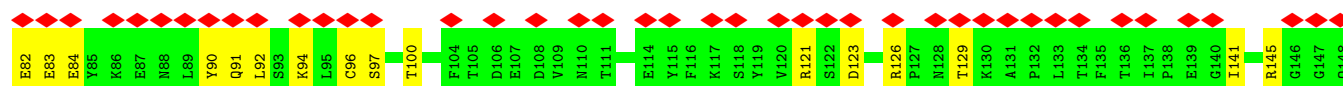
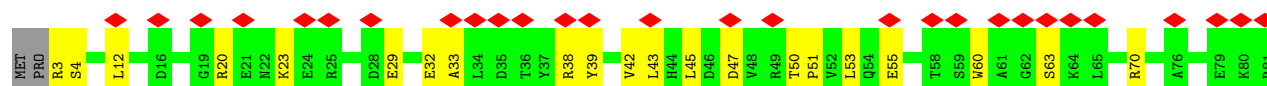
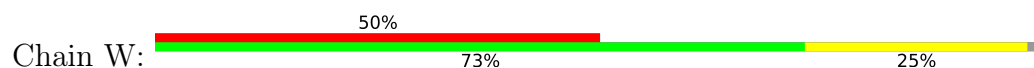
Chain S:  12% 84% 15%



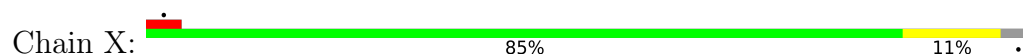
• Molecule 18: 60S ribosomal protein L21-A



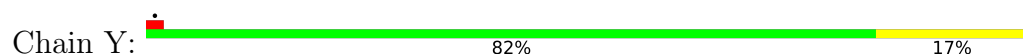
• Molecule 19: Ribosome assembly factor MRT4



• Molecule 20: 60S ribosomal protein L25

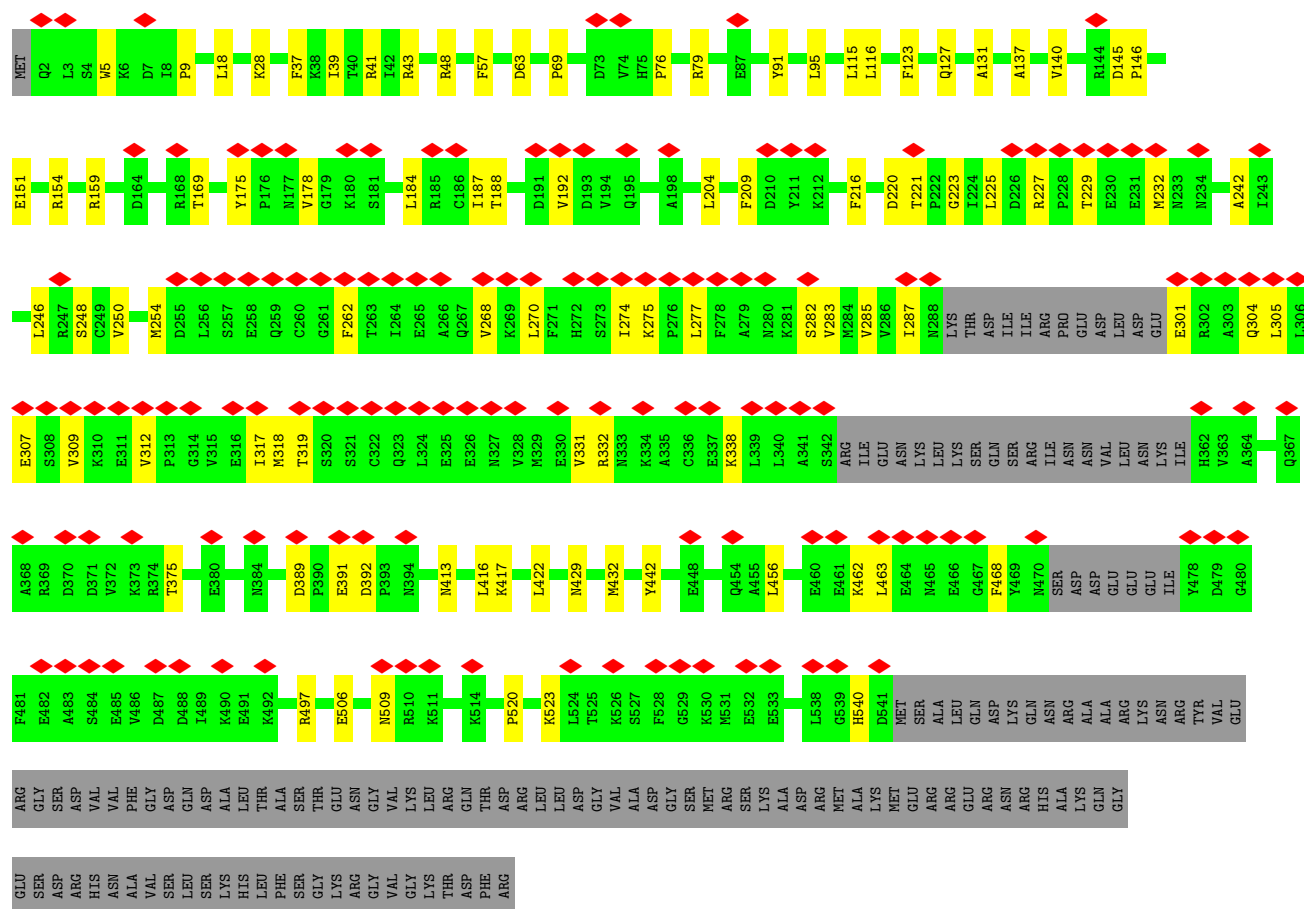


• Molecule 21: 60S ribosomal protein L26-A

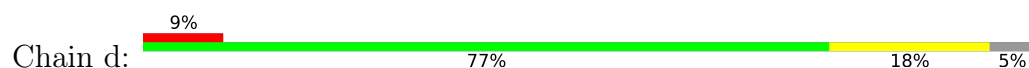




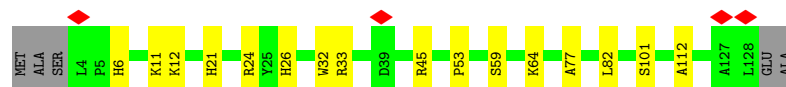
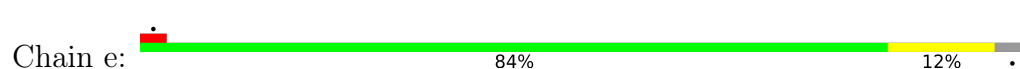
• Molecule 22: Nucleolar GTP-binding protein 1



• Molecule 23: 60S ribosomal protein L31-A



• Molecule 24: 60S ribosomal protein L32

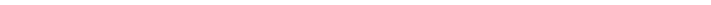


• Molecule 25: 60S ribosomal protein L33-A

MET
A2
Y16
R21
I49
Y53
R54
R65
V66
M67
V71
H75
V80
L89
P90
R99
L102
I107

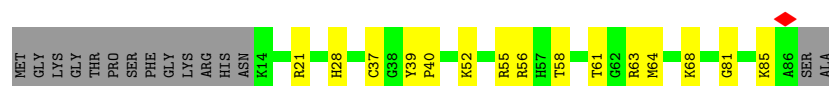
- Chain h: 86% 13%



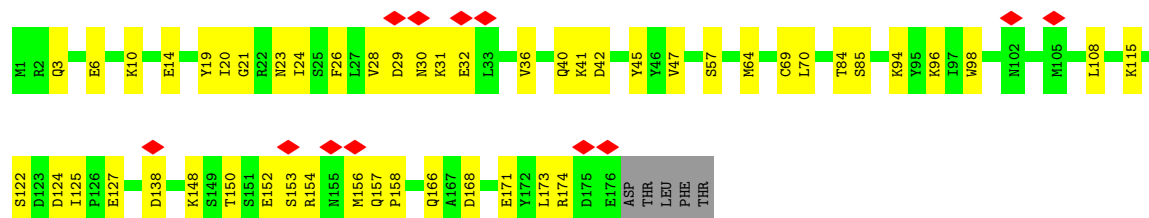
- Chain i:  7% 66% 13% 21%

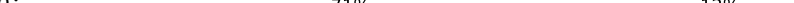


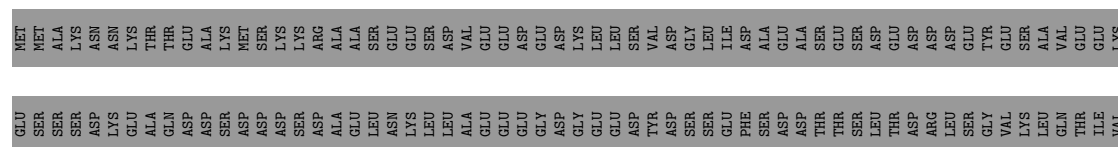
- Chain j:

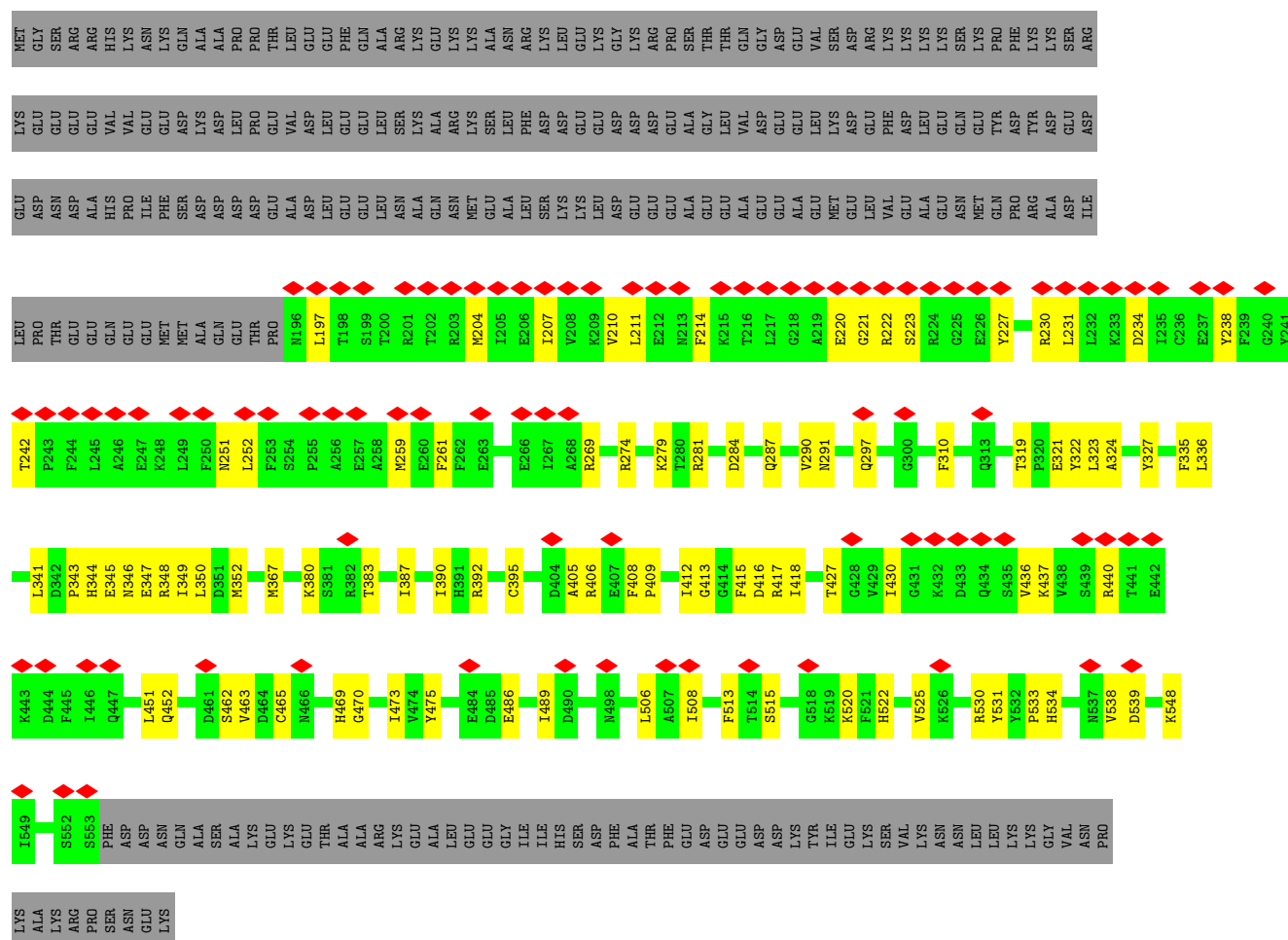


- Chain 1: 7% 70% 28%

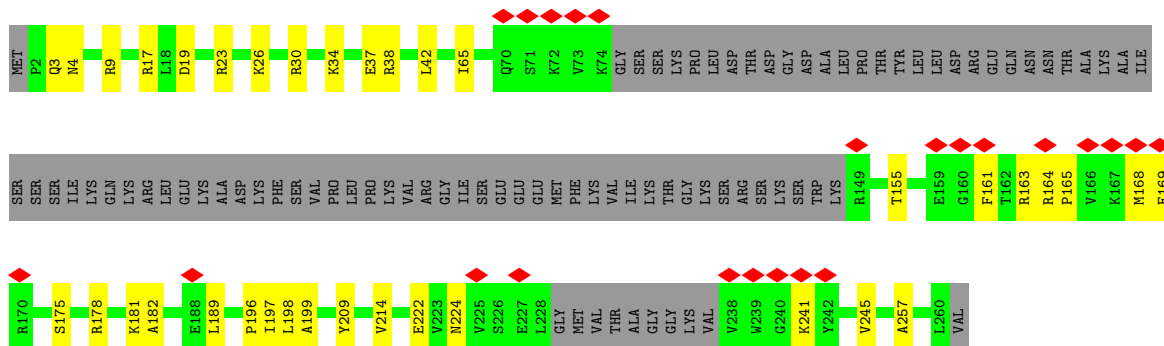


- Chain m: 

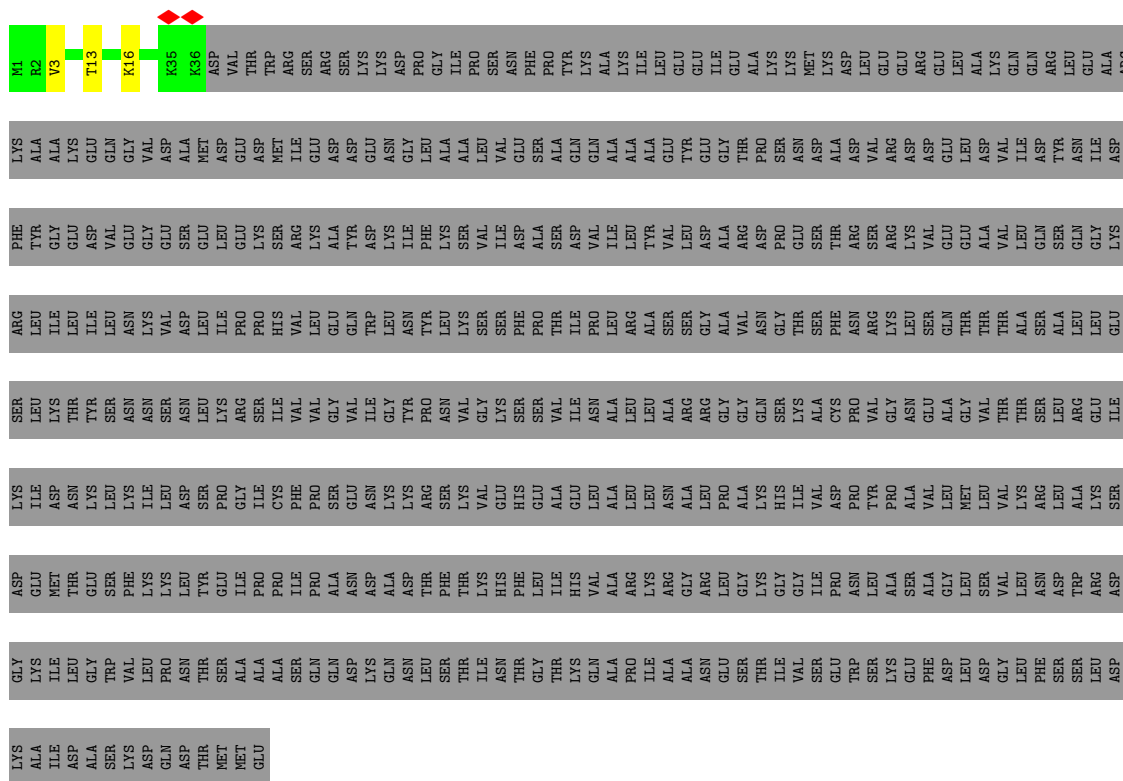




Chain r:

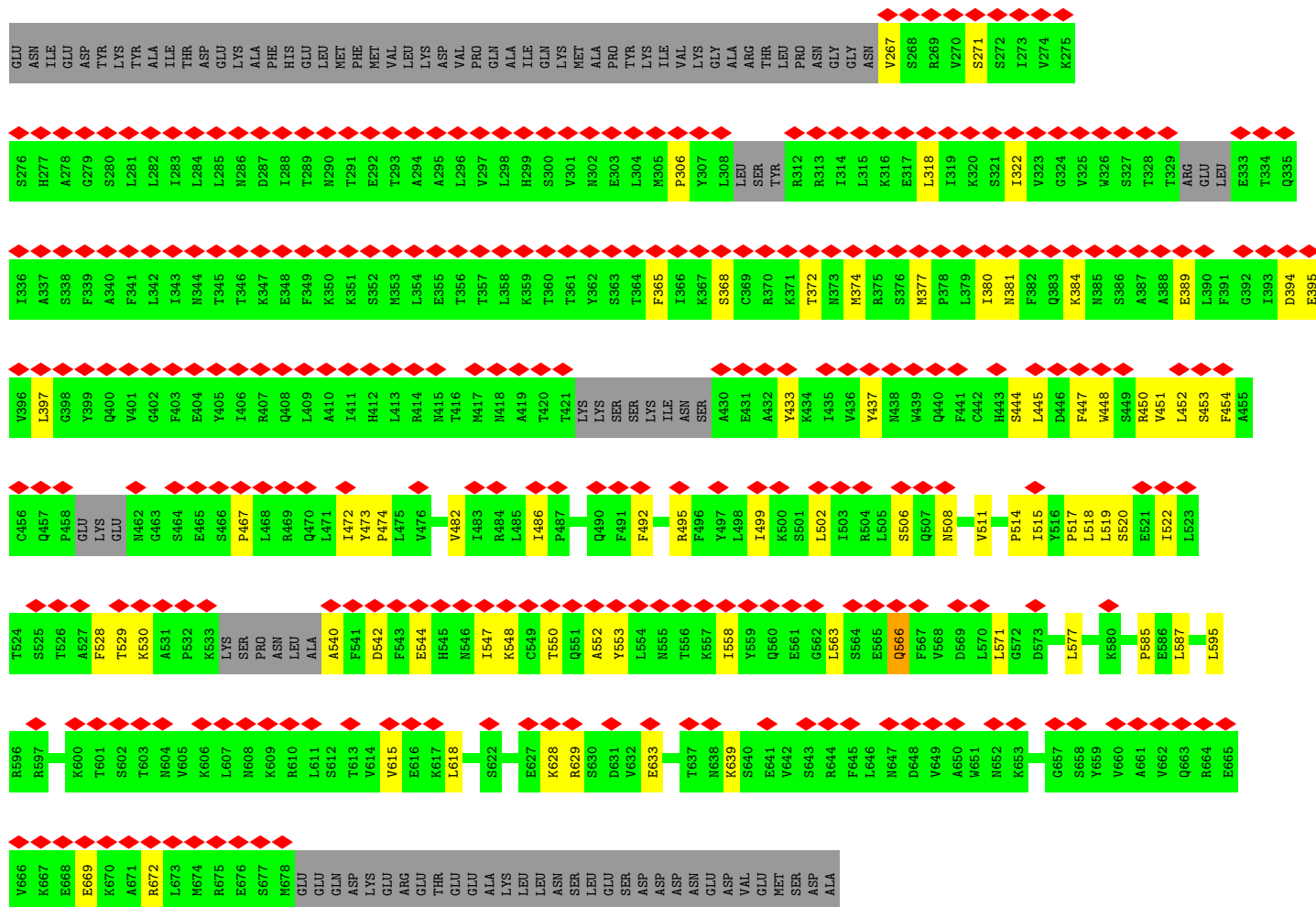


Chain s: 6% 93%

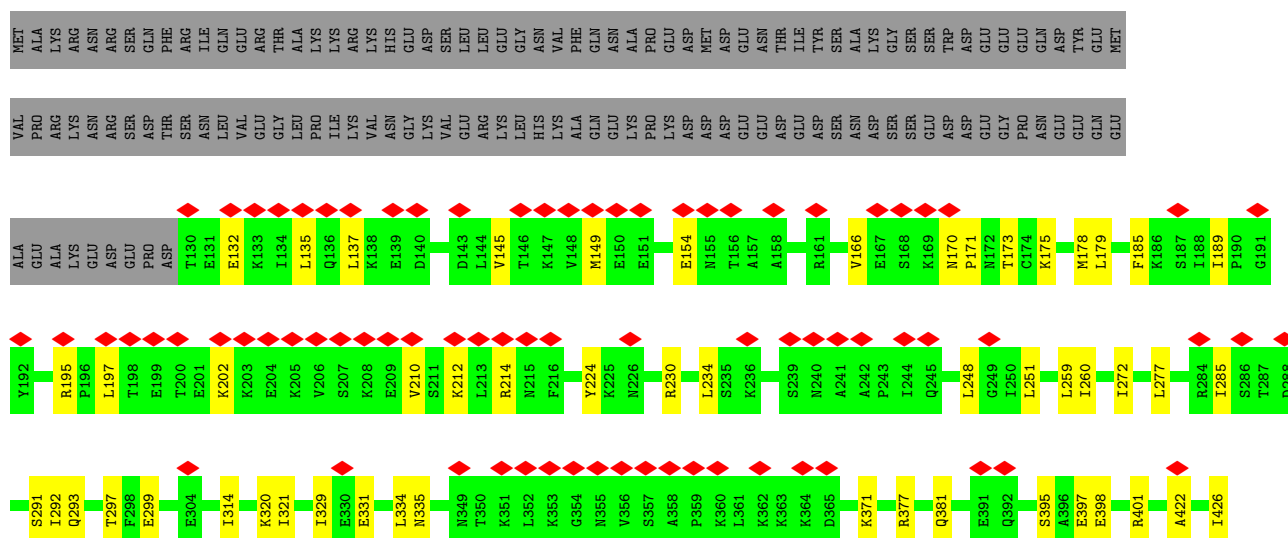


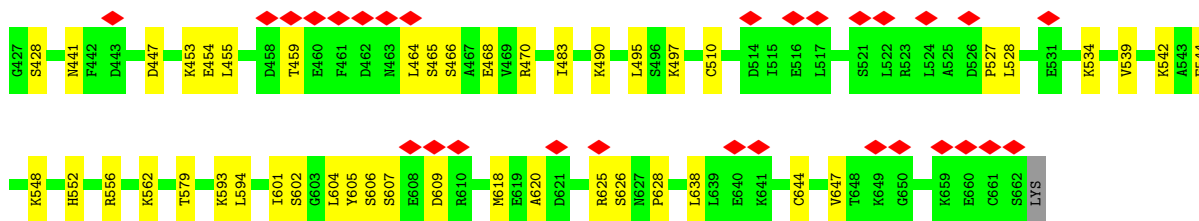
Chain u: 58% 13% 30%



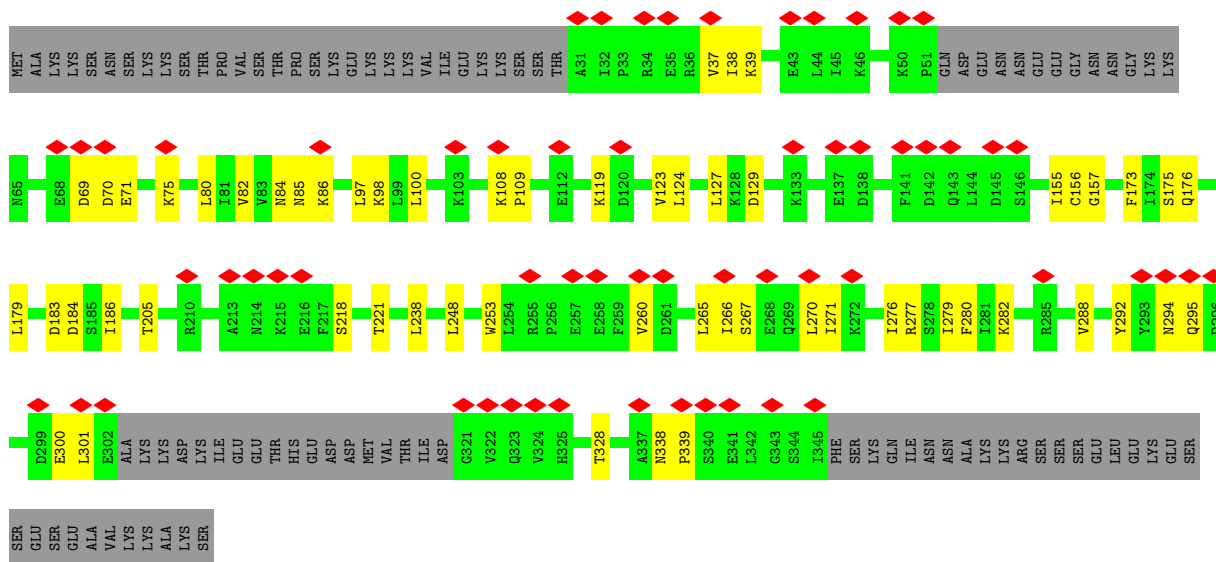


• Molecule 39: Nucleolar complex-associated protein 3

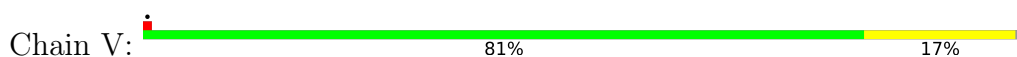




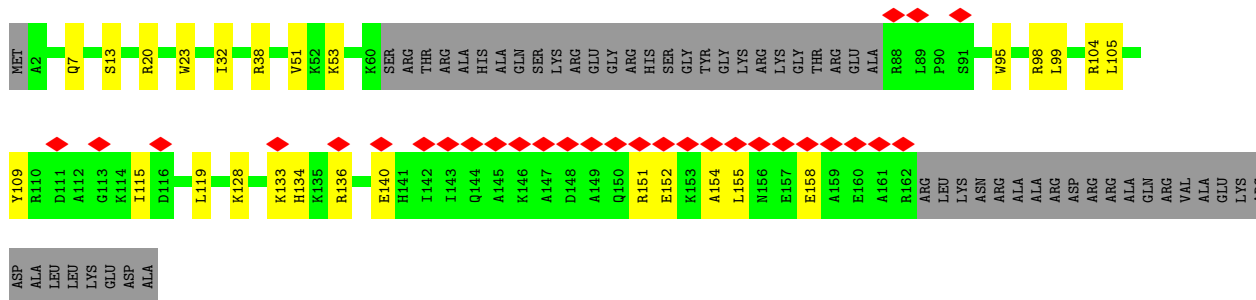
• Molecule 40: Proteasome-interacting protein CIC1



• Molecule 41: 60S ribosomal protein L23-A

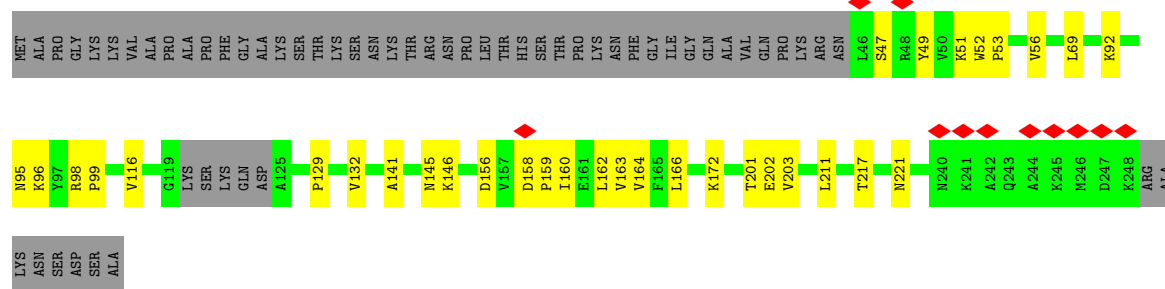


• Molecule 42: 60S ribosomal protein L19-A



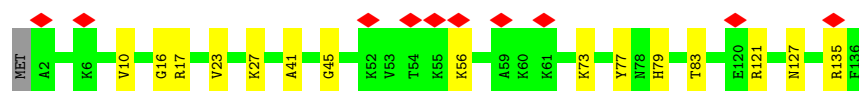
• Molecule 43: 60S ribosomal protein L8-A

Chain G: 



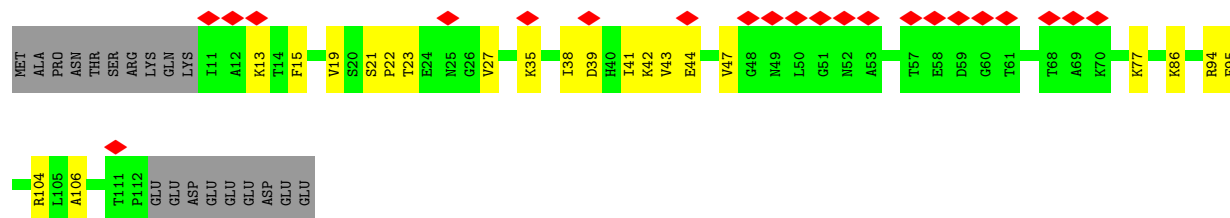
- Molecule 44: 60S ribosomal protein L27-A

Chain Z: 



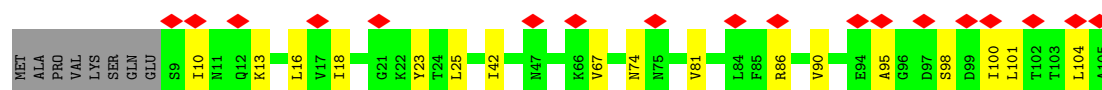
- Molecule 45: 60S ribosomal protein L22-A

Chain U: 



- Molecule 46: 60S ribosomal protein L30

Chain c: 



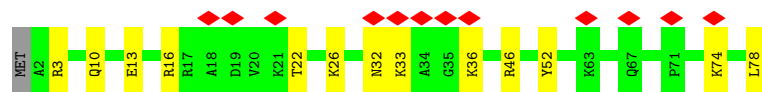
- Molecule 47: 60S ribosomal protein L34-A

Chain g: 

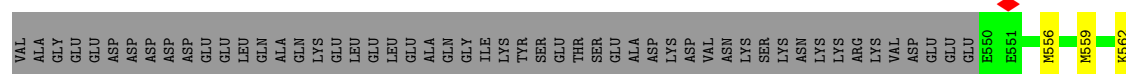
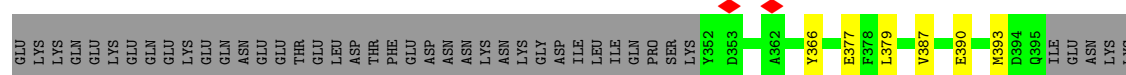
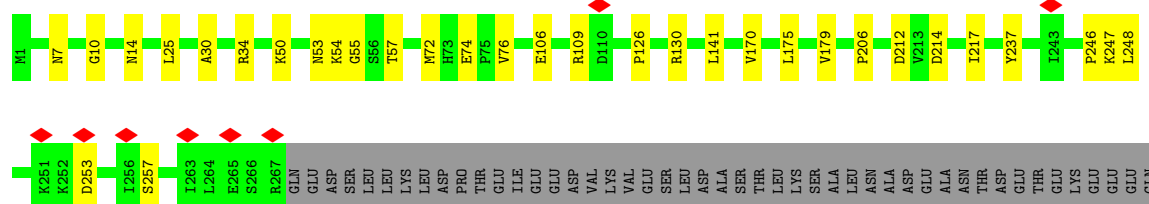


- Molecule 48: 60S ribosomal protein L38

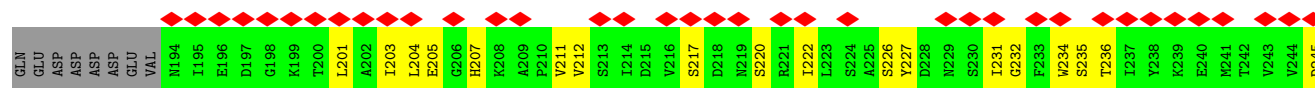
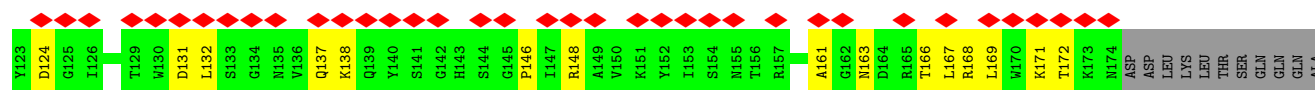
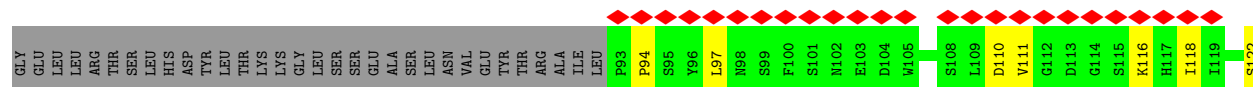
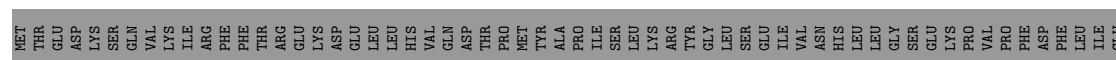
Chain k: 

