



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:35 AM UTC

PDB ID : 6EM1 / pdb_00006em1
EMDB ID : EMD-3893
Title : State C (Nsa1-TAP Flag-Ytm1) - Visualizing the assembly pathway of nuclear pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-10-01
Resolution : 3.60 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:

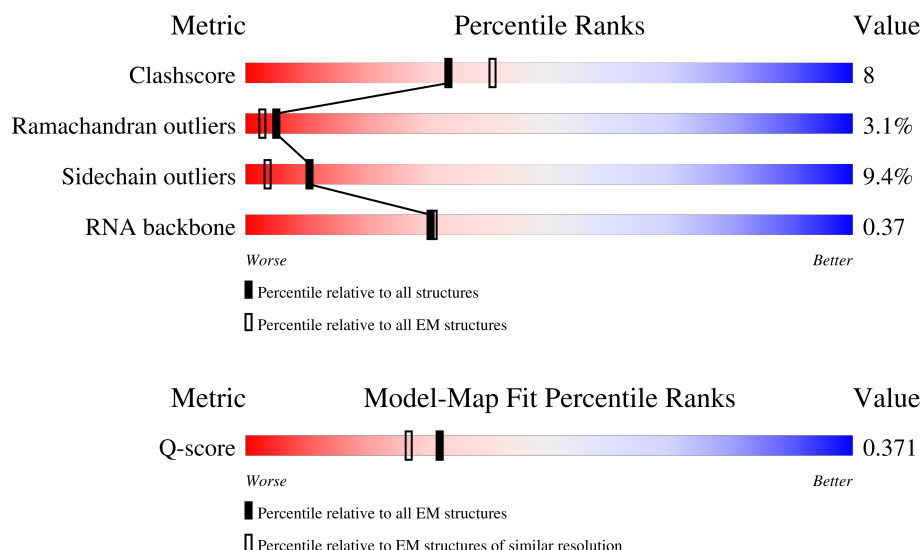
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	x	295	
2	F	244	
3	3	306	

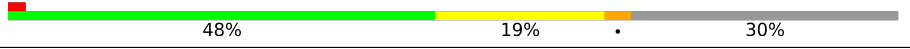
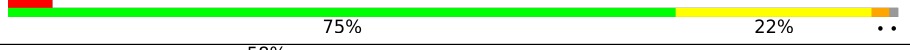
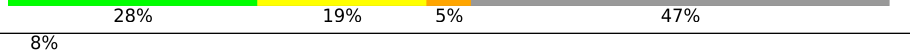
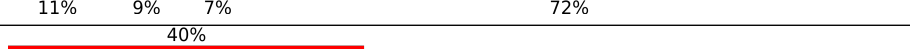
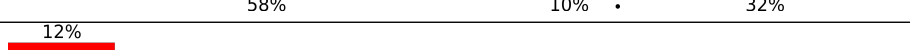
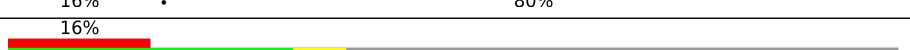
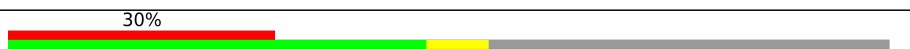
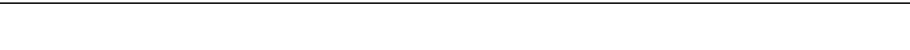
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Mol	Chain	Length	Quality of chain
4	4	278	
5	5	463	
6	A	291	
7	b	647	
8	J	427	
9	r	261	
10	s	520	
11	u	199	
12	v	231	
13	W	236	
14	y	245	
15	z	106	
16	B	387	
17	C	362	
18	e	130	
19	E	176	
20	f	107	
21	G	256	
22	h	120	
23	H	191	
24	i	100	
25	j	88	
26	L	199	
27	M	138	
28	N	204	

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Mol	Chain	Length	Quality of chain
29	O	199	
30	P	184	
31	Q	186	
32	S	172	
33	V	137	
34	Y	127	
35	1	3396	
36	2	158	
37	6	232	
38	K	376	
39	m	807	
40	D	505	
41	o	220	
42	n	605	
43	t	322	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 99980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	267	Total	C	N	O	S	0	0
			2268	1444	413	407	4		

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	241	Total	C	N	O	S	0	0
			1936	1246	351	338	1		

- Molecule 3 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	173	Total	C	N	O	S	0	0
			1434	901	274	250	9		

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	217	Total	C	N	O	S	0	0
			1853	1208	319	323	3		

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	385	Total	C	N	O	S	0	0
			3055	1957	514	573	11		

- Molecule 6 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	145	Total	C	N	O	S	0	0
			1211	780	218	210	3		

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	421	Total	C	N	O	S	0	0
			3410	2180	585	627	18		

- Molecule 8 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			549	341	97	110	1		

- Molecule 9 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	73	Total	C	N	O	S	0	0
			628	388	133	106	1		

- Molecule 10 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	s	27	Total	C	N	O	S	0	0
			224	136	51	37			

- Molecule 11 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	u	116	Total	C	N	O	S	0	0
			976	612	200	155	9		

- Molecule 12 is a protein called Nucleolar protein 16.

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

- Molecule 13 is a protein called Ribosome assembly factor MRT4.

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

- Molecule 14 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 15 is a protein called UPF0642 protein YBL028C.

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

- Molecule 16 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	333	Total	C	N	O	S	0	0
			2646	1680	490	470	6		

- Molecule 17 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	343	Total	C	N	O	S	0	0
			2611	1643	499	466	3		

- Molecule 18 is a protein called 60S ribosomal protein L32.

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

- Molecule 19 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	151	Total	C	N	O	S	0	0
			1205	780	215	209	1		

- Molecule 20 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	159	Total	C	N	O	S	0	0
			1231	794	209	226	2		

- Molecule 22 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L36-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	74	Total	C	N	O	S	0	0
			594	367	125	101	1		

- Molecule 25 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	71	Total	C	N	O	S	0	0
			566	344	123	94	5		

- Molecule 26 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	108	Total	C	N	O		0	0
			864	541	180	143			

- Molecule 27 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	134	Total	C	N	O	S	0	0
			1041	668	197	174	2		

- Molecule 28 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	177	Total	C	N	O	S	0	0
			1513	948	320	244	1		

- Molecule 29 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P	137	Total	C	N	O	S	0	0
			1062	666	198	198			

- Molecule 31 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	131	Total	C	N	O	S	0	0
			1009	645	190	173	1		

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	126	Total	C	N	O	S	0	0
			936	588	176	165	7		

- Molecule 34 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 35 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	1785	Total	C	N	O	P	0	0
			38221	17064	6918	12454	1785		

- Molecule 36 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 37 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 38 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	K	257	Total	C	N	O	S	0	0
			2073	1337	341	392	3		

- Molecule 39 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	161	Total	C	N	O	S	0	0
			1362	867	238	253	4		

- Molecule 40 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D	194	Total	C	N	O	S	0	0
			1590	1030	268	287	5		

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

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

- Molecule 42 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	334	Total	C	N	O	S	0	0
			2734	1787	457	482	8		

- Molecule 43 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	244	Total	C	N	O	S	0	0
			1935	1233	345	354	3		

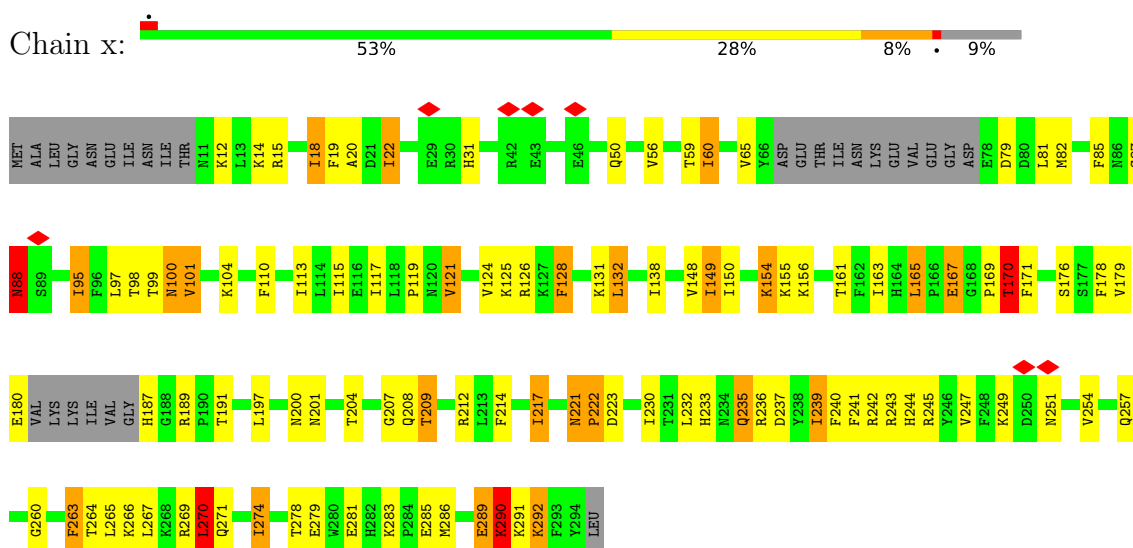
- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	u	1	Total	Zn	0
			1	1	
44	j	1	Total	Zn	0
			1	1	

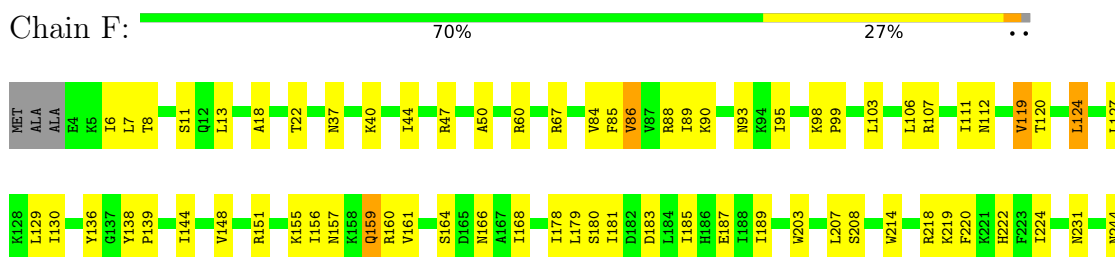
3 Residue-property plots

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.