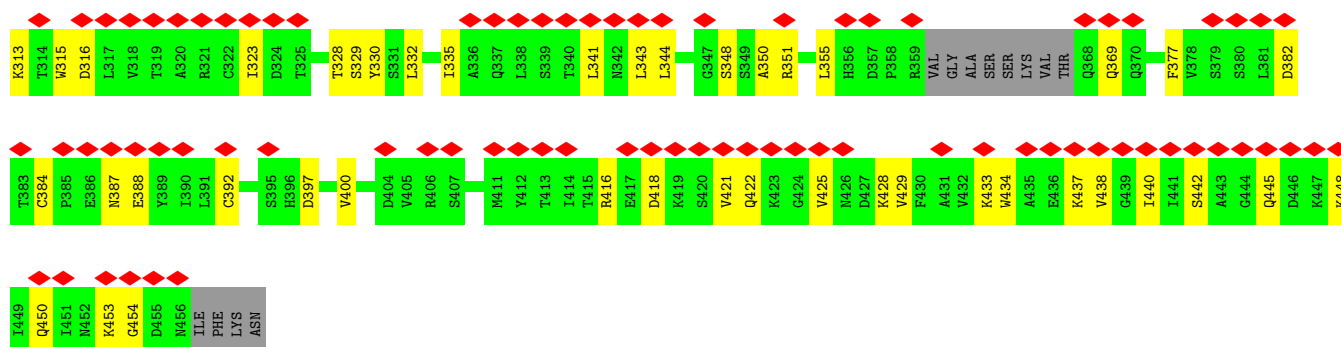


• Molecule 49: Pescadillo homolog

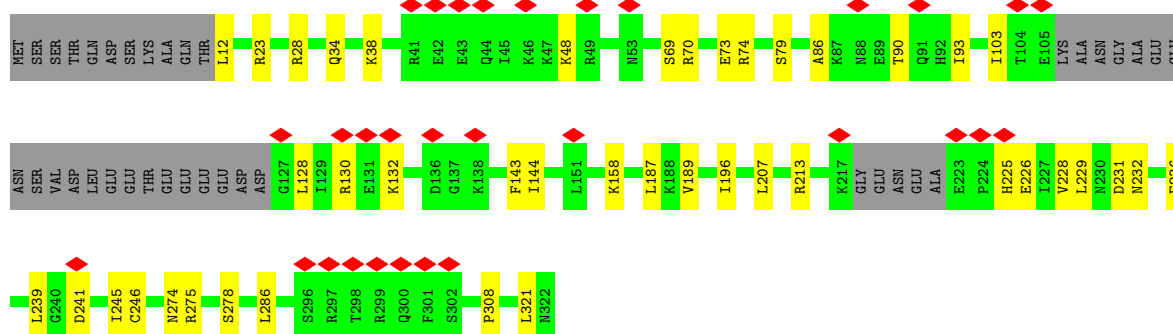
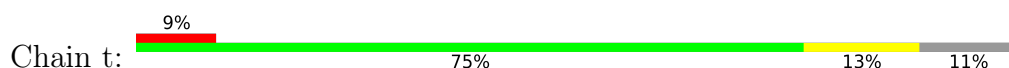


• Molecule 50: YTM1 isoform 1

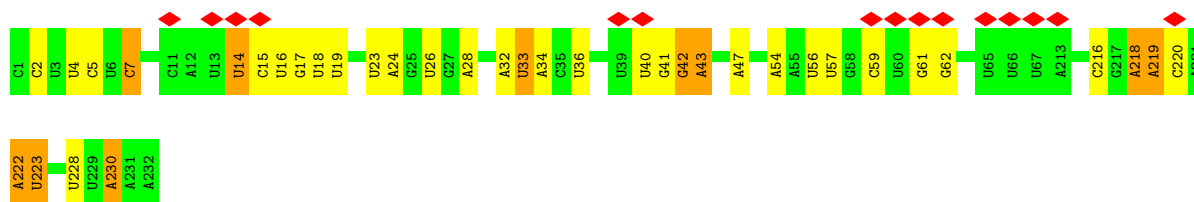




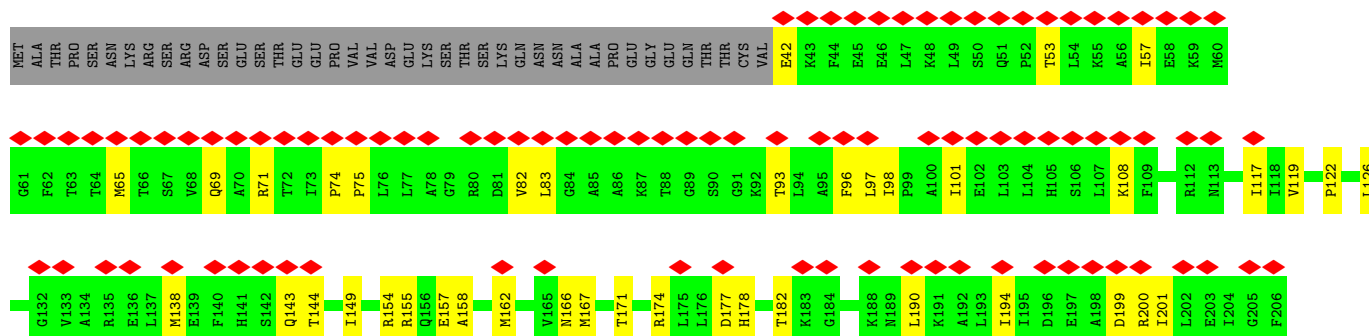
• Molecule 51: Ribosome biogenesis protein RLP7

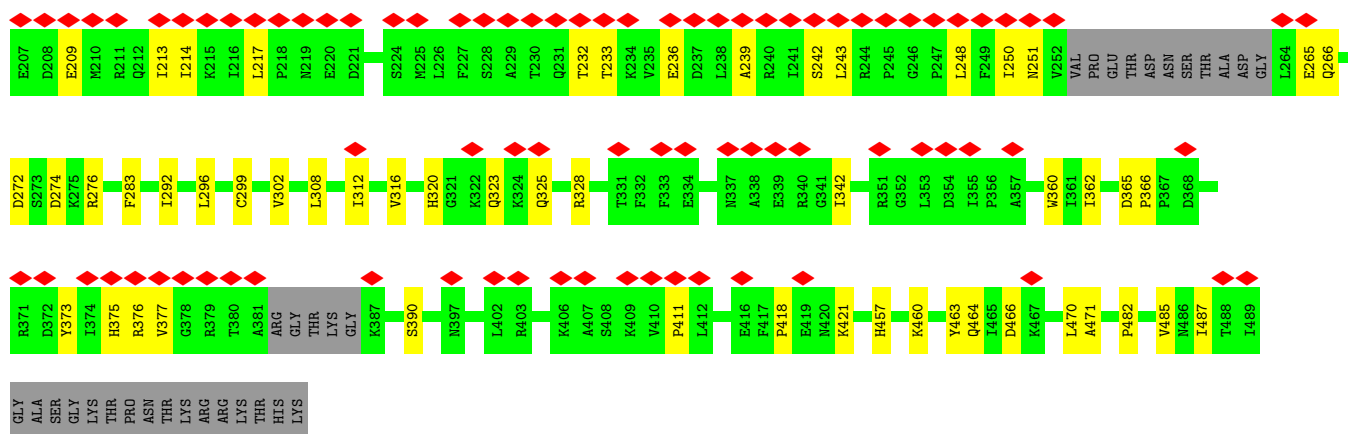


• Molecule 52: 5.8S ribosomal RNA gene and internal transcribed spacer 2

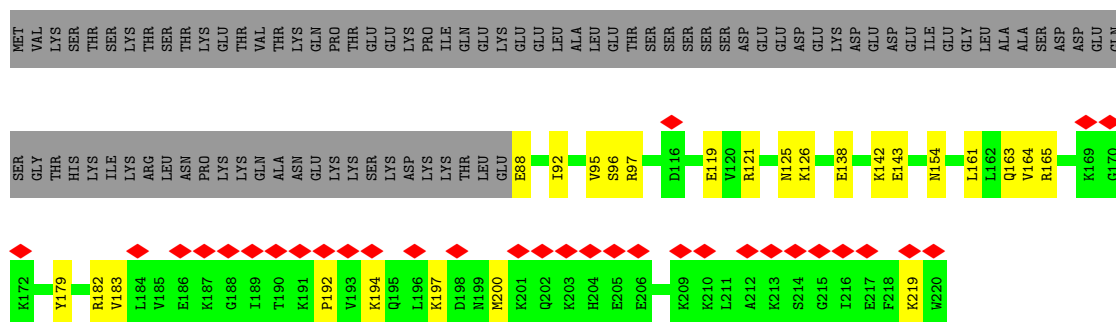


• Molecule 53: ATP-dependent RNA helicase HAS1

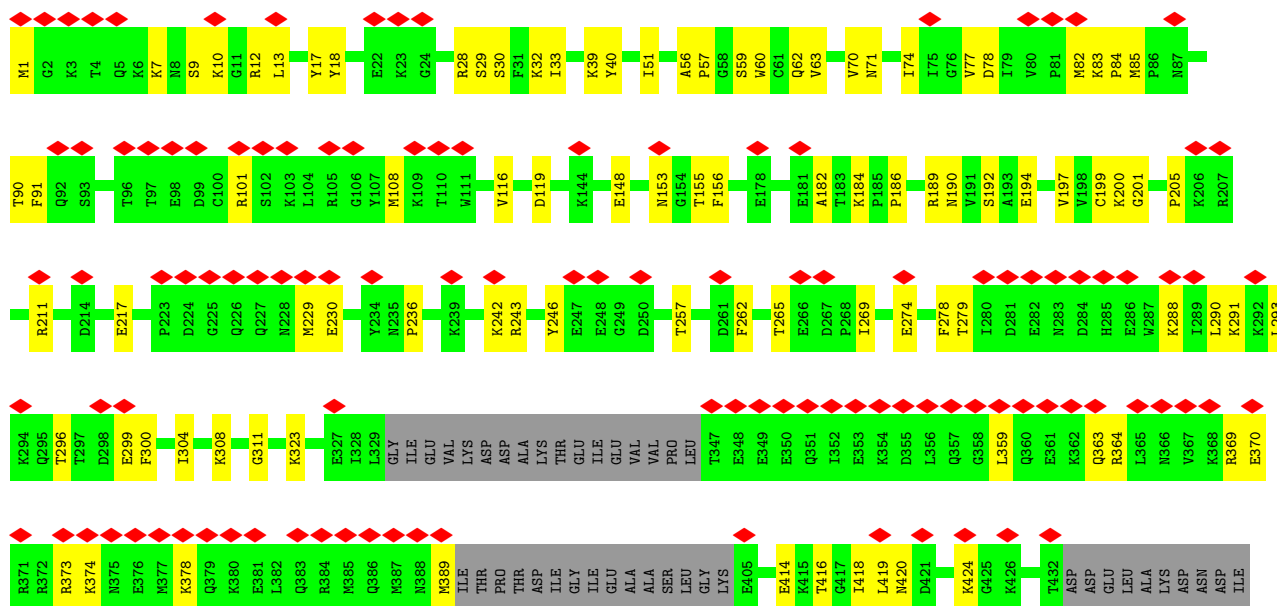


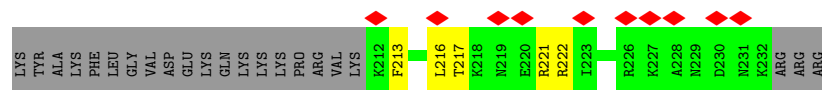


• Molecule 54: Ribosome biogenesis protein 15

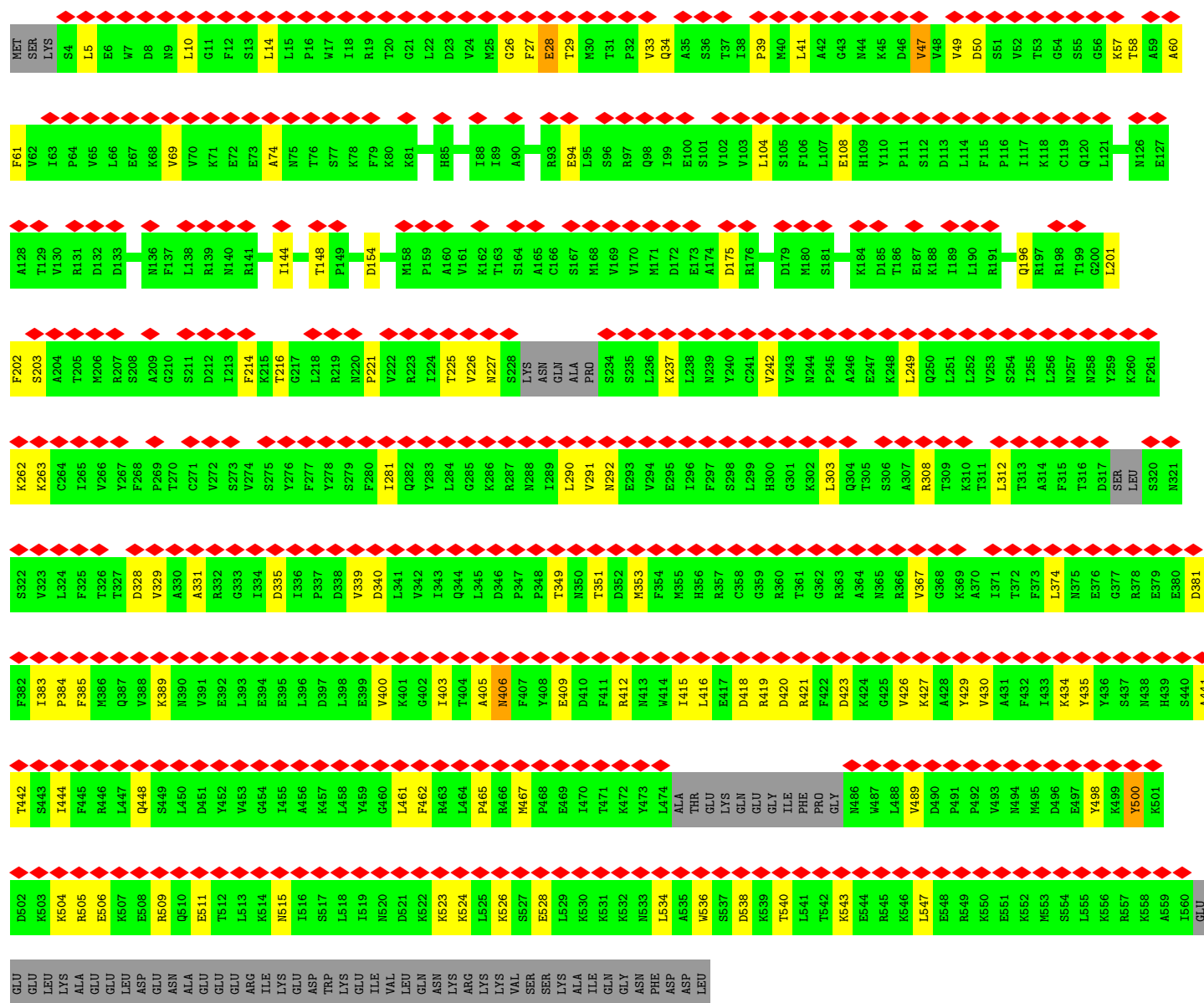
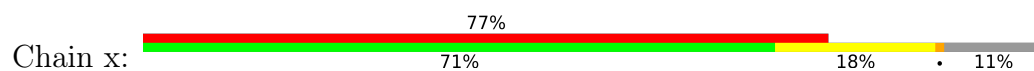


• Molecule 55: 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase





• Molecule 58: ATP-dependent rRNA helicase SPB4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0275	Depositor
Map size ($\text{\AA}$)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, OMU, SAH, OMG, A2M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.19	0/63625	0.30	4/99173 (0.0%)
2	2	0.22	0/3746	0.33	0/5832
3	7	0.16	0/1056	0.31	0/1408
4	A	0.16	0/2222	0.32	0/2998
5	B	0.20	0/2715	0.34	0/3647
6	C	0.18	0/2782	0.30	0/3766
7	E	0.16	0/1332	0.29	0/1791
8	F	0.17	0/1821	0.32	0/2451
9	H	0.17	0/1531	0.31	0/2062
10	J	0.13	0/1232	0.27	0/1642
11	L	0.19	0/1009	0.33	0/1355
12	M	0.16	0/1068	0.28	0/1438
13	N	0.20	0/1654	0.28	0/2212
14	O	0.18	0/1585	0.29	0/2128
15	P	0.17	0/1465	0.32	0/1968
16	Q	0.15	0/1050	0.26	0/1419
17	S	0.16	0/1468	0.33	0/1973
18	T	0.12	0/404	0.33	0/542
19	W	0.13	0/1902	0.33	0/2564
20	X	0.17	0/1083	0.30	0/1458
21	Y	0.20	0/1004	0.35	0/1341
22	b	0.14	0/4141	0.30	0/5575
23	d	0.16	0/887	0.32	0/1191
24	e	0.17	0/1030	0.29	0/1379
25	f	0.20	0/868	0.31	0/1168
26	h	0.17	0/978	0.29	0/1301
27	i	0.17	0/633	0.32	0/839
28	j	0.22	0/592	0.40	0/785
29	l	0.15	0/1425	0.32	0/1922
30	m	0.15	0/5511	0.31	0/7471
31	q	0.15	0/2854	0.35	0/3860
32	r	0.15	0/1462	0.30	0/1952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	s	0.18	0/301	0.26	0/386
34	u	0.14	0/1205	0.26	0/1603
35	v	0.17	0/1100	0.31	0/1456
36	y	0.15	0/1722	0.31	0/2343
37	z	0.13	0/445	0.26	0/585
38	8	0.14	0/3624	0.32	1/4891 (0.0%)
39	I	0.13	0/4310	0.29	0/5807
40	K	0.14	0/2310	0.31	0/3118
41	V	0.16	0/1008	0.34	0/1356
42	R	0.14	0/1095	0.26	0/1465
43	G	0.18	0/1575	0.28	0/2125
44	Z	0.14	0/1118	0.26	0/1497
45	U	0.14	0/825	0.29	0/1120
46	c	0.13	0/751	0.29	0/1008
47	g	0.16	0/891	0.28	0/1191
48	k	0.19	0/618	0.33	0/826
49	n	0.16	0/3544	0.29	0/4766
50	p	0.13	0/2674	0.34	0/3623
51	t	0.14	0/2319	0.27	0/3108
52	6	0.15	0/2050	0.30	0/3186
53	D	0.13	0/3516	0.30	0/4741
54	o	0.14	0/1129	0.30	0/1502
55	w	0.13	0/5531	0.31	0/7389
56	a	0.12	0/1722	0.35	0/2313
57	5	0.10	0/1217	0.28	0/1613
58	x	0.15	0/4419	0.31	0/5958
All	All	0.17	0/167154	0.31	5/239587 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2600	C	C2'-C3'-O3'	7.84	121.25	109.50
1	1	906	A	C2'-C3'-O3'	7.19	124.49	113.70
1	1	906	A	C3'-C2'-O2'	6.67	120.71	110.70
38	8	306	PRO	N-CA-CB	6.55	110.13	103.25
1	1	2600	C	C4'-C3'-O3'	5.29	117.34	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	56944	0	28630	609	0
2	2	3353	0	1695	30	0
3	7	1048	0	1117	15	0
4	A	2174	0	2179	48	0
5	B	2661	0	2738	58	0
6	C	2731	0	2852	41	0
7	E	1309	0	1394	17	0
8	F	1784	0	1862	24	0
9	H	1510	0	1576	17	0
10	J	1215	0	1245	22	0
11	L	991	0	1044	13	0
12	M	1053	0	1149	6	0
13	N	1621	0	1678	22	0
14	O	1555	0	1659	8	0
15	P	1442	0	1485	23	0
16	Q	1035	0	1115	6	0
17	S	1432	0	1470	24	0
18	T	401	0	418	16	0
19	W	1870	0	1902	40	0
20	X	1068	0	1153	11	0
21	Y	993	0	1081	17	0
22	b	4066	0	4111	66	0
23	d	873	0	914	14	0
24	e	1009	0	1080	15	0
25	f	850	0	880	9	0
26	h	969	0	1078	15	0
27	i	628	0	675	11	0
28	j	580	0	584	14	0
29	l	1394	0	1426	42	0
30	m	5377	0	5366	65	0
31	q	2799	0	2834	61	0
32	r	1438	0	1515	31	0
33	s	301	0	359	2	0
34	u	1183	0	1227	20	0
35	v	1087	0	1133	16	0
36	y	1701	0	1697	27	0
37	z	444	0	478	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	8	3567	0	3408	68	0
39	I	4247	0	4386	67	0
40	K	2274	0	2352	38	0
41	V	993	0	1040	17	0
42	R	1082	0	1160	28	0
43	G	1549	0	1637	23	0
44	Z	1092	0	1155	12	0
45	U	808	0	822	14	0
46	c	743	0	797	12	0
47	g	881	0	945	15	0
48	k	612	0	682	8	0
49	n	3470	0	3586	35	0
50	p	2628	0	2612	68	0
51	t	2293	0	2449	30	0
52	6	1838	0	927	21	0
53	D	3451	0	3578	59	0
54	o	1107	0	1159	19	0
55	w	5451	0	5578	102	0
56	a	1695	0	1781	41	0
57	5	1208	0	1228	31	0
58	x	4340	0	4468	85	0
59	g	1	0	0	0	0
59	j	1	0	0	0	0
60	w	26	0	19	3	0
All	All	158246	0	130568	1904	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 7.

All (1904) 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)
57:5:156:GLU:HG3	58:x:225:THR:OG1	1.48	1.10
42:R:105:LEU:HD11	42:R:109:TYR:CZ	1.95	1.02
1:1:909:G:H4'	55:w:750:ARG:HH22	1.28	0.97
1:1:909:G:C5'	55:w:750:ARG:HH22	1.79	0.96
31:q:269:ARG:HH21	31:q:533:PRO:HB2	1.32	0.94
42:R:151:ARG:NH2	58:x:442:THR:HB	1.83	0.94
1:1:909:G:H4'	55:w:750:ARG:NH2	1.82	0.94
1:1:909:G:C4'	55:w:750:ARG:HH22	1.82	0.92
40:K:295:GLN:HE21	54:o:197:LYS:HB3	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:155:VAL:HG11	58:x:226:VAL:HG22	1.59	0.84
1:1:2103:U:H3'	1:1:2103:U:OP2	1.78	0.83
55:w:549:HIS:HB2	55:w:556:ARG:HH21	1.44	0.82
39:I:132:GLU:HA	39:I:135:LEU:HD12	1.62	0.82
29:l:127:GLU:HG3	29:l:148:LYS:HA	1.62	0.82
1:1:815:G:N2	1:1:925:A:N1	2.29	0.80
57:5:155:VAL:HG12	58:x:226:VAL:HA	1.62	0.80
1:1:461:U:H3	1:1:469:G:H1	1.29	0.80
50:p:316:ASP:HB2	50:p:323:ILE:HD11	1.64	0.80
57:5:155:VAL:CG1	58:x:226:VAL:HG22	2.12	0.80
1:1:441:U:H3	1:1:493:G:H22	1.27	0.79
6:C:34:ILE:HG21	6:C:120:TYR:HD2	1.47	0.79
19:W:70:ARG:HD2	19:W:97:SER:HA	1.63	0.78
31:q:204:MET:HG2	31:q:259:MET:HE1	1.64	0.78
23:d:88:PRO:HB2	23:d:89:LEU:HD12	1.65	0.78
1:1:815:G:H1	1:1:925:A:H61	1.31	0.78
56:a:31:THR:HA	56:a:171:ASN:HA	1.64	0.77
1:1:959:C:H2'	1:1:960:U:H4'	1.66	0.77
38:8:515:ILE:HG13	38:8:518:LEU:HD12	1.65	0.77
1:1:2393:G:N2	1:1:2394:G:O6	2.16	0.77
21:Y:3:LYS:HD2	21:Y:8:VAL:HG13	1.67	0.77
56:a:76:ARG:HB2	56:a:144:LEU:HD13	1.65	0.76
23:d:25:PHE:HB3	23:d:65:LYS:HG2	1.68	0.75
31:q:409:PRO:HB3	31:q:462:SER:HB3	1.69	0.75
1:1:916:G:H5''	1:1:916:G:H8	1.50	0.75
22:b:506:GLU:HB2	23:d:97:LEU:HD21	1.68	0.75
58:x:263:LYS:HB2	58:x:339:VAL:HA	1.66	0.75
1:1:1504:A:OP1	15:P:23:ARG:NH1	2.20	0.74
42:R:134:HIS:CE1	42:R:136:ARG:HB3	2.22	0.74
1:1:711:A:N6	1:1:755:A:OP1	2.21	0.74
13:N:68:ARG:NH1	13:N:124:ASP:O	2.21	0.74
38:8:64:GLU:OE2	39:I:534:LYS:NZ	2.21	0.74
35:v:62:PRO:HG2	35:v:66:LYS:HE3	1.69	0.73
38:8:587:LEU:HD12	39:I:638:LEU:HD21	1.69	0.73
1:1:351:A:H1'	2:2:53:A:H1'	1.70	0.73
1:1:909:G:C5'	55:w:750:ARG:NH2	2.51	0.73
32:r:4:ASN:O	32:r:9:ARG:NH1	2.21	0.73
44:Z:56:LYS:HD2	51:t:28:ARG:HD2	1.69	0.73
55:w:370:GLU:OE1	55:w:373:ARG:NH2	2.21	0.73
1:1:1896:A:H61	1:1:2339:C:H42	1.37	0.73
11:L:62:THR:HG22	11:L:64:LYS:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:R:105:LEU:HD11	42:R:109:TYR:CE2	2.23	0.73
1:1:713:U:O4	4:A:255:GLN:NE2	2.22	0.72
4:A:142:ARG:HB2	4:A:181:ILE:HD13	1.70	0.72
5:B:115:LYS:NZ	5:B:129:ALA:O	2.23	0.72
30:m:378:PRO:HB3	51:t:231:ASP:HB3	1.69	0.72
1:1:2922:OMG:HM22	1:1:2923:PSU:H5''	1.70	0.72
51:t:144:ILE:HG12	51:t:196:ILE:HG12	1.71	0.72
22:b:187:ILE:HD11	22:b:332:ARG:HD3	1.72	0.72
55:w:230:GLU:HG2	55:w:269:ILE:HG21	1.71	0.72
1:1:1949:G:H5''	30:m:577:LYS:HD2	1.72	0.72
36:y:68:ARG:NH2	36:y:112:ASP:O	2.23	0.72
29:l:174:ARG:HD2	32:r:165:PRO:HA	1.71	0.71
40:K:338:ASN:OD1	40:K:339:PRO:HD3	1.91	0.71
45:U:35:LYS:NZ	45:U:39:ASP:OD2	2.22	0.71
1:1:1661:G:H2'	1:1:1662:G:C8	2.26	0.71
1:1:1807:G:H5''	44:Z:135:ARG:HH12	1.53	0.71
29:l:157:GLN:HG3	29:l:158:PRO:HD2	1.73	0.71
1:1:2375:G:N2	1:1:2375:G:OP2	2.23	0.71
20:X:26:VAL:HG22	55:w:450:ILE:HG12	1.72	0.71
58:x:57:LYS:HD3	58:x:202:PHE:HB3	1.71	0.71
3:7:100:ILE:HD11	29:l:6:GLU:HA	1.72	0.71
49:n:556:MET:HG3	49:n:559:MET:HE2	1.70	0.71
1:1:1320:C:O2'	17:S:115:ARG:NH1	2.23	0.71
12:M:19:ARG:NH1	12:M:66:THR:O	2.24	0.70
1:1:2949:U:OP1	1:1:2950:G:N2	2.25	0.70
4:A:140:ASP:HB2	4:A:180:SER:HA	1.74	0.70
5:B:95:THR:HG22	5:B:97:ARG:H	1.56	0.70
6:C:226:GLU:OE1	6:C:237:GLN:NE2	2.25	0.70
6:C:334:PHE:HA	6:C:339:LEU:HD12	1.72	0.70
36:y:112:ASP:OD2	36:y:156:ASN:ND2	2.24	0.70
48:k:3:ARG:NH2	48:k:52:TYR:OH	2.24	0.70
5:B:358:TRP:HB2	34:u:1:MET:HE1	1.74	0.69
1:1:40:A:O2'	1:1:41:G:N7	2.25	0.69
19:W:55:GLU:OE2	19:W:121:ARG:NH2	2.23	0.69
1:1:164:A:H3'	1:1:165:A:H4'	1.75	0.69
29:l:138:ASP:OD2	39:I:562:LYS:NZ	2.24	0.69
55:w:9:SER:HB2	55:w:12:ARG:HG2	1.74	0.69
1:1:3268:A:OP1	7:E:46:ARG:NH2	2.25	0.69
5:B:57:VAL:HG13	5:B:357:LYS:HB3	1.73	0.69
58:x:418:ASP:HB3	58:x:421:ARG:HG3	1.75	0.69
1:1:1724:U:OP1	42:R:128:LYS:NZ	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:m:385:ARG:NH1	49:n:212:ASP:OD2	2.26	0.68
1:1:1904:C:OP2	55:w:1:MET:N	2.26	0.68
1:1:2457:G:O2'	1:1:2481:G:N2	2.27	0.68
2:2:63:G:O2'	26:h:49:LYS:NZ	2.27	0.68
31:q:350:LEU:HB3	31:q:418:ILE:HG12	1.76	0.68
1:1:1945:A:H1'	58:x:154:ASP:HB2	1.73	0.68
57:5:156:GLU:HG3	58:x:225:THR:HG1	1.58	0.68
1:1:1097:G:H8	18:T:112:ASN:HD22	1.42	0.68
50:p:222:ILE:HB	50:p:234:TRP:HB2	1.73	0.68
57:5:156:GLU:CG	58:x:225:THR:OG1	2.35	0.68
1:1:3056:U:H4'	1:1:3057:U:H5'	1.75	0.67
55:w:278:PHE:HB2	55:w:304:ILE:HG23	1.76	0.67
57:5:156:GLU:OE2	58:x:225:THR:CG2	2.42	0.67
1:1:2830:G:H2'	1:1:2831:G:C8	2.29	0.67
54:o:119:GLU:OE2	54:o:121:ARG:NH1	2.27	0.67
1:1:760:G:H1	1:1:770:G:H21	1.42	0.67
31:q:417:ARG:NH1	31:q:469:HIS:O	2.26	0.67
31:q:347:GLU:OE2	31:q:417:ARG:NH1	2.28	0.67
9:H:57:VAL:HG23	9:H:68:LEU:HD13	1.77	0.67
19:W:145:ARG:NH1	19:W:206:PHE:O	2.28	0.67
20:X:50:ALA:HB1	26:h:66:VAL:HG11	1.76	0.67
38:8:517:PRO:HA	38:8:520:SER:HB3	1.76	0.67
53:D:82:VAL:HG12	53:D:248:LEU:HD11	1.76	0.67
57:5:153:THR:HG23	58:x:227:ASN:O	1.94	0.67
1:1:2931:C:OP1	41:V:40:LYS:NZ	2.27	0.67
38:8:365:PHE:HA	38:8:368:SER:HB3	1.77	0.67
58:x:430:VAL:HG22	58:x:467:MET:HE2	1.75	0.67
6:C:325:LEU:O	8:F:41:ARG:NH2	2.24	0.67
31:q:197:LEU:HD12	31:q:238:TYR:HD1	1.60	0.67
1:1:1728:G:OP1	46:c:86:ARG:NH2	2.27	0.66
39:I:398:GLU:OE1	39:I:401:ARG:NH2	2.29	0.66
1:1:459:G:H1	1:1:471:U:H3	1.44	0.66
39:I:197:LEU:HG	39:I:202:LYS:HE3	1.76	0.66
50:p:235:SER:HB2	50:p:280:LEU:HD11	1.78	0.66
19:W:29:GLU:HA	19:W:32:GLU:HG3	1.78	0.66
31:q:538:VAL:HG23	31:q:539:ASP:H	1.61	0.66
40:K:97:LEU:HD11	40:K:205:THR:HG23	1.78	0.66
1:1:1924:U:H1'	1:1:2110:G:N2	2.11	0.66
13:N:31:ARG:NH1	13:N:124:ASP:OD2	2.28	0.66
23:d:41:LYS:NZ	23:d:47:ASP:OD1	2.29	0.66
50:p:418:ASP:HB3	50:p:421:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:890:C:H5	38:8:37:ARG:HE	1.42	0.65
1:1:1684:U:OP1	45:U:86:LYS:NZ	2.26	0.65
4:A:167:ARG:NH1	30:m:150:ASP:O	2.29	0.65
19:W:96:CYS:HB2	19:W:100:THR:HG21	1.77	0.65
1:1:2482:U:H3	1:1:2486:A:H62	1.44	0.65
51:t:90:THR:HG23	51:t:93:ILE:HD11	1.79	0.65
55:w:556:ARG:O	55:w:560:ASN:ND2	2.27	0.65
38:8:448:TRP:HA	38:8:451:VAL:HG12	1.77	0.65
23:d:13:THR:OG1	23:d:72:ARG:NH1	2.29	0.65
31:q:327:TYR:O	31:q:392:ARG:NH2	2.30	0.65
6:C:3:ARG:HD2	6:C:22:LEU:HB2	1.77	0.65
38:8:492:PHE:HD2	38:8:563:LEU:HD11	1.62	0.65
40:K:82:VAL:HG21	40:K:270:LEU:HD13	1.78	0.65
55:w:808:ARG:NH2	55:w:814:GLY:O	2.29	0.65
1:1:707:U:O2'	1:1:754:G:N3	2.30	0.65
23:d:55:LEU:HB2	23:d:95:PRO:HD3	1.78	0.65
38:8:65:VAL:O	39:I:593:LYS:NZ	2.30	0.65
1:1:1385:C:HO2'	7:E:2:SER:N	1.95	0.64
30:m:387:ARG:HG3	49:n:141:LEU:HD22	1.79	0.64
30:m:789:ARG:NH2	50:p:308:GLN:OE1	2.30	0.64
58:x:506:GLU:OE2	58:x:509:ARG:NH2	2.30	0.64
4:A:141:GLN:NE2	10:J:225:SER:O	2.28	0.64
1:1:1634:G:N7	44:Z:17:ARG:NH2	2.45	0.64
1:1:3014:U:H3	1:1:3040:A:H62	1.46	0.64
26:h:119:LYS:HB2	35:v:56:ARG:HG2	1.79	0.64
56:a:39:LYS:HG3	56:a:202:GLY:HA2	1.80	0.64
1:1:728:G:H5'	16:Q:43:PRO:HB2	1.77	0.64
5:B:29:VAL:HG22	5:B:218:ILE:HD12	1.78	0.64
52:6:28:A:OP1	54:o:125:ASN:ND2	2.31	0.64
8:F:168:ILE:O	8:F:172:ASN:ND2	2.31	0.63
38:8:377:MET:HA	38:8:380:ILE:HG22	1.80	0.63
41:V:61:THR:HG22	41:V:73:VAL:HG12	1.80	0.63
1:1:3295:A:H2'	1:1:3296:A:C8	2.33	0.63
4:A:103:LYS:HB2	4:A:107:GLY:HA3	1.80	0.63
21:Y:74:TYR:HE2	21:Y:77:LYS:HG3	1.63	0.63
34:u:119:ASP:OD1	34:u:122:ARG:NH2	2.32	0.63
38:8:529:THR:HG22	38:8:530:LYS:H	1.63	0.63
44:Z:121:ARG:NH2	44:Z:127:ASN:OD1	2.32	0.63
1:1:870:C:H2'	1:1:871:G:H8	1.62	0.63
4:A:238:GLU:OE1	10:J:196:ASN:ND2	2.31	0.63
29:l:173:LEU:HB2	31:q:323:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:a:209:SER:OG	56:a:210:MET:N	2.32	0.63
51:t:103:ILE:HG12	51:t:130:ARG:HG2	1.80	0.63
1:1:412:G:OP1	15:P:62:ARG:NH1	2.31	0.63
53:D:471:ALA:HA	53:D:482:PRO:HG3	1.79	0.63
1:1:114:A:N3	13:N:50:ARG:NH1	2.47	0.63
57:5:216:LEU:O	57:5:221:ARG:NH2	2.32	0.62
1:1:3151:U:OP2	5:B:132:LYS:NZ	2.30	0.62
31:q:319:THR:HG22	31:q:321:GLU:H	1.64	0.62
31:q:465:CYS:HB3	31:q:548:LYS:HE2	1.80	0.62
56:a:68:PHE:HB2	56:a:112:ALA:HA	1.81	0.62
17:S:23:LYS:HA	18:T:146:ASN:HD21	1.65	0.62
21:Y:87:LYS:HB3	21:Y:97:ILE:HD11	1.80	0.62
1:1:3008:A:OP2	14:O:74:ARG:NH1	2.32	0.62
9:H:4:ILE:HG13	17:S:142:GLN:NE2	2.15	0.62
51:t:232:ASN:HB3	51:t:246:CYS:HA	1.80	0.62
38:8:453:SER:HB2	38:8:508:ASN:HB2	1.82	0.62
1:1:1964:C:H3'	1:1:1965:C:H5''	1.81	0.62
23:d:47:ASP:H	23:d:86:LYS:HE2	1.65	0.62
3:7:117:ASP:OD1	29:l:94:LYS:NZ	2.33	0.62
53:D:292:ILE:HG12	53:D:360:TRP:HB2	1.81	0.62
1:1:2129:U:H5''	57:5:221:ARG:HD3	1.81	0.62
1:1:2454:G:N2	31:q:251:ASN:O	2.33	0.62
1:1:316:U:O2'	27:i:29:LYS:NZ	2.28	0.62
4:A:116:ASN:HB2	4:A:220:VAL:HG12	1.82	0.61
43:G:163:VAL:HG12	43:G:166:LEU:HD12	1.81	0.61
38:8:32:ARG:O	38:8:36:ARG:NH1	2.33	0.61
46:c:18:ILE:HD13	46:c:81:VAL:HG13	1.81	0.61
50:p:306:VAL:HG12	50:p:312:ILE:HG12	1.82	0.61
55:w:155:THR:HG22	55:w:200:LYS:HG2	1.82	0.61
1:1:869:G:OP2	57:5:222:ARG:NH1	2.34	0.61
4:A:143:PHE:HA	4:A:149:TYR:HB3	1.83	0.61
22:b:287:ILE:HB	22:b:319:THR:HG22	1.83	0.61
5:B:216:ASP:OD1	5:B:339:ARG:HB3	2.00	0.61
1:1:2493:U:OP1	56:a:215:ARG:NH2	2.34	0.61
43:G:69:LEU:HG	55:w:695:LEU:HD11	1.82	0.61
1:1:806:A:H2'	1:1:807:A:C2	2.35	0.61
5:B:50:LYS:NZ	5:B:330:GLY:O	2.29	0.61
29:l:174:ARG:HB2	32:r:163:ARG:HD3	1.81	0.61
32:r:175:SER:HA	32:r:178:ARG:HD2	1.81	0.61
56:a:205:VAL:HB	56:a:213:ALA:HB1	1.81	0.61
4:A:113:TYR:HB2	4:A:224:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:142:ARG:HG2	10:J:229:THR:HB	1.82	0.61
1:1:1204:A:H2'	1:1:1205:A:O4'	2.00	0.61
34:u:66:ASP:OD1	34:u:103:ARG:NH1	2.32	0.61
38:8:514:PRO:O	38:8:517:PRO:HD2	2.00	0.61
39:I:285:ILE:HD12	39:I:291:SER:HB2	1.83	0.61
39:I:453:LYS:HD3	39:I:497:LYS:HD3	1.82	0.61
1:1:92:G:H5'	1:1:93:C:H5''	1.83	0.61
5:B:57:VAL:HG12	5:B:358:TRP:HB3	1.83	0.61
31:q:279:LYS:NZ	31:q:324:ALA:O	2.34	0.61
34:u:127:VAL:HG13	34:u:134:LEU:HD11	1.83	0.61
1:1:484:C:H2'	1:1:485:A:C4	2.36	0.60
1:1:645:A:OP1	1:1:1116:G:N2	2.32	0.60
3:7:110:ARG:NH2	29:l:6:GLU:OE2	2.34	0.60
19:W:43:LEU:HD23	19:W:217:VAL:HB	1.82	0.60
22:b:497:ARG:NH2	34:u:123:ASP:OD1	2.34	0.60
30:m:165:TYR:O	30:m:182:ARG:NH2	2.31	0.60
55:w:288:LYS:HA	55:w:291:LYS:HE2	1.83	0.60
55:w:732:PRO:HD2	55:w:735:LYS:HD2	1.82	0.60
1:1:216:G:OP1	21:Y:16:ARG:NH1	2.34	0.60
1:1:2889:C:OP1	22:b:28:LYS:NZ	2.33	0.60
30:m:285:GLU:OE1	30:m:287:ARG:NH1	2.34	0.60
39:I:320:LYS:NZ	55:w:642:GLU:OE2	2.25	0.60
56:a:10:ARG:HG2	56:a:180:VAL:HG21	1.83	0.60
1:1:447:U:H2'	1:1:448:U:C6	2.37	0.60
4:A:27:PHE:O	4:A:30:LYS:NZ	2.35	0.60
54:o:92:ILE:HG13	54:o:138:GLU:HG3	1.83	0.60
1:1:3233:C:H2'	1:1:3234:A:C8	2.36	0.60
51:t:132:LYS:HE3	51:t:308:PRO:HG3	1.84	0.60
2:2:127:U:O2	49:n:14:ASN:ND2	2.31	0.60
19:W:145:ARG:HG3	19:W:149:ILE:HD12	1.83	0.60
42:R:105:LEU:HD11	42:R:109:TYR:OH	2.02	0.60
50:p:148:ARG:HE	50:p:212:VAL:HG12	1.65	0.60
1:1:257:U:H2'	1:1:258:G:H8	1.67	0.60
1:1:2395:G:H2'	1:1:2396:G:C8	2.37	0.60
9:H:4:ILE:HG13	17:S:142:GLN:HE21	1.64	0.60
39:I:594:LEU:HD22	39:I:601:ILE:HD11	1.84	0.60
45:U:77:LYS:NZ	45:U:95:PHE:O	2.35	0.60
50:p:207:HIS:HE2	50:p:232:GLY:HA3	1.67	0.60
1:1:1786:G:H2'	1:1:1787:A:C8	2.37	0.60
1:1:2123:G:H5''	1:1:2123:G:H8	1.66	0.60
25:f:67:MET:HE1	25:f:90:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:m:127:LYS:HD3	30:m:128:TYR:O	2.01	0.60
39:I:441:ASN:HD21	55:w:726:LYS:HE2	1.65	0.60
1:1:835:G:O2'	1:1:857:G:N2	2.31	0.59
30:m:248:THR:HA	43:G:172:LYS:HD3	1.84	0.59
53:D:154:ARG:HH22	53:D:182:THR:HG23	1.67	0.59
1:1:252:U:O2'	35:v:218:ARG:NH1	2.35	0.59
1:1:1635:G:N2	1:1:1638:A:OP2	2.29	0.59
1:1:469:G:H2'	1:1:470:G:C8	2.37	0.59
1:1:3343:G:O2'	1:1:3362:A:N6	2.25	0.59
9:H:4:ILE:H	17:S:142:GLN:HE21	1.51	0.59
56:a:128:LEU:HD21	56:a:134:PHE:HA	1.84	0.59
1:1:1060:U:H2'	1:1:1061:A:C8	2.37	0.59
1:1:2428:U:H2'	1:1:2429:G:C8	2.38	0.59
41:V:97:ASP:OD2	55:w:246:TYR:OH	2.20	0.59
1:1:1592:G:OP1	47:g:58:ARG:NH2	2.35	0.59
23:d:80:ASN:ND2	23:d:84:ASP:OD2	2.36	0.59
52:6:42:G:H2'	52:6:43:A:H8	1.68	0.59
1:1:1553:U:H4'	1:1:1554:U:H5'	1.82	0.59
1:1:3259:U:H5''	1:1:3261:C:H5	1.67	0.59
2:2:29:U:H5''	11:L:27:ASP:HB3	1.83	0.59
4:A:86:VAL:HG23	4:A:104:PRO:HG3	1.85	0.59
30:m:466:ILE:HG13	30:m:467:LEU:HD22	1.85	0.59
51:t:48:LYS:NZ	52:6:228:U:O2'	2.23	0.59
1:1:331:G:OP1	35:v:3:SER:OG	2.20	0.59
5:B:216:ASP:HB3	5:B:278:ILE:HA	1.83	0.59
1:1:299:G:N7	27:i:30:LYS:HB3	2.18	0.59
1:1:1679:A:H4'	22:b:520:PRO:HB3	1.85	0.59
1:1:2924:U:OP1	55:w:28:ARG:HG2	2.03	0.59
4:A:119:THR:OG1	4:A:121:ASP:OD1	2.21	0.59
53:D:154:ARG:NH2	53:D:177:ASP:OD1	2.26	0.59
6:C:2:SER:OG	6:C:3:ARG:N	2.36	0.59
30:m:375:ARG:O	51:t:232:ASN:ND2	2.25	0.59
38:8:389:GLU:HG2	38:8:454:PHE:HE2	1.67	0.59
40:K:84:ASN:HB3	40:K:276:ILE:HD13	1.84	0.59
40:K:119:LYS:NZ	40:K:175:SER:O	2.32	0.59
42:R:152:GLU:OE2	55:w:363:GLN:NE2	2.36	0.59
1:1:871:G:O2'	55:w:744:ARG:NH1	2.34	0.58
22:b:76:PRO:HA	22:b:79:ARG:HG2	1.85	0.58
1:1:707:U:O2	1:1:712:G:N2	2.31	0.58
1:1:3139:A:OP2	5:B:30:LYS:NZ	2.28	0.58
41:V:74:MET:HG3	41:V:102:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1639:C:OP2	47:g:74:ARG:NH1	2.32	0.58
4:A:148:HIS:HB3	10:J:201:MET:HE1	1.85	0.58
28:j:64:MET:O	28:j:68:LYS:HG3	2.03	0.58
29:l:98:TRP:NE1	29:l:138:ASP:OD1	2.31	0.58
29:l:108:LEU:O	32:r:163:ARG:NH1	2.36	0.58
1:1:1766:G:HO2'	1:1:1767:C:H6	1.51	0.58
1:1:2491:A:H1'	56:a:207:LYS:HE2	1.84	0.58
26:h:64:GLU:OE2	26:h:68:GLN:NE2	2.36	0.58
40:K:71:GLU:OE2	40:K:75:LYS:NZ	2.36	0.58
6:C:261:VAL:O	6:C:269:SER:OG	2.21	0.58
1:1:3313:U:H4'	5:B:173:GLN:HG3	1.85	0.58
10:J:226:GLU:HG2	10:J:227:THR:HG23	1.84	0.58
42:R:158:GLU:OE2	58:x:441:ALA:HB1	2.02	0.58
34:u:74:ARG:HH12	36:y:74:THR:HG23	1.69	0.58
1:1:780:A:H2'	1:1:780:A:N3	2.17	0.58
1:1:1300:G:H5''	1:1:1301:A:H5'	1.86	0.58
1:1:2982:A:O2'	1:1:2984:C:OP2	2.22	0.58
58:x:420:ASP:OD2	58:x:505:ARG:NH2	2.37	0.58
1:1:1210:U:H5	19:W:3:ARG:HG2	1.68	0.58
41:V:23:MET:HE3	41:V:100:GLY:HA3	1.86	0.58
1:1:842:G:H5'	55:w:369:ARG:HD2	1.86	0.58
1:1:2496:C:O2'	1:1:2497:U:OP1	2.20	0.57
10:J:205:LEU:O	10:J:209:GLN:HG3	2.04	0.57
49:n:106:GLU:OE2	51:t:286:LEU:HD23	2.04	0.57
1:1:711:A:H5'	4:A:248:VAL:HG13	1.86	0.57
22:b:509:ASN:O	23:d:61:LYS:NZ	2.37	0.57
31:q:341:LEU:O	31:q:417:ARG:NE	2.36	0.57
53:D:57:ILE:HD11	53:D:98:ILE:HD11	1.85	0.57
1:1:351:A:O2'	2:2:53:A:O2'	2.22	0.57
1:1:531:G:H2'	1:1:532:A:C8	2.39	0.57
1:1:873:U:H3'	39:I:490:LYS:HD2	1.87	0.57
1:1:2429:G:H2'	1:1:2430:A:C8	2.39	0.57
2:2:75:G:OP2	21:Y:74:TYR:OH	2.21	0.57
8:F:165:ASP:OD1	8:F:166:ASN:N	2.38	0.57
29:l:31:LYS:NZ	39:I:625:ARG:HH12	2.01	0.57
30:m:160:ILE:HD12	30:m:161:PRO:HD2	1.85	0.57
34:u:66:ASP:HB3	34:u:69:LEU:HD13	1.86	0.57
1:1:1366:A:O2'	24:e:45:ARG:NH2	2.36	0.57
17:S:77:VAL:HG11	17:S:106:LEU:HD22	1.84	0.57
39:I:299:GLU:HB3	39:I:528:LEU:HD22	1.87	0.57
1:1:441:U:H3	1:1:493:G:N2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:7:LEU:HD21	43:G:162:LEU:HA	1.87	0.57
30:m:409:PRO:HG3	49:n:570:MET:HB3	1.86	0.57
42:R:105:LEU:CD1	42:R:109:TYR:CZ	2.79	0.57
56:a:148:VAL:HA	56:a:151:VAL:HG12	1.86	0.57
57:5:156:GLU:OE2	58:x:225:THR:HG21	2.03	0.57
1:1:3275:U:O2'	25:f:99:ARG:NH1	2.38	0.57
15:P:30:ARG:HA	15:P:119:VAL:HG11	1.85	0.57
1:1:3277:U:O4	15:P:172:GLN:NE2	2.33	0.57
1:1:3295:A:H2'	1:1:3296:A:H8	1.69	0.57
39:I:185:PHE:O	39:I:189:ILE:HG12	2.05	0.57
1:1:1943:C:H5''	58:x:329:VAL:HB	1.85	0.57
3:7:108:LEU:O	3:7:112:ILE:HG12	2.05	0.57
6:C:143:GLU:HG2	6:C:144:LYS:HD2	1.84	0.57
39:I:179:LEU:HD11	39:I:251:LEU:HD12	1.86	0.57
38:8:540:ALA:HA	38:8:558:ILE:HD12	1.87	0.57
1:1:1353:U:O2'	7:E:8:LYS:O	2.22	0.57
9:H:90:MET:HE2	9:H:179:ILE:HG22	1.87	0.57
17:S:26:ARG:HB2	18:T:148:PRO:HB2	1.85	0.57
20:X:2:ALA:N	54:o:143:GLU:OE1	2.38	0.57
28:j:63:ARG:O	28:j:68:LYS:HE3	2.05	0.57
40:K:109:PRO:HB2	40:K:253:TRP:HB3	1.85	0.57
50:p:110:ASP:OD1	50:p:433:LYS:NZ	2.38	0.57
52:6:42:G:H2'	52:6:43:A:C8	2.40	0.57
55:w:414:GLU:HG2	55:w:419:LEU:HD11	1.86	0.57
56:a:10:ARG:HH11	56:a:180:VAL:HG11	1.70	0.57
38:8:12:GLN:HG2	38:8:16:LEU:HD22	1.87	0.56
40:K:328:THR:HG21	51:t:86:ALA:HB1	1.86	0.56
53:D:485:VAL:HG12	53:D:487:ILE:HG12	1.87	0.56
1:1:3343:G:H21	1:1:3362:A:H2	1.52	0.56
4:A:135:PRO:HB3	4:A:175:HIS:NE2	2.19	0.56
6:C:34:ILE:HG13	6:C:120:TYR:CE2	2.40	0.56
53:D:265:GLU:HA	53:D:411:PRO:HG2	1.86	0.56
1:1:3278:C:OP1	25:f:54:ARG:NH2	2.24	0.56
9:H:175:PHE:O	32:r:17:ARG:NH1	2.37	0.56
19:W:175:ILE:HG22	19:W:180:ILE:HA	1.87	0.56
47:g:20:ILE:HD11	47:g:32:ALA:HB1	1.87	0.56
47:g:22:VAL:HG12	47:g:30:LEU:HD22	1.87	0.56
53:D:71:ARG:NH1	53:D:251:ASN:O	2.38	0.56
53:D:323:GLN:O	53:D:328:ARG:NH1	2.37	0.56
1:1:487:U:H3'	1:1:488:U:H5''	1.87	0.56
1:1:1696:A:H2'	1:1:1697:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:m:580:GLN:HA	30:m:583:LEU:HD23	1.87	0.56
38:8:550:THR:HG22	38:8:553:TYR:HB2	1.87	0.56
39:I:166:VAL:HG12	39:I:230:ARG:HG2	1.85	0.56
55:w:51:ILE:HD11	55:w:108:MET:HE3	1.88	0.56
56:a:69:GLY:HA2	56:a:113:SER:HB3	1.87	0.56
1:1:1954:G:O2'	1:1:1955:U:OP1	2.22	0.56
22:b:389:ASP:HB3	22:b:392:ASP:HB2	1.88	0.56
30:m:192:LEU:HD13	39:I:447:ASP:HB3	1.87	0.56
30:m:545:SER:HB2	30:m:628:LYS:HD2	1.88	0.56
30:m:751:HIS:NE2	30:m:753:THR:OG1	2.39	0.56
56:a:55:LEU:HB2	56:a:153:SER:HB3	1.88	0.56
1:1:655:C:H5''	24:e:26:HIS:HB3	1.87	0.56
6:C:206:LEU:HD12	6:C:226:GLU:HB2	1.86	0.56
31:q:287:GLN:NE2	31:q:291:ASN:OD1	2.38	0.56
50:p:252:ASN:HB3	50:p:253:PRO:HD3	1.88	0.56
1:1:156:G:H22	11:L:91:ARG:HH12	1.53	0.56
1:1:870:C:H2'	1:1:871:G:C8	2.40	0.56
20:X:133:LEU:O	20:X:137:ASN:ND2	2.32	0.56
39:I:470:ARG:HB2	39:I:542:LYS:HE2	1.87	0.56
40:K:39:LYS:HZ3	54:o:219:LYS:HB2	1.70	0.56
49:n:170:VAL:HG13	49:n:175:LEU:HB2	1.88	0.56
55:w:558:ILE:HG23	55:w:559:PHE:HD1	1.71	0.56
1:1:455:C:N3	1:1:476:G:N1	2.54	0.56
5:B:54:THR:OG1	5:B:360:ASP:O	2.24	0.56
38:8:506:SER:OG	38:8:511:VAL:O	2.23	0.56
1:1:909:G:H5'	55:w:750:ARG:NH2	2.20	0.56
3:7:81:ASN:HB3	4:A:128:ASN:HB3	1.86	0.56
1:1:818:C:H42	1:1:907:G:N2	2.03	0.56
6:C:34:ILE:HG21	6:C:120:TYR:CD2	2.36	0.56
55:w:416:THR:HG23	55:w:418:ILE:H	1.70	0.56
1:1:2104:A:H4'	1:1:2105:G:H4'	1.87	0.55
1:1:872:G:H1	1:1:889:U:H3	1.53	0.55
1:1:1353:U:OP2	1:1:1354:G:N2	2.37	0.55
1:1:2894:C:OP1	9:H:168:ARG:NH1	2.39	0.55
2:2:57:C:H4'	2:2:63:G:N7	2.21	0.55
5:B:303:LYS:HD2	5:B:361:THR:HG21	1.87	0.55
31:q:452:GLN:OE1	31:q:475:TYR:OH	2.24	0.55
1:1:2130:G:H2'	1:1:2131:A:C8	2.41	0.55
46:c:104:LEU:HB2	55:w:543:LYS:HD2	1.88	0.55
1:1:424:G:H21	24:e:24:ARG:NH2	2.04	0.55
1:1:2434:U:H5''	1:1:2435:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3119:U:OP1	32:r:26:LYS:NZ	2.39	0.55
8:F:74:SER:HB2	18:T:141:VAL:O	2.06	0.55
30:m:252:GLU:O	43:G:146:LYS:NZ	2.38	0.55
1:1:1596:C:H2'	1:1:1597:C:C6	2.41	0.55
1:1:2610:G:N2	1:1:2611:U:O2'	2.40	0.55
39:I:321:ILE:HG23	55:w:637:TYR:HE1	1.70	0.55
39:I:395:SER:OG	55:w:490:ARG:NH2	2.40	0.55
50:p:285:SER:OG	50:p:313:LYS:NZ	2.38	0.55
6:C:126:ILE:O	6:C:129:THR:OG1	2.24	0.55
6:C:156:LEU:HD12	6:C:159:ILE:HD12	1.88	0.55
26:h:22:VAL:HG12	26:h:26:LYS:HE3	1.88	0.55
53:D:316:VAL:HG12	53:D:342:ILE:HB	1.89	0.55
1:1:209:A:O2'	1:1:211:A:OP2	2.23	0.55
1:1:449:U:N3	1:1:450:G:O6	2.40	0.55
1:1:754:G:O6	1:1:779:G:O6	2.25	0.55
50:p:416:ARG:NH2	50:p:448:LYS:O	2.40	0.55
1:1:2343:C:O2'	1:1:3056:U:OP1	2.24	0.55
1:1:3099:C:H42	1:1:3135:U:H3	1.54	0.55
1:1:3164:C:HO2'	1:1:3165:A:H8	1.54	0.55
38:8:445:LEU:HD11	38:8:482:VAL:HG21	1.88	0.55
58:x:47:VAL:HG13	58:x:49:VAL:HG23	1.87	0.55
1:1:364:G:OP2	28:j:52:LYS:NZ	2.39	0.55
6:C:31:ARG:NH2	6:C:33:ASP:OD2	2.30	0.55
6:C:68:GLY:HA2	55:w:820:ASP:HB2	1.88	0.55
21:Y:102:SER:OG	21:Y:103:LYS:NZ	2.40	0.55
39:I:644:CYS:HB3	39:I:647:VAL:HG12	1.88	0.55
24:e:82:LEU:HD11	24:e:112:ALA:HB2	1.89	0.55
1:1:1643:A:H5''	1:1:1644:C:C4	2.42	0.54
16:Q:90:ASP:OD2	16:Q:92:ARG:NH2	2.28	0.54
38:8:437:TYR:HE2	38:8:486:ILE:HB	1.71	0.54
46:c:16:LEU:HB3	46:c:98:SER:HB2	1.89	0.54
56:a:38:LEU:HD23	56:a:163:LEU:HB2	1.89	0.54
1:1:1290:A:H2'	1:1:1291:A:C8	2.42	0.54
1:1:3085:G:OP2	34:u:38:LYS:NZ	2.41	0.54
1:1:3165:A:H2'	1:1:3166:C:C6	2.43	0.54
1:1:3294:A:H2'	1:1:3295:A:O4'	2.08	0.54
34:u:100:ARG:NH2	34:u:101:GLN:OE1	2.40	0.54
40:K:85:ASN:HB2	40:K:301:LEU:HD11	1.88	0.54
50:p:392:CYS:HB3	50:p:434:TRP:HE1	1.71	0.54
58:x:426:VAL:HA	58:x:461:LEU:HD11	1.89	0.54
1:1:3358:U:H3'	1:1:3359:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:85:VAL:HG12	5:B:202:THR:HG22	1.89	0.54
30:m:393:ASP:OD1	51:t:23:ARG:NH1	2.39	0.54
31:q:390:ILE:HG23	31:q:395:CYS:HB2	1.90	0.54
1:1:548:G:H2'	1:1:549:U:O4'	2.07	0.54
1:1:819:U:O2	1:1:819:U:H2'	2.08	0.54
1:1:3180:A:OP1	14:O:171:LYS:NZ	2.41	0.54
31:q:416:ASP:OD1	31:q:470:GLY:HA3	2.07	0.54
48:k:32:ASN:HD21	48:k:36:LYS:HE3	1.73	0.54
53:D:232:THR:HG22	53:D:233:THR:H	1.73	0.54
1:1:528:U:H2'	1:1:529:A:C8	2.42	0.54
1:1:918:C:O2	1:1:918:C:H2'	2.07	0.54
1:1:1194:G:H2'	1:1:1195:A:C8	2.42	0.54
1:1:3252:G:H2'	1:1:3253:G:C8	2.42	0.54
13:N:19:LEU:O	13:N:23:GLN:HG3	2.08	0.54
21:Y:5:SER:HB3	21:Y:8:VAL:HG12	1.90	0.54
29:l:40:GLN:HB3	29:l:45:TYR:HE2	1.72	0.54
43:G:158:ASP:HB3	43:G:159:PRO:HD3	1.90	0.54
1:1:1637:A:OP1	44:Z:73:LYS:NZ	2.40	0.54
1:1:3036:G:OP1	37:z:17:LYS:HD2	2.08	0.54
4:A:110:ILE:HG12	4:A:152:ILE:HG22	1.90	0.54
42:R:134:HIS:HE1	42:R:136:ARG:HB3	1.69	0.54
53:D:178:HIS:O	53:D:182:THR:OG1	2.26	0.54
55:w:29:SER:OG	60:w:901:SAH:N	2.39	0.54
55:w:32:LYS:NZ	55:w:194:GLU:OE2	2.41	0.54
1:1:498:A:O2'	1:1:3273:A:N1	2.37	0.54
19:W:29:GLU:O	19:W:33:ALA:N	2.27	0.54
22:b:254:MET:HB2	22:b:287:ILE:HG13	1.88	0.54
35:v:157:GLU:O	35:v:161:LYS:HG2	2.08	0.54
38:8:495:ARG:HD2	38:8:522:ILE:HD11	1.90	0.54
1:1:1757:A:OP1	45:U:94:ARG:NH2	2.26	0.54
1:1:1947:G:OP2	1:1:1947:G:N2	2.24	0.54
2:2:57:C:OP2	28:j:68:LYS:NZ	2.39	0.54
40:K:100:LEU:HD13	40:K:266:ILE:HG23	1.89	0.54
53:D:199:ASP:OD1	53:D:200:ARG:N	2.41	0.54
55:w:418:ILE:HG13	55:w:418:ILE:O	2.08	0.54
22:b:209:PHE:CE1	22:b:332:ARG:HD2	2.42	0.54
51:t:236:GLU:HG3	51:t:245:ILE:HG22	1.90	0.54
1:1:2420:C:H2'	1:1:2421:U:H6	1.73	0.54
1:1:2469:G:H2'	1:1:2470:C:C6	2.43	0.54
31:q:463:VAL:HG21	31:q:473:ILE:HG12	1.90	0.54
45:U:13:LYS:HE3	45:U:15:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:p:392:CYS:HG	50:p:434:TRP:CD1	2.25	0.54
1:1:1447:G:N7	15:P:25:SER:OG	2.40	0.53
1:1:1717:U:H2'	1:1:1718:G:C8	2.44	0.53
29:l:148:LYS:HD3	29:l:152:GLU:HG2	1.90	0.53
50:p:428:LYS:HB2	50:p:445:GLN:HB2	1.89	0.53
1:1:121:A:C6	43:G:129:PRO:HG3	2.42	0.53
1:1:257:U:H2'	1:1:258:G:C8	2.43	0.53
1:1:655:C:H2'	1:1:656:A:H8	1.73	0.53
1:1:1920:U:H3'	1:1:1921:A:H8	1.73	0.53
1:1:3120:C:OP1	32:r:30:ARG:NH1	2.40	0.53
4:A:225:LEU:HG	4:A:235:LYS:HE2	1.89	0.53
13:N:114:ARG:NH1	13:N:151:ILE:O	2.42	0.53
43:G:217:THR:HG23	54:o:161:LEU:HD21	1.90	0.53
50:p:335:ILE:HD11	50:p:344:LEU:HD11	1.91	0.53
50:p:350:ALA:C	50:p:351:ARG:HD3	2.33	0.53
52:6:218:A:O2'	52:6:219:A:OP1	2.23	0.53
58:x:10:LEU:HD11	58:x:39:PRO:HG3	1.90	0.53
58:x:423:ASP:OD2	58:x:500:TYR:OH	2.22	0.53
6:C:114:ASN:HB2	6:C:117:GLU:HG3	1.91	0.53
11:L:48:PRO:HG3	35:v:33:ASN:HD22	1.73	0.53
18:T:112:ASN:HA	18:T:115:LYS:HB2	1.91	0.53
31:q:406:ARG:HH11	31:q:451:LEU:HD11	1.73	0.53
32:r:165:PRO:HD2	32:r:168:MET:HE3	1.90	0.53
38:8:33:ILE:HA	38:8:36:ARG:HD2	1.90	0.53
39:I:466:SER:O	39:I:542:LYS:NZ	2.38	0.53
49:n:214:ASP:HB3	49:n:217:ILE:HD12	1.91	0.53
50:p:422:GLN:HB2	50:p:425:VAL:HB	1.90	0.53
57:5:67:ILE:HG22	57:5:70:ARG:HH12	1.73	0.53
1:1:744:A:OP1	16:Q:66:ARG:NH1	2.33	0.53
1:1:1624:G:OP2	49:n:562:LYS:HE3	2.08	0.53
1:1:2831:G:H2'	1:1:2832:C:C6	2.44	0.53
6:C:328:ASN:OD1	8:F:48:ASN:ND2	2.41	0.53
9:H:92:TYR:HB3	9:H:179:ILE:HG12	1.89	0.53
40:K:69:ASP:OD1	40:K:70:ASP:N	2.41	0.53
1:1:863:C:H2'	1:1:864:G:C8	2.44	0.53
30:m:304:GLU:HA	30:m:307:GLN:HG3	1.90	0.53
37:z:14:LYS:HA	37:z:17:LYS:HD3	1.91	0.53
1:1:890:C:H41	38:8:37:ARG:HH21	1.57	0.53
1:1:1355:A:H4'	1:1:1356:U:O5'	2.09	0.53
30:m:218:LYS:NZ	30:m:222:GLU:OE2	2.41	0.53
37:z:49:LEU:HD23	37:z:52:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:x:426:VAL:HG23	58:x:465:PRO:HG3	1.90	0.53
1:1:870:C:O2'	1:1:871:G:OP1	2.24	0.53
19:W:141:ILE:HD12	19:W:179:LYS:HD3	1.91	0.53
1:1:909:G:H2'	1:1:910:G:C8	2.43	0.53
18:T:136:ARG:HD2	18:T:139:ARG:HH21	1.73	0.53
42:R:158:GLU:OE2	58:x:441:ALA:CB	2.57	0.53
50:p:122:SER:OG	50:p:124:ASP:OD1	2.24	0.53
58:x:409:GLU:OE1	58:x:412:ARG:NH2	2.40	0.53
1:1:358:G:N2	1:1:361:A:OP2	2.36	0.53
1:1:808:A:H2'	1:1:809:G:C8	2.44	0.53
2:2:128:U:OP1	2:2:129:C:N4	2.35	0.53
9:H:1:MET:HE1	17:S:138:GLN:HG3	1.89	0.53
17:S:8:GLN:HB2	17:S:64:ILE:HD11	1.89	0.53
31:q:281:ARG:NH1	31:q:284:ASP:OD2	2.42	0.53
32:r:245:VAL:HA	32:r:257:ALA:HA	1.90	0.53
34:u:47:ARG:HH11	55:w:299:GLU:HB2	1.74	0.53
46:c:42:ILE:HD11	46:c:67:VAL:HG22	1.91	0.53
53:D:366:PRO:HB3	53:D:463:TYR:CE1	2.44	0.53
1:1:891:G:H2'	1:1:892:U:C6	2.43	0.53
1:1:1132:C:H2'	1:1:1133:A:H8	1.73	0.53
1:1:3193:C:H2'	1:1:3194:C:C6	2.43	0.53
5:B:292:ALA:HB1	5:B:295:ALA:HB3	1.90	0.53
12:M:135:LEU:HD21	14:O:178:VAL:HG22	1.90	0.53
50:p:290:VAL:HG22	50:p:307:SER:HB3	1.90	0.53
1:1:909:G:H5''	55:w:750:ARG:HH22	1.72	0.52
1:1:2491:A:N3	56:a:35:GLN:NE2	2.57	0.52
15:P:127:ARG:HG3	15:P:139:TYR:HB2	1.89	0.52
17:S:96:ASP:OD1	17:S:97:VAL:N	2.41	0.52
38:8:452:LEU:HD21	38:8:472:ILE:HA	1.91	0.52
53:D:71:ARG:NH1	53:D:250:ILE:HG23	2.25	0.52
58:x:303:LEU:HB2	58:x:308:ARG:HG3	1.90	0.52
1:1:483:G:H2'	1:1:484:C:C6	2.45	0.52
1:1:1612:A:P	48:k:46:ARG:HH21	2.32	0.52
28:j:68:LYS:HD3	35:v:14:VAL:HG21	1.90	0.52
41:V:120:LYS:HB2	41:V:137:VAL:HG22	1.90	0.52
45:U:42:LYS:HA	45:U:47:VAL:HA	1.90	0.52
50:p:341:LEU:HD23	50:p:388:GLU:OE1	2.09	0.52
1:1:528:U:H2'	1:1:529:A:H8	1.74	0.52
1:1:1203:A:C2	1:1:1300:G:H2'	2.45	0.52
19:W:126:ARG:O	19:W:129:THR:OG1	2.26	0.52
43:G:141:ALA:O	43:G:145:ASN:ND2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:5:20:GLN:O	57:5:22:LYS:N	2.41	0.52
1:1:900:G:H1'	1:1:1589:A:N6	2.24	0.52
1:1:2370:G:H5''	1:1:2371:G:H5'	1.92	0.52
1:1:3267:A:H2'	7:E:69:PHE:CZ	2.44	0.52
9:H:162:GLN:NE2	32:r:19:ASP:OD2	2.42	0.52
17:S:69:PRO:O	17:S:97:VAL:HG22	2.10	0.52
31:q:348:ARG:NH2	31:q:413:GLY:O	2.30	0.52
51:t:79:SER:OG	51:t:158:LYS:NZ	2.35	0.52
1:1:585:A:H2'	1:1:586:C:C6	2.45	0.52
1:1:646:A:H2'	1:1:647:A:O4'	2.10	0.52
1:1:775:A:H2'	1:1:776:U:C6	2.44	0.52
1:1:1528:G:O2'	1:1:1588:A:N3	2.39	0.52
13:N:5:LYS:HG2	27:i:40:VAL:HG11	1.92	0.52
29:l:122:SER:HB3	29:l:125:ILE:HD11	1.91	0.52
31:q:211:LEU:HD11	31:q:227:TYR:HB3	1.91	0.52
51:t:70:ARG:NH2	52:6:2:C:O2	2.21	0.52
1:1:953:G:H2'	1:1:1116:G:N7	2.24	0.52
38:8:12:GLN:HA	38:8:16:LEU:HB2	1.91	0.52
38:8:547:ILE:HG13	38:8:548:LYS:H	1.74	0.52
39:I:145:VAL:HG11	55:w:558:ILE:HD12	1.91	0.52
50:p:307:SER:OG	50:p:309:ASP:OD1	2.21	0.52
58:x:249:LEU:HD11	58:x:281:ILE:HD11	1.92	0.52
1:1:503:C:H2'	1:1:504:A:H8	1.75	0.52
1:1:734:C:O2'	1:1:735:A:OP1	2.28	0.52
47:g:54:ILE:HD11	47:g:78:GLY:HA2	1.92	0.52
50:p:146:PRO:HD2	50:p:163:ASN:HB2	1.92	0.52
1:1:63:A:N3	1:1:78:U:O2'	2.39	0.52
1:1:524:U:OP1	12:M:77:ARG:NH2	2.42	0.52
1:1:662:U:H2'	1:1:663:C:C6	2.44	0.52
1:1:850:U:OP1	57:5:70:ARG:NH1	2.43	0.52
1:1:1329:U:O2'	1:1:1330:A:OP1	2.22	0.52
1:1:2942:C:H1'	22:b:41:ARG:NH1	2.25	0.52
43:G:221:ASN:ND2	54:o:154:ASN:O	2.42	0.52
38:8:444:SER:O	38:8:448:TRP:HD1	1.92	0.52
39:I:539:VAL:HG11	39:I:548:LYS:HD2	1.91	0.52
55:w:364:ARG:HG2	55:w:364:ARG:HH11	1.75	0.52
1:1:406:G:N3	2:2:16:G:C2	2.78	0.52
30:m:407:ILE:HD13	51:t:12:LEU:HD22	1.91	0.52
1:1:705:A:O4'	1:1:715:A:N6	2.43	0.51
10:J:284:HIS:O	10:J:287:LYS:HG2	2.10	0.51
34:u:16:GLY:N	41:V:90:GLY:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:R:105:LEU:CD1	42:R:109:TYR:CE2	2.92	0.51
22:b:417:LYS:HD3	22:b:429:ASN:HA	1.93	0.51
1:1:3166:C:H2'	1:1:3167:A:H8	1.75	0.51
58:x:462:PHE:HB2	58:x:489:VAL:HG12	1.92	0.51
19:W:12:LEU:HD11	32:r:65:ILE:HD13	1.91	0.51
22:b:43:ARG:HD2	22:b:116:LEU:O	2.11	0.51
23:d:75:ILE:HG23	23:d:93:VAL:HG22	1.92	0.51
29:l:168:ASP:O	29:l:171:GLU:HG3	2.10	0.51
48:k:22:THR:HG22	48:k:74:LYS:HB3	1.92	0.51
49:n:179:VAL:HG21	49:n:379:LEU:HD11	1.93	0.51
1:1:3192:U:H2'	1:1:3193:C:C6	2.46	0.51
32:r:209:TYR:HB3	32:r:214:VAL:HB	1.93	0.51
55:w:82:MET:SD	55:w:90:THR:OG1	2.68	0.51
1:1:12:A:H2'	1:1:13:A:C8	2.46	0.51
1:1:43:A:H5''	3:7:42:GLN:HG2	1.93	0.51
1:1:1657:C:O2'	1:1:1796:G:O2'	2.28	0.51
30:m:785:ILE:HG22	30:m:794:PHE:HB2	1.91	0.51
31:q:352:MET:HE2	31:q:405:ALA:HB1	1.92	0.51
1:1:678:G:H5''	1:1:678:G:H8	1.76	0.51
1:1:1498:A:H2'	1:1:1499:C:C6	2.45	0.51
4:A:234:PRO:HG3	30:m:128:TYR:HB3	1.93	0.51
7:E:126:GLN:HG3	7:E:127:ASN:H	1.75	0.51
49:n:50:LYS:HE2	49:n:57:THR:HG22	1.92	0.51
53:D:209:GLU:O	53:D:213:ILE:HG12	2.09	0.51
1:1:689:U:O4	6:C:209:TYR:OH	2.27	0.51
2:2:69:U:H2'	2:2:70:G:O4'	2.10	0.51
6:C:31:ARG:HD3	6:C:120:TYR:OH	2.09	0.51
49:n:7:ASN:HB3	49:n:54:LYS:HB3	1.92	0.51
55:w:62:GLN:HG3	55:w:85:MET:HE3	1.93	0.51
1:1:475:G:H2'	1:1:476:G:C8	2.46	0.51
1:1:490:A:H2'	1:1:491:C:C6	2.46	0.51
1:1:1195:A:H5''	1:1:1196:C:H5''	1.92	0.51
1:1:1260:A:HO2'	1:1:1279:C:HO2'	1.59	0.51
1:1:2924:U:OP2	1:1:2924:U:H6	1.93	0.51
13:N:36:ILE:HG12	13:N:64:VAL:HG23	1.93	0.51
15:P:42:THR:HG22	15:P:46:LYS:HE3	1.93	0.51
43:G:99:PRO:HD3	43:G:132:VAL:HG22	1.92	0.51
55:w:182:ALA:HA	55:w:197:VAL:HA	1.93	0.51
1:1:1899:G:O2'	1:1:2334:U:O4	2.25	0.51
5:B:284:ARG:NH1	5:B:293:ASN:O	2.42	0.51
19:W:38:ARG:NH1	19:W:39:TYR:OH	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:l:28:VAL:HG23	29:l:29:ASP:H	1.76	0.51
29:l:148:LYS:HD2	29:l:156:MET:HE2	1.93	0.51
30:m:473:TYR:OH	30:m:586:ASP:OD2	2.28	0.51
1:1:1404:G:N2	1:1:1407:A:OP2	2.31	0.50
1:1:2942:C:O2	22:b:41:ARG:NH1	2.41	0.50
1:1:2952:G:N7	1:1:2953:U:N3	2.58	0.50
22:b:175:TYR:H	22:b:178:VAL:HG11	1.76	0.50
34:u:2:ARG:NH1	36:y:78:ASP:OD2	2.44	0.50