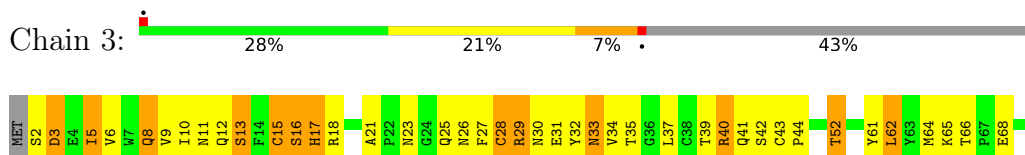
• Molecule 1: Ribosome production factor 1

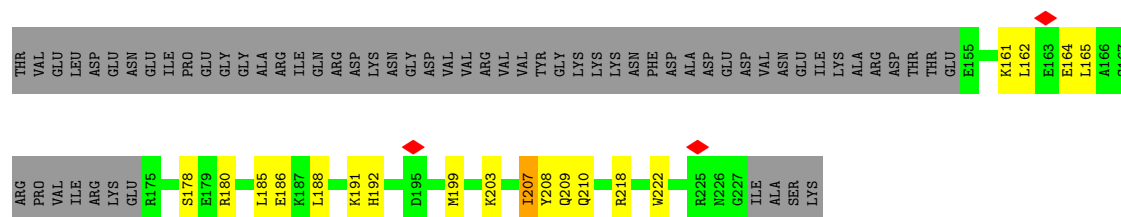


• Molecule 2: 60S ribosomal protein L7-A

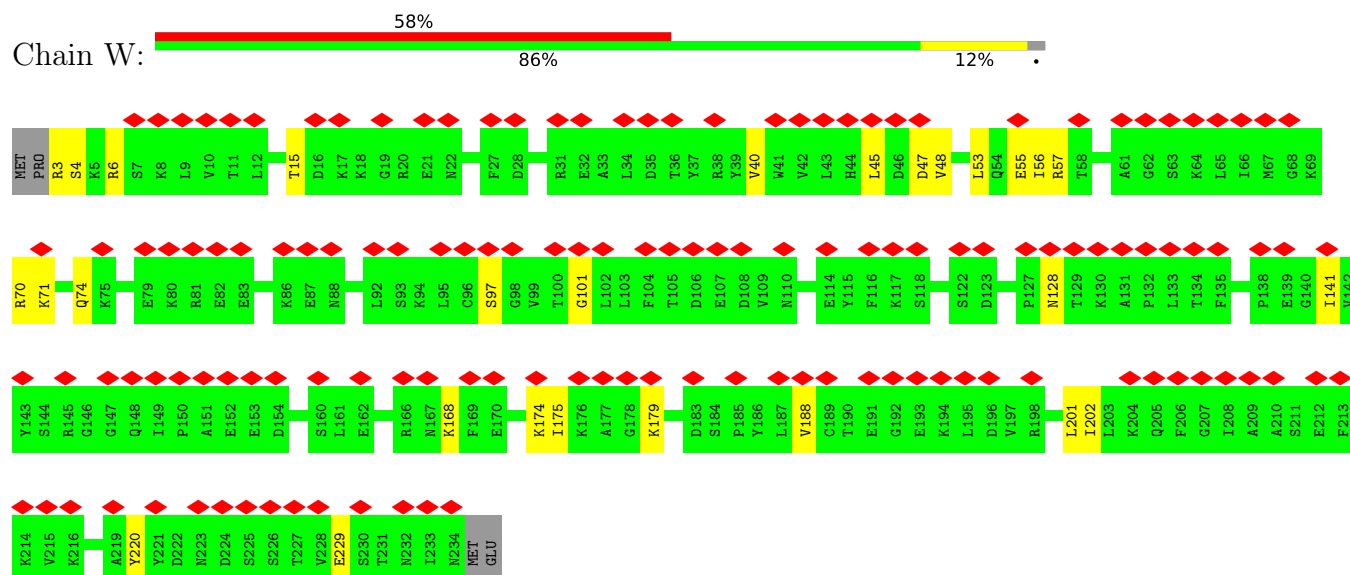


• Molecule 3: Protein MAK16

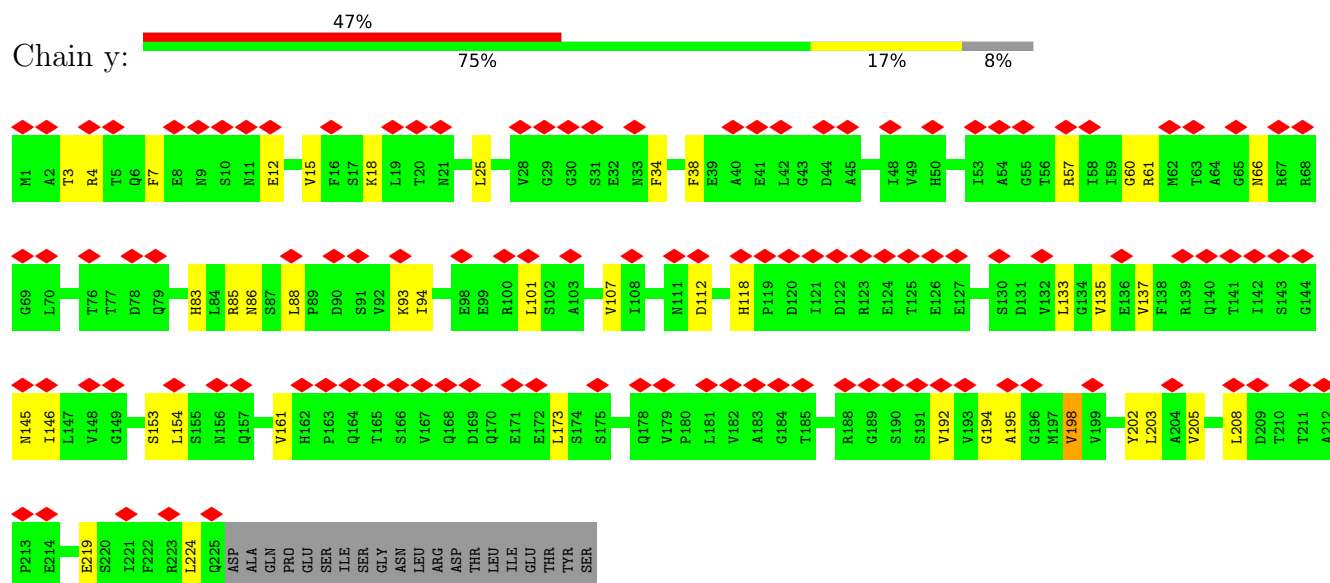




• Molecule 13: Ribosome assembly factor MRT4

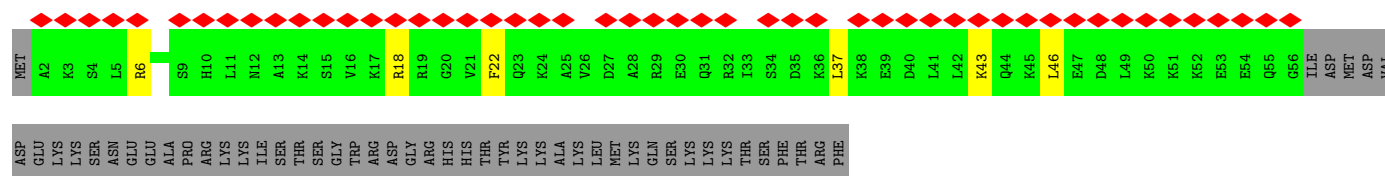


• Molecule 14: Eukaryotic translation initiation factor 6

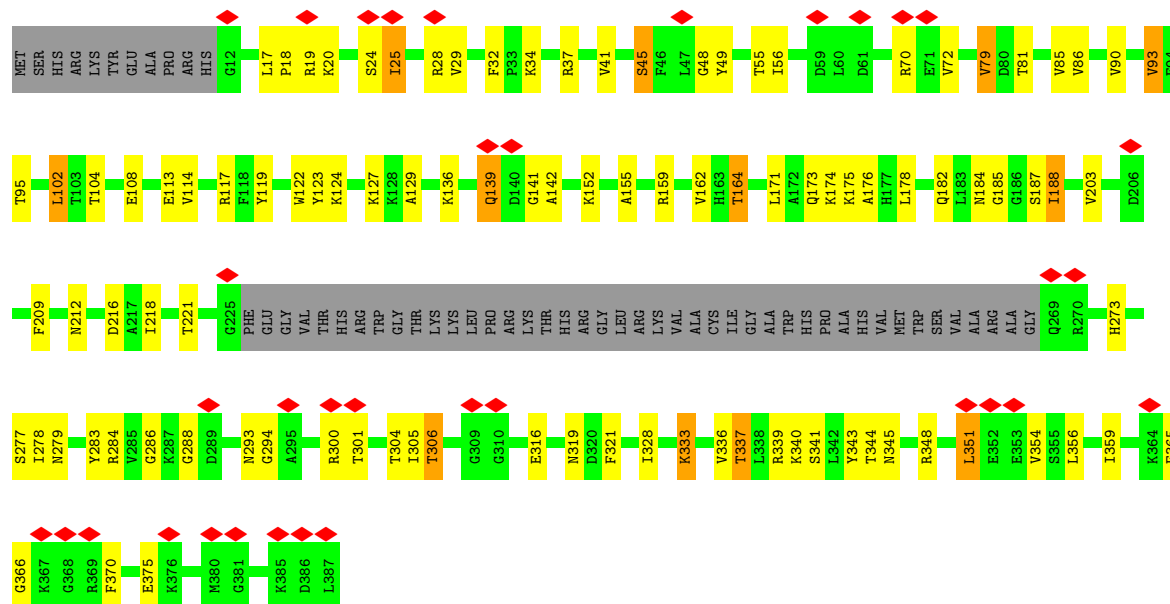


• Molecule 15: UPF0642 protein YBL028C

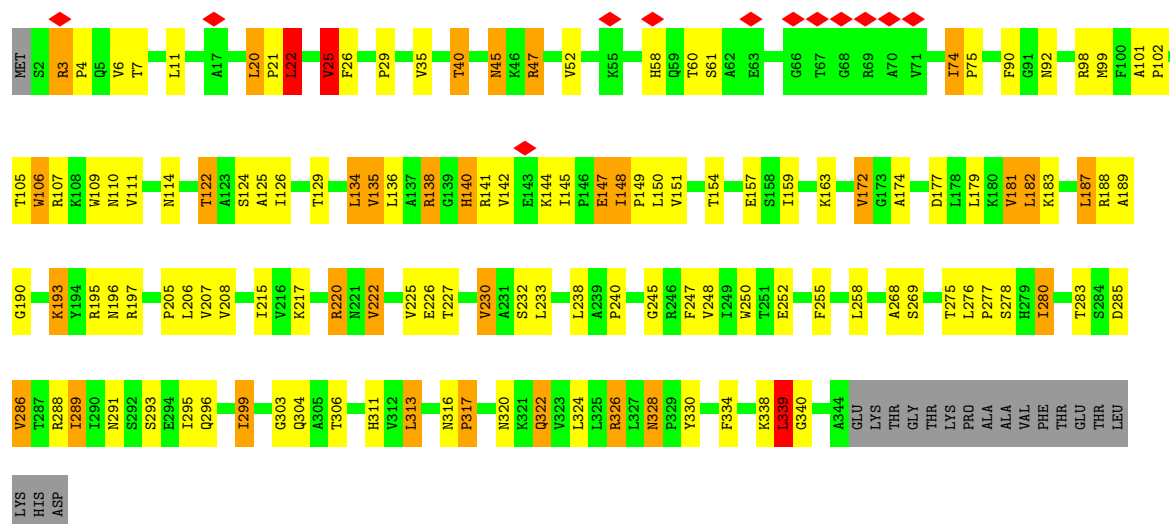




• Molecule 16: 60S ribosomal protein L3



• Molecule 17: 60S ribosomal protein L4-A



• Molecule 18: 60S ribosomal protein L32

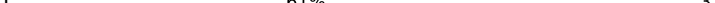
- Chain E:  70% 15% 14%

Top Chart (MET highlighted in grey):

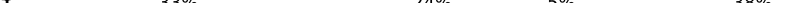
Amino Acid	Frequency (approx.)	Significance
MET	100	Highly Significant (Red Diamond)
SER	10	
ALA	10	
GLN	10	
LYS	10	
ALA	10	
P7	10	Significant (Red Diamond)
R8	10	Significant (Red Diamond)
H9	10	
Y10	10	Significant (Red Diamond)
V15	10	
A16	10	Significant (Red Diamond)
A17	10	
R22	10	Significant (Red Diamond)
R26	10	Significant (Red Diamond)
K29	10	Significant (Red Diamond)
L30	10	Significant (Red Diamond)
R31	10	Significant (Red Diamond)
V39	10	Significant (Red Diamond)
L40	10	
L41	10	Significant (Red Diamond)
V52	10	Significant (Red Diamond)
V53	10	Significant (Red Diamond)
Y54	10	
L58	10	
L63	10	Significant (Red Diamond)
L64	10	
T65	10	
S66	10	
L76	10	Significant (Red Diamond)
V79	10	
N80	10	
Y83	10	
R84	10	
L85	10	Significant (Red Diamond)
A86	10	
Q95	10	Significant (Red Diamond)
V98	10	Significant (Red Diamond)
E99	10	Significant (Red Diamond)
K100	10	
F101	10	
E109	10	Significant (Red Diamond)
LYS	10	
LEU	10	
THR	10	

Bottom Chart (E129 highlighted in grey):

Amino Acid	Frequency (approx.)	Significance
LYS	10	
LYS	10	
GLU	10	
LYS	10	
LYS	10	
GLU	10	
ALA	10	
ASN	10	
LEU	10	
PHE	10	
PRO	10	
GLN	10	
GLN	10	
ASN	10	
LYS	10	
E129	10	Highly Significant (Red Diamond)
L155	10	Significant (Red Diamond)
K170	10	Significant (Red Diamond)