39:I:331:GLU:HG3	39:I:428:SER:HB2	1.93	0.50
45:U:35:LYS:HA	45:U:38:ILE:HD12	1.91	0.50
56:a:55:LEU:HD11	56:a:155:ILE:HG12	1.94	0.50
57:5:153:THR:CG2	58:x:227:ASN:O	2.59	0.50
58:x:381:ASP:HB3	58:x:444:ILE:HG12	1.93	0.50
1:1:475:G:H2'	1:1:476:G:H8	1.76	0.50
1:1:1176:C:H2'	1:1:1177:G:N2	2.25	0.50
22:b:18:LEU:HD21	22:b:137:ALA:HA	1.94	0.50
30:m:446:ASP:OD2	30:m:448:SER:OG	2.28	0.50
31:q:322:TYR:HB2	31:q:327:TYR:CZ	2.47	0.50
36:y:63:THR:HG22	36:y:72:VAL:HG12	1.93	0.50
36:y:97:VAL:HG12	36:y:128:LEU:HD12	1.93	0.50
48:k:26:LYS:HD2	48:k:78:LEU:HD13	1.93	0.50
50:p:250:ILE:HD12	50:p:262:ARG:HG3	1.92	0.50
1:1:239:G:H2'	1:1:240:U:C6	2.45	0.50
1:1:2951:G:N3	1:1:2951:G:H5''	2.26	0.50
9:H:89:LYS:HG2	9:H:145:VAL:HG22	1.93	0.50
31:q:221:GLY:O	31:q:222:ARG:HG2	2.11	0.50
38:8:628:LYS:HG3	38:8:629:ARG:HG3	1.93	0.50
44:Z:23:VAL:HG12	44:Z:45:GLY:HA3	1.93	0.50
53:D:299:CYS:HB3	53:D:320:HIS:HB2	1.93	0.50
57:5:155:VAL:HG12	58:x:226:VAL:HG22	1.92	0.50
1:1:1062:A:O4'	18:T:108:ARG:NH2	2.44	0.50
1:1:2830:G:H2'	1:1:2831:G:H8	1.76	0.50
9:H:86:TYR:CZ	9:H:151:VAL:HG22	2.46	0.50
22:b:523:LYS:HD3	42:R:51:VAL:HG13	1.94	0.50
36:y:72:VAL:HG23	36:y:96:ARG:HG2	1.92	0.50
39:I:602:SER:HA	39:I:605:TYR:HD2	1.77	0.50
43:G:203:VAL:HG21	43:G:211:LEU:HD22	1.93	0.50
53:D:119:VAL:HG22	53:D:194:ILE:HB	1.92	0.50
53:D:308:LEU:O	53:D:312:ILE:HG12	2.12	0.50
1:1:481:U:H3	1:1:484:C:H41	1.59	0.50
1:1:953:G:H2'	1:1:1116:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:984:G:H22	1:1:1138:U:H5''	1.76	0.50
50:p:332:LEU:HA	50:p:348:SER:HA	1.91	0.50
1:1:916:G:H5''	1:1:916:G:C8	2.38	0.50
1:1:2328:U:H2'	1:1:2329:C:C6	2.47	0.50
1:1:2604:U:H2'	1:1:2605:G:O4'	2.12	0.50
38:8:547:ILE:HG13	38:8:548:LYS:N	2.26	0.50
42:R:151:ARG:NH2	58:x:442:THR:CB	2.67	0.50
53:D:296:LEU:HD12	53:D:302:VAL:HA	1.94	0.50
58:x:405:ALA:O	58:x:406:ASN:HB2	2.11	0.50
1:1:907:G:H8	1:1:907:G:O5'	1.94	0.50
4:A:98:TYR:CD2	4:A:111:LYS:HE2	2.47	0.50
5:B:47:LEU:HD12	5:B:335:ILE:HD11	1.94	0.50
5:B:61:ASP:HB3	22:b:413:ASN:HD21	1.75	0.50
26:h:117:ALA:HB1	35:v:55:LEU:HD22	1.93	0.50
38:8:68:ASP:OD1	38:8:69:MET:N	2.45	0.50
1:1:363:G:OP2	28:j:56:ARG:NH2	2.38	0.50
22:b:204:LEU:O	32:r:4:ASN:ND2	2.38	0.50
25:f:16:TYR:OH	25:f:89:LEU:O	2.21	0.50
35:v:225:ARG:NH2	35:v:226:ASN:OD1	2.45	0.50
50:p:309:ASP:OD1	50:p:311:THR:OG1	2.30	0.50
58:x:5:LEU:O	58:x:29:THR:OG1	2.30	0.50
1:1:394:G:N1	1:1:397:A:OP2	2.39	0.50
1:1:910:G:H2'	1:1:911:C:H6	1.77	0.50
1:1:1283:C:HO2'	1:1:1284:C:P	2.33	0.50
1:1:1799:A:H2'	1:1:1800:A:C8	2.46	0.50
1:1:2367:A:H2'	1:1:2368:A:C8	2.46	0.50
1:1:2842:U:OP1	1:1:2844:C:N4	2.45	0.50
1:1:3322:A:H2'	1:1:3323:A:C8	2.46	0.50
4:A:214:GLU:OE2	4:A:218:ARG:HD3	2.12	0.50
5:B:165:GLN:OE1	5:B:167:ARG:NH2	2.44	0.50
38:8:595:LEU:HD23	38:8:615:VAL:HB	1.93	0.50
55:w:39:LYS:HD3	55:w:40:TYR:CE2	2.47	0.50
58:x:420:ASP:OD1	58:x:505:ARG:NH1	2.40	0.50
4:A:185:LYS:HG2	4:A:222:THR:HB	1.94	0.49
11:L:70:ARG:NH1	11:L:71:ALA:O	2.45	0.49
1:1:3194:C:O2'	1:1:3195:U:O2	2.30	0.49
3:7:112:ILE:HG23	29:l:24:ILE:HG13	1.94	0.49
5:B:152:LYS:HG2	5:B:189:SER:HA	1.93	0.49
6:C:69:ARG:NH1	55:w:807:GLY:O	2.43	0.49
30:m:255:PRO:HB3	43:G:145:ASN:HA	1.93	0.49
30:m:732:HIS:HD2	30:m:786:TRP:CE3	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:566:GLN:HA	38:8:566:GLN:HE21	1.75	0.49
50:p:285:SER:HB3	50:p:315:TRP:CH2	2.47	0.49
54:o:126:LYS:HG3	54:o:179:TYR:CD2	2.46	0.49
1:1:1551:C:O2'	1:1:1552:G:OP1	2.24	0.49
4:A:287:ASP:O	6:C:266:THR:OG1	2.29	0.49
4:A:287:ASP:OD2	6:C:24:ALA:HB2	2.12	0.49
8:F:98:LYS:HB3	8:F:99:PRO:HD3	1.92	0.49
22:b:375:THR:O	36:y:113:TYR:OH	2.24	0.49
38:8:628:LYS:HE3	38:8:629:ARG:HE	1.78	0.49
38:8:669:GLU:HB2	38:8:672:ARG:HH21	1.78	0.49
58:x:33:VAL:HG22	58:x:226:VAL:HG21	1.93	0.49
3:7:86:PRO:HG2	10:J:272:LEU:HA	1.95	0.49
5:B:117:ARG:HA	5:B:175:LYS:HE3	1.95	0.49
36:y:155:SER:OG	36:y:156:ASN:N	2.46	0.49
1:1:406:G:H1'	2:2:16:G:N2	2.27	0.49
1:1:1799:A:H2'	1:1:1800:A:H8	1.77	0.49
1:1:2461:A:H62	1:1:2483:G:H21	1.60	0.49
1:1:3165:A:H2'	1:1:3166:C:H6	1.77	0.49
43:G:92:LYS:O	43:G:96:LYS:NZ	2.45	0.49
58:x:34:GLN:HG2	58:x:60:ALA:HB2	1.95	0.49
1:1:651:G:O2'	1:1:1435:A:OP1	2.31	0.49
6:C:138:ARG:HD3	6:C:245:GLY:O	2.13	0.49
10:J:223:VAL:HG11	10:J:253:ALA:HA	1.95	0.49
38:8:437:TYR:HE1	38:8:482:VAL:HG13	1.76	0.49
40:K:37:VAL:HG12	40:K:260:VAL:HG12	1.95	0.49
51:t:74:ARG:NH2	51:t:189:VAL:O	2.40	0.49
39:I:260:ILE:HD13	39:I:272:ILE:HB	1.95	0.49
1:1:155:G:H4'	1:1:156:G:H2'	1.94	0.49
1:1:820:A:H61	1:1:905:U:H3	1.59	0.49
1:1:952:A:H2'	1:1:953:G:O4'	2.11	0.49
1:1:1896:A:H61	1:1:2339:C:N4	2.07	0.49
1:1:2328:U:H2'	1:1:2329:C:H6	1.78	0.49
1:1:2830:G:H1'	22:b:131:ALA:HA	1.95	0.49
13:N:7:LEU:HD11	43:G:162:LEU:HD23	1.94	0.49
19:W:20:ARG:HA	19:W:23:LYS:HD3	1.94	0.49
22:b:221:THR:HG22	22:b:223:GLY:H	1.78	0.49
50:p:226:SER:OG	50:p:227:TYR:N	2.46	0.49
4:A:270:ARG:HH11	4:A:273:LYS:NZ	2.10	0.49
5:B:95:THR:HB	5:B:98:GLY:O	2.12	0.49
5:B:138:ALA:O	5:B:139:GLN:HG3	2.13	0.49
40:K:277:ARG:NH1	52:6:36:U:O3'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:g:51:LEU:HB3	47:g:54:ILE:HD12	1.94	0.49
50:p:355:LEU:HD12	50:p:369:GLN:HB2	1.94	0.49
50:p:416:ARG:HH11	50:p:429:VAL:HG22	1.78	0.49
55:w:39:LYS:HG3	57:5:213:PHE:CD1	2.48	0.49
12:M:12:TRP:CZ2	17:S:153:PRO:HB3	2.48	0.49
19:W:82:GLU:HG2	19:W:83:GLU:OE1	2.13	0.49
32:r:198:LEU:HB2	32:r:222:GLU:HG3	1.93	0.49
42:R:98:ARG:HD2	42:R:133:LYS:O	2.12	0.49
47:g:15:THR:HG22	47:g:17:SER:H	1.78	0.49
50:p:434:TRP:CH2	50:p:440:ILE:HD11	2.48	0.49
55:w:211:ARG:NH2	57:5:31:PHE:O	2.46	0.49
58:x:262:LYS:N	58:x:340:ASP:OD2	2.38	0.49
1:1:424:G:N3	24:e:24:ARG:NH2	2.58	0.48
1:1:1062:A:H1'	18:T:130:ARG:HH22	1.77	0.48
5:B:112:ASP:O	5:B:116:ARG:HG3	2.13	0.48
5:B:218:ILE:HG12	5:B:276:THR:HG23	1.95	0.48
18:T:104:GLU:O	18:T:108:ARG:HG2	2.12	0.48
22:b:422:LEU:HD13	34:u:81:TYR:HD2	1.77	0.48
30:m:789:ARG:HG3	30:m:790:GLU:HG2	1.95	0.48
49:n:417:LEU:HD11	49:n:420:LYS:HB2	1.95	0.48
1:1:754:G:C6	1:1:779:G:C6	3.01	0.48
22:b:301:GLU:O	22:b:304:GLN:HG3	2.14	0.48
49:n:237:TYR:CE2	49:n:246:PRO:HG3	2.48	0.48
50:p:111:VAL:HG22	50:p:118:ILE:HG22	1.95	0.48
55:w:794:THR:HG23	55:w:813:LYS:HE3	1.94	0.48
1:1:92:G:H5''	1:1:94:G:N7	2.28	0.48
1:1:655:C:H2'	1:1:656:A:C8	2.47	0.48
1:1:2428:U:H5'	31:q:412:ILE:HD11	1.95	0.48
39:I:195:ARG:NH2	55:w:488:GLN:O	2.46	0.48
1:1:759:U:H3'	1:1:760:G:H5''	1.94	0.48
14:O:59:ARG:NH1	33:s:3:VAL:O	2.44	0.48
22:b:250:VAL:HG13	22:b:283:VAL:HG13	1.96	0.48
38:8:550:THR:HG23	38:8:552:ALA:H	1.77	0.48
39:I:175:LYS:HA	39:I:178:MET:HE2	1.95	0.48
58:x:58:THR:HA	58:x:61:PHE:CE2	2.48	0.48
1:1:275:U:H2'	1:1:276:U:C6	2.49	0.48
1:1:1544:G:O2'	3:7:12:LEU:O	2.31	0.48
1:1:1857:C:OP1	38:8:6:LYS:NZ	2.42	0.48
1:1:2318:U:OP2	57:5:53:LYS:NZ	2.47	0.48
1:1:2909:U:H2'	1:1:2910:A:O4'	2.14	0.48
2:2:111:A:O2'	2:2:112:U:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:387:LEU:HD11	34:u:109:LYS:HG2	1.96	0.48
6:C:292:SER:OG	6:C:294:GLU:OE1	2.32	0.48
8:F:73:GLY:O	18:T:143:THR:OG1	2.31	0.48
8:F:79:ALA:HB2	18:T:138:SER:HB3	1.95	0.48
30:m:467:LEU:HD21	50:p:308:GLN:HE22	1.78	0.48
39:I:277:LEU:HD11	39:I:314:ILE:HG23	1.94	0.48
46:c:74:ASN:ND2	46:c:86:ARG:HD2	2.28	0.48
55:w:551:LEU:O	55:w:556:ARG:NH2	2.47	0.48
1:1:377:A:H1'	1:1:392:G:N2	2.29	0.48
1:1:490:A:H2'	1:1:491:C:H6	1.79	0.48
1:1:754:G:C6	1:1:779:G:O6	2.66	0.48
1:1:2125:A:OP1	57:5:47:LYS:HD3	2.13	0.48
1:1:2942:C:H5'	1:1:2943:G:O3'	2.14	0.48
1:1:2976:A:HO2'	1:1:2977:G:H8	1.62	0.48
15:P:175:ARG:O	15:P:179:GLN:HG2	2.13	0.48
29:l:20:ILE:HG13	29:l:21:GLY:H	1.78	0.48
38:8:633:GLU:HA	39:I:607:SER:HB3	1.96	0.48
39:I:464:LEU:HA	39:I:468:GLU:HB2	1.96	0.48
39:I:510:CYS:HB2	39:I:579:THR:HG23	1.94	0.48
49:n:30:ALA:O	49:n:34:ARG:HG3	2.13	0.48
54:o:163:GLN:HB3	54:o:165:ARG:NH1	2.29	0.48
58:x:94:GLU:HG2	58:x:312:LEU:HD22	1.95	0.48
58:x:331:ALA:HB3	58:x:353:MET:HE2	1.96	0.48
1:1:2103:U:O2	58:x:526:LYS:HD3	2.14	0.48
9:H:9:GLN:HB3	9:H:52:LEU:HD11	1.95	0.48
20:X:108:LEU:HD23	20:X:125:ARG:HD3	1.95	0.48
22:b:463:LEU:HD23	22:b:468:PHE:CG	2.48	0.48
23:d:26:LYS:NZ	23:d:65:LYS:HD2	2.29	0.48
34:u:47:ARG:HG3	34:u:54:ALA:HB1	1.95	0.48
49:n:402:ILE:HG13	49:n:403:ASP:N	2.29	0.48
53:D:276:ARG:NH2	53:D:365:ASP:OD1	2.45	0.48
55:w:71:ASN:HB2	57:5:11:THR:O	2.14	0.48
55:w:186:PRO:HG2	57:5:216:LEU:HG	1.96	0.48
57:5:160:LEU:HB2	58:x:221:PRO:HG2	1.94	0.48
1:1:952:A:H4'	1:1:968:G:N2	2.29	0.48
1:1:3204:C:H2'	1:1:3205:G:C8	2.48	0.48
5:B:71:GLU:HG2	5:B:357:LYS:HE3	1.96	0.48
19:W:39:TYR:HB3	19:W:220:TYR:HE1	1.78	0.48
29:l:69:CYS:O	29:l:84:THR:OG1	2.23	0.48
31:q:486:GLU:HA	31:q:489:ILE:HG22	1.95	0.48
36:y:4:ARG:HH11	36:y:215:LEU:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:I:234:LEU:HD22	39:I:248:LEU:HB3	1.95	0.48
50:p:246:PRO:HG3	50:p:276:ARG:NH1	2.29	0.48
55:w:809:PRO:HG2	55:w:812:VAL:HG21	1.96	0.48
1:1:375:A:OP2	21:Y:89:LYS:NZ	2.45	0.48
1:1:383:G:N2	1:1:386:A:OP2	2.37	0.48
1:1:847:A:H2'	1:1:848:A:O4'	2.14	0.48
1:1:3291:G:H2'	1:1:3292:A:C8	2.48	0.48
19:W:84:GLU:OE2	19:W:90:TYR:N	2.45	0.48
30:m:426:PRO:HA	30:m:807:THR:HA	1.96	0.48
39:I:601:ILE:O	39:I:604:LEU:HD23	2.14	0.48
46:c:13:LYS:HB3	46:c:100:ILE:HB	1.96	0.48
49:n:420:LYS:HA	49:n:426:TYR:HE2	1.78	0.48
1:1:599:C:OP1	6:C:332:LYS:HE3	2.13	0.48
1:1:644:G:H4'	1:1:1116:G:N2	2.28	0.48
1:1:1643:A:H2'	1:1:1644:C:C2	2.49	0.48
1:1:2926:A:C2	55:w:7:LYS:HB3	2.49	0.48
1:1:3166:C:H2'	1:1:3167:A:C8	2.49	0.48
12:M:15:VAL:HG23	12:M:35:ILE:HD13	1.94	0.48
22:b:37:PHE:HB3	22:b:41:ARG:HD3	1.96	0.48
29:l:31:LYS:HZ3	39:I:625:ARG:HH12	1.60	0.48
39:I:320:LYS:HG2	55:w:642:GLU:OE2	2.13	0.48
42:R:136:ARG:HG2	42:R:136:ARG:HH11	1.78	0.48
53:D:122:PRO:HB3	53:D:201:ILE:HG12	1.96	0.48
55:w:374:LYS:O	55:w:378:LYS:HG2	2.13	0.48
58:x:524:LYS:O	58:x:528:GLU:HG2	2.14	0.48
1:1:119:U:H5'	30:m:265:ARG:HG2	1.94	0.47
1:1:501:A:H2'	1:1:502:U:C6	2.49	0.47
1:1:1228:C:H2'	1:1:1229:G:H8	1.79	0.47
1:1:2855:U:H2'	1:1:2856:G:H8	1.79	0.47
1:1:3047:U:O2'	1:1:3048:A:H5'	2.14	0.47
3:7:124:GLU:OE1	3:7:128:GLU:HB3	2.14	0.47
13:N:63:ARG:NH2	13:N:131:GLU:OE2	2.46	0.47
19:W:123:ASP:N	19:W:211:SER:O	2.44	0.47
22:b:169:THR:HB	22:b:248:SER:HB3	1.95	0.47
22:b:187:ILE:HG23	22:b:188:THR:HG23	1.95	0.47
22:b:285:VAL:HB	22:b:317:ILE:HD13	1.97	0.47
29:l:40:GLN:HB3	29:l:45:TYR:CE2	2.49	0.47
46:c:74:ASN:HD21	55:w:389:MET:HE3	1.79	0.47
56:a:148:VAL:HB	56:a:152:ARG:HH21	1.79	0.47
1:1:190:U:H2'	21:Y:60:ARG:HH22	1.79	0.47
1:1:2419:A:H2'	1:1:2420:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2420:C:H2'	1:1:2421:U:C6	2.48	0.47
1:1:2923:PSU:H2'	1:1:2924:U:C6	2.49	0.47
6:C:349:THR:HG21	8:F:67:ARG:HB3	1.96	0.47
11:L:47:ALA:HB1	35:v:36:ILE:HG21	1.95	0.47
28:j:52:LYS:HE3	28:j:52:LYS:HB2	1.68	0.47
39:I:483:ILE:HG13	39:I:495:LEU:HD11	1.95	0.47
56:a:74:VAL:HG12	56:a:78:LYS:HZ2	1.78	0.47
1:1:631:U:H2'	1:1:632:G:C8	2.49	0.47
1:1:1480:G:O2'	1:1:1871:U:O4	2.29	0.47
3:7:99:PHE:HB3	29:l:3:GLN:HG3	1.96	0.47
4:A:31:GLN:HB2	4:A:163:PRO:HG3	1.97	0.47
7:E:51:ARG:O	7:E:72:ASN:ND2	2.48	0.47
8:F:85:PHE:HB2	8:F:139:PRO:HG3	1.95	0.47
13:N:60:VAL:HB	13:N:134:LEU:HB2	1.95	0.47
29:l:124:ASP:H	29:l:150:THR:HG21	1.79	0.47
31:q:508:ILE:HG13	31:q:531:TYR:HE1	1.79	0.47
39:I:137:LEU:HD21	39:I:173:THR:HG22	1.95	0.47
40:K:173:PHE:O	40:K:176:GLN:HG2	2.14	0.47
45:U:41:ILE:HG23	45:U:43:VAL:HG23	1.96	0.47
52:6:61:G:H2'	52:6:62:G:C8	2.50	0.47
1:1:492:U:H2'	1:1:493:G:C8	2.49	0.47
1:1:707:U:H2'	1:1:708:G:O4'	2.14	0.47
4:A:106:ASN:HD22	30:m:136:ILE:HG23	1.80	0.47
25:f:49:ILE:HD11	25:f:71:VAL:HG22	1.97	0.47
31:q:336:LEU:HD12	31:q:506:LEU:HD13	1.95	0.47
55:w:30:SER:HB3	55:w:59:SER:HB2	1.96	0.47
55:w:156:PHE:HB3	55:w:199:CYS:SG	2.54	0.47
58:x:69:VAL:HG21	58:x:144:ILE:HD11	1.95	0.47
1:1:1654:A:OP2	39:I:371:LYS:NZ	2.48	0.47
5:B:286:GLY:HA3	5:B:321:PHE:CE2	2.49	0.47
27:i:45:ARG:NH2	27:i:49:GLY:O	2.42	0.47
42:R:155:LEU:HD13	55:w:359:LEU:HD23	1.96	0.47
58:x:543:LYS:HE2	58:x:547:LEU:HG	1.96	0.47
1:1:157:A:H2'	1:1:158:G:O4'	2.14	0.47
1:1:444:U:H2'	1:1:445:G:C8	2.49	0.47
19:W:50:THR:N	19:W:51:PRO:HD2	2.28	0.47
22:b:175:TYR:HE2	22:b:262:PHE:HD2	1.63	0.47
30:m:277:MET:HE1	43:G:116:VAL:HG11	1.96	0.47
31:q:297:GLN:HG2	31:q:310:PHE:HE2	1.78	0.47
43:G:95:ASN:OD1	43:G:98:ARG:NH2	2.24	0.47
50:p:274:ILE:H	50:p:274:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D:190:LEU:HD22	53:D:217:LEU:HD22	1.96	0.47
56:a:43:PRO:HB3	56:a:159:LEU:HD21	1.97	0.47
1:1:656:A:H2'	1:1:657:A:C8	2.50	0.47
1:1:748:U:H2'	1:1:749:C:C6	2.50	0.47
1:1:1669:C:H5'	47:g:30:LEU:HD11	1.97	0.47
1:1:1894:U:O2'	1:1:3054:U:OP1	2.32	0.47
1:1:1940:G:N3	58:x:434:LYS:HB2	2.30	0.47
2:2:63:G:H22	2:2:97:A:H2	1.61	0.47
23:d:79:ARG:HG2	23:d:79:ARG:HH11	1.79	0.47
31:q:214:PHE:CE2	31:q:223:SER:HB2	2.50	0.47
32:r:182:ALA:HB2	32:r:197:ILE:HD11	1.96	0.47
38:8:318:LEU:O	38:8:322:ILE:N	2.43	0.47
39:I:335:ASN:HD22	39:I:527:PRO:HG3	1.80	0.47
40:K:80:LEU:HB2	40:K:248:LEU:HD11	1.96	0.47
41:V:30:GLY:HA3	41:V:66:LYS:HE2	1.96	0.47
41:V:80:ARG:HH12	41:V:116:GLY:HA3	1.80	0.47
49:n:206:PRO:HB2	51:t:228:VAL:HB	1.95	0.47
53:D:65:MET:HE3	53:D:69:GLN:HG3	1.96	0.47
55:w:257:THR:O	55:w:279:THR:N	2.40	0.47
1:1:1448:U:O2'	1:1:2983:C:O2	2.22	0.47
1:1:1615:C:H2'	1:1:1616:U:C6	2.50	0.47
8:F:103:LEU:HD23	8:F:108:LEU:HD12	1.97	0.47
22:b:462:LYS:HG3	22:b:463:LEU:HD12	1.97	0.47
27:i:54:GLU:HG2	27:i:90:MET:SD	2.55	0.47
31:q:380:LYS:O	31:q:383:THR:HG22	2.15	0.47
41:V:22:ILE:HB	55:w:243:ARG:HD2	1.96	0.47
1:1:8:C:H2'	1:1:9:U:C6	2.50	0.47
1:1:616:G:H2'	1:1:617:G:C8	2.50	0.47
1:1:1213:G:OP1	17:S:139:TYR:OH	2.27	0.47
17:S:132:THR:HG23	17:S:144:LEU:HD13	1.96	0.47
20:X:131:ASP:O	20:X:135:ILE:HG12	2.15	0.47
31:q:210:VAL:HG23	31:q:211:LEU:HD12	1.97	0.47
38:8:528:PHE:HE1	38:8:563:LEU:HD22	1.80	0.47
39:I:465:SER:OG	39:I:466:SER:N	2.48	0.47
40:K:279:ILE:HB	40:K:292:TYR:HB3	1.95	0.47
56:a:50:SER:OG	56:a:158:GLN:OE1	2.33	0.47
1:1:893:C:H41	38:8:39:ASN:HD21	1.61	0.47
1:1:1895:A:O2'	1:1:3053:G:H4'	2.14	0.47
1:1:2396:G:H1	1:1:2984:C:H42	1.62	0.47
2:2:95:G:O2'	28:j:81:GLY:O	2.27	0.47
3:7:45:PRO:HB2	3:7:50:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:540:HIS:CD2	45:U:27:VAL:HA	2.49	0.47
26:h:118:ILE:HG22	26:h:119:LYS:H	1.80	0.47
40:K:85:ASN:OD1	40:K:86:LYS:N	2.47	0.47
53:D:457:HIS:O	53:D:460:LYS:NZ	2.43	0.47
58:x:419:ARG:NH1	58:x:498:TYR:HB3	2.30	0.47
1:1:41:G:O6	1:1:43:A:C6	2.68	0.46
1:1:1534:A:H2'	1:1:1535:A:C8	2.51	0.46
22:b:275:LYS:NZ	22:b:312:VAL:HG22	2.30	0.46
44:Z:41:ALA:HB2	44:Z:77:TYR:HE1	1.79	0.46
46:c:10:ILE:HA	46:c:13:LYS:HE2	1.96	0.46
55:w:83:LYS:HG3	55:w:84:PRO:HD2	1.97	0.46
1:1:1312:C:O2'	14:O:83:ALA:O	2.33	0.46
1:1:2597:U:H3'	1:1:2598:G:C8	2.51	0.46
1:1:2831:G:H2'	1:1:2832:C:H6	1.81	0.46
30:m:375:ARG:HH21	49:n:415:PRO:HD3	1.80	0.46
32:r:199:ALA:H	32:r:222:GLU:HB3	1.78	0.46
35:v:208:TYR:O	35:v:210:GLN:N	2.46	0.46
38:8:377:MET:HB3	38:8:381:ASN:OD1	2.15	0.46
51:t:143:PHE:CZ	51:t:207:LEU:HD21	2.51	0.46
1:1:737:G:H2'	1:1:738:A:C8	2.50	0.46
1:1:782:U:H2'	1:1:783:A:O4'	2.16	0.46
1:1:834:U:H2'	1:1:835:G:O4'	2.15	0.46
1:1:1717:U:H2'	1:1:1718:G:H8	1.78	0.46
1:1:2097:U:H2'	1:1:2098:C:C6	2.50	0.46
5:B:322:ILE:HG22	5:B:324:VAL:HG23	1.97	0.46
33:s:13:THR:HA	33:s:16:LYS:HE3	1.98	0.46
40:K:183:ASP:HB3	40:K:186:ILE:HG22	1.96	0.46
50:p:217:SER:HB2	50:p:300:ASN:OD1	2.15	0.46
58:x:69:VAL:HG13	58:x:74:ALA:HB3	1.97	0.46
1:1:364:G:OP1	6:C:60:THR:OG1	2.26	0.46
1:1:520:U:O4	6:C:349:THR:HG22	2.16	0.46
1:1:700:C:OP1	11:L:65:TYR:OH	2.31	0.46
1:1:733:G:N2	1:1:736:A:OP2	2.43	0.46
1:1:794:U:H2'	1:1:795:G:H8	1.81	0.46
1:1:1507:G:C6	15:P:129:THR:HG21	2.51	0.46
1:1:1873:U:OP2	42:R:20:ARG:NH2	2.48	0.46
1:1:2951:G:C8	55:w:10:LYS:HA	2.50	0.46
4:A:96:ASP:OD1	4:A:249:ARG:NH2	2.49	0.46
10:J:289:LYS:O	10:J:293:ILE:HG12	2.14	0.46
29:l:21:GLY:C	29:l:23:ASN:H	2.24	0.46
30:m:648:HIS:ND1	30:m:649:PRO:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:q:204:MET:HG3	31:q:234:ASP:OD1	2.14	0.46
40:K:156:CYS:SG	40:K:157:GLY:N	2.89	0.46
47:g:58:ARG:HB2	47:g:61:GLN:HG3	1.97	0.46
53:D:157:GLU:OE1	53:D:174:ARG:NH1	2.48	0.46
55:w:101:ARG:NE	55:w:148:GLU:OE2	2.46	0.46
1:1:276:U:O2'	13:N:93:LYS:HE2	2.15	0.46
1:1:1965:C:OP1	1:1:1965:C:H4'	2.14	0.46
1:1:2395:G:H2'	1:1:2396:G:H8	1.78	0.46
1:1:2466:G:H3'	1:1:2467:G:H8	1.80	0.46
7:E:40:LEU:HD11	7:E:54:TYR:HB2	1.97	0.46
9:H:41:ILE:HG22	9:H:43:VAL:HG13	1.98	0.46
19:W:97:SER:O	19:W:100:THR:OG1	2.34	0.46
26:h:31:LEU:HB3	26:h:44:ILE:HG12	1.97	0.46
29:l:19:TYR:OH	29:l:166:GLN:OE1	2.33	0.46
38:8:502:LEU:HB2	38:8:515:ILE:HD12	1.97	0.46
38:8:529:THR:HG22	38:8:530:LYS:N	2.30	0.46
51:t:239:LEU:HD12	51:t:239:LEU:O	2.15	0.46
53:D:158:ALA:O	53:D:162:MET:HG2	2.16	0.46
55:w:549:HIS:HB2	55:w:556:ARG:NH2	2.21	0.46
1:1:29:C:H4'	1:1:62:A:H4'	1.97	0.46
1:1:806:A:O2'	1:1:807:A:H5'	2.16	0.46
1:1:1348:U:H4'	1:1:1349:G:OP1	2.15	0.46
1:1:1383:G:O2'	6:C:138:ARG:NH1	2.48	0.46
1:1:3218:A:O2'	1:1:3278:C:H5	1.99	0.46
1:1:3322:A:H2'	1:1:3323:A:H8	1.79	0.46
4:A:80:LEU:HD12	27:i:67:LYS:HG3	1.98	0.46
4:A:191:TYR:HB3	4:A:212:LEU:HB3	1.96	0.46
50:p:166:THR:HG22	50:p:205:GLU:HG2	1.97	0.46
52:6:61:G:H2'	52:6:62:G:H8	1.81	0.46
1:1:634:C:H5'	25:f:21:ARG:O	2.16	0.46
1:1:1679:A:OP1	45:U:94:ARG:NE	2.45	0.46
1:1:1688:U:H2'	1:1:1689:U:C6	2.51	0.46
1:1:2440:G:H2'	1:1:2441:A:C8	2.51	0.46
5:B:216:ASP:CB	5:B:278:ILE:HA	2.46	0.46
22:b:184:LEU:HD23	22:b:192:VAL:HG21	1.98	0.46
30:m:123:ASN:HB3	30:m:137:LYS:HA	1.97	0.46
38:8:267:VAL:O	38:8:271:SER:N	2.45	0.46
38:8:550:THR:HG23	38:8:552:ALA:N	2.31	0.46
55:w:420:ASN:O	55:w:424:LYS:HG2	2.16	0.46
6:C:187:LEU:HG	6:C:193:LYS:HD3	1.98	0.46
8:F:40:LYS:NZ	8:F:170:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:318:MET:HE2	22:b:331:VAL:HG22	1.97	0.46
29:l:26:PHE:O	29:l:30:ASN:ND2	2.49	0.46
35:v:50:TYR:CG	35:v:57:ALA:HB2	2.51	0.46
38:8:395:GLU:HB3	38:8:467:PRO:HB2	1.97	0.46
50:p:138:LYS:HD3	50:p:172:THR:HG21	1.96	0.46
1:1:696:C:H1'	35:v:65:GLY:H	1.80	0.46
4:A:173:ILE:HD13	10:J:261:LEU:HD13	1.97	0.46
10:J:212:TRP:CZ3	10:J:220:HIS:HB3	2.51	0.46
19:W:92:LEU:HD22	19:W:221:TYR:HB2	1.98	0.46
27:i:57:LEU:HD21	27:i:73:ALA:HB2	1.98	0.46
31:q:204:MET:HE1	31:q:238:TYR:CD2	2.51	0.46
31:q:290:VAL:HG13	55:w:70:VAL:HG21	1.97	0.46
45:U:43:VAL:HG12	45:U:44:GLU:HG2	1.98	0.46
1:1:316:U:HO2'	27:i:29:LYS:NZ	2.13	0.46
1:1:913:A:H8	1:1:913:A:O5'	1.99	0.46
1:1:2344:U:H2'	1:1:2345:A:C8	2.51	0.46
1:1:2855:U:H2'	1:1:2856:G:C8	2.51	0.46
38:8:73:THR:HA	38:8:76:GLU:HG2	1.98	0.46
38:8:585:PRO:HB2	39:I:618:MET:HE1	1.98	0.46
50:p:97:LEU:HD21	50:p:453:LYS:HG3	1.98	0.46
50:p:382:ASP:OD2	50:p:433:LYS:HA	2.15	0.46
56:a:63:MET:HG2	56:a:65:ILE:HG12	1.98	0.46
1:1:1256:G:H2'	1:1:1257:C:C6	2.51	0.45
1:1:1282:G:H2'	1:1:1283:C:C6	2.51	0.45
1:1:1448:U:H5''	15:P:66:SER:HB2	1.96	0.45
1:1:1798:A:H2'	1:1:1799:A:C8	2.51	0.45
1:1:1936:A:N3	1:1:1936:A:H2'	2.32	0.45
2:2:74:U:C4	21:Y:74:TYR:CD1	3.04	0.45
19:W:42:VAL:HG13	19:W:92:LEU:HD12	1.98	0.45
54:o:88:GLU:OE1	54:o:142:LYS:NZ	2.32	0.45
55:w:205:PRO:HG3	57:5:29:VAL:HG22	1.98	0.45
1:1:595:G:OP1	8:F:33:ARG:NH2	2.49	0.45
1:1:1227:C:HO2'	1:1:1228:C:P	2.39	0.45
1:1:1269:U:H4'	19:W:158:ILE:HD11	1.98	0.45
1:1:1304:A:N1	1:1:2938:G:O2'	2.39	0.45
1:1:1658:G:OP2	1:1:1796:G:O2'	2.30	0.45
1:1:3163:A:H2'	1:1:3164:C:C6	2.50	0.45
7:E:126:GLN:HE22	15:P:181:ARG:HG3	1.80	0.45
8:F:185:ILE:O	8:F:189:ILE:HG22	2.15	0.45
13:N:114:ARG:NH2	13:N:157:LYS:HG2	2.32	0.45
17:S:96:ASP:CG	17:S:97:VAL:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:282:SER:OG	22:b:338:LYS:NZ	2.27	0.45
27:i:74:LYS:HD3	27:i:80:PHE:HD1	1.81	0.45
40:K:280:PHE:HB3	40:K:288:VAL:HB	1.97	0.45
50:p:131:ASP:OD2	50:p:137:GLN:NE2	2.49	0.45
52:6:222:A:H2'	52:6:223:U:O2	2.15	0.45
55:w:236:PRO:HG2	55:w:311:GLY:HA2	1.98	0.45
55:w:643:LYS:O	55:w:646:THR:OG1	2.33	0.45
1:1:446:U:H2'	1:1:447:U:C6	2.51	0.45
1:1:1299:U:O2'	32:r:42:LEU:O	2.32	0.45
1:1:1456:A:N1	1:1:1476:G:O2'	2.40	0.45
1:1:2995:A:H2'	1:1:2996:U:C2	2.52	0.45
31:q:252:LEU:HB2	31:q:513:PHE:HE2	1.82	0.45
34:u:50:LYS:HG3	34:u:55:PHE:CE1	2.51	0.45
39:I:377:ARG:O	39:I:381:GLN:HG3	2.17	0.45
50:p:97:LEU:HD21	50:p:453:LYS:HE2	1.98	0.45
53:D:144:THR:HB	53:D:166:ASN:H	1.82	0.45
58:x:351:THR:HG21	58:x:385:PHE:HE2	1.80	0.45
58:x:415:ILE:O	58:x:498:TYR:OH	2.35	0.45
1:1:835:G:H1'	1:1:858:A:H61	1.81	0.45
1:1:3228:C:H4'	1:1:3229:G:O5'	2.16	0.45
8:F:189:ILE:HG23	8:F:190:THR:HG23	1.99	0.45
19:W:60:TRP:CD1	19:W:63:SER:HB2	2.51	0.45
32:r:199:ALA:N	32:r:222:GLU:HB3	2.31	0.45
1:1:20:A:H2'	1:1:21:G:C8	2.51	0.45
1:1:761:A:H1'	1:1:771:A:C8	2.51	0.45
1:1:863:C:H2'	1:1:864:G:H8	1.81	0.45
1:1:1243:G:O6	1:1:1244:A:N6	2.50	0.45
1:1:1618:G:H2'	1:1:1619:A:C8	2.52	0.45
1:1:2419:A:H8	1:1:2420:C:C5	2.35	0.45
1:1:3291:G:H2'	1:1:3292:A:H8	1.81	0.45
8:F:86:VAL:O	8:F:114:GLY:HA2	2.17	0.45
17:S:131:LYS:HB3	17:S:134:ASP:OD2	2.16	0.45
30:m:415:GLU:HG2	30:m:415:GLU:O	2.16	0.45
31:q:515:SER:HA	31:q:520:LYS:H	1.82	0.45
36:y:116:LEU:HD13	36:y:177:LEU:HD21	1.99	0.45
40:K:123:VAL:HG22	40:K:179:LEU:HB3	1.98	0.45
41:V:11:PHE:HZ	41:V:121:GLU:HG2	1.80	0.45
43:G:51:LYS:HG3	43:G:52:TRP:CD1	2.51	0.45
46:c:23:TYR:O	58:x:196:GLN:NE2	2.27	0.45
49:n:53:ASN:O	49:n:55:GLY:N	2.50	0.45
49:n:438:LYS:HG2	49:n:440:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:t:69:SER:O	51:t:73:GLU:HG3	2.17	0.45
52:6:17:G:H2'	52:6:18:U:C6	2.51	0.45
53:D:274:ASP:OD1	53:D:274:ASP:N	2.48	0.45
55:w:56:ALA:HB2	55:w:78:ASP:OD2	2.16	0.45
1:1:909:G:H2'	1:1:910:G:H8	1.81	0.45
1:1:1182:A:H2'	1:1:1183:C:C6	2.52	0.45
1:1:3164:C:O2'	1:1:3165:A:H8	1.99	0.45
7:E:85:ILE:HD11	25:f:102:LEU:HD23	1.98	0.45
19:W:158:ILE:HG12	19:W:160:SER:H	1.82	0.45
30:m:351:LYS:HB2	30:m:351:LYS:HE3	1.67	0.45
36:y:42:LEU:HD22	36:y:46:ILE:HG12	1.99	0.45
45:U:21:SER:OG	45:U:22:PRO:HD3	2.16	0.45
49:n:126:PRO:O	49:n:130:ARG:HG3	2.17	0.45
50:p:257:ILE:O	50:p:262:ARG:NH2	2.49	0.45
51:t:274:ASN:O	51:t:321:LEU:HD22	2.17	0.45
52:6:230:A:H2'	52:6:230:A:N3	2.32	0.45
57:5:156:GLU:OE2	58:x:225:THR:HG23	2.15	0.45
1:1:2417:U:HO2'	1:1:2418:G:P	2.40	0.45
10:J:291:LYS:O	10:J:294:GLU:HG2	2.16	0.45
22:b:57:PHE:CE1	22:b:140:VAL:HG21	2.52	0.45
28:j:39:TYR:CD1	28:j:40:PRO:HA	2.51	0.45
29:l:30:ASN:O	29:l:32:GLU:N	2.47	0.45
29:l:42:ASP:OD1	29:l:42:ASP:N	2.48	0.45
30:m:225:SER:O	30:m:229:ARG:HG2	2.17	0.45
37:z:52:LYS:HA	37:z:55:GLN:CD	2.41	0.45
39:I:397:GLU:OE2	55:w:483:LYS:NZ	2.38	0.45
50:p:217:SER:HB3	50:p:295:PHE:CE2	2.51	0.45
52:6:61:G:C8	54:o:182:ARG:NH1	2.85	0.45
1:1:1863:G:O2'	1:1:1867:A:N6	2.50	0.45
15:P:168:LEU:HB3	15:P:172:GLN:HB2	1.98	0.45
30:m:754:VAL:HG12	30:m:762:PRO:HB3	1.99	0.45
39:I:626:SER:O	39:I:628:PRO:HD3	2.17	0.45
40:K:282:LYS:NZ	52:6:33:U:O2'	2.37	0.45
44:Z:27:LYS:HE3	44:Z:27:LYS:HB2	1.80	0.45
1:1:628:A:H2'	1:1:629:U:O4'	2.17	0.45
1:1:1362:G:H2'	1:1:1363:A:C8	2.51	0.45
1:1:1646:G:H1'	1:1:1809:A:N6	2.31	0.45
1:1:2901:G:O2'	1:1:3024:A:N1	2.46	0.45
1:1:3298:C:C2	1:1:3299:A:C8	3.04	0.45
4:A:236:ILE:HD12	10:J:201:MET:HG2	1.98	0.45
6:C:34:ILE:HG13	6:C:120:TYR:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:322:THR:O	10:J:326:ARG:HG3	2.17	0.45
31:q:274:ARG:HB2	31:q:335:PHE:CZ	2.52	0.45
42:R:109:TYR:HB3	42:R:115:ILE:HD13	1.98	0.45
55:w:17:TYR:HA	55:w:28:ARG:HB3	1.98	0.45
56:a:41:TYR:HB2	56:a:200:ASN:HD21	1.81	0.45
1:1:428:A:H2'	1:1:429:U:C6	2.52	0.45
1:1:707:U:H3	1:1:712:G:H1	1.65	0.45
1:1:1227:C:O2'	1:1:1228:C:OP1	2.29	0.45
1:1:1259:A:H2'	1:1:1260:A:C8	2.52	0.45
1:1:2982:A:H2'	1:1:2984:C:C5	2.51	0.45
31:q:538:VAL:HG23	31:q:539:ASP:N	2.30	0.45
39:I:224:TYR:HE1	39:I:259:LEU:HD21	1.82	0.45
40:K:127:LEU:HA	40:K:183:ASP:HB2	1.99	0.45
50:p:161:ALA:HB1	50:p:211:VAL:HB	1.98	0.45
58:x:335:ASP:OD1	58:x:335:ASP:N	2.49	0.45
1:1:1240:A:N6	1:1:1241:U:O4	2.50	0.44
1:1:1452:A:N6	1:1:1507:G:O2'	2.44	0.44
1:1:2489:C:H2'	1:1:2490:C:H6	1.82	0.44
1:1:2938:G:OP1	22:b:48:ARG:NH1	2.47	0.44
1:1:2961:G:H2'	1:1:2962:U:C6	2.52	0.44
2:2:40:A:H2'	2:2:41:A:C8	2.52	0.44
2:2:76:C:H2'	2:2:77:A:H8	1.82	0.44
14:O:127:LEU:HD22	17:S:156:VAL:HG13	1.99	0.44
35:v:52:LYS:HB3	35:v:52:LYS:HE3	1.76	0.44
39:I:329:ILE:HD11	39:I:334:LEU:HD13	1.99	0.44
41:V:136:VAL:HG12	41:V:137:VAL:HG23	1.97	0.44
47:g:91:ARG:O	47:g:95:ILE:HG13	2.18	0.44
50:p:132:LEU:HD22	50:p:438:VAL:HG11	1.98	0.44
50:p:167:LEU:HB2	50:p:204:LEU:HB2	1.99	0.44
50:p:341:LEU:HD12	50:p:343:LEU:HB2	1.98	0.44
53:D:93:THR:HA	53:D:96:PHE:CE1	2.52	0.44
1:1:226:C:H2'	1:1:227:G:O4'	2.17	0.44
1:1:641:C:H2'	1:1:642:U:C6	2.52	0.44
1:1:685:G:OP1	11:L:39:ARG:NH2	2.50	0.44
1:1:985:U:H2'	1:1:986:U:H6	1.81	0.44
1:1:1062:A:N3	18:T:130:ARG:NH2	2.60	0.44
1:1:2463:G:N2	56:a:164:CYS:SG	2.81	0.44
5:B:48:GLY:HA3	5:B:81:THR:HG22	1.99	0.44
5:B:289:ASP:OD1	5:B:290:ASP:N	2.50	0.44
21:Y:53:ASP:HA	21:Y:69:LYS:HG2	1.99	0.44
22:b:229:THR:HA	22:b:232:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:270:LEU:O	22:b:274:ILE:HG12	2.17	0.44
30:m:698:SER:HB3	30:m:729:VAL:HG13	1.99	0.44
31:q:522:HIS:HB3	31:q:525:VAL:HG23	1.98	0.44
36:y:102:SER:HB2	41:V:136:VAL:H	1.82	0.44
38:8:519:LEU:HD23	38:8:519:LEU:H	1.83	0.44
42:R:95:TRP:CZ2	42:R:99:LEU:HD22	2.52	0.44
43:G:156:ASP:OD1	43:G:156:ASP:N	2.49	0.44
47:g:58:ARG:HD2	47:g:58:ARG:HA	1.84	0.44
50:p:169:LEU:O	50:p:201:LEU:N	2.46	0.44
51:t:213:ARG:NH1	51:t:228:VAL:HG12	2.32	0.44
53:D:214:ILE:HD11	53:D:242:SER:HB3	1.98	0.44
56:a:116:LEU:O	56:a:120:VAL:HG23	2.17	0.44
1:1:1124:U:H2'	1:1:1125:U:C6	2.51	0.44
1:1:1209:G:H5'	19:W:4:SER:HB2	1.98	0.44
1:1:1621:A:H2'	1:1:1622:U:C6	2.52	0.44
1:1:1646:G:H4'	49:n:57:THR:HG21	1.99	0.44
1:1:1896:A:N6	1:1:2339:C:H42	2.11	0.44
1:1:2423:U:O2'	1:1:2424:A:H8	2.00	0.44
1:1:2958:A:H2'	1:1:2959:C:C6	2.52	0.44
8:F:75:TYR:HE2	18:T:143:THR:HG21	1.82	0.44
19:W:47:ASP:N	19:W:47:ASP:OD1	2.50	0.44
22:b:151:GLU:CD	22:b:154:ARG:HH21	2.25	0.44
39:I:422:ALA:O	39:I:426:ILE:HG12	2.17	0.44
50:p:416:ARG:HA	50:p:450:GLN:OE1	2.17	0.44
54:o:192:PRO:HB2	54:o:194:LYS:HG2	1.98	0.44
55:w:119:ASP:HB3	60:w:901:SAH:HB2	1.98	0.44
56:a:49:PHE:CE2	56:a:159:LEU:HD13	2.51	0.44
58:x:383:ILE:HB	58:x:384:PRO:HD3	2.00	0.44
1:1:1244:A:H5''	1:1:1271:A:H4'	2.00	0.44
1:1:1590:G:O2'	1:1:1797:A:N6	2.50	0.44
1:1:3281:U:H2'	1:1:3282:U:C6	2.52	0.44
2:2:142:C:H2'	2:2:143:U:C6	2.52	0.44
7:E:87:THR:HG22	7:E:89:THR:H	1.83	0.44
40:K:267:SER:O	40:K:271:ILE:HG12	2.17	0.44
50:p:171:LYS:HB2	50:p:201:LEU:HB2	1.99	0.44
50:p:306:VAL:HG13	50:p:335:ILE:HD12	2.00	0.44
56:a:158:GLN:HG2	56:a:160:LYS:HE2	1.99	0.44
1:1:761:A:H62	1:1:769:G:H2'	1.81	0.44
3:7:115:ILE:HG12	29:l:14:GLU:HG2	1.99	0.44
4:A:36:ILE:HD11	4:A:65:LEU:HD13	1.99	0.44
5:B:280:HIS:HB3	5:B:324:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:36:HIS:O	6:C:40:THR:HG23	2.17	0.44
17:S:40:ARG:HD2	17:S:40:ARG:HA	1.71	0.44
25:f:53:TYR:CZ	25:f:65:ARG:HB2	2.52	0.44
29:l:20:ILE:O	29:l:94:LYS:HB2	2.17	0.44
30:m:792:TRP:HB3	30:m:804:LEU:HD11	2.00	0.44
32:r:164:ARG:NH2	32:r:169:GLU:O	2.37	0.44
38:8:437:TYR:OH	38:8:482:VAL:O	2.21	0.44
51:t:187:LEU:HD13	51:t:196:ILE:HD13	1.99	0.44
1:1:386:A:C5	1:1:387:A:H1'	2.53	0.44
1:1:1127:G:N1	1:1:1128:U:O4	2.51	0.44
1:1:1927:G:OP1	42:R:104:ARG:NH2	2.48	0.44
1:1:3270:U:OP2	7:E:128:LYS:HE2	2.18	0.44
1:1:3333:G:OP2	1:1:3333:G:H8	1.99	0.44
7:E:170:LYS:HB3	7:E:172:HIS:CE1	2.52	0.44
13:N:183:THR:HG22	13:N:187:ARG:HB2	1.99	0.44
22:b:274:ILE:O	22:b:277:LEU:HG	2.18	0.44
23:d:26:LYS:HA	23:d:26:LYS:HD3	1.82	0.44
38:8:372:THR:HB	38:8:374:MET:HE1	1.98	0.44
39:I:210:VAL:O	39:I:214:ARG:HG3	2.18	0.44
50:p:400:VAL:HG21	50:p:442:SER:OG	2.17	0.44
53:D:266:GLN:HG3	53:D:377:VAL:HG11	2.00	0.44
55:w:217:GLU:OE1	55:w:217:GLU:N	2.51	0.44
1:1:508:U:OP1	8:F:211:SER:OG	2.25	0.44
1:1:1466:G:N2	1:1:1510:G:H5''	2.32	0.44
1:1:1945:A:OP1	58:x:148:THR:OG1	2.36	0.44
2:2:52:A:H2'	2:2:53:A:C8	2.53	0.44
5:B:67:PHE:HA	5:B:70:ARG:HD2	2.00	0.44
49:n:564:LYS:HG2	49:n:568:LYS:HE3	2.00	0.44
1:1:353:G:O6	28:j:55:ARG:NH2	2.51	0.44
1:1:1104:G:H2'	1:1:1105:A:C8	2.53	0.44
1:1:1393:A:N6	1:1:1417:G:H1'	2.32	0.44
1:1:1963:G:OP2	50:p:275:ARG:NH2	2.43	0.44
8:F:86:VAL:HG21	8:F:127:LEU:HD21	1.99	0.44
15:P:82:ARG:HE	15:P:82:ARG:HB3	1.67	0.44
30:m:187:SER:OG	39:I:454:GLU:OE2	2.25	0.44
53:D:149:ILE:HG22	53:D:171:THR:HG23	2.00	0.44
55:w:211:ARG:HB2	55:w:217:GLU:OE2	2.18	0.44
56:a:131:ALA:HB1	56:a:133:LYS:HE3	1.99	0.44
56:a:207:LYS:HB2	56:a:211:GLY:O	2.17	0.44
1:1:26:A:N3	1:1:328:U:O2'	2.45	0.44
1:1:155:G:N2	53:D:155:ARG:HH22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:523:A:O2'	17:S:69:PRO:HD2	2.18	0.44
1:1:761:A:N6	1:1:769:G:H2'	2.32	0.44
1:1:1797:A:H2'	1:1:1798:A:C8	2.53	0.44
1:1:1828:A:H2'	1:1:1829:G:C8	2.52	0.44
1:1:2946:A2M:H5'	1:1:2947:G:C8	2.53	0.44
7:E:40:LEU:HD13	7:E:84:VAL:HG11	1.99	0.44
8:F:75:TYR:CE2	18:T:143:THR:HG21	2.52	0.44
19:W:141:ILE:HD11	19:W:156:PRO:HB3	2.00	0.44
22:b:159:ARG:O	32:r:3:GLN:HA	2.18	0.44
29:l:70:LEU:HA	29:l:85:SER:HB3	2.00	0.44
31:q:349:ILE:HD12	31:q:417:ARG:HB2	2.00	0.44
50:p:245:ASP:OD1	50:p:248:GLU:N	2.49	0.44
53:D:266:GLN:HG2	53:D:390:SER:OG	2.18	0.44
1:1:1392:G:H1'	1:1:1418:A:N6	2.33	0.43
1:1:1551:C:HO2'	1:1:1552:G:P	2.40	0.43
1:1:1616:U:H2'	1:1:1617:G:C8	2.53	0.43
1:1:1930:A:H3'	1:1:1931:U:C6	2.53	0.43
15:P:30:ARG:HD2	15:P:63:PHE:HE2	1.82	0.43
19:W:45:LEU:HD11	19:W:53:LEU:HD21	1.99	0.43
22:b:242:ALA:HA	22:b:246:LEU:HD13	1.99	0.43
31:q:214:PHE:HE2	31:q:223:SER:HB2	1.83	0.43
38:8:380:ILE:O	38:8:384:LYS:HG2	2.18	0.43
40:K:86:LYS:NZ	40:K:300:GLU:O	2.34	0.43
40:K:277:ARG:HE	54:o:200:MET:HE3	1.82	0.43
1:1:210:U:C2	1:1:230:U:H4'	2.53	0.43
1:1:893:C:H42	38:8:36:ARG:HD3	1.83	0.43
1:1:2832:C:H2'	1:1:2833:A:C8	2.53	0.43
10:J:306:ARG:NH1	10:J:309:ARG:HH22	2.16	0.43
39:I:552:HIS:HA	39:I:556:ARG:HB2	2.00	0.43
40:K:129:ASP:HA	40:K:156:CYS:SG	2.58	0.43
42:R:136:ARG:NH1	42:R:140:GLU:OE1	2.52	0.43