F176	10	Significant (Red Diamond)

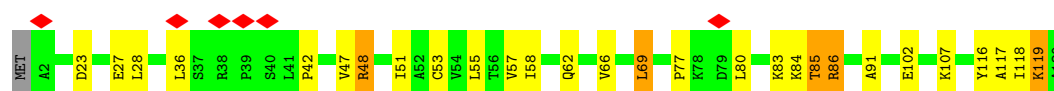
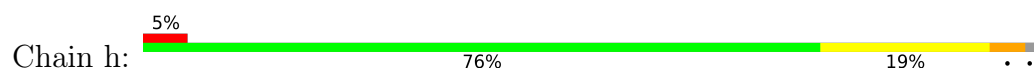
- Chain f:  61% 32% 7%

Amino Acid	Category	Frequency (approx.)
S97	Amino acids in the protein	10
V98	Amino acids in the protein	10
R99	Amino acids in the protein	10
I100	Amino acids in the protein	10
F101	Amino acids in the protein	10
L102	Amino acids in the protein	10
Y103	Amino acids in the protein	10
P104	Amino acids in the protein	10
S105	Amino acids in the protein	10
N106	Amino acids in the protein	10
I107	Amino acids in the protein	10
MET	Amino acids in the database	10
A2	Amino acids in the database	10
E3	Amino acids in the database	10
Y8	Amino acids in the database	10
V9	Amino acids in the database	10
K10	Amino acids in the database	10
L14	Amino acids in the database	10
S15	Amino acids in the database	10
Y16	Amino acids in the database	10
K20	Amino acids in the database	10
N23	Amino acids in the database	10
N24	Amino acids in the database	10
N25	Amino acids in the database	10
P26	Amino acids in the database	10
V27	Amino acids in the database	10
K31	Amino acids in the database	10
G34	Amino acids in the database	10
P38	Amino acids in the database	10
K47	Amino acids in the database	10
R48	Amino acids in the database	10
L49	Amino acids in the database	10
V52	Amino acids in the database	10
Y53	Amino acids in the database	10
E58	Amino acids in the database	10
V59	Amino acids in the database	10
R60	Amino acids in the database	10
T64	Amino acids in the database	10
R65	Amino acids in the database	10
V66	Amino acids in the database	10
M67	Amino acids in the database	10
V68	Amino acids in the database	10
V71	Amino acids in the database	10
G76	Amino acids in the database	10
N77	Amino acids in the database	10
V80	Amino acids in the database	10
R81	Amino acids in the database	10
R82	Amino acids in the database	10
R86	Amino acids in the database	10
R87	Amino acids in the database	10
R88	Amino acids in the database	10
L89	Amino acids in the database	10
P90	Amino acids in the database	10
A91	Amino acids in the database	10
K92	Amino acids in the database	10

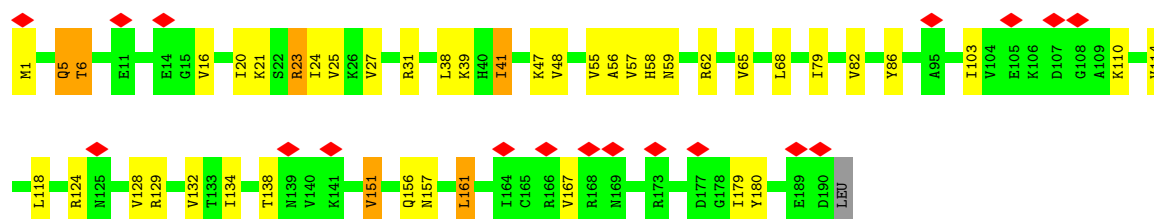
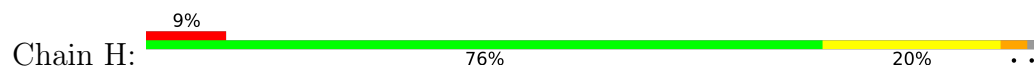
- Chain G: 

MET	ALA	GLY	LYS	VAL	ALA	ALA	PRO	PRO	PHE	GLY	LYS	SER	THR	LYS	ASN	SER	THR	HIS	THR	PRO	LYS	ASN	PHE	GLY	ILE	GLY	GLN	ALA	VAL	GLN	LYS	ASN	SER	THR	VAL	LYS	TRP	PRO	GLU	TYR	VAL	ARG	GLN	ARG				
V132	K133	Y134	G135	L136	N137	V140	A141	L142	I143	A144	N145	K146	K147	A148	K149	L150	V157	D158	P159	V162	L163	L166	K172	M173	G174	V175	P176	I179	V180	L186	L189	V190	N191	V197	L200	T201	E202	V203	R204	A205	E206	K213	L214	T217	A220	N221		
D224	V229	K230	K231	H232	H233	GLY	GLY	GLY	ILE	LEU	GLY	ASN	LYS	ALA	GLN	ALA	LYS	MET	ASP	LYS	ARG	ALA	LYS	SER	ASP	SER	ALA																					
GLN	LYS	LYS	ILE	LEU	SER	K70	V71	P72	P73	T74	I75	A76	Q77	F78	Y80	N85	T90	F91	K92	L93	F94	N95	K96	Y97	N98	T101	E104	K105	R108	L109	F110	K111	E112	A113	A114	A115	V116	G119	LYS	SER	LYS	GLN	ASP	A125	K128	P129	Y130	A131

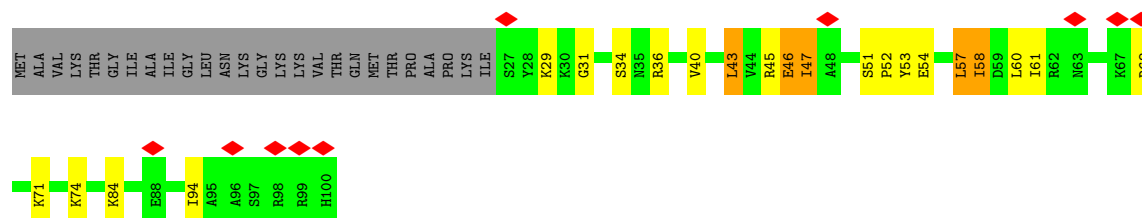
- 



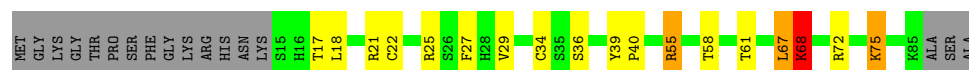
- Molecule 23: 60S ribosomal protein L9-A



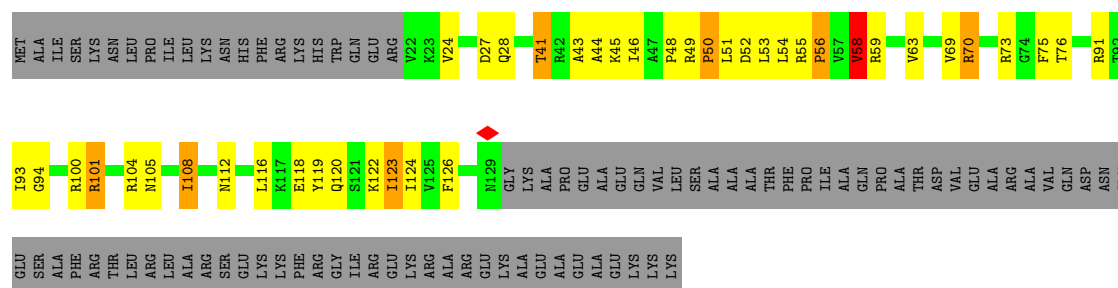
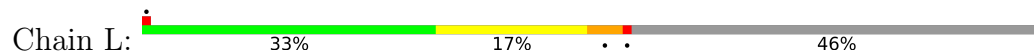
- Molecule 24: 60S ribosomal protein L36-B