49:n:106:GLU:O	49:n:109:ARG:HG2	2.17	0.43
50:p:168:ARG:HG2	50:p:203:ILE:HG12	1.99	0.43
51:t:241:ASP:N	51:t:241:ASP:OD1	2.50	0.43
55:w:153:ASN:HA	55:w:201:GLY:HA2	2.00	0.43
55:w:290:LEU:HA	55:w:293:LEU:HD13	2.00	0.43
58:x:427:LYS:HE3	58:x:427:LYS:HB2	1.63	0.43
1:1:737:G:H2'	1:1:738:A:H8	1.83	0.43
1:1:1620:U:H2'	1:1:1621:A:C8	2.54	0.43
1:1:1807:G:H5''	44:Z:135:ARG:NH1	2.29	0.43
1:1:2470:C:H5''	56:a:26:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2493:U:O2'	56:a:163:LEU:HD11	2.18	0.43
1:1:2924:U:OP2	1:1:2924:U:C6	2.70	0.43
1:1:2933:A:C6	1:1:3014:U:H4'	2.53	0.43
1:1:3013:U:H2'	1:1:3014:U:C6	2.53	0.43
1:1:3315:G:P	5:B:116:ARG:HH22	2.41	0.43
2:2:83:C:H5''	2:2:85:G:H5'	2.00	0.43
5:B:222:LYS:HD3	5:B:331:ASN:HB3	2.00	0.43
22:b:184:LEU:HA	22:b:187:ILE:HG22	2.00	0.43
30:m:128:TYR:CD1	30:m:134:ARG:HD2	2.54	0.43
30:m:174:ASP:HB3	30:m:180:ILE:HD11	1.99	0.43
38:8:63:GLU:OE2	39:I:548:LYS:NZ	2.44	0.43
40:K:124:LEU:HD11	40:K:155:ILE:HG12	2.00	0.43
44:Z:10:VAL:O	44:Z:83:THR:OG1	2.24	0.43
52:6:18:U:H2'	52:6:19:U:C6	2.53	0.43
58:x:10:LEU:HD12	58:x:10:LEU:HA	1.85	0.43
58:x:10:LEU:HD23	58:x:14:LEU:HD11	2.00	0.43
1:1:348:A:N3	1:1:352:A:O2'	2.51	0.43
1:1:2490:C:H2'	1:1:2491:A:O4'	2.18	0.43
1:1:3343:G:N2	1:1:3362:A:OP2	2.51	0.43
2:2:79:A:H2'	2:2:80:A:O4'	2.18	0.43
4:A:57:PRO:HD3	4:A:132:GLY:HA2	2.00	0.43
4:A:107:GLY:HA2	10:J:207:ARG:NH2	2.33	0.43
5:B:46:PHE:CE2	5:B:205:VAL:HG22	2.53	0.43
15:P:25:SER:HB3	15:P:28:ASN:HB2	2.01	0.43
15:P:176:ILE:HG22	15:P:180:LYS:HE3	2.00	0.43
19:W:165:MET:HA	19:W:169:PHE:HB2	2.00	0.43
37:z:18:ARG:O	37:z:23:GLN:HB2	2.18	0.43
53:D:373:TYR:O	53:D:377:VAL:HG13	2.18	0.43
56:a:159:LEU:O	56:a:159:LEU:HD23	2.17	0.43
58:x:50:ASP:HA	58:x:203:SER:O	2.18	0.43
58:x:242:VAL:HG22	58:x:374:LEU:HD12	2.00	0.43
1:1:495:G:H5''	24:e:6:HIS:CG	2.53	0.43
1:1:761:A:C6	1:1:770:G:H5'	2.54	0.43
1:1:1060:U:H2'	1:1:1061:A:H8	1.81	0.43
1:1:1132:C:H2'	1:1:1133:A:C8	2.52	0.43
1:1:2410:U:H2'	1:1:2411:U:C6	2.53	0.43
1:1:3006:A:H2'	1:1:3007:U:O4'	2.19	0.43
5:B:211:GLN:HG2	5:B:212:ASN:N	2.33	0.43
7:E:51:ARG:HE	7:E:163:PHE:HB2	1.84	0.43
22:b:91:TYR:O	22:b:95:LEU:HD23	2.19	0.43
22:b:304:GLN:O	22:b:307:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:l:156:MET:HG3	29:l:157:GLN:N	2.33	0.43
31:q:344:HIS:N	31:q:347:GLU:OE1	2.50	0.43
35:v:178:SER:O	35:v:182:GLU:HG3	2.18	0.43
53:D:464:GLN:HG2	53:D:466:ASP:H	1.83	0.43
54:o:96:SER:OG	54:o:97:ARG:N	2.51	0.43
55:w:56:ALA:HA	55:w:57:PRO:HA	1.84	0.43
1:1:129:U:H2'	1:1:130:A:C8	2.54	0.43
1:1:2406:C:OP1	10:J:326:ARG:NH1	2.41	0.43
1:1:2430:A:C2	1:1:2601:A:H2	2.37	0.43
4:A:36:ILE:HG23	4:A:88:PHE:HD1	1.83	0.43
22:b:391:GLU:HG2	22:b:391:GLU:O	2.19	0.43
24:e:59:SER:HB2	24:e:64:LYS:HG3	2.00	0.43
36:y:53:ILE:O	36:y:56:THR:OG1	2.35	0.43
36:y:118:HIS:NE2	36:y:146:ILE:HD12	2.34	0.43
45:U:104:ARG:NH1	45:U:106:ALA:HB2	2.33	0.43
51:t:275:ARG:HG3	51:t:278:SER:OG	2.18	0.43
53:D:375:HIS:HB2	53:D:376:ARG:HH11	1.82	0.43
54:o:95:VAL:HG12	54:o:164:VAL:HG22	1.99	0.43
1:1:293:C:H2'	1:1:294:U:O4'	2.19	0.43
1:1:659:G:H5''	1:1:660:A:OP1	2.19	0.43
1:1:1245:A:H2'	1:1:1272:C:OP1	2.18	0.43
1:1:1694:U:O2'	1:1:1695:U:H5'	2.18	0.43
1:1:2122:G:H2'	1:1:2123:G:H5''	2.00	0.43
1:1:2469:G:N2	1:1:2477:G:H1'	2.33	0.43
11:L:124:ILE:HD11	26:h:120:ALA:HB3	2.00	0.43
28:j:58:THR:O	28:j:61:THR:OG1	2.31	0.43
31:q:530:ARG:HE	31:q:530:ARG:HB3	1.73	0.43
39:I:170:ASN:OD1	39:I:173:THR:HG23	2.18	0.43
53:D:101:ILE:HG12	53:D:138:MET:HG2	2.00	0.43
56:a:35:GLN:HG2	56:a:166:ALA:HB2	1.99	0.43
1:1:1178:G:N3	1:1:1328:C:O2'	2.50	0.43
1:1:3045:G:H2'	1:1:3046:A:O4'	2.19	0.43
4:A:93:LYS:HZ1	4:A:246:ASN:HA	1.83	0.43
21:Y:70:ILE:HD13	21:Y:82:VAL:HG22	2.01	0.43
36:y:166:SER:HB2	36:y:169:ASP:OD1	2.19	0.43
42:R:136:ARG:HG2	42:R:136:ARG:NH1	2.34	0.43
48:k:13:GLU:HG2	48:k:16:ARG:HH21	1.83	0.43
49:n:390:GLU:HA	49:n:393:MET:HE2	2.00	0.43
50:p:205:GLU:O	50:p:234:TRP:HH2	2.01	0.43
50:p:328:THR:HG22	50:p:330:TYR:H	1.84	0.43
53:D:122:PRO:HD2	53:D:126:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D:325:GLN:O	53:D:325:GLN:NE2	2.51	0.43
58:x:94:GLU:OE1	58:x:94:GLU:N	2.46	0.43
1:1:13:A:H4'	20:X:39:LYS:HD3	2.01	0.43
1:1:551:A:O2'	1:1:552:G:H8	2.01	0.43
1:1:757:C:H42	1:1:775:A:H61	1.67	0.43
1:1:1202:A:H2'	1:1:1203:A:C2	2.53	0.43
1:1:2496:C:HO2'	1:1:2497:U:P	2.39	0.43
1:1:3023:U:H5	1:1:3032:A:N7	2.17	0.43
4:A:235:LYS:HD3	4:A:238:GLU:HB3	2.00	0.43
6:C:132:ALA:HB2	6:C:148:ILE:HG21	1.99	0.43
18:T:105:PHE:HA	18:T:108:ARG:NE	2.34	0.43
30:m:682:TRP:HB3	30:m:700:PHE:HB2	2.01	0.43
38:8:377:MET:HE1	38:8:544:GLU:O	2.19	0.43
42:R:115:ILE:HG23	42:R:119:LEU:HB3	2.00	0.43
46:c:25:LEU:HD23	46:c:90:VAL:HG12	2.01	0.43
53:D:239:ALA:HB1	53:D:243:LEU:HD12	2.01	0.43
55:w:308:LYS:HA	55:w:308:LYS:HD3	1.77	0.43
1:1:165:A:O2'	1:1:166:C:OP2	2.28	0.43
1:1:1313:G:O2'	1:1:1318:A:N1	2.38	0.43
1:1:1655:G:N7	39:I:371:LYS:HE2	2.34	0.43
2:2:76:C:H2'	2:2:77:A:C8	2.53	0.43
3:7:84:ILE:HG13	3:7:85:VAL:HG23	2.01	0.43
4:A:146:SER:O	4:A:150:GLN:HG3	2.18	0.43
22:b:184:LEU:HD22	22:b:220:ASP:HB2	2.00	0.43
31:q:345:GLU:O	31:q:346:ASN:HB2	2.19	0.43
53:D:42:GLU:O	53:D:65:MET:HB2	2.18	0.43
57:5:217:THR:O	57:5:221:ARG:N	2.41	0.43
1:1:1255:C:H2'	1:1:1256:G:H8	1.84	0.42
1:1:2430:A:C2	1:1:2601:A:C2	3.07	0.42
1:1:2970:C:H3'	1:1:2971:A:H4'	2.00	0.42
1:1:3140:G:N7	5:B:28:ARG:NH2	2.64	0.42
2:2:67:U:OP1	28:j:85:LYS:HE2	2.18	0.42
4:A:130:LEU:HB3	4:A:170:LYS:HD2	2.00	0.42
5:B:36:ASP:CB	5:B:39:LYS:HD2	2.48	0.42
6:C:6:VAL:N	6:C:20:LEU:O	2.47	0.42
13:N:192:LYS:O	13:N:196:THR:HG23	2.19	0.42
22:b:225:LEU:HD23	22:b:225:LEU:HA	1.84	0.42
23:d:87:ASN:N	23:d:88:PRO:HD2	2.34	0.42
32:r:34:LYS:NZ	32:r:37:GLU:OE2	2.48	0.42
37:z:41:LEU:HG	37:z:45:LYS:NZ	2.33	0.42
49:n:366:TYR:HD2	49:n:410:GLN:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:184:LYS:NZ	55:w:192:SER:O	2.47	0.42
1:1:94:G:H2'	1:1:95:A:C8	2.55	0.42
1:1:297:G:OP2	1:1:297:G:N2	2.32	0.42
1:1:784:A:O2'	16:Q:92:ARG:NH1	2.49	0.42
1:1:2098:C:H2'	1:1:2099:A:O4'	2.19	0.42
1:1:2810:C:H2'	1:1:2811:A:C8	2.55	0.42
1:1:2840:C:H2'	1:1:2841:G:O4'	2.19	0.42
39:I:292:ILE:H	39:I:292:ILE:HD12	1.84	0.42
40:K:292:TYR:CE2	40:K:294:ASN:HB2	2.54	0.42
49:n:377:GLU:HA	49:n:387:VAL:HG21	2.00	0.42
52:6:32:A:C6	52:6:47:A:C8	3.07	0.42
53:D:138:MET:HE3	53:D:143:GLN:HB2	2.01	0.42
58:x:175:ASP:OD1	58:x:203:SER:OG	2.26	0.42
1:1:422:A:N1	1:1:2362:C:O2'	2.37	0.42
1:1:424:G:H22	1:1:637:C:P	2.42	0.42
1:1:472:A:H2'	1:1:473:G:C8	2.54	0.42
1:1:1174:G:N2	14:O:87:MET:HE2	2.35	0.42
1:1:2962:U:H2'	1:1:2963:C:C6	2.54	0.42
1:1:3138:U:OP2	5:B:30:LYS:HD2	2.19	0.42
1:1:3205:G:OP2	1:1:3206:C:N4	2.48	0.42
12:M:77:ARG:O	12:M:81:VAL:HG23	2.18	0.42
21:Y:74:TYR:HE2	21:Y:77:LYS:CG	2.30	0.42
22:b:145:ASP:HB2	22:b:146:PRO:HD3	2.01	0.42
31:q:343:PRO:HB2	31:q:367:MET:HG3	2.01	0.42
49:n:248:LEU:HD21	49:n:253:ASP:OD2	2.19	0.42
1:1:906:A:H2'	1:1:907:G:C8	2.55	0.42
1:1:985:U:H5''	8:F:98:LYS:HD3	2.00	0.42
1:1:1192:C:N4	14:O:56:ASP:OD1	2.32	0.42
1:1:1209:G:C8	19:W:3:ARG:HD2	2.55	0.42
1:1:1936:A:N1	58:x:523:LYS:HD2	2.35	0.42
1:1:2096:A:OP1	58:x:504:LYS:HD2	2.19	0.42
1:1:2434:U:H5''	1:1:2435:G:C8	2.52	0.42
19:W:38:ARG:HG2	19:W:39:TYR:CE1	2.54	0.42
22:b:227:ARG:NH1	22:b:232:MET:HA	2.35	0.42
30:m:462:ARG:HG2	30:m:474:ARG:HG3	2.00	0.42
41:V:11:PHE:CZ	41:V:121:GLU:HG2	2.53	0.42
42:R:7:GLN:HG2	42:R:32:ILE:HG22	2.00	0.42
47:g:12:PRO:HD2	47:g:13:TYR:CD2	2.54	0.42
53:D:117:ILE:HB	53:D:167:MET:HG3	2.01	0.42
55:w:189:ARG:O	55:w:192:SER:OG	2.36	0.42
1:1:2976:A:O2'	1:1:2977:G:H8	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3393:U:H2'	1:1:3394:U:C6	2.55	0.42
17:S:131:LYS:HG3	17:S:133:ALA:H	1.83	0.42
24:e:32:TRP:O	24:e:33:ARG:NH1	2.51	0.42
25:f:75:HIS:HB3	25:f:80:VAL:HG12	2.01	0.42
29:l:64:MET:HB3	31:q:387:ILE:HD11	2.00	0.42
49:n:25:LEU:HD23	49:n:72:MET:SD	2.59	0.42
52:6:61:G:H1	54:o:183:VAL:HG22	1.84	0.42
1:1:406:G:H1'	2:2:17:A:N6	2.35	0.42
1:1:1102:A:O2'	1:1:1103:A:OP1	2.34	0.42
1:1:1593:A:H2'	1:1:1594:A:C8	2.54	0.42
1:1:1930:A:H3'	1:1:1931:U:H6	1.83	0.42
1:1:2883:U:H2'	1:1:2884:C:C6	2.54	0.42
5:B:280:HIS:HB3	5:B:324:VAL:CG1	2.50	0.42
5:B:295:ALA:HB2	5:B:301:THR:O	2.19	0.42
21:Y:39:LEU:HD22	21:Y:43:TYR:HE2	1.84	0.42
30:m:254:MET:HE3	53:D:470:LEU:HD13	2.01	0.42
30:m:806:THR:HG21	50:p:377:PHE:HZ	1.84	0.42
31:q:230:ARG:NH1	31:q:234:ASP:HB3	2.35	0.42
31:q:242:THR:OG1	31:q:437:LYS:O	2.30	0.42
32:r:181:LYS:HA	32:r:196:PRO:HA	2.02	0.42
36:y:200:ASN:OD1	36:y:203:LEU:N	2.52	0.42
49:n:74:GLU:HG3	49:n:76:VAL:H	1.83	0.42
52:6:216:C:C5	54:o:183:VAL:HG11	2.54	0.42
56:a:34:LEU:HD12	56:a:205:VAL:O	2.20	0.42
57:5:162:PRO:HB3	58:x:214:PHE:CD1	2.55	0.42
58:x:237:LYS:NZ	58:x:367:VAL:HG13	2.34	0.42
1:1:1234:G:H2'	1:1:1235:U:C5	2.55	0.42
5:B:198:HIS:CE1	37:z:41:LEU:HD13	2.54	0.42
19:W:91:GLN:O	19:W:94:LYS:HG2	2.20	0.42
24:e:21:HIS:ND1	24:e:24:ARG:HD2	2.34	0.42
29:l:148:LYS:HG3	29:l:153:SER:HB3	2.02	0.42
32:r:155:THR:HG22	32:r:214:VAL:HG22	2.01	0.42
51:t:103:ILE:HG23	51:t:128:LEU:HD11	2.00	0.42
53:D:74:PRO:HB2	53:D:75:PRO:HD3	2.01	0.42
55:w:60:TRP:CD1	60:w:901:SAH:HN2	2.37	0.42
55:w:828:ARG:HH21	55:w:832:ARG:NH2	2.17	0.42
58:x:104:LEU:O	58:x:108:GLU:HG2	2.20	0.42
1:1:144:A:H2'	1:1:145:G:O4'	2.20	0.42
1:1:429:U:H2'	1:1:430:U:H6	1.84	0.42
1:1:846:A:H2'	1:1:847:A:N3	2.35	0.42
1:1:1310:G:O2'	1:1:2380:U:O2'	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1963:G:H2'	1:1:1964:C:C6	2.55	0.42
1:1:2467:G:N2	1:1:2487:U:OP2	2.44	0.42
1:1:2475:G:H2'	1:1:2476:C:C6	2.54	0.42
1:1:3084:C:H2'	1:1:3085:G:O4'	2.19	0.42
11:L:122:LYS:HB3	26:h:119:LYS:H	1.84	0.42
31:q:427:THR:HA	31:q:430:ILE:HD11	2.02	0.42
32:r:34:LYS:O	32:r:38:ARG:HB2	2.20	0.42
34:u:80:ARG:NH1	36:y:85:ARG:O	2.53	0.42
38:8:394:ASP:OD2	38:8:397:LEU:N	2.51	0.42
40:K:38:ILE:HA	40:K:260:VAL:HG11	2.01	0.42
55:w:323:LYS:HD3	55:w:323:LYS:HA	1.77	0.42
55:w:499:THR:OG1	55:w:500:GLY:N	2.52	0.42
1:1:573:C:H2'	1:1:574:U:C6	2.55	0.42
1:1:786:A:P	16:Q:146:SER:HB2	2.60	0.42
1:1:1222:G:H8	1:1:1222:G:OP2	2.03	0.42
1:1:1229:G:O3'	19:W:126:ARG:NH1	2.52	0.42
1:1:1597:C:H5'	1:1:1696:A:H1'	2.02	0.42
1:1:1877:U:H4'	1:1:1878:G:C5	2.55	0.42
1:1:1951:C:H2'	1:1:1952:G:H8	1.84	0.42
1:1:2438:A:OP2	1:1:2438:A:H8	2.03	0.42
1:1:2457:G:HO2'	1:1:2481:G:N2	2.15	0.42
1:1:2975:U:O2'	1:1:2976:A:H5'	2.20	0.42
1:1:3163:A:N6	1:1:3288:G:O6	2.51	0.42
5:B:115:LYS:HA	5:B:118:PHE:HD2	1.85	0.42
8:F:176:TYR:HB3	8:F:194:HIS:CG	2.55	0.42
21:Y:126:LEU:HD12	21:Y:127:GLU:HG2	2.01	0.42
30:m:747:ILE:HG21	30:m:793:LEU:HD21	2.02	0.42
32:r:34:LYS:HA	32:r:34:LYS:HD2	1.75	0.42
32:r:161:PHE:CZ	32:r:164:ARG:HG2	2.54	0.42
38:8:473:TYR:HB3	38:8:474:PRO:HD3	2.02	0.42
39:I:455:LEU:O	39:I:459:THR:HG23	2.20	0.42
40:K:70:ASP:CG	53:D:421:LYS:HZ1	2.28	0.42
43:G:47:SER:HB2	43:G:49:TYR:HE1	1.85	0.42
51:t:34:GLN:O	51:t:38:LYS:HG3	2.19	0.42
58:x:201:LEU:HD21	58:x:216:THR:HG21	2.02	0.42
58:x:290:LEU:H	58:x:290:LEU:HD23	1.85	0.42
1:1:3375:A:O2'	1:1:3378:C:OP2	2.26	0.42
6:C:174:ALA:O	6:C:178:LEU:HG	2.20	0.42
15:P:41:LEU:HD22	15:P:150:VAL:HG21	2.02	0.42
17:S:79:VAL:HG21	17:S:106:LEU:HD21	2.02	0.42
22:b:209:PHE:CE1	22:b:216:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:32:TRP:CZ2	24:e:53:PRO:HD2	2.55	0.42
30:m:751:HIS:HB2	30:m:767:LEU:HD11	2.02	0.42
36:y:163:PRO:HG3	36:y:185:THR:HG22	2.01	0.42
37:z:29:ARG:HA	37:z:32:ARG:HE	1.85	0.42
42:R:154:ALA:O	42:R:158:GLU:HG2	2.20	0.42
43:G:160:ILE:O	43:G:164:VAL:HG13	2.19	0.42
43:G:201:THR:HG22	43:G:202:GLU:HG2	2.01	0.42
52:6:14:U:O4	52:6:17:G:H1'	2.20	0.42
55:w:51:ILE:HB	55:w:116:VAL:HG22	2.02	0.42
57:5:62:GLU:O	57:5:65:ARG:HG2	2.19	0.42
58:x:27:PHE:C	58:x:29:THR:H	2.27	0.42
58:x:351:THR:HG21	58:x:385:PHE:CE2	2.55	0.42
1:1:753:C:C2	1:1:781:G:C2	3.08	0.41
1:1:818:C:N4	1:1:907:G:H22	2.18	0.41
1:1:2890:A:O2'	1:1:2933:A:N3	2.41	0.41
6:C:23:PRO:HD2	6:C:26:PHE:CD2	2.55	0.41
13:N:72:LYS:HD3	13:N:94:TYR:CE2	2.54	0.41
13:N:193:ARG:NH1	13:N:194:GLN:OE1	2.53	0.41
15:P:64:ASN:O	15:P:80:LYS:NZ	2.50	0.41
16:Q:19:PRO:HD3	16:Q:53:PHE:CE1	2.55	0.41
19:W:38:ARG:HG3	19:W:223:ASN:OD1	2.20	0.41
22:b:309:VAL:O	22:b:312:VAL:HG23	2.19	0.41
38:8:447:PHE:HA	38:8:450:ARG:HH21	1.85	0.41
38:8:639:LYS:HA	38:8:639:LYS:HD2	1.79	0.41
39:I:170:ASN:ND2	39:I:171:PRO:HD2	2.35	0.41
50:p:116:LYS:HG3	50:p:437:LYS:HD3	2.00	0.41
50:p:231:ILE:O	50:p:283:LEU:N	2.49	0.41
55:w:229:MET:HE3	55:w:274:GLU:OE2	2.20	0.41
55:w:262:PHE:O	55:w:265:THR:HG22	2.20	0.41
56:a:26:ARG:HD2	56:a:28:PHE:CE2	2.55	0.41
1:1:959:C:H1'	10:J:309:ARG:HE	1.85	0.41
1:1:1126:G:H4'	10:J:324:GLN:OE1	2.20	0.41
1:1:1675:G:H2'	1:1:1676:A:H8	1.84	0.41
1:1:1821:U:C4	47:g:67:LYS:HE3	2.54	0.41
1:1:3072:C:H2'	1:1:3073:A:O4'	2.20	0.41
1:1:3099:C:H2'	37:z:5:LEU:HD21	2.01	0.41
2:2:26:U:H2'	2:2:27:U:C6	2.55	0.41
5:B:197:GLU:OE1	37:z:41:LEU:HD21	2.20	0.41
6:C:315:LYS:HD3	6:C:320:ASN:ND2	2.34	0.41
19:W:171:ILE:HG22	19:W:186:TYR:CZ	2.55	0.41
22:b:9:PRO:HG2	22:b:63:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:268:VAL:HG11	22:b:305:LEU:HD13	2.01	0.41
30:m:128:TYR:CD2	30:m:132:SER:HB2	2.55	0.41
31:q:207:ILE:HG21	31:q:231:LEU:HB2	2.01	0.41
38:8:542:ASP:OD1	38:8:542:ASP:N	2.53	0.41
38:8:571:LEU:HD21	38:8:618:LEU:HD11	2.01	0.41
41:V:18:PRO:HA	41:V:51:ALA:HA	2.00	0.41
51:t:225:HIS:ND1	51:t:226:GLU:N	2.68	0.41
53:D:108:LYS:HD2	53:D:108:LYS:HA	1.89	0.41
1:1:266:A:N6	27:i:28:TYR:O	2.52	0.41
1:1:455:C:N4	1:1:476:G:O6	2.51	0.41
1:1:3297:U:O4	5:B:124:LYS:NZ	2.53	0.41
2:2:9:A:H2'	2:2:10:A:C8	2.55	0.41
30:m:217:THR:OG1	30:m:220:GLU:HG3	2.20	0.41
30:m:680:ALA:CB	30:m:699:SER:OG	2.69	0.41
30:m:711:LEU:O	48:k:10:GLN:HB2	2.20	0.41
31:q:408:PHE:HE2	31:q:415:PHE:CE2	2.39	0.41
39:I:594:LEU:CD2	39:I:601:ILE:HD11	2.49	0.41
40:K:108:LYS:HB3	40:K:109:PRO:HD3	2.02	0.41
51:t:229:LEU:HD23	51:t:229:LEU:HA	1.93	0.41
53:D:418:PRO:HG2	53:D:421:LYS:HB2	2.02	0.41
55:w:13:LEU:HD12	55:w:18:TYR:CZ	2.55	0.41
58:x:448:GLN:H	58:x:448:GLN:CD	2.29	0.41
1:1:421:G:O6	1:1:2383:C:O2'	2.31	0.41
1:1:532:A:O2'	1:1:533:A:H8	2.03	0.41
1:1:2367:A:H2'	1:1:2368:A:H8	1.84	0.41
5:B:219:ALA:HB2	5:B:336:VAL:HG12	2.03	0.41
5:B:294:GLY:HA2	5:B:359:ILE:HD12	2.03	0.41
5:B:306:THR:HA	5:B:307:PRO:HD3	1.90	0.41
8:F:173:LEU:HB3	8:F:178:ILE:HB	2.02	0.41
30:m:678:PRO:HB2	30:m:705:LEU:HD13	2.02	0.41
38:8:577:LEU:HD23	38:8:577:LEU:H	1.86	0.41
40:K:218:SER:HG	40:K:221:THR:HG1	1.59	0.41
41:V:87:ARG:HH12	41:V:137:VAL:HG13	1.86	0.41
43:G:53:PRO:HG2	43:G:56:VAL:HG23	2.02	0.41
44:Z:16:GLY:O	47:g:74:ARG:HG3	2.20	0.41
45:U:19:VAL:O	45:U:23:THR:OG1	2.32	0.41
50:p:94:PRO:HA	50:p:454:GLY:H	1.85	0.41
55:w:33:ILE:HG23	55:w:63:VAL:HG11	2.02	0.41
57:5:78:LYS:HE3	57:5:78:LYS:HB3	1.84	0.41
58:x:511:GLU:OE2	58:x:515:ASN:ND2	2.53	0.41
1:1:431:U:H2'	1:1:432:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:695:C:H5''	6:C:119:ARG:HH21	1.86	0.41
1:1:2328:U:H5'	55:w:190:ASN:O	2.19	0.41
2:2:81:U:O3'	2:2:82:U:H4'	2.20	0.41
6:C:116:ASN:O	6:C:116:ASN:ND2	2.52	0.41
9:H:27:VAL:HG12	9:H:82:VAL:HG11	2.01	0.41
10:J:306:ARG:HD3	10:J:309:ARG:NH2	2.36	0.41
22:b:39:ILE:O	22:b:43:ARG:HG3	2.21	0.41
22:b:432:MET:HG2	22:b:442:TYR:OH	2.20	0.41
29:l:96:LYS:O	29:l:122:SER:HB2	2.20	0.41
30:m:423:ARG:HB3	30:m:424:PRO:HA	2.03	0.41
36:y:57:ARG:HE	36:y:57:ARG:HB2	1.68	0.41
39:I:154:GLU:HG2	39:I:212:LYS:NZ	2.35	0.41
53:D:236:GLU:HA	53:D:239:ALA:HB3	2.02	0.41
53:D:366:PRO:HB3	53:D:463:TYR:CZ	2.56	0.41
56:a:114:GLU:HG2	56:a:137:PRO:HB2	2.02	0.41
58:x:351:THR:OG1	58:x:389:LYS:NZ	2.52	0.41
1:1:618:C:H5'	15:P:169:THR:HG22	2.03	0.41
1:1:816:A:OP2	28:j:28:HIS:NE2	2.46	0.41
1:1:1389:G:H5''	24:e:101:SER:HB3	2.03	0.41
1:1:2320:A:H2'	1:1:2321:A:O4'	2.21	0.41
7:E:3:ALA:HB2	24:e:77:ALA:HB2	2.01	0.41
19:W:216:LYS:NZ	19:W:218:SER:HB3	2.36	0.41
30:m:568:VAL:HG23	30:m:632:GLN:HA	2.01	0.41
31:q:341:LEU:HD23	31:q:341:LEU:H	1.85	0.41
31:q:436:VAL:HG22	31:q:440:ARG:HG2	2.02	0.41
34:u:46:PRO:O	34:u:52:THR:OG1	2.28	0.41
38:8:433:TYR:CG	38:8:486:ILE:HD11	2.56	0.41
46:c:95:ALA:HB2	46:c:101:LEU:HG	2.02	0.41
1:1:1618:G:O3'	49:n:10:GLY:HA3	2.21	0.41
1:1:1831:U:O2'	2:2:114:G:OP1	2.24	0.41
4:A:88:PHE:HB3	4:A:100:TRP:HB2	2.03	0.41
7:E:126:GLN:HG3	7:E:127:ASN:N	2.35	0.41
11:L:61:PRO:O	11:L:62:THR:OG1	2.34	0.41
20:X:77:GLU:HB2	20:X:133:LEU:HD22	2.02	0.41
22:b:456:LEU:HD21	34:u:68:THR:HG22	2.02	0.41
32:r:189:LEU:H	32:r:189:LEU:HD23	1.85	0.41
41:V:15:LEU:HD13	41:V:51:ALA:HB3	2.03	0.41
47:g:54:ILE:CD1	47:g:78:GLY:HA2	2.50	0.41
49:n:247:LYS:HD3	49:n:247:LYS:HA	1.95	0.41
53:D:83:LEU:HD23	53:D:83:LEU:O	2.20	0.41
53:D:232:THR:HG22	53:D:233:THR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D:272:ASP:O	53:D:276:ARG:HG3	2.20	0.41
1:1:69:C:OP1	13:N:178:HIS:ND1	2.50	0.41
1:1:247:C:H2'	1:1:248:U:O4'	2.21	0.41
1:1:454:C:C2	1:1:455:C:H5	2.38	0.41
1:1:1583:A:H2'	1:1:1584:U:O4'	2.21	0.41
1:1:1940:G:H1'	58:x:434:LYS:HD2	2.03	0.41
1:1:2466:G:H4'	56:a:33:GLU:OE2	2.21	0.41
1:1:2493:U:H2'	1:1:2494:A:C8	2.55	0.41
5:B:37:ARG:HD2	5:B:186:GLY:O	2.20	0.41
27:i:30:LYS:HB3	27:i:30:LYS:HE2	1.84	0.41
30:m:229:ARG:HG3	30:m:231:GLU:HG3	2.02	0.41
30:m:724:LYS:HD3	30:m:744:ASP:HB3	2.03	0.41
31:q:261:PHE:HA	31:q:534:HIS:HB3	2.02	0.41
31:q:515:SER:HB3	31:q:520:LYS:HD2	2.02	0.41
39:l:293:GLN:O	39:l:297:THR:HG23	2.21	0.41
48:k:33:LYS:HA	48:k:33:LYS:HD2	1.74	0.41
53:D:97:LEU:HD23	53:D:97:LEU:HA	1.93	0.41
55:w:74:ILE:HD12	55:w:74:ILE:H	1.86	0.41
55:w:296:THR:HA	55:w:300:PHE:CD2	2.56	0.41
56:a:208:SER:O	56:a:210:MET:N	2.54	0.41
57:5:162:PRO:HB3	58:x:214:PHE:HD1	1.86	0.41
1:1:201:A:H2'	1:1:202:G:H8	1.85	0.41
1:1:393:U:H2'	1:1:394:G:O4'	2.21	0.41
1:1:424:G:H21	24:e:24:ARG:HH22	1.66	0.41
1:1:599:C:H2'	1:1:600:G:O4'	2.20	0.41
1:1:748:U:H2'	1:1:749:C:H6	1.85	0.41
1:1:760:G:H22	1:1:770:G:H1'	1.86	0.41
1:1:893:C:H41	38:8:39:ASN:ND2	2.19	0.41
1:1:928:C:H2'	1:1:929:A:C8	2.56	0.41
1:1:1738:C:H2'	1:1:1739:U:C6	2.55	0.41
1:1:2363:A:H2'	1:1:2364:G:O4'	2.20	0.41
1:1:2503:G:H2'	1:1:2503:G:N3	2.35	0.41
1:1:2603:G:H21	29:l:57:SER:HA	1.86	0.41
1:1:2930:A:H2'	1:1:2931:C:C6	2.56	0.41
1:1:3115:C:OP1	9:H:62:ARG:NH1	2.53	0.41
3:7:14:ARG:HH12	13:N:94:TYR:HB2	1.85	0.41
6:C:35:VAL:HG21	6:C:244:LEU:HD21	2.02	0.41
11:L:60:ALA:HA	11:L:61:PRO:HD3	1.92	0.41
13:N:99:ARG:NE	13:N:167:THR:HG21	2.36	0.41
13:N:115:VAL:HA	13:N:134:LEU:HD23	2.02	0.41
15:P:16:SER:O	15:P:101:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:110:MET:HB3	17:S:116:ALA:HB3	2.01	0.41
19:W:221:TYR:HD1	19:W:228:VAL:HG22	1.86	0.41
20:X:16:LYS:HD3	20:X:16:LYS:HA	1.85	0.41
20:X:110:VAL:HG22	20:X:124:VAL:HG22	2.03	0.41
22:b:175:TYR:H	22:b:178:VAL:CG1	2.34	0.41
22:b:416:LEU:HB3	36:y:83:HIS:HE1	1.84	0.41
29:l:115:LYS:NZ	29:l:154:ARG:O	2.29	0.41
30:m:330:PRO:HA	30:m:331:PRO:HD3	1.94	0.41
36:y:109:CYS:HB2	36:y:149:GLY:HA2	2.03	0.41
40:K:98:LYS:HE2	40:K:238:LEU:HD11	2.03	0.41
49:n:253:ASP:O	49:n:257:SER:HB2	2.21	0.41
50:p:273:THR:O	50:p:273:THR:HG22	2.21	0.41
50:p:296:ASP:HB2	50:p:302:VAL:HB	2.02	0.41
50:p:350:ALA:O	50:p:351:ARG:HD3	2.21	0.41
52:6:17:G:H2'	52:6:18:U:H6	1.86	0.41
53:D:283:PHE:CE2	53:D:362:ILE:HD11	2.55	0.41
55:w:77:VAL:HG22	55:w:91:PHE:CE1	2.56	0.41
55:w:664:THR:HG21	55:w:713:ILE:HA	2.03	0.41
58:x:328:ASP:HB3	58:x:353:MET:HE1	2.02	0.41
1:1:127:G:H2'	1:1:128:G:H8	1.86	0.41
1:1:165:A:HO2'	1:1:166:C:P	2.40	0.41
1:1:357:A:O4'	6:C:81:GLY:HA3	2.21	0.41
1:1:374:A:N3	1:1:376:G:H5''	2.36	0.41
1:1:424:G:N2	24:e:24:ARG:HH22	2.19	0.41
1:1:640:U:H2'	1:1:641:C:C6	2.56	0.41
1:1:1283:C:O2'	1:1:1284:C:OP1	2.30	0.41
1:1:1302:A:O2'	1:1:1303:A:OP1	2.35	0.41
1:1:2128:C:H2'	1:1:2129:U:O4'	2.21	0.41
1:1:2445:A:H4'	1:1:2446:U:OP1	2.20	0.41
1:1:3112:G:O6	1:1:3120:C:H5''	2.21	0.41
1:1:3233:C:H2'	1:1:3234:A:H8	1.82	0.41
5:B:110:LEU:HD23	5:B:114:VAL:HG11	2.02	0.41
24:e:11:LYS:O	24:e:12:LYS:HB2	2.20	0.41
30:m:341:PRO:HD3	49:n:455:PRO:HB3	2.02	0.41
32:r:23:ARG:HE	32:r:23:ARG:HB3	1.70	0.41
32:r:196:PRO:HG2	32:r:224:ASN:HB3	2.03	0.41
42:R:13:SER:HB3	42:R:38:ARG:HH22	1.85	0.41
58:x:412:ARG:O	58:x:416:LEU:HG	2.20	0.41
58:x:536:TRP:O	58:x:540:THR:HG23	2.21	0.41
1:1:305:U:H3'	4:A:246:ASN:HD21	1.86	0.40
1:1:1120:A:H2'	1:1:1121:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2469:G:O2'	56:a:28:PHE:HZ	2.05	0.40
1:1:2922:OMG:HM22	1:1:2923:PSU:C5'	2.44	0.40
4:A:92:ARG:HA	4:A:92:ARG:HD3	1.87	0.40
4:A:116:ASN:O	4:A:219:PHE:HA	2.21	0.40
8:F:110:ARG:O	8:F:113:SER:OG	2.33	0.40
17:S:12:ARG:HB3	17:S:24:LEU:HD23	2.03	0.40
19:W:198:ARG:HH21	19:W:199:GLN:HG3	1.86	0.40
22:b:5:TRP:CD1	22:b:69:PRO:HB3	2.56	0.40
29:l:29:ASP:OD1	29:l:30:ASN:N	2.48	0.40
34:u:109:LYS:HE3	34:u:109:LYS:HB3	1.86	0.40
36:y:19:LEU:HA	36:y:24:CYS:HA	2.03	0.40
36:y:175:SER:O	36:y:178:GLN:NE2	2.44	0.40
39:I:606:SER:OG	39:I:609:ASP:OD2	2.40	0.40
50:p:220:SER:HB3	50:p:236:THR:HB	2.02	0.40
50:p:384:CYS:HB3	50:p:387:ASN:O	2.21	0.40
56:a:61:PRO:HG2	56:a:62:ASN:OD1	2.22	0.40
1:1:710:A:H2'	1:1:711:A:C8	2.57	0.40
1:1:1636:U:O2'	44:Z:79:HIS:ND1	2.51	0.40
1:1:2356:A:H61	1:1:2983:C:H42	1.68	0.40
2:2:12:A:OP1	15:P:3:ARG:HD3	2.21	0.40
5:B:92:TYR:HB2	5:B:157:VAL:HB	2.02	0.40
5:B:210:GLU:OE2	37:z:29:ARG:HG3	2.22	0.40
21:Y:39:LEU:HD22	21:Y:43:TYR:CE2	2.57	0.40
22:b:123:PHE:O	22:b:127:GLN:HG2	2.21	0.40
29:l:10:LYS:O	29:l:14:GLU:HG3	2.21	0.40
30:m:171:ILE:HD12	30:m:171:ILE:HA	1.96	0.40
36:y:4:ARG:HB3	36:y:208:LEU:HA	2.02	0.40
36:y:5:THR:O	36:y:13:ILE:HD11	2.21	0.40
38:8:499:ILE:HA	38:8:515:ILE:HD11	2.02	0.40
38:8:519:LEU:HA	38:8:522:ILE:HG12	2.03	0.40
42:R:23:TRP:HB2	42:R:53:LYS:HE2	2.03	0.40
53:D:53:THR:O	53:D:57:ILE:HG12	2.21	0.40
54:o:126:LYS:HG2	54:o:182:ARG:HH21	1.87	0.40
1:1:643:U:O2'	1:1:645:A:N7	2.48	0.40
1:1:918:C:O2	1:1:918:C:C2'	2.70	0.40
1:1:1104:G:H2'	1:1:1105:A:H8	1.87	0.40
1:1:1954:G:H2'	1:1:1955:U:C6	2.56	0.40
5:B:286:GLY:HA3	5:B:321:PHE:CZ	2.56	0.40
9:H:2:LYS:HA	9:H:60:GLY:O	2.21	0.40
11:L:124:ILE:HD11	26:h:120:ALA:CB	2.51	0.40
17:S:12:ARG:HH12	18:T:141:VAL:HB	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:115:LEU:HA	22:b:115:LEU:HD23	1.85	0.40
26:h:100:VAL:HG22	26:h:104:GLN:HB3	2.03	0.40
35:v:33:ASN:HD21	35:v:161:LYS:HE3	1.87	0.40
55:w:242:LYS:HE2	55:w:242:LYS:HB2	1.92	0.40
55:w:364:ARG:HG2	55:w:364:ARG:NH1	2.36	0.40
56:a:41:TYR:HB2	56:a:200:ASN:ND2	2.37	0.40
58:x:26:GLY:C	58:x:28:GLU:H	2.29	0.40
58:x:534:LEU:HD23	58:x:534:LEU:HA	1.97	0.40
1:1:1392:G:H1'	1:1:1418:A:H61	1.86	0.40
1:1:1667:A:H2'	1:1:1668:G:H8	1.86	0.40
1:1:1827:C:H2'	1:1:1828:A:C8	2.57	0.40
1:1:2832:C:H2'	1:1:2833:A:H8	1.85	0.40
1:1:2974:U:H2'	1:1:2975:U:O4'	2.22	0.40
1:1:3098:G:OP1	5:B:279:ASN:ND2	2.49	0.40
5:B:35:ASP:OD1	5:B:185:GLY:N	2.48	0.40
7:E:64:LEU:HD11	7:E:76:LEU:HD22	2.01	0.40
10:J:258:ARG:O	10:J:262:LYS:HG2	2.21	0.40
15:P:30:ARG:HD2	15:P:63:PHE:CE2	2.56	0.40
21:Y:40:ARG:NH1	21:Y:46:LYS:HZ2	2.20	0.40
26:h:62:GLN:O	26:h:66:VAL:HG23	2.22	0.40
26:h:94:LYS:HB2	26:h:94:LYS:HE2	1.88	0.40
26:h:118:ILE:HG22	26:h:119:LYS:N	2.36	0.40
28:j:21:ARG:HD2	28:j:37:CYS:SG	2.61	0.40
29:l:36:VAL:HG23	29:l:47:VAL:HG13	2.02	0.40
31:q:220:GLU:OE2	31:q:222:ARG:NH1	2.51	0.40
37:z:51:LYS:O	37:z:55:GLN:HG3	2.22	0.40
39:I:149:MET:HE3	39:I:149:MET:HB3	1.92	0.40
39:I:544:GLU:O	39:I:548:LYS:HG3	2.21	0.40
39:I:620:ALA:HB3	39:I:626:SER:HB3	2.03	0.40
55:w:721:ILE:O	55:w:725:ILE:HG12	2.22	0.40
58:x:41:LEU:HD13	58:x:47:VAL:HB	2.03	0.40
58:x:429:TYR:HE2	58:x:465:PRO:HD2	1.87	0.40
1:1:263:C:H2'	1:1:264:G:O4'	2.21	0.40
1:1:297:G:O6	13:N:12:ARG:NH1	2.54	0.40
1:1:385:A:H2'	1:1:386:A:C8	2.55	0.40
1:1:786:A:H4'	1:1:787:G:H5'	2.03	0.40
1:1:818:C:O2	1:1:818:C:H2'	2.20	0.40
1:1:2092:A:H5''	1:1:2094:C:O4'	2.21	0.40
1:1:2934:A:H2'	1:1:2935:U:O4'	2.21	0.40
4:A:90:GLU:O	4:A:98:TYR:N	2.53	0.40
4:A:183:ASP:OD1	4:A:183:ASP:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:124:LYS:HB2	15:P:126:ARG:HH12	1.87	0.40
20:X:115:ARG:HD3	20:X:121:LYS:HE2	2.02	0.40
31:q:347:GLU:HG2	31:q:416:ASP:OD2	2.21	0.40
32:r:222:GLU:OE2	32:r:241:LYS:HE3	2.22	0.40
36:y:18:LYS:HE3	36:y:63:THR:O	2.22	0.40
40:K:184:ASP:CG	52:6:7:C:H41	2.29	0.40
40:K:265:LEU:HD12	40:K:265:LEU:HA	1.93	0.40
50:p:328:THR:HG22	50:p:329:SER:N	2.37	0.40
55:w:77:VAL:HG22	55:w:91:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	7	125/204 (61%)	117 (94%)	8 (6%)	0	100	100
4	A	264/291 (91%)	245 (93%)	19 (7%)	0	100	100
5	B	331/387 (86%)	315 (95%)	16 (5%)	0	100	100
6	C	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
7	E	160/176 (91%)	150 (94%)	10 (6%)	0	100	100
8	F	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
9	H	188/191 (98%)	179 (95%)	9 (5%)	0	100	100
10	J	143/427 (34%)	136 (95%)	7 (5%)	0	100	100
11	L	119/199 (60%)	113 (95%)	6 (5%)	0	100	100
12	M	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
13	N	185/204 (91%)	181 (98%)	4 (2%)	0	100	100
14	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
15	P	181/184 (98%)	173 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	132/186 (71%)	130 (98%)	2 (2%)	0	100	100
17	S	168/172 (98%)	162 (96%)	6 (4%)	0	100	100
18	T	50/160 (31%)	45 (90%)	5 (10%)	0	100	100
19	W	230/236 (98%)	217 (94%)	13 (6%)	0	100	100
20	X	135/142 (95%)	127 (94%)	8 (6%)	0	100	100
21	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
22	b	494/647 (76%)	473 (96%)	21 (4%)	0	100	100
23	d	105/113 (93%)	102 (97%)	3 (3%)	0	100	100
24	e	123/130 (95%)	119 (97%)	4 (3%)	0	100	100
25	f	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
26	h	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
27	i	75/100 (75%)	69 (92%)	6 (8%)	0	100	100
28	j	71/88 (81%)	69 (97%)	2 (3%)	0	100	100
29	l	174/181 (96%)	164 (94%)	9 (5%)	1 (1%)	21	53
30	m	658/807 (82%)	629 (96%)	29 (4%)	0	100	100
31	q	356/618 (58%)	330 (93%)	26 (7%)	0	100	100
32	r	170/261 (65%)	165 (97%)	5 (3%)	0	100	100
33	s	34/520 (6%)	34 (100%)	0	0	100	100
34	u	138/199 (69%)	137 (99%)	1 (1%)	0	100	100
35	v	124/231 (54%)	119 (96%)	5 (4%)	0	100	100
36	y	223/245 (91%)	213 (96%)	10 (4%)	0	100	100
37	z	53/106 (50%)	53 (100%)	0	0	100	100
38	8	456/710 (64%)	435 (95%)	21 (5%)	0	100	100
39	I	531/663 (80%)	511 (96%)	20 (4%)	0	100	100
40	K	278/376 (74%)	267 (96%)	11 (4%)	0	100	100
41	V	132/137 (96%)	128 (97%)	4 (3%)	0	100	100
42	R	130/189 (69%)	128 (98%)	2 (2%)	0	100	100
43	G	194/256 (76%)	190 (98%)	4 (2%)	0	100	100
44	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
45	U	100/121 (83%)	94 (94%)	6 (6%)	0	100	100
46	c	95/105 (90%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	g	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
48	k	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
49	n	417/605 (69%)	401 (96%)	16 (4%)	0	100	100
50	p	331/460 (72%)	303 (92%)	28 (8%)	0	100	100
51	t	279/322 (87%)	271 (97%)	8 (3%)	0	100	100
53	D	426/505 (84%)	413 (97%)	13 (3%)	0	100	100
54	o	131/220 (60%)	128 (98%)	3 (2%)	0	100	100
55	w	656/841 (78%)	614 (94%)	42 (6%)	0	100	100
56	a	212/217 (98%)	192 (91%)	17 (8%)	3 (1%)	9	33
57	5	133/235 (57%)	126 (95%)	7 (5%)	0	100	100
58	x	531/606 (88%)	508 (96%)	22 (4%)	1 (0%)	43	73
All	All	11810/15605 (76%)	11302 (96%)	503 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	a	63	MET
58	x	406	ASN
56	a	209	SER
56	a	65	ILE
29	l	41	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7	114/181 (63%)	114 (100%)	0	100	100
4	A	242/263 (92%)	242 (100%)	0	100	100
5	B	281/323 (87%)	281 (100%)	0	100	100
6	C	286/289 (99%)	286 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	142/153 (93%)	142 (100%)	0	100	100
8	F	186/205 (91%)	186 (100%)	0	100	100
9	H	170/171 (99%)	170 (100%)	0	100	100
10	J	133/383 (35%)	133 (100%)	0	100	100
11	L	100/159 (63%)	100 (100%)	0	100	100
12	M	107/109 (98%)	107 (100%)	0	100	100
13	N	165/176 (94%)	165 (100%)	0	100	100
14	O	160/162 (99%)	160 (100%)	0	100	100
15	P	145/146 (99%)	145 (100%)	0	100	100
16	Q	110/151 (73%)	110 (100%)	0	100	100
17	S	155/156 (99%)	155 (100%)	0	100	100
18	T	41/137 (30%)	41 (100%)	0	100	100
19	W	209/213 (98%)	209 (100%)	0	100	100
20	X	114/118 (97%)	114 (100%)	0	100	100
21	Y	109/110 (99%)	109 (100%)	0	100	100
22	b	447/573 (78%)	447 (100%)	0	100	100
23	d	94/97 (97%)	94 (100%)	0	100	100
24	e	108/111 (97%)	108 (100%)	0	100	100
25	f	90/91 (99%)	90 (100%)	0	100	100
26	h	104/105 (99%)	104 (100%)	0	100	100
27	i	65/82 (79%)	65 (100%)	0	100	100
28	j	60/71 (84%)	60 (100%)	0	100	100
29	l	151/156 (97%)	151 (100%)	0	100	100
30	m	599/722 (83%)	599 (100%)	0	100	100
31	q	304/535 (57%)	304 (100%)	0	100	100
32	r	156/229 (68%)	156 (100%)	0	100	100
33	s	32/445 (7%)	32 (100%)	0	100	100
34	u	125/180 (69%)	125 (100%)	0	100	100
35	v	116/205 (57%)	116 (100%)	0	100	100
36	y	193/211 (92%)	193 (100%)	0	100	100
37	z	48/95 (50%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	8	351/647 (54%)	350 (100%)	1 (0%)	86	88
39	I	484/602 (80%)	484 (100%)	0	100	100
40	K	261/346 (75%)	261 (100%)	0	100	100
41	V	103/105 (98%)	103 (100%)	0	100	100
42	R	112/154 (73%)	112 (100%)	0	100	100
43	G	161/208 (77%)	161 (100%)	0	100	100
44	Z	115/116 (99%)	115 (100%)	0	100	100
45	U	89/107 (83%)	89 (100%)	0	100	100
46	c	81/88 (92%)	81 (100%)	0	100	100
47	g	95/103 (92%)	95 (100%)	0	100	100
48	k	68/69 (99%)	68 (100%)	0	100	100
49	n	381/548 (70%)	381 (100%)	0	100	100
50	p	300/413 (73%)	299 (100%)	1 (0%)	86	88
51	t	256/287 (89%)	256 (100%)	0	100	100
53	D	378/440 (86%)	378 (100%)	0	100	100
54	o	118/199 (59%)	118 (100%)	0	100	100
55	w	592/745 (80%)	592 (100%)	0	100	100
56	a	195/198 (98%)	195 (100%)	0	100	100
57	5	133/217 (61%)	133 (100%)	0	100	100
58	x	489/548 (89%)	479 (98%)	10 (2%)	48	73
All	All	10423/13653 (76%)	10411 (100%)	12 (0%)	87	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	8	566	GLN
50	p	397	ASP
58	x	28	GLU
58	x	47	VAL
58	x	291	VAL
58	x	292	ASN
58	x	349	THR
58	x	400	VAL
58	x	403	ILE
58	x	435	TYR