- Molecule 25: 60S ribosomal protein L37-A

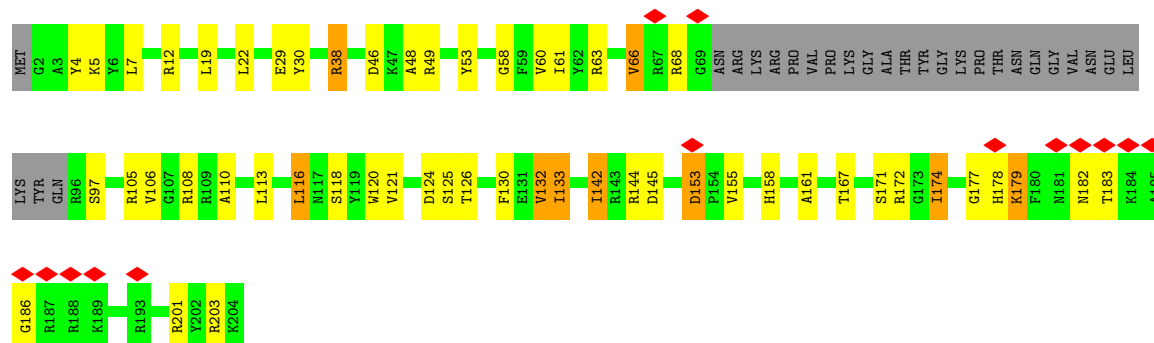


- Molecule 26: 60S ribosomal protein L13-A

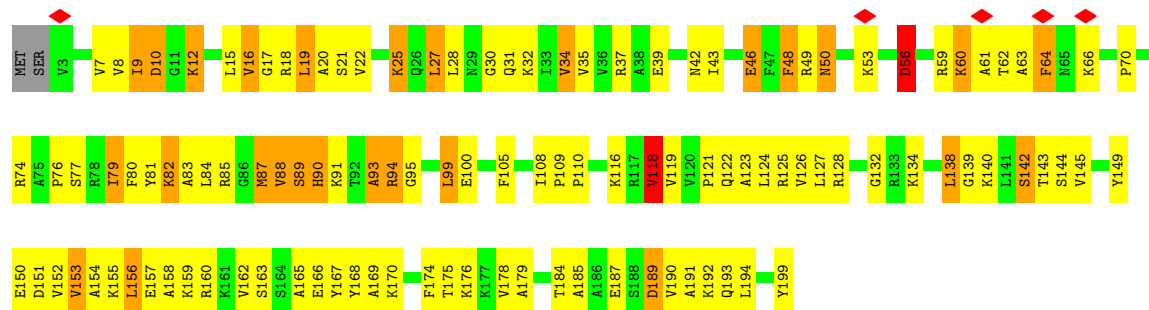


- Molecule 27: 60S ribosomal protein L14-A

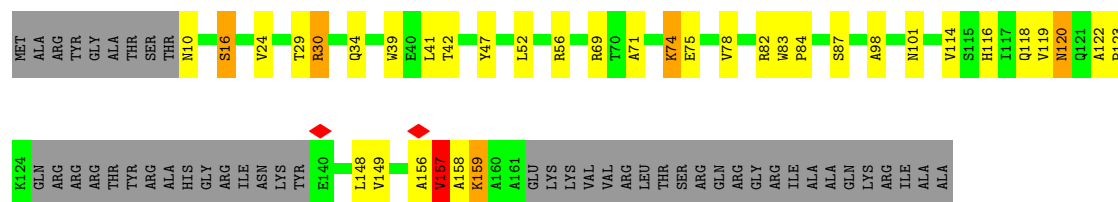
Chain N: 7% 60% 22% 13%



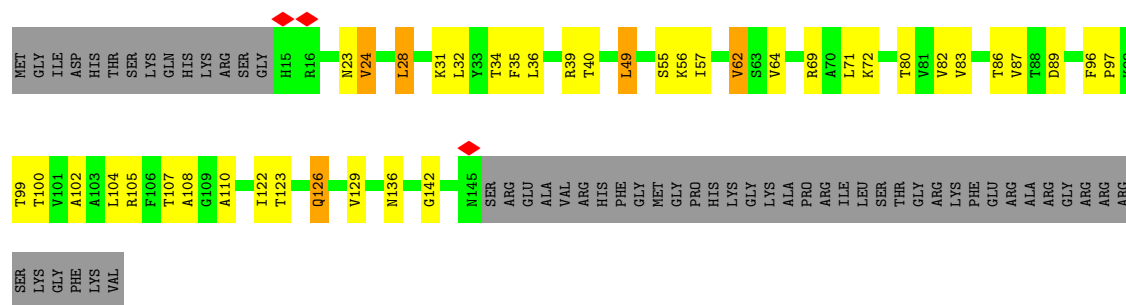
Chain 0: 40% 45% 14%



Chain P: 55% 16% 26%

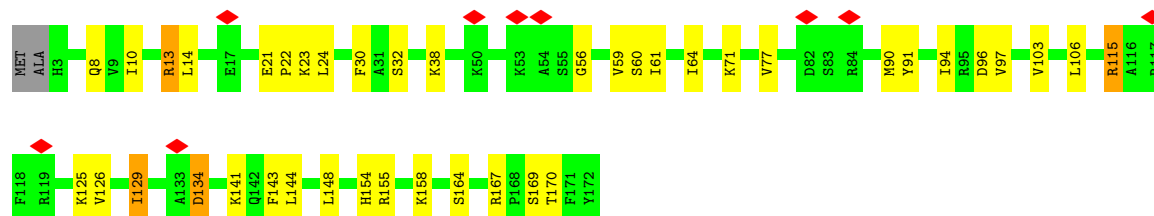


Chain Q: 



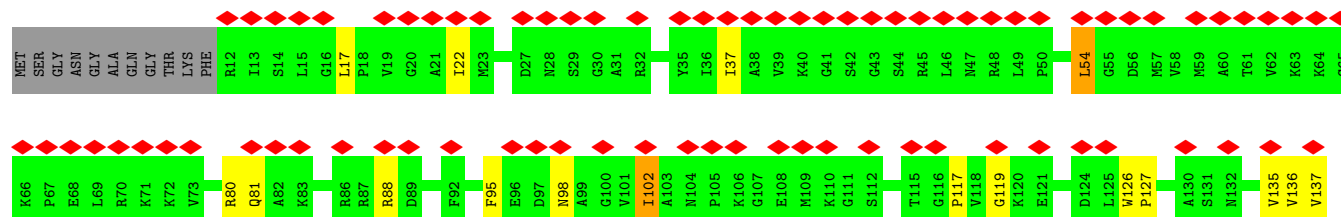
• Molecule 32: 60S ribosomal protein L20-A

Chain S: 



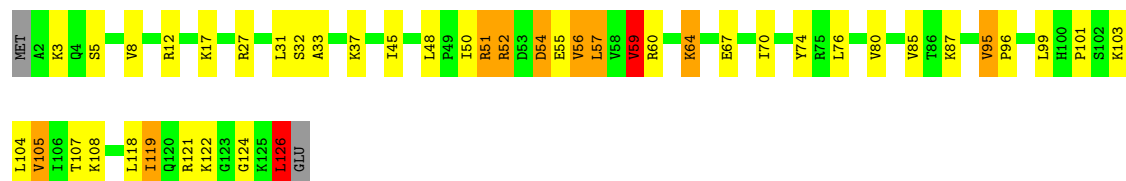
• Molecule 33: 60S ribosomal protein L23-A

Chain V: 

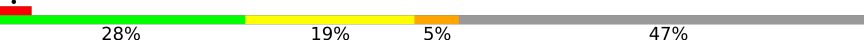


• Molecule 34: 60S ribosomal protein L26-A

Chain Y: 

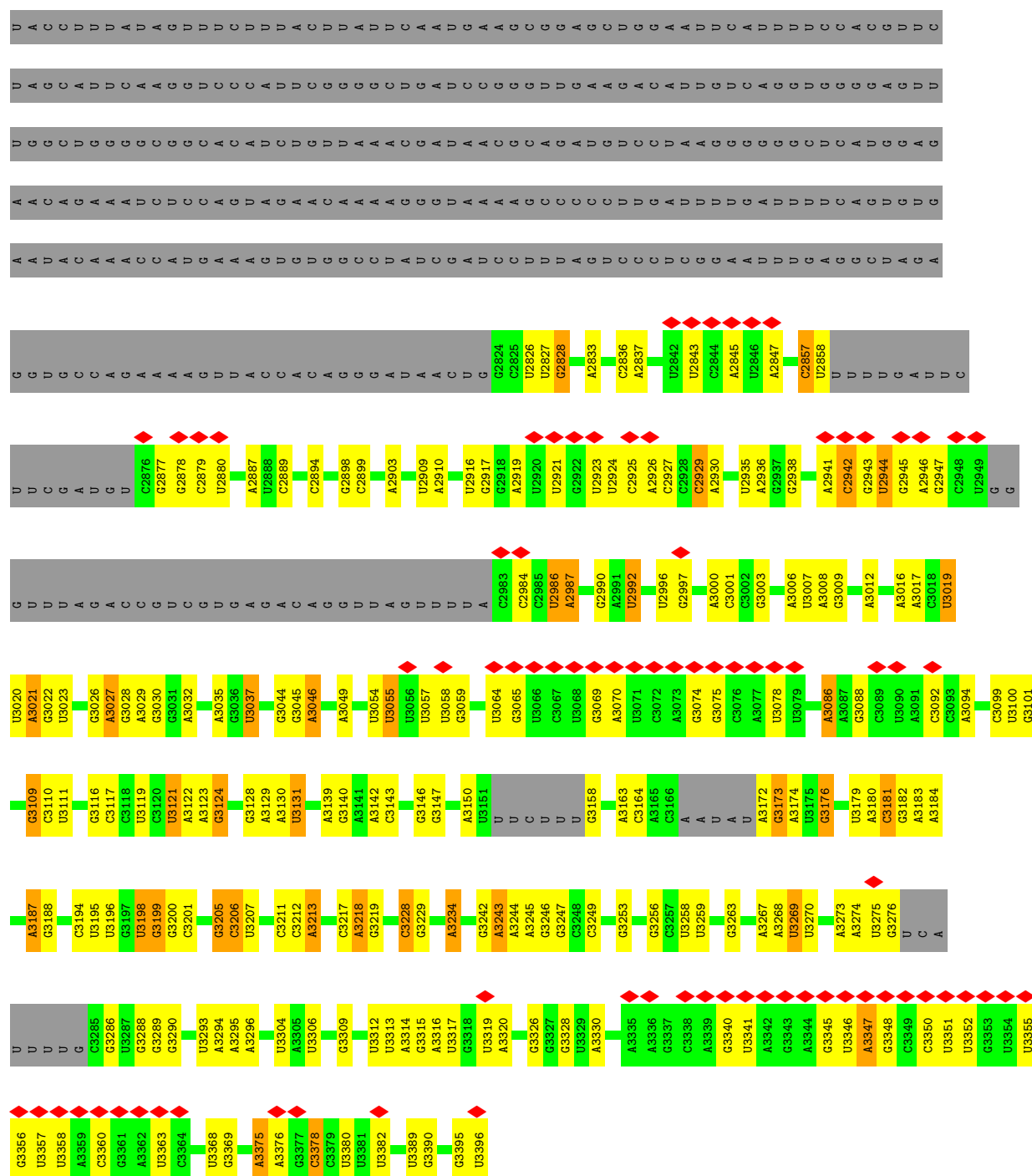


• Molecule 35: 25S ribosomal RNA

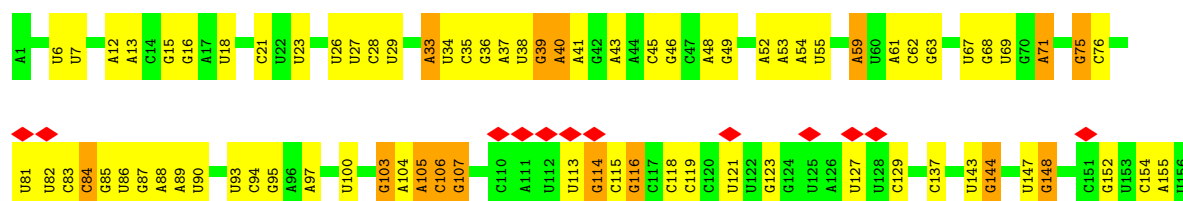
Chain 1: 





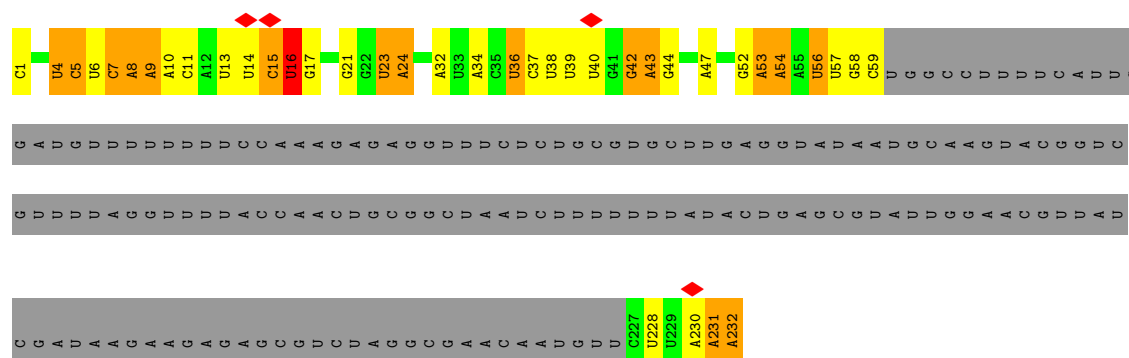


• Molecule 36: 5.8S ribosomal RNA

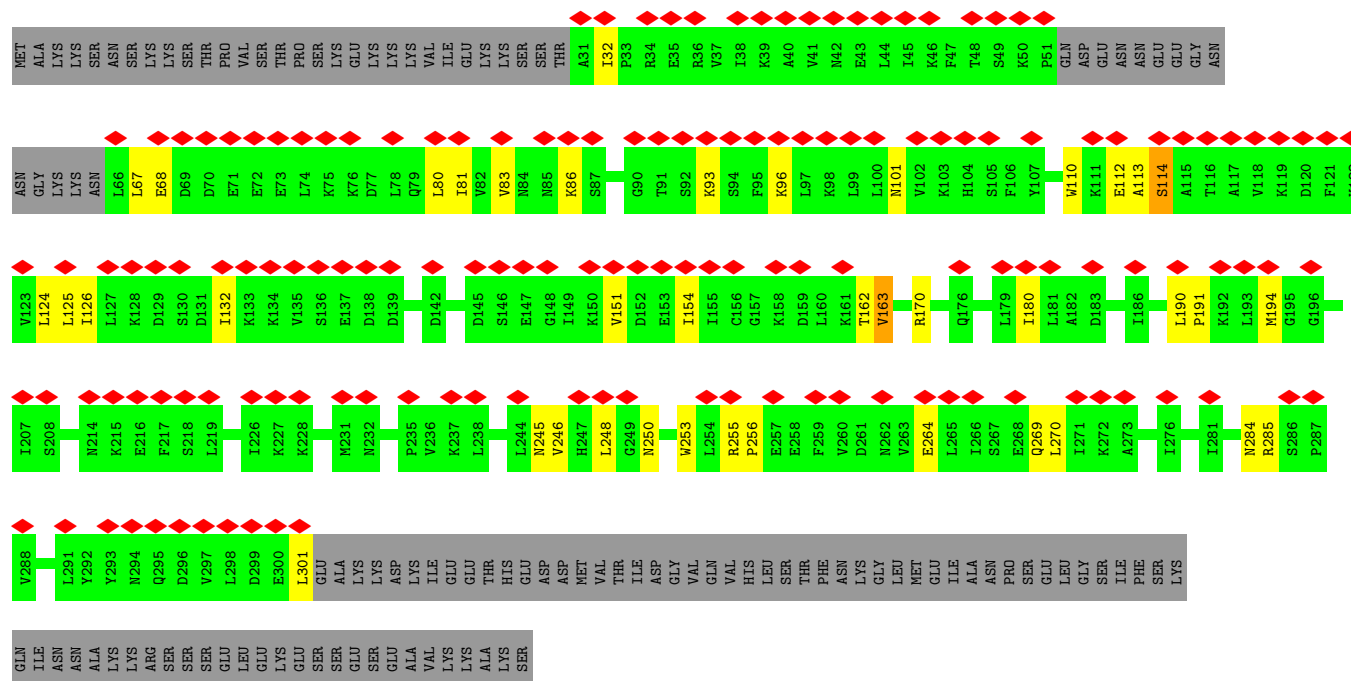




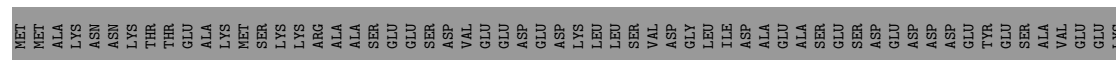
• Molecule 37: 5.8S ribosomal RNA



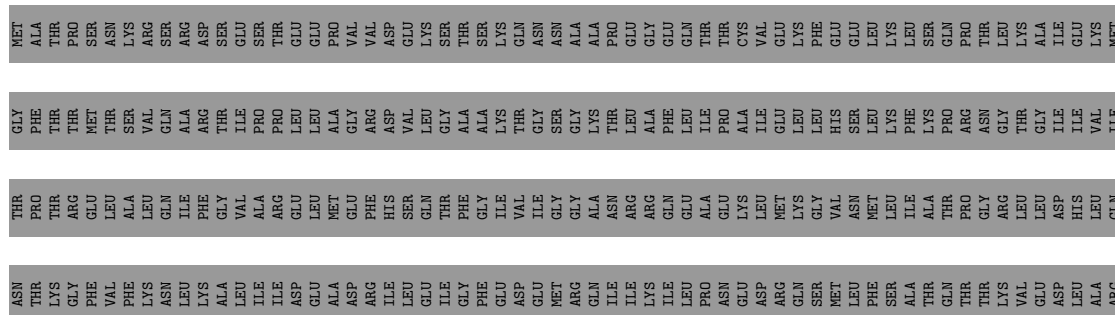
• Molecule 38: Proteasome-interacting protein CIC1