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Mol	Chain	Res	Type
58	x	500	TYR
58	x	538	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
3	7	32	ASN
3	7	42	GLN
4	A	73	GLN
4	A	95	GLN
4	A	150	GLN
4	A	286	ASN
5	B	121	ASN
5	B	173	GLN
5	B	371	GLN
6	C	237	GLN
6	C	322	GLN
8	F	64	GLN
8	F	93	ASN
8	F	231	ASN
10	J	308	GLN
11	L	12	ASN
11	L	17	HIS
12	M	105	GLN
13	N	123	GLN
13	N	138	GLN
13	N	175	ASN
14	O	26	GLN
14	O	31	GLN
15	P	55	GLN
15	P	125	GLN
16	Q	73	GLN
17	S	138	GLN
17	S	142	GLN
18	T	103	GLN
19	W	74	GLN
19	W	88	ASN
22	b	23	ASN
22	b	72	ASN
22	b	406	ASN
22	b	454	GLN
23	d	21	HIS

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Mol	Chain	Res	Type
23	d	105	GLN
24	e	49	ASN
24	e	71	HIS
26	h	76	GLN
30	m	318	ASN
30	m	483	ASN
32	r	256	ASN
35	v	10	ASN
35	v	60	GLN
35	v	210	GLN
37	z	55	GLN
39	I	155	ASN
39	I	254	GLN
39	I	335	ASN
39	I	373	GLN
39	I	381	GLN
40	K	214	ASN
40	K	295	GLN
40	K	323	GLN
42	R	27	ASN
42	R	134	HIS
43	G	61	GLN
44	Z	122	HIS
45	U	40	HIS
48	k	57	ASN
49	n	11	ASN
49	n	165	GLN
49	n	428	GLN
49	n	580	GLN
49	n	590	GLN
50	p	352	HIS
50	p	370	GLN
50	p	452	ASN
51	t	51	ASN
51	t	92	HIS
51	t	157	ASN
51	t	172	ASN
53	D	105	HIS
53	D	153	ASN
53	D	287	ASN
53	D	325	GLN
53	D	337	ASN