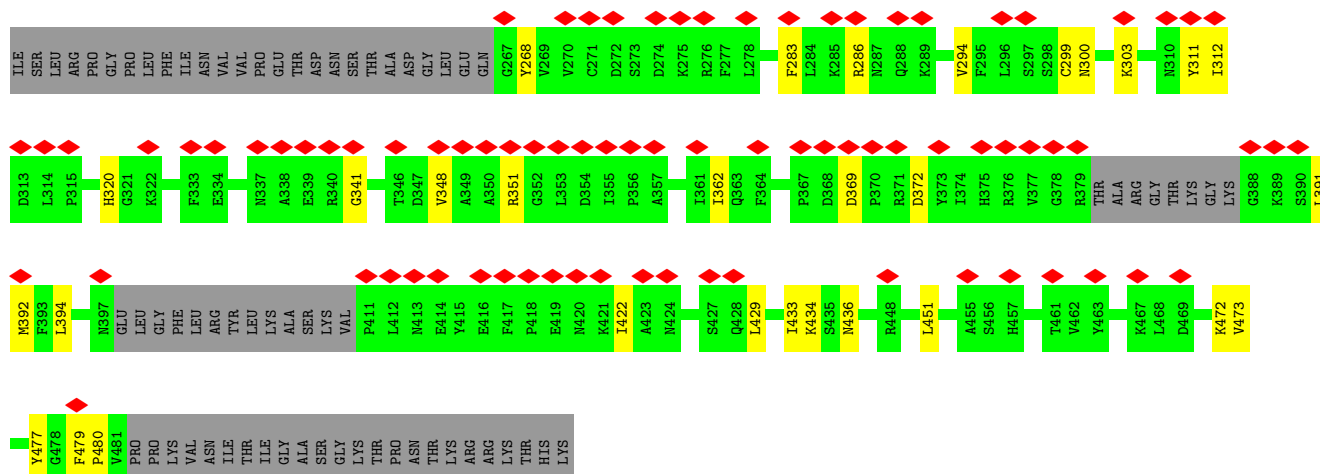


• Molecule 39: Ribosome biogenesis protein ERB1

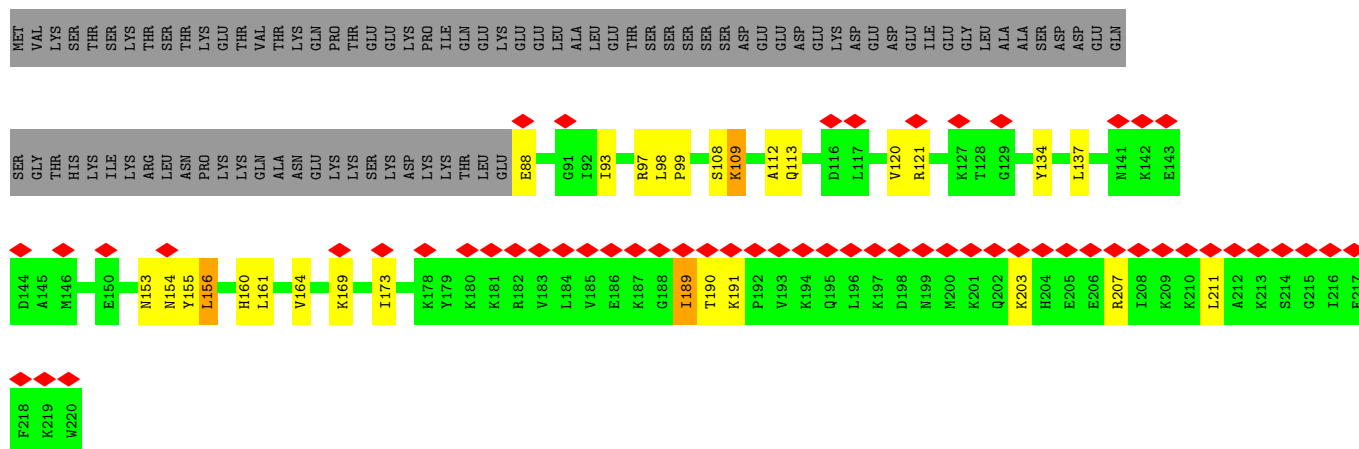


- Molecule 40: ATP-dependent RNA helicase HAS1

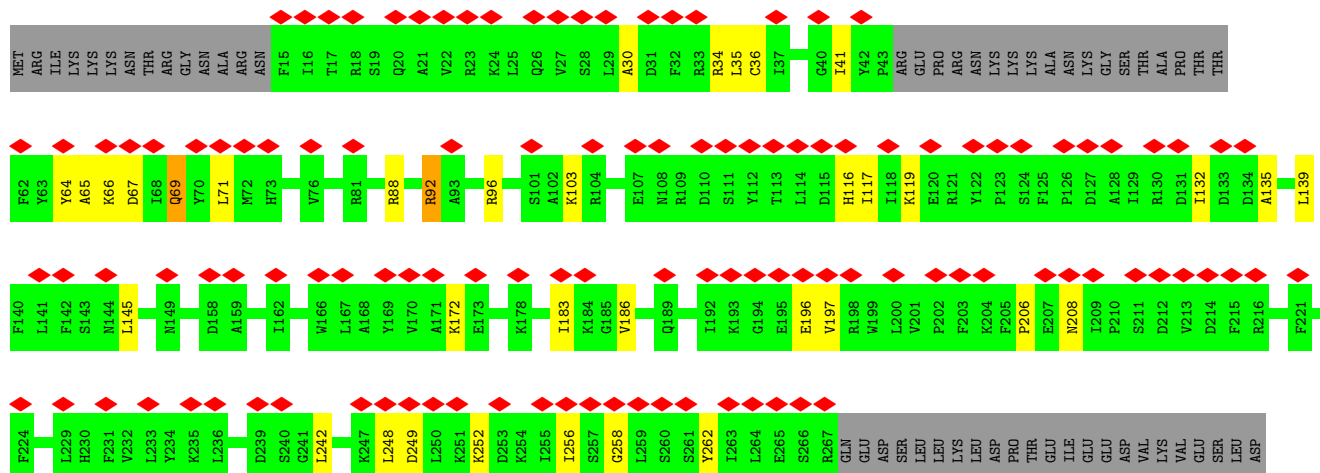


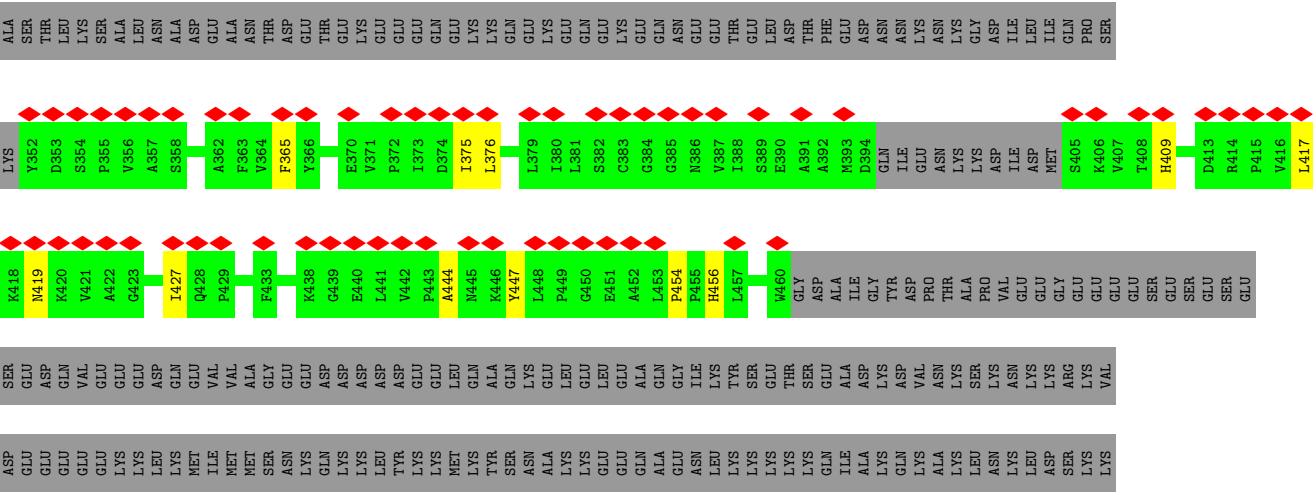


• Molecule 41: Ribosome biogenesis protein 15

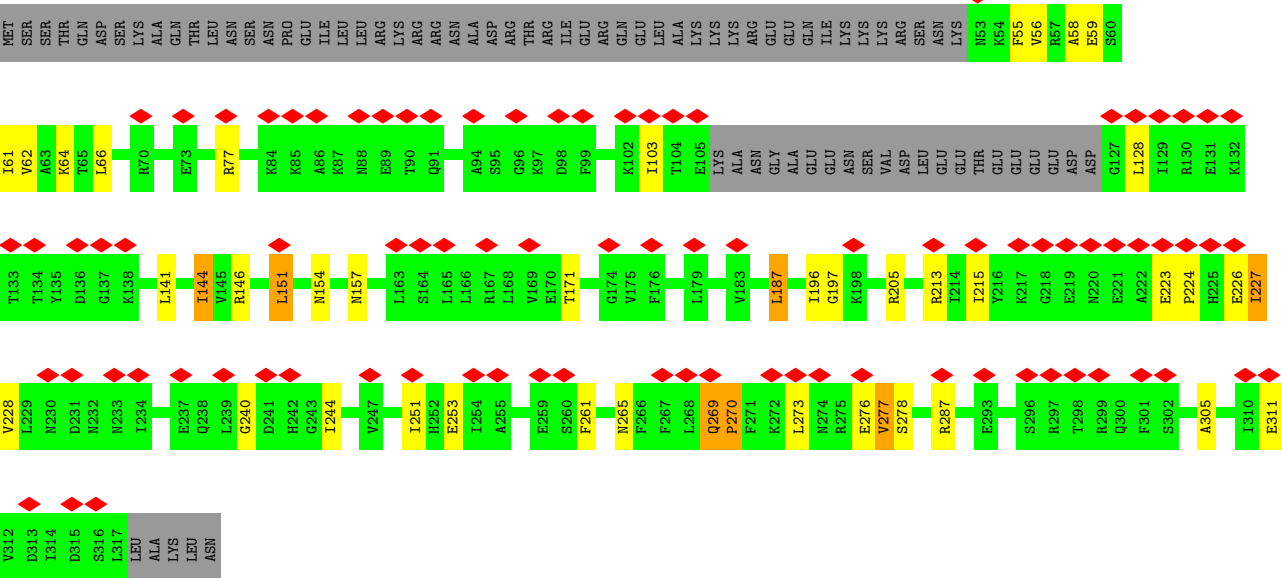


• Molecule 42: Pescadillo homolog





• Molecule 43: Ribosome biogenesis protein RLP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156937	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 ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.082	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	x	0.70	1/2312 (0.0%)	1.11	13/3097 (0.4%)
2	F	0.60	0/1974	1.09	4/2654 (0.2%)
3	3	0.81	0/1461	1.20	9/1958 (0.5%)
4	4	0.57	0/1895	1.15	10/2549 (0.4%)
5	5	0.53	0/3109	0.89	6/4187 (0.1%)
6	A	0.65	0/1243	0.92	1/1679 (0.1%)
7	b	0.57	0/3474	0.96	1/4683 (0.0%)
8	J	0.59	0/559	0.87	0/754
9	r	0.47	0/638	0.95	0/837
10	s	0.59	0/224	0.99	0/288
11	u	0.52	0/996	0.92	0/1324
12	v	0.53	0/1100	0.97	0/1456
13	W	0.57	0/1902	0.91	1/2564 (0.0%)
14	y	0.58	0/1722	0.92	0/2343
15	z	0.55	0/445	0.92	0/585
16	B	0.57	0/2699	0.96	1/3626 (0.0%)
17	C	0.73	0/2660	1.19	17/3601 (0.5%)
18	e	0.70	0/1030	1.09	4/1379 (0.3%)
19	E	0.55	0/1226	1.00	1/1648 (0.1%)
20	f	0.70	0/868	1.08	5/1168 (0.4%)
21	G	0.57	0/1252	1.07	3/1695 (0.2%)
22	h	0.50	0/978	1.05	0/1301
23	H	0.53	0/1531	0.90	0/2062
24	i	0.51	0/599	1.09	0/793
25	j	0.66	0/578	1.02	0/767
26	L	0.64	0/877	1.11	1/1179 (0.1%)
27	M	0.52	0/1056	1.06	3/1421 (0.2%)
28	N	0.66	2/1544 (0.1%)	1.04	5/2065 (0.2%)
29	O	0.86	0/1585	1.13	11/2128 (0.5%)
30	P	0.60	0/1080	0.99	3/1455 (0.2%)
31	Q	0.62	0/1024	1.06	3/1385 (0.2%)
32	S	0.56	0/1468	0.97	1/1973 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	V	0.61	0/950	0.90	0/1279
34	Y	0.71	1/995 (0.1%)	1.03	2/1329 (0.2%)
35	1	0.44	2/42777 (0.0%)	0.78	71/66679 (0.1%)
36	2	0.43	0/3740	0.80	7/5808 (0.1%)
37	6	0.38	0/1527	0.77	4/2371 (0.2%)
38	K	0.58	0/2107	0.97	3/2845 (0.1%)
39	m	0.57	0/1401	0.99	2/1895 (0.1%)
40	D	0.57	0/1626	0.92	1/2193 (0.0%)
41	o	0.54	0/1129	0.94	1/1502 (0.1%)
42	n	0.54	1/2802 (0.0%)	0.96	0/3791
43	t	0.57	0/1961	0.96	1/2639 (0.0%)
All	All	0.54	7/106124 (0.0%)	0.91	195/152935 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	1
4	4	0	3
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	126	LEU	C-O	10.58	1.44	1.23
28	N	105	ARG	CZ-NH1	6.77	1.42	1.32
28	N	105	ARG	NE-CZ	5.91	1.39	1.33
35	1	1159	A	O5'-C5'	5.89	1.51	1.42
42	n	454	PRO	CA-C	5.13	1.54	1.51
35	1	2942	C	C1'-N1	5.08	1.56	1.48
1	x	180	GLU	C-O	5.00	1.33	1.23

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1	649	A	C2'-C3'-O3'	10.38	129.27	113.70
35	1	1347	U	C4'-C3'-O3'	10.19	128.28	113.00
35	1	480	C	C2'-C3'-O3'	10.00	124.50	109.50
2	F	95	ILE	CA-C-N	9.60	126.67	119.66
2	F	95	ILE	C-N-CA	9.60	126.67	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O	100	GLU	N-CA-C	-9.35	101.43	113.12
35	1	1356	U	C4'-C3'-O3'	-9.11	99.33	113.00
1	x	165	LEU	CA-C-N	-8.80	111.56	120.98
1	x	165	LEU	C-N-CA	-8.80	111.56	120.98
35	1	1352	A	C2'-C3'-O3'	-8.77	100.54	113.70
20	f	106	ASN	N-CA-C	-8.49	103.05	113.50
20	f	89	LEU	CA-C-N	8.43	128.64	119.87
20	f	89	LEU	C-N-CA	8.43	128.64	119.87
35	1	3218	A	C4'-C3'-O3'	8.41	122.02	109.40
20	f	90	PRO	N-CA-C	7.90	123.75	114.03
4	4	91	ASN	N-CA-C	-7.83	102.27	112.68
17	C	101	ALA	CA-C-N	7.70	128.17	119.93
17	C	101	ALA	C-N-CA	7.70	128.17	119.93
17	C	25	VAL	N-CA-C	-7.68	101.49	111.09
35	1	3228	C	C4'-C3'-O3'	7.57	120.75	109.40
35	1	1102	A	C2'-C3'-O3'	7.55	125.03	113.70
35	1	3269	U	C4'-C3'-O3'	7.49	120.64	109.40
37	6	16	U	C2'-C3'-O3'	7.43	120.64	109.50
35	1	2857	C	C2'-C3'-O3'	7.42	120.64	109.50
21	G	71	VAL	N-CA-C	7.36	115.91	107.89
1	x	221	ASN	CA-C-N	7.32	128.99	119.84
1	x	221	ASN	C-N-CA	7.32	128.99	119.84
35	1	588	G	C2'-C3'-O3'	7.18	120.27	109.50
35	1	1307	G	C2'-C3'-O3'	7.14	120.21	109.50
35	1	1356	U	C2'-C3'-O3'	7.10	124.35	113.70
35	1	1385	C	C2'-C3'-O3'	-7.10	103.05	113.70
35	1	93	C	C2'-C3'-O3'	7.05	120.07	109.50
29	O	109	PRO	CA-C-N	7.01	124.78	119.66
29	O	109	PRO	C-N-CA	7.01	124.78	119.66
35	1	618	C	C2'-C3'-O3'	6.96	119.94	109.50
36	2	114	G	C2'-C3'-O3'	6.93	124.09	113.70
4	4	36	GLU	N-CA-C	-6.93	105.45	114.04
21	G	77	GLN	N-CA-C	-6.91	104.11	112.54
1	x	244	HIS	N-CA-C	6.76	116.97	108.45
37	6	56	U	C2'-C3'-O3'	6.67	119.51	109.50
6	A	104	PRO	N-CA-C	6.66	118.83	110.70
17	C	22	LEU	CA-C-N	6.65	126.24	119.19
17	C	22	LEU	C-N-CA	6.65	126.24	119.19
28	N	66	VAL	N-CA-C	6.59	117.31	108.27
35	1	1241	U	C2'-C3'-O3'	6.58	119.38	109.50
17	C	20	LEU	CA-C-N	6.52	126.54	119.89
17	C	20	LEU	C-N-CA	6.52	126.54	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	165	LEU	N-CA-C	6.47	121.02	112.35
35	1	658	G	C3'-C2'-O2'	6.43	120.34	110.70
35	1	1166	G	C3'-C2'-O2'	6.42	120.33	110.70
35	1	64	G	C4'-C3'-O3'	-6.41	103.38	113.00
35	1	696	C	C4'-C3'-O3'	-6.41	103.39	113.00
35	1	403	C	C2'-C3'-O3'	-6.40	104.11	113.70
35	1	1128	U	C4'-C3'-O3'	6.39	118.98	109.40
17	C	293	SER	N-CA-C	-6.38	105.62	113.41
36	2	89	A	C4'-C3'-O3'	-6.37	103.44	113.00
38	K	255	ARG	CA-C-N	6.35	127.78	119.84
38	K	255	ARG	C-N-CA	6.35	127.78	119.84
18	e	67	SER	CA-C-N	6.28	126.76	119.47
18	e	67	SER	C-N-CA	6.28	126.76	119.47
35	1	720	A	C4'-C3'-O3'	6.28	118.81	109.40
3	3	118	VAL	CB-CA-C	6.27	116.91	110.70
17	C	3	ARG	CA-C-N	-6.26	112.02	119.84
17	C	3	ARG	C-N-CA	-6.26	112.02	119.84
5	5	12	SER	N-CA-C	6.20	116.62	108.07
35	1	720	A	C2'-C3'-O3'	6.14	118.71	109.50
35	1	229	G	C4'-C3'-O3'	-6.14	103.79	113.00
3	3	72	THR	CA-C-N	6.13	127.51	119.84
3	3	72	THR	C-N-CA	6.13	127.51	119.84
27	M	9	ALA	N-CA-C	6.12	118.43	108.08
3	3	43	CYS	CA-C-N	-6.11	114.60	120.83
3	3	43	CYS	C-N-CA	-6.11	114.60	120.83
4	4	95	PHE	N-CA-C	6.11	117.94	111.28
28	N	153	ASP	CA-C-N	6.10	125.80	119.82
28	N	153	ASP	C-N-CA	6.10	125.80	119.82
35	1	398	A	C4'-C3'-O3'	6.10	122.15	113.00
36	2	88	A	C4'-C3'-O3'	-6.09	103.87	113.00
35	1	107	A	C4'-C3'-O3'	-6.06	103.91	113.00
18	e	121	ASN	CA-C-N	-6.04	114.52	120.98
18	e	121	ASN	C-N-CA	-6.04	114.52	120.98
27	M	8	LYS	N-CA-C	6.00	118.97	110.50
31	Q	126	GLN	N-CA-C	-5.93	104.82	111.28
29	O	19	LEU	CA-CB-CG	-5.92	95.58	116.30
5	5	301	GLU	CA-C-N	5.91	127.22	119.84
5	5	301	GLU	C-N-CA	5.91	127.22	119.84
36	2	103	G	C4'-C3'-O3'	-5.90	104.15	113.00
35	1	397	A	C4'-C3'-O3'	-5.89	104.16	113.00
2	F	203	TRP	CA-C-N	5.85	127.15	119.84
2	F	203	TRP	C-N-CA	5.85	127.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1	694	C	C2'-C3'-O3'	5.84	122.45	113.70
30	P	157	VAL	N-CA-C	5.83	115.92	107.88
29	O	119	VAL	CB-CA-C	-5.81	103.21	111.34
31	Q	142	GLY	CA-C-N	5.79	127.08	119.84
31	Q	142	GLY	C-N-CA	5.79	127.08	119.84
35	1	239	G	C4'-C3'-O3'	5.79	121.68	113.00
37	6	53	A	C4'-C3'-O3'	-5.77	104.35	113.00
40	D	341	GLY	N-CA-C	5.75	119.96	112.25
1	x	88	ASN	N-CA-C	5.71	117.66	109.14
17	C	197	ARG	N-CA-C	-5.69	104.09	111.71
35	1	1302	A	C4'-C3'-O3'	5.68	117.92	109.40
35	1	1162	U	C3'-C2'-O2'	5.67	119.21	110.70
3	3	118	VAL	N-CA