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Mol	Chain	Res	Type
54	o	100	HIS
55	w	42	HIS
55	w	137	GLN
55	w	175	GLN
55	w	366	ASN
55	w	549	HIS
56	a	21	ASN
56	a	27	ASN
56	a	140	HIS
57	5	55	GLN
58	x	98	GLN
58	x	375	ASN
58	x	486	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2643/3396 (77%)	555 (20%)	38 (1%)
2	2	157/158 (99%)	24 (15%)	1 (0%)
52	6	85/87 (97%)	24 (28%)	4 (4%)
All	All	2885/3641 (79%)	603 (20%)	43 (1%)

All (603) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	U
1	1	6	A
1	1	7	C
1	1	14	U
1	1	40	A
1	1	42	C
1	1	43	A
1	1	49	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	72	C
1	1	96	G
1	1	105	C

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Mol	Chain	Res	Type
1	1	109	A
1	1	110	G
1	1	111	C
1	1	116	A
1	1	118	U
1	1	122	A
1	1	135	C
1	1	136	G
1	1	143	G
1	1	148	G
1	1	165	A
1	1	166	C
1	1	170	G
1	1	190	U
1	1	191	U
1	1	192	C
1	1	200	C
1	1	206	G
1	1	210	U
1	1	211	A
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	240	U
1	1	241	G
1	1	252	U
1	1	255	A
1	1	265	A
1	1	266	A
1	1	268	A
1	1	269	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	339	C

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Mol	Chain	Res	Type
1	1	368	G
1	1	370	U
1	1	376	G
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	406	G
1	1	407	A
1	1	421	G
1	1	422	A
1	1	439	C
1	1	440	A
1	1	446	U
1	1	449	U
1	1	451	U
1	1	454	C
1	1	457	C
1	1	459	G
1	1	463	C
1	1	464	U
1	1	466	G
1	1	468	G
1	1	469	G
1	1	472	A
1	1	478	A
1	1	479	U
1	1	480	C
1	1	481	U
1	1	482	C
1	1	483	G
1	1	485	A
1	1	486	U
1	1	487	U
1	1	488	U
1	1	521	A
1	1	530	G
1	1	533	A
1	1	535	G
1	1	543	C
1	1	544	C
1	1	547	G

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Mol	Chain	Res	Type
1	1	550	A
1	1	552	G
1	1	557	A
1	1	559	A
1	1	560	G
1	1	578	A
1	1	579	G
1	1	591	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	636	C
1	1	642	U
1	1	645	A
1	1	660	A
1	1	677	A
1	1	681	U
1	1	691	A
1	1	695	C
1	1	705	A
1	1	706	A
1	1	715	A
1	1	716	A
1	1	719	U
1	1	721	G
1	1	722	G
1	1	725	G
1	1	734	C
1	1	735	A
1	1	742	G
1	1	757	C
1	1	760	G
1	1	761	A
1	1	770	G
1	1	774	G
1	1	776	U
1	1	777	U
1	1	779	G
1	1	784	A
1	1	785	G
1	1	807	A

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Mol	Chain	Res	Type
1	1	808	A
1	1	817	A
1	1	818	C
1	1	819	U
1	1	820	A
1	1	822	G
1	1	830	A
1	1	845	G
1	1	860	G
1	1	861	C
1	1	862	U
1	1	871	G
1	1	887	G
1	1	894	G
1	1	895	A
1	1	896	A
1	1	906	A
1	1	907	G
1	1	908	G
1	1	909	G
1	1	910	G
1	1	912	G
1	1	913	A
1	1	917	A
1	1	936	A
1	1	944	C
1	1	958	C
1	1	959	C
1	1	960	U
1	1	961	C
1	1	962	A
1	1	963	G
1	1	978	G
1	1	979	U
1	1	980	A
1	1	982	C
1	1	985	U
1	1	991	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A

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Mol	Chain	Res	Type
1	1	1112	A
1	1	1115	G
1	1	1116	G
1	1	1127	G
1	1	1129	A
1	1	1132	C
1	1	1143	A
1	1	1145	G
1	1	1151	U
1	1	1153	A
1	1	1160	C
1	1	1174	G
1	1	1179	A
1	1	1180	A
1	1	1181	U
1	1	1191	U
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1204	A
1	1	1217	A
1	1	1222	G
1	1	1228	C
1	1	1235	U
1	1	1241	U
1	1	1242	G
1	1	1245	A
1	1	1251	A
1	1	1252	A
1	1	1258	U
1	1	1259	A
1	1	1261	G
1	1	1262	G
1	1	1263	A
1	1	1265	U
1	1	1272	C
1	1	1279	C
1	1	1284	C

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Mol	Chain	Res	Type
1	1	1286	A
1	1	1287	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1330	A
1	1	1332	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1392	G
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1450	G
1	1	1452	A
1	1	1454	A
1	1	1455	U
1	1	1469	C
1	1	1481	A
1	1	1483	G
1	1	1484	U
1	1	1485	G
1	1	1496	C
1	1	1525	G
1	1	1539	A
1	1	1552	G

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Mol	Chain	Res	Type
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1571	A
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1587	A
1	1	1589	A
1	1	1590	G
1	1	1593	A
1	1	1604	G
1	1	1627	U
1	1	1628	C
1	1	1629	U
1	1	1630	U
1	1	1633	C
1	1	1639	C
1	1	1643	A
1	1	1694	U
1	1	1724	U
1	1	1725	C
1	1	1741	A
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1761	C
1	1	1762	C
1	1	1763	U
1	1	1764	U
1	1	1766	G
1	1	1767	C
1	1	1773	C
1	1	1780	G
1	1	1795	U
1	1	1797	A
1	1	1806	A
1	1	1808	G

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Mol	Chain	Res	Type
1	1	1813	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1821	U
1	1	1858	A
1	1	1863	G
1	1	1864	A
1	1	1865	A
1	1	1866	C
1	1	1867	A
1	1	1868	G
1	1	1876	U
1	1	1878	G
1	1	1886	A
1	1	1906	G
1	1	1918	C
1	1	1921	A
1	1	1922	A
1	1	1923	C
1	1	1927	G
1	1	1929	G
1	1	1930	A
1	1	1932	A
1	1	1935	G
1	1	1939	G
1	1	1940	G
1	1	1955	U
1	1	1962	G
1	1	1965	C
1	1	1971	C
1	1	2057	G
1	1	2091	U
1	1	2092	A
1	1	2102	U
1	1	2103	U
1	1	2104	A
1	1	2105	G
1	1	2110	G
1	1	2111	G
1	1	2113	A
1	1	2114	C

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Mol	Chain	Res	Type
1	1	2118	C
1	1	2119	A
1	1	2120	A
1	1	2122	G
1	1	2123	G
1	1	2131	A
1	1	2319	U
1	1	2320	A
1	1	2324	A
1	1	2329	C
1	1	2335	G
1	1	2336	U
1	1	2370	G
1	1	2371	G
1	1	2373	A
1	1	2374	C
1	1	2376	G
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2394	G
1	1	2395	G
1	1	2405	C
1	1	2416	U
1	1	2418	G
1	1	2419	A
1	1	2420	C
1	1	2421	U
1	1	2422	C
1	1	2423	U
1	1	2424	A
1	1	2430	A
1	1	2433	U
1	1	2434	U
1	1	2435	G
1	1	2437	G
1	1	2438	A
1	1	2440	G
1	1	2445	A
1	1	2446	U
1	1	2448	G
1	1	2450	G

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Mol	Chain	Res	Type
1	1	2452	G
1	1	2453	U
1	1	2460	U
1	1	2461	A
1	1	2462	A
1	1	2463	G
1	1	2469	G
1	1	2472	U
1	1	2473	C
1	1	2474	G
1	1	2475	G
1	1	2487	U
1	1	2491	A
1	1	2494	A
1	1	2495	C
1	1	2497	U
1	1	2501	U
1	1	2503	G
1	1	2504	U
1	1	2505	U
1	1	2507	C
1	1	2596	U
1	1	2598	G
1	1	2599	U
1	1	2600	C
1	1	2601	A
1	1	2602	G
1	1	2603	G
1	1	2606	G
1	1	2611	U
1	1	2803	A
1	1	2818	U
1	1	2821	C
1	1	2822	U
1	1	2824	G
1	1	2836	C
1	1	2838	A
1	1	2844	C
1	1	2845	A
1	1	2879	C
1	1	2887	A
1	1	2898	G

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Mol	Chain	Res	Type
1	1	2899	C
1	1	2904	U
1	1	2907	G
1	1	2916	U
1	1	2922	OMG
1	1	2925	C
1	1	2927	C
1	1	2935	U
1	1	2936	A
1	1	2941	A
1	1	2942	C
1	1	2943	G
1	1	2945	G
1	1	2946	A2M
1	1	2947	G
1	1	2948	C
1	1	2949	U
1	1	2950	G
1	1	2951	G
1	1	2952	G
1	1	2953	U
1	1	2955	U
1	1	2956	A
1	1	2971	A
1	1	2972	G
1	1	2976	A
1	1	2977	G
1	1	2978	U
1	1	2979	U
1	1	2980	U
1	1	2982	A
1	1	2983	C
1	1	2984	C
1	1	2990	G
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3022	G
1	1	3023	U
1	1	3026	G
1	1	3027	A
1	1	3028	G

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Mol	Chain	Res	Type
1	1	3030	G
1	1	3032	A
1	1	3050	U
1	1	3057	U
1	1	3058	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3092	C
1	1	3093	C
1	1	3100	U
1	1	3109	G
1	1	3122	A
1	1	3127	A
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3156	U
1	1	3157	U
1	1	3165	A
1	1	3167	A
1	1	3168	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3224	G

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Mol	Chain	Res	Type
1	1	3227	A
1	1	3228	C
1	1	3229	G
1	1	3238	G
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3259	U
1	1	3270	U
1	1	3276	G
1	1	3278	C
1	1	3279	A
1	1	3280	U
1	1	3287	U
1	1	3289	G
1	1	3294	A
1	1	3304	U
1	1	3313	U
1	1	3314	A
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3334	U
1	1	3335	A
1	1	3341	U
1	1	3349	C
1	1	3358	U
1	1	3362	A
1	1	3369	G
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3386	G
1	1	3389	U
1	1	3396	U
2	2	23	U
2	2	34	U
2	2	35	C
2	2	48	A
2	2	59	A
2	2	62	C
2	2	63	G

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Mol	Chain	Res	Type
2	2	79	A
2	2	81	U
2	2	82	U
2	2	84	C
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	104	A
2	2	105	A
2	2	106	C
2	2	107	G
2	2	111	A
2	2	113	U
2	2	116	G
2	2	124	G
2	2	148	G
52	6	4	U
52	6	5	C
52	6	7	C
52	6	14	U
52	6	15	C
52	6	16	U
52	6	23	U
52	6	24	A
52	6	26	U
52	6	33	U
52	6	34	A
52	6	40	U
52	6	41	G
52	6	42	G
52	6	43	A
52	6	54	A
52	6	56	U
52	6	57	U
52	6	59	C
52	6	218	A
52	6	219	A
52	6	220	C
52	6	223	U
52	6	230	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	165	A
1	1	239	G
1	1	406	G
1	1	480	C
1	1	487	U
1	1	644	G
1	1	720	A
1	1	734	C
1	1	817	A
1	1	870	C
1	1	906	A
1	1	908	G
1	1	1102	A
1	1	1104	G
1	1	1128	U
1	1	1159	A
1	1	1227	C
1	1	1241	U
1	1	1283	C
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1355	A
1	1	1551	C
1	1	1954	G
1	1	2417	U
1	1	2419	A
1	1	2445	A
1	1	2496	C
1	1	2500	A
1	1	2597	U
1	1	2600	C
1	1	2602	G
1	1	2954	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
2	2	123	G
52	6	42	G
52	6	56	U
52	6	218	A
52	6	222	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	2923	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	OMU	1	2921	1	19,22,23	0.73	0	25,31,34	1.00	2 (8%)
1	A2M	1	2946	1	22,25,26	1.45	3 (13%)	30,36,39	1.04	2 (6%)
1	OMG	1	2922	1	23,26,27	1.14	3 (13%)	32,38,41	0.88	1 (3%)

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
1	PSU	1	2923	1	-	1/7/25/26	0/2/2/2
1	OMU	1	2921	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2946	1	-	1/9/27/28	0/3/3/3
1	OMG	1	2922	1	-	1/9/27/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2946	A2M	O5'-C5'	-3.43	1.34	1.44
1	1	2923	PSU	C6-C5	3.28	1.38	1.35
1	1	2922	OMG	C6-N1	2.80	1.44	1.38
1	1	2923	PSU	C4-N3	-2.62	1.33	1.38
1	1	2922	OMG	C2-N2	2.62	1.40	1.34
1	1	2922	OMG	C4-N3	2.39	1.39	1.34
1	1	2946	A2M	C5-C4	2.29	1.43	1.39
1	1	2946	A2M	C8-N9	2.04	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2923	PSU	N1-C2-N3	6.31	121.83	115.17
1	1	2923	PSU	C4-N3-C2	-4.08	120.75	126.37
1	1	2923	PSU	O2-C2-N1	-3.54	119.14	122.79
1	1	2921	OMU	CM2-O2'-C2'	-2.56	107.89	114.47
1	1	2921	OMU	C4-N3-C2	-2.43	123.60	126.61
1	1	2946	A2M	N3-C4-N9	2.30	131.08	127.17
1	1	2946	A2M	C2-N1-C6	-2.13	115.23	118.73
1	1	2922	OMG	O6-C6-N1	-2.05	116.27	120.11
1	1	2923	PSU	C5-C6-N1	-2.02	119.33	122.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2922	OMG	O4'-C4'-C5'-O5'
1	1	2923	PSU	O4'-C1'-C5-C4
1	1	2946	A2M	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2923	PSU	3	0
1	1	2946	A2M	1	0
1	1	2922	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SAH	w	901	-	27,28,28	1.10	4 (14%)	36,40,40	2.02	9 (25%)

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
60	SAH	w	901	-	-	6/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	901	SAH	C2-N3	2.53	1.38	1.33
60	w	901	SAH	C2-N1	2.51	1.38	1.33
60	w	901	SAH	OXT-C	-2.24	1.23	1.30
60	w	901	SAH	C8-N7	2.09	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	w	901	SAH	N3-C2-N1	-5.50	120.26	128.58
60	w	901	SAH	C5-C4-N3	-4.52	120.50	126.72
60	w	901	SAH	C5'-SD-CG	-3.89	90.71	102.26
60	w	901	SAH	N9-C8-N7	-3.81	108.52	113.94
60	w	901	SAH	C2-N3-C4	3.42	120.19	111.83
60	w	901	SAH	C5-N7-C8	3.35	108.72	103.45
60	w	901	SAH	N3-C4-N9	2.91	132.12	127.17
60	w	901	SAH	OXT-C-O	-2.55	118.30	124.08
60	w	901	SAH	C4-C5-N7	-2.44	107.79	110.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

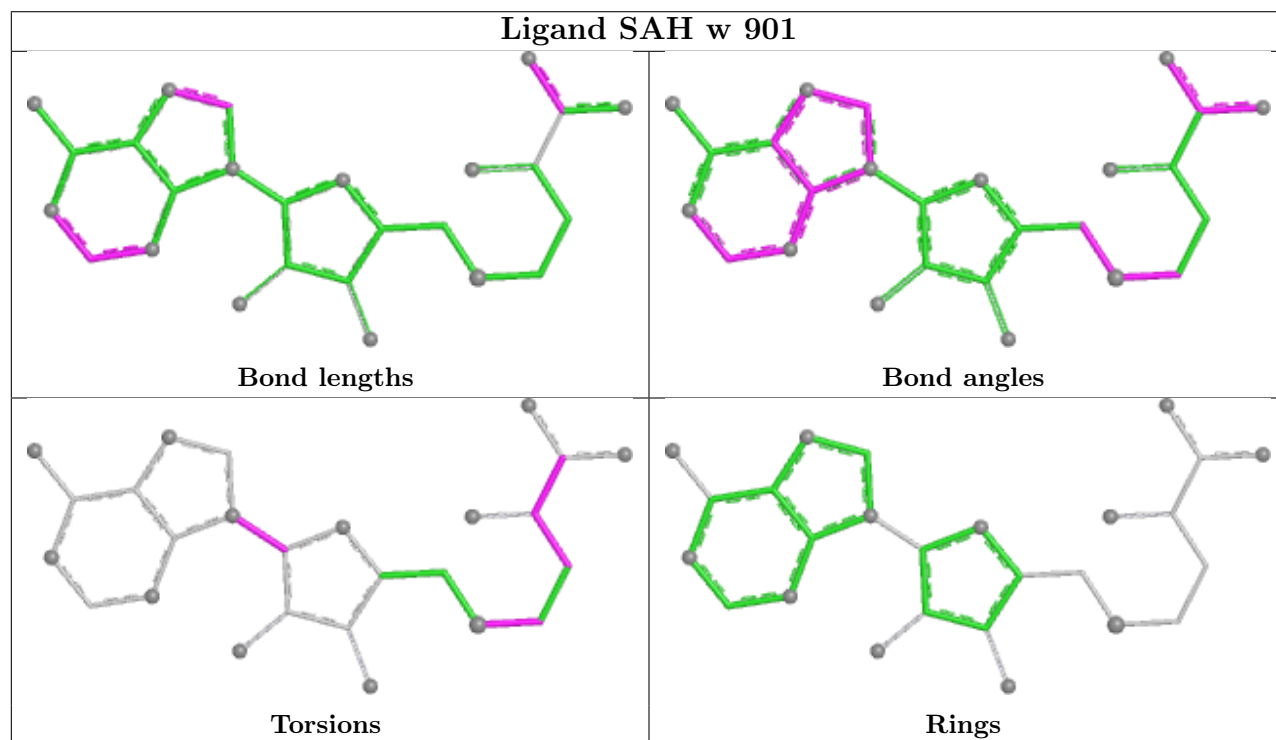
Mol	Chain	Res	Type	Atoms
60	w	901	SAH	C-CA-CB-CG
60	w	901	SAH	N-CA-CB-CG
60	w	901	SAH	OXT-C-CA-N
60	w	901	SAH	CB-CG-SD-C5'
60	w	901	SAH	C2'-C1'-N9-C8
60	w	901	SAH	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	w	901	SAH	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	6	67:U	O3'	213:A	P	14.86

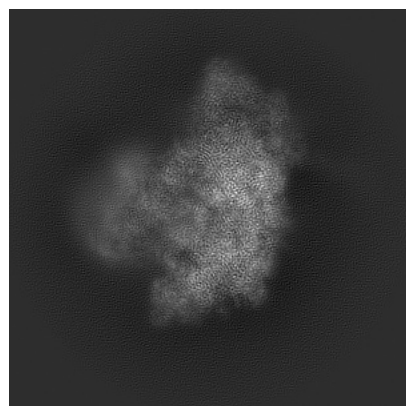
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24269. These allow visual inspection of the internal detail of the map and identification of artifacts.

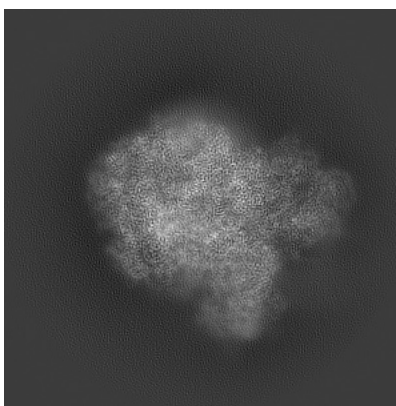
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

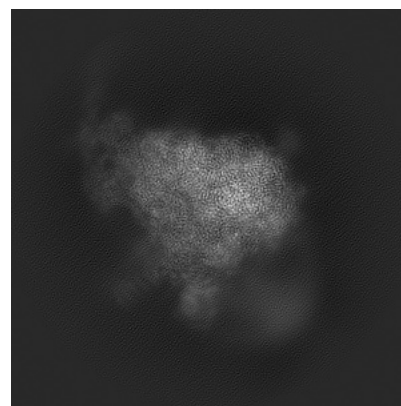
6.1.1 Primary map



X

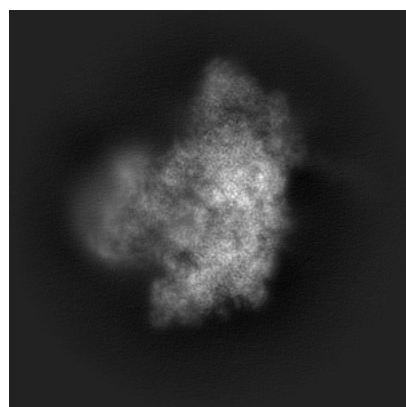


Y

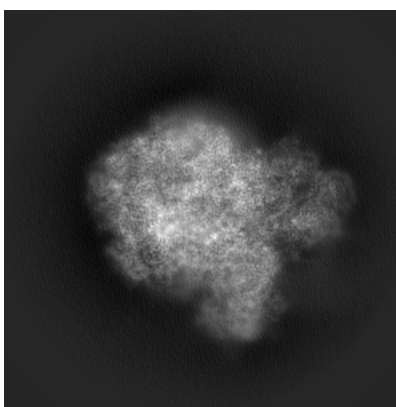


Z

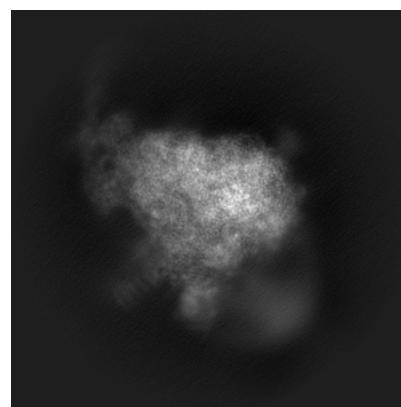
6.1.2 Raw map



X



Y

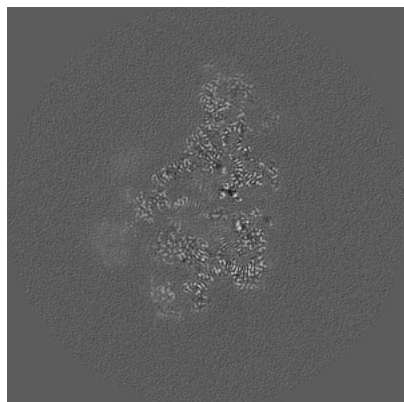


Z

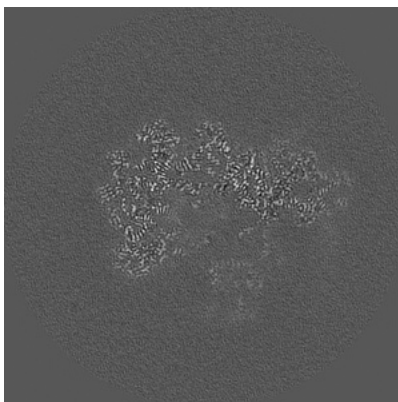
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

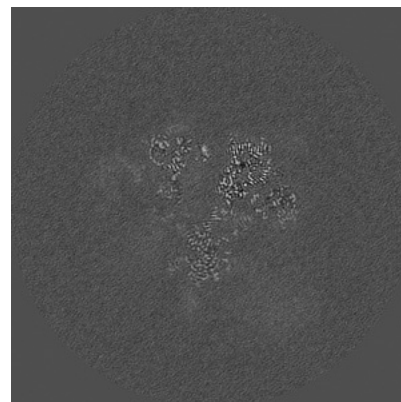
6.2.1 Primary map



X Index: 210

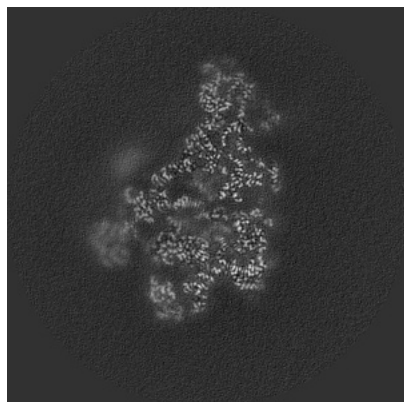


Y Index: 210

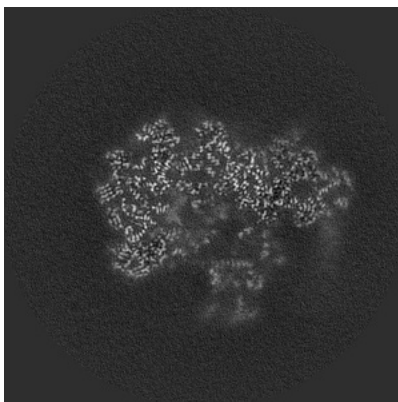


Z Index: 210

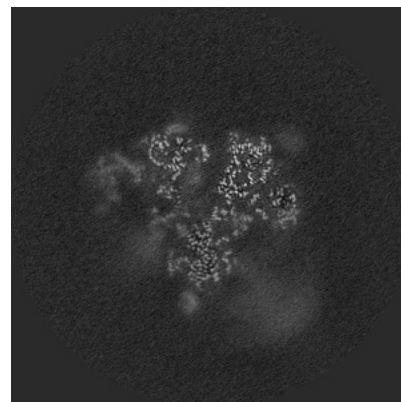
6.2.2 Raw map



X Index: 210



Y Index: 210

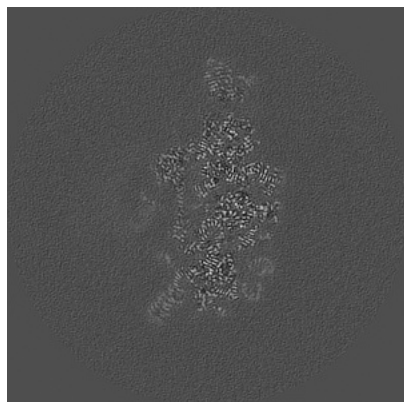


Z Index: 210

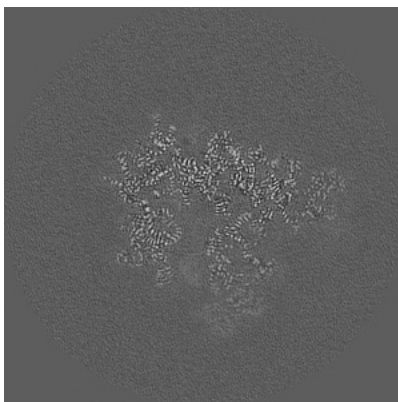
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

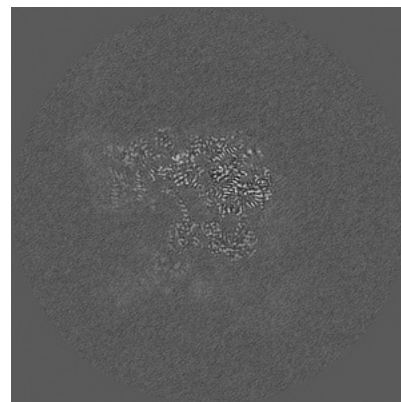
6.3.1 Primary map



X Index: 234

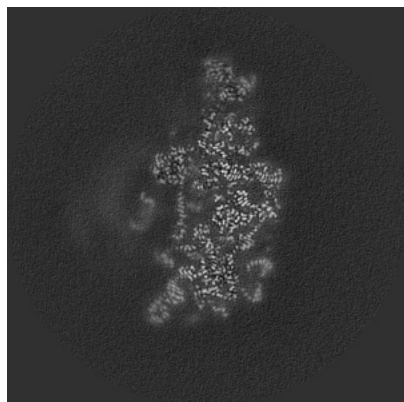


Y Index: 233

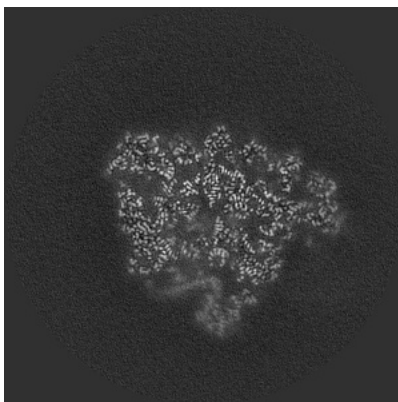


Z Index: 247

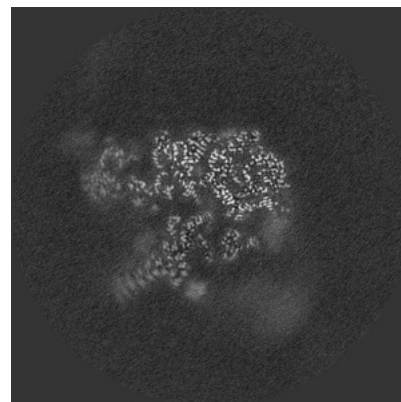
6.3.2 Raw map



X Index: 236



Y Index: 246

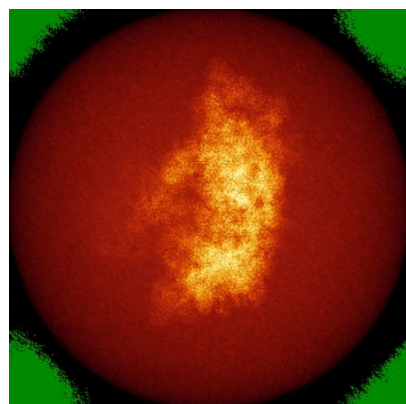


Z Index: 235

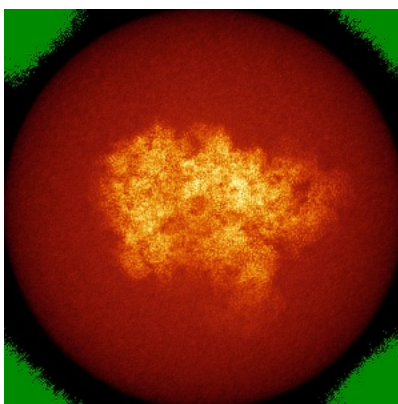
The images above show the largest variance slices of the map in three orthogonal directions.

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

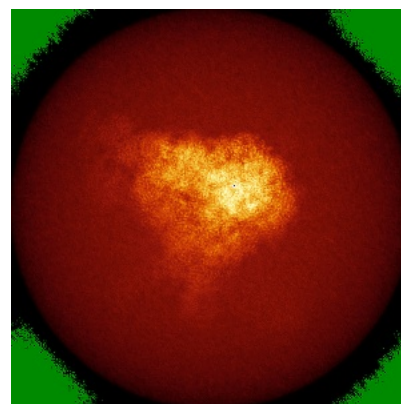
6.4.1 Primary map



X

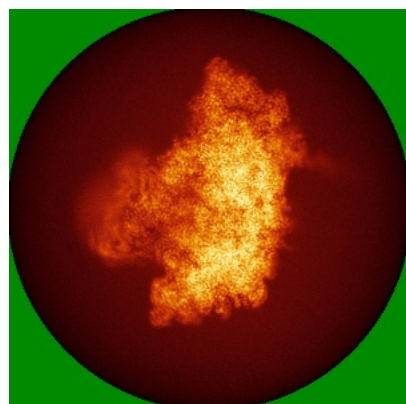


Y

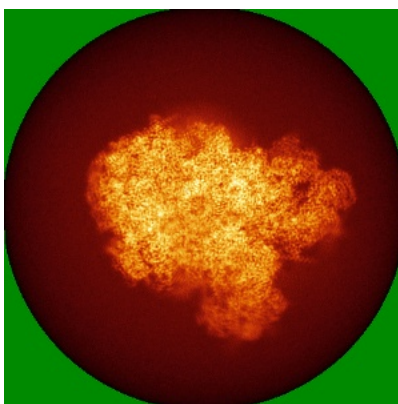


Z

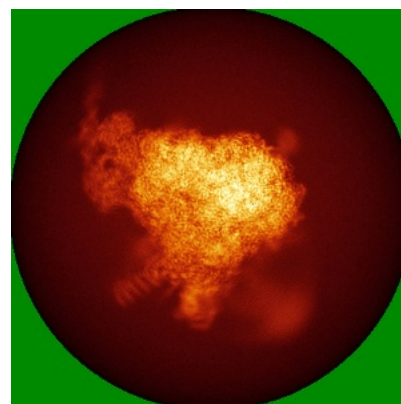
6.4.2 Raw map



X



Y

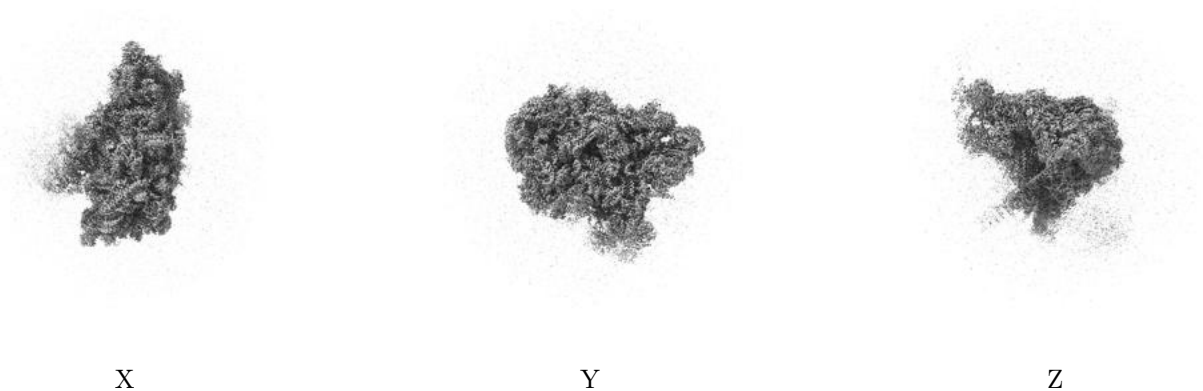


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

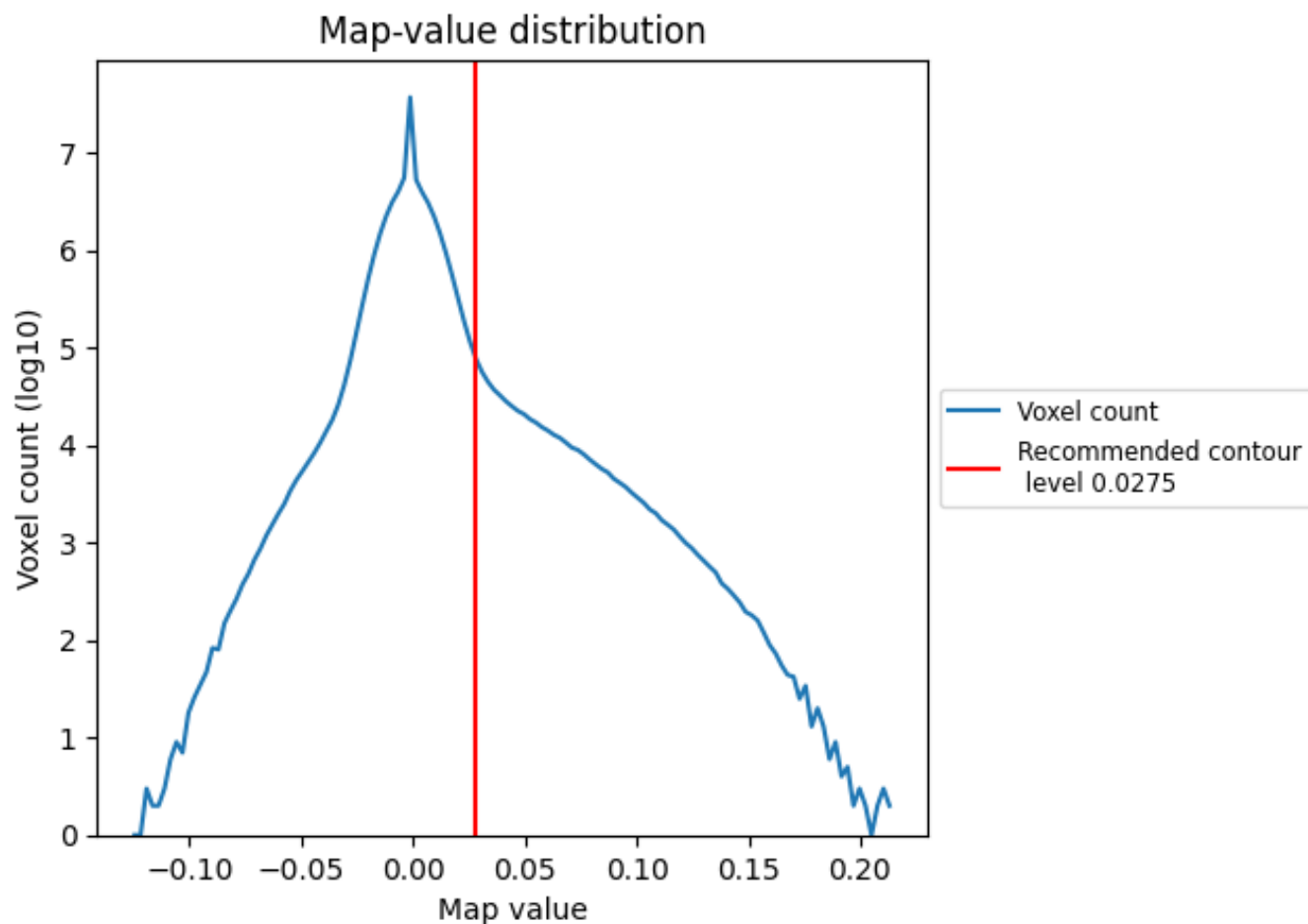
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

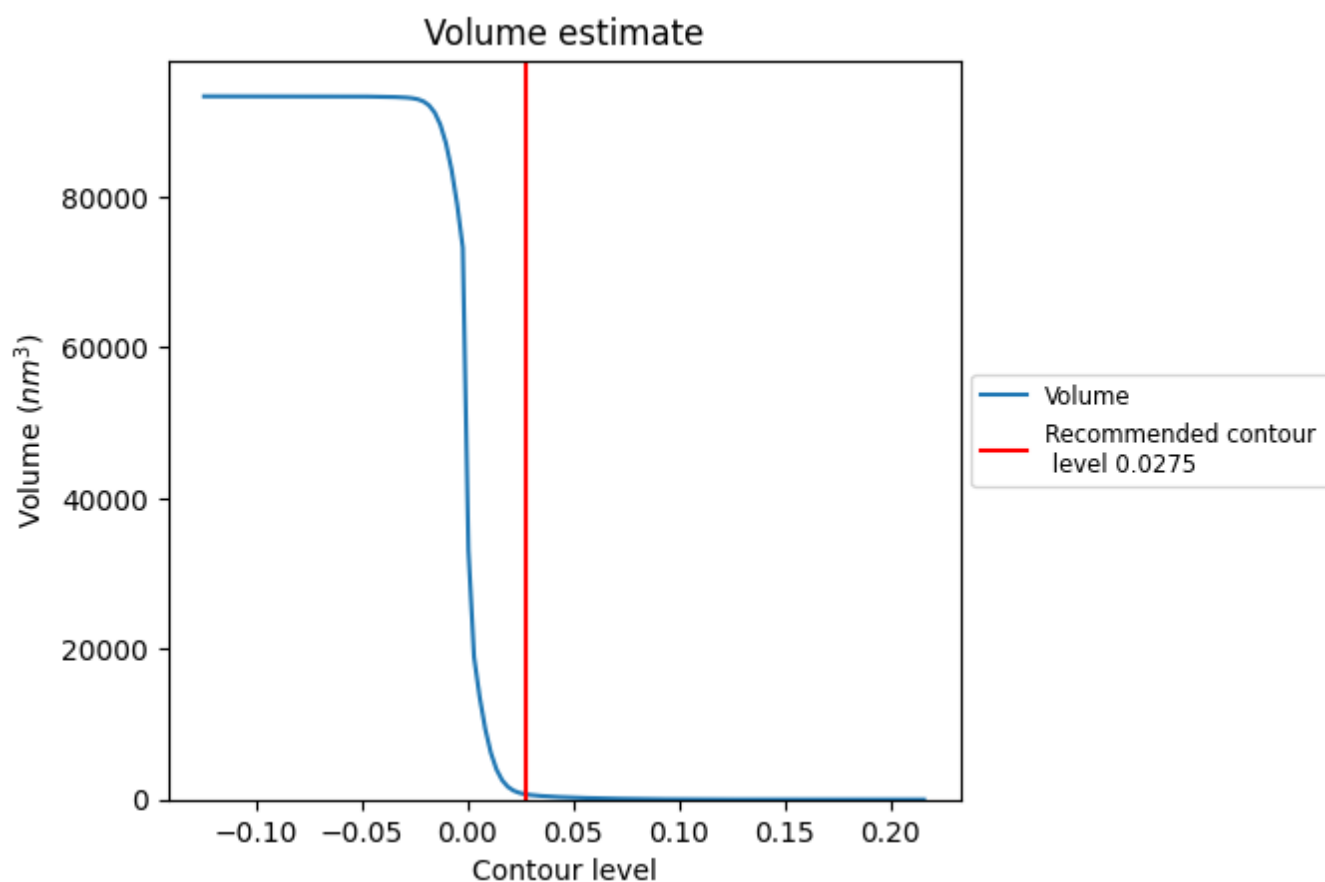
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

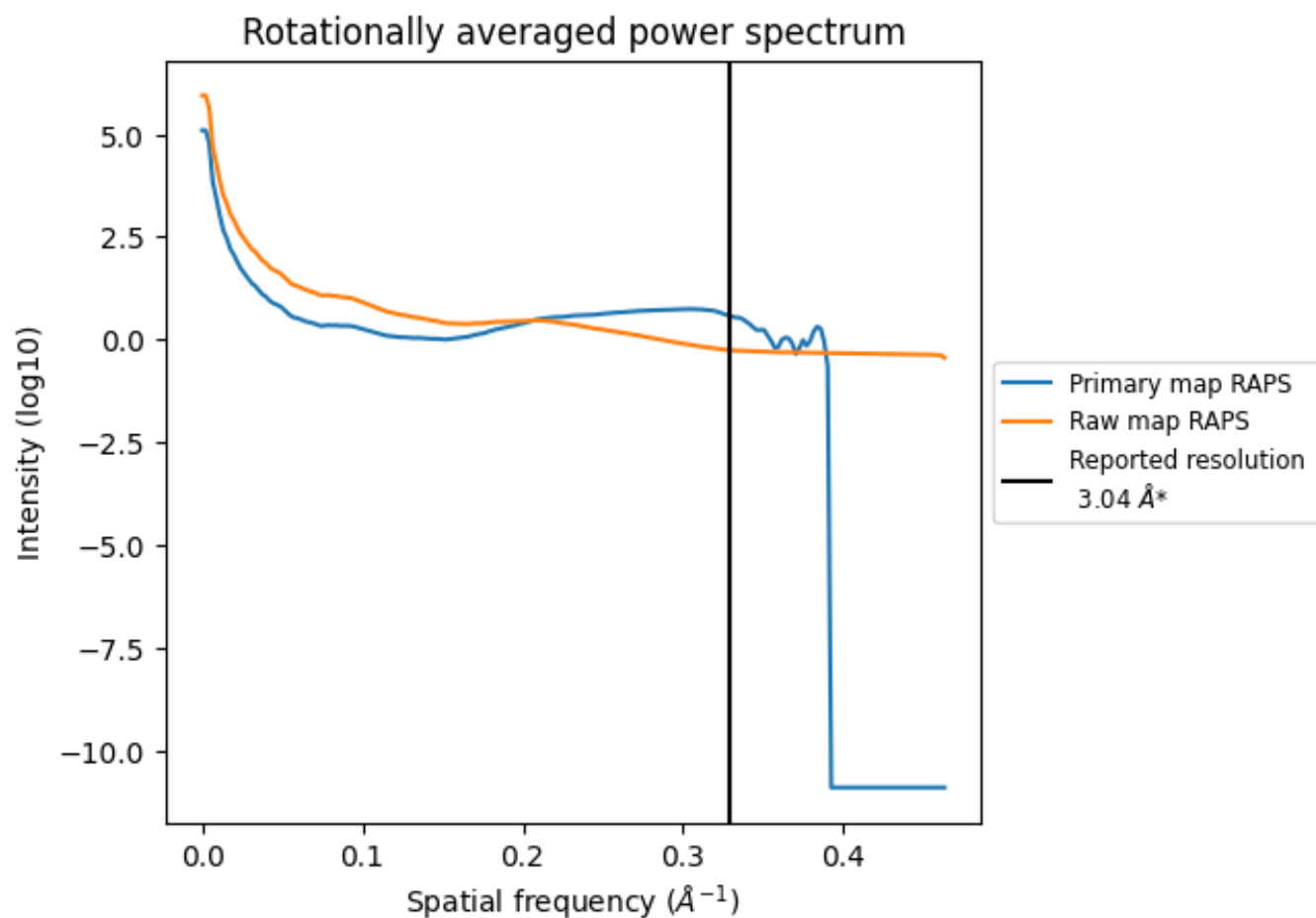
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 704 nm^3 ; this corresponds to an approximate mass of 636 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 ⓘ

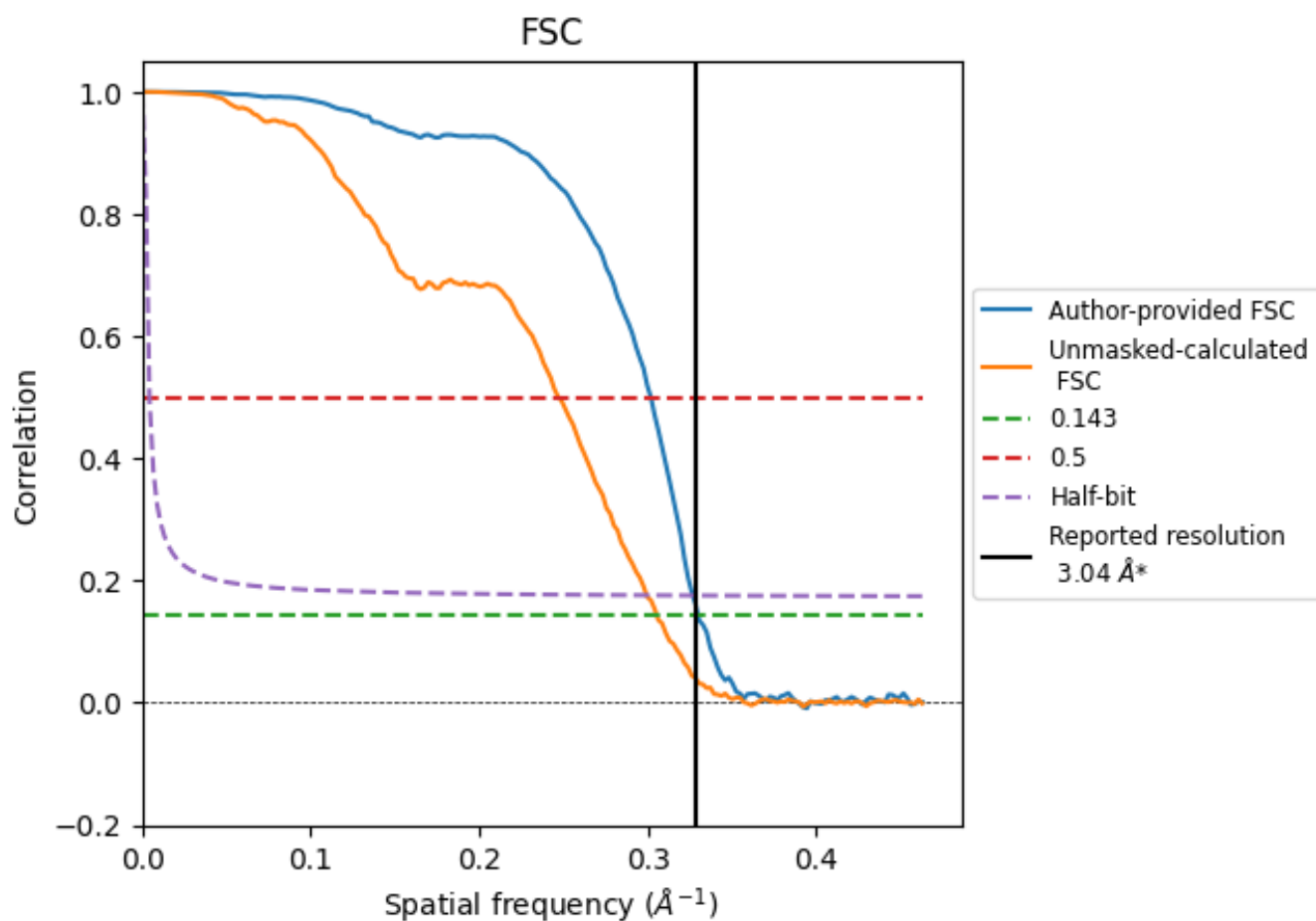


*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.329 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

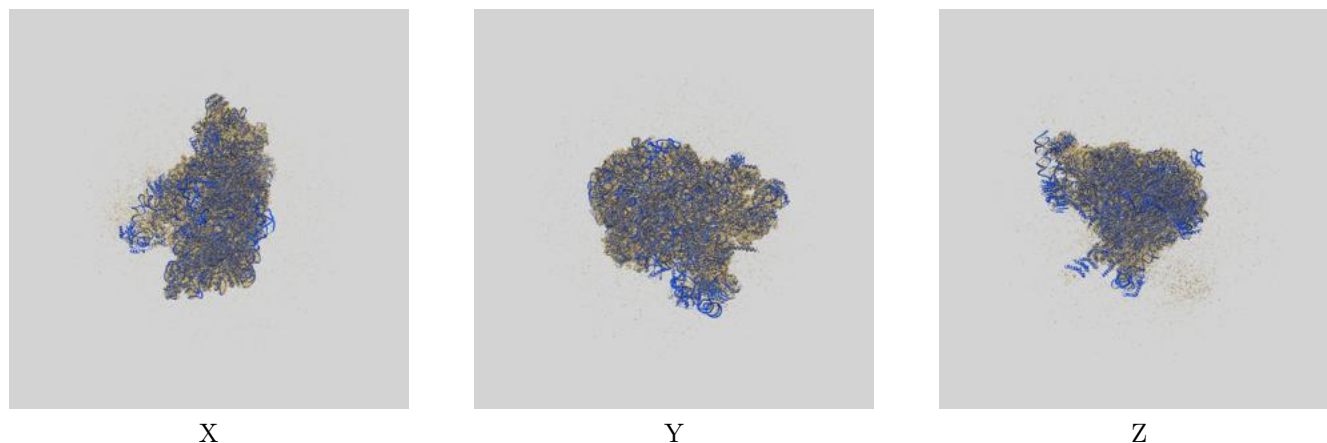
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.03	3.31	3.06
Unmasked-calculated*	3.27	4.05	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

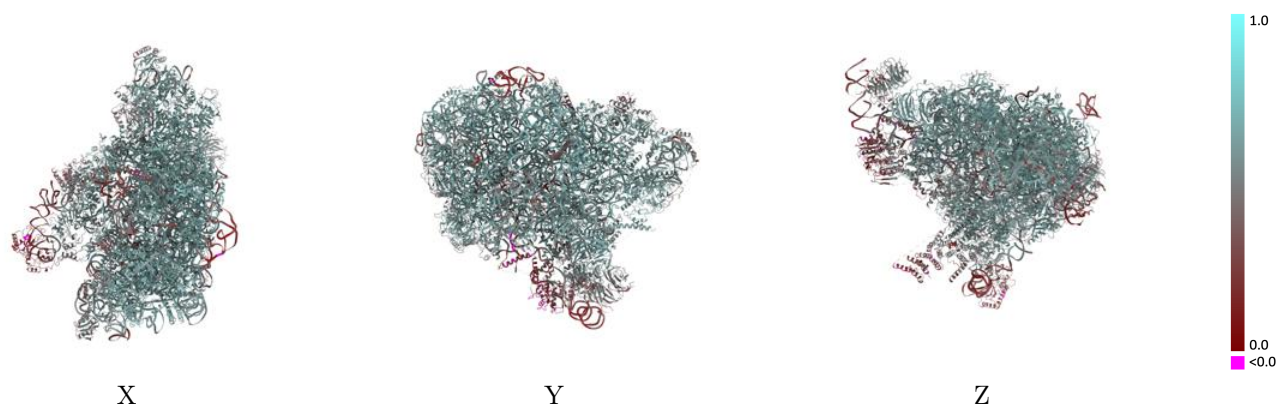
This section contains information regarding the fit between EMDB map EMD-24269 and PDB model 7NAC. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0275 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](#)

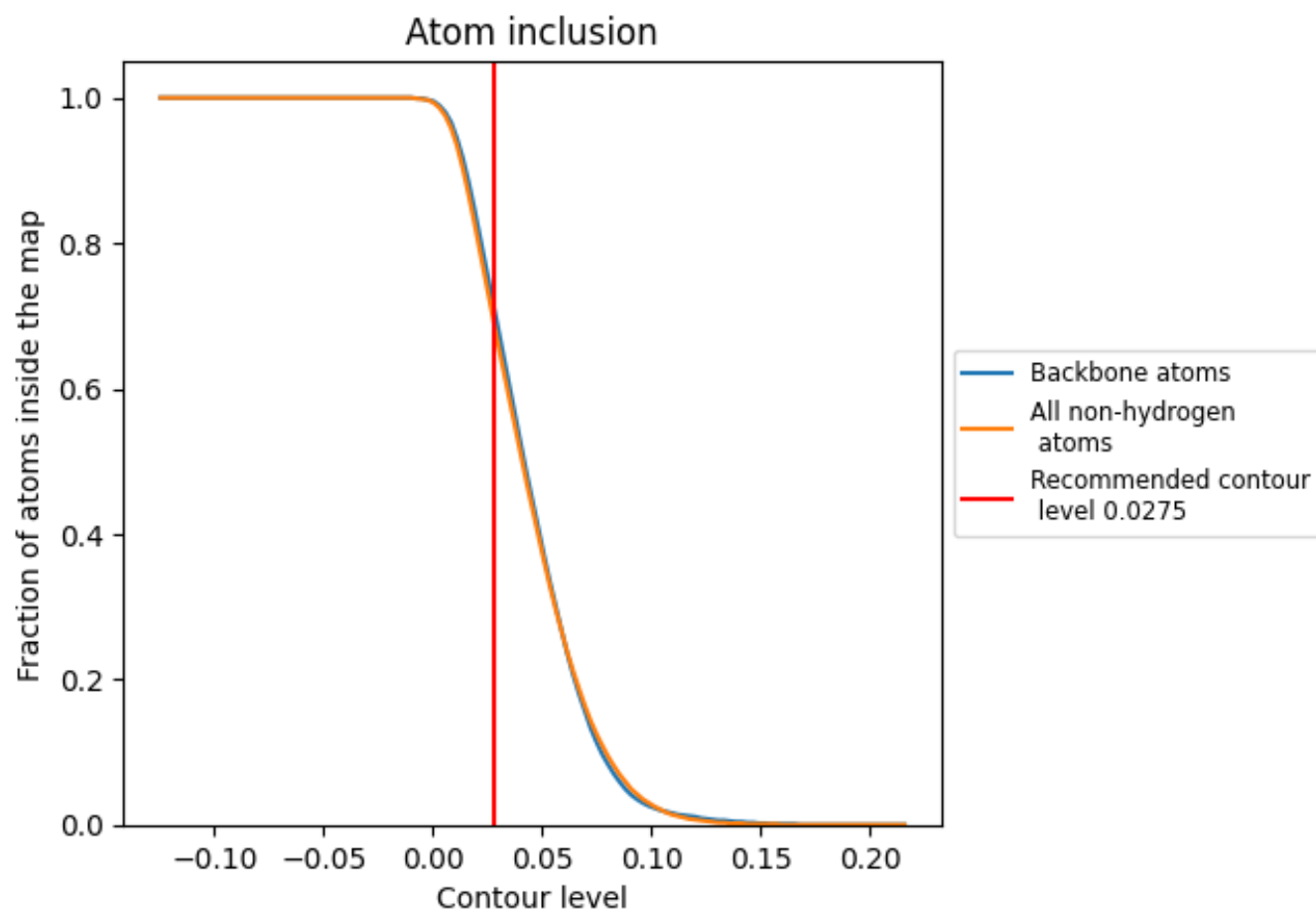


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.0275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.5490
1	 0.7670	 0.5470
2	 0.9030	 0.6080
5	 0.2830	 0.4650
6	 0.7140	 0.5480
7	 0.6390	 0.5610
8	 0.3090	 0.4270
A	 0.6680	 0.5390
B	 0.8900	 0.6200
C	 0.8700	 0.6250
D	 0.4970	 0.5230
E	 0.7690	 0.5870
F	 0.8230	 0.6100
G	 0.8380	 0.6120
H	 0.8040	 0.6050
I	 0.6150	 0.5450
J	 0.6210	 0.5550
K	 0.6280	 0.5510
L	 0.8710	 0.6240
M	 0.8310	 0.6110
N	 0.9340	 0.6420
O	 0.9030	 0.6290
P	 0.7790	 0.5880
Q	 0.8090	 0.6090
R	 0.6550	 0.5550
S	 0.7390	 0.5850
T	 0.0330	 0.3610
U	 0.6250	 0.5490
V	 0.8300	 0.6170
W	 0.4160	 0.4790
X	 0.8200	 0.6170
Y	 0.8850	 0.6230
Z	 0.7620	 0.5990
a	 0.0230	 0.2310
b	 0.5820	 0.5370



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Chain	Atom inclusion	Q-score
c	 0.6210	 0.5600
d	 0.7530	 0.5810
e	 0.8820	 0.6320
f	 0.9460	 0.6500
g	 0.8280	 0.6130
h	 0.8660	 0.6260
i	 0.7870	 0.5850
j	 0.9080	 0.6390
k	 0.6930	 0.5830
l	 0.7590	 0.5940
m	 0.7530	 0.5940
n	 0.7830	 0.6010
o	 0.6510	 0.5500
p	 0.3150	 0.4580
q	 0.5830	 0.5280
r	 0.6930	 0.5770
s	 0.7750	 0.6040
t	 0.7190	 0.5860
u	 0.7490	 0.5890
v	 0.8220	 0.6080
w	 0.5630	 0.5320
x	 0.1590	 0.3020
y	 0.8050	 0.5930
z	 0.4950	 0.5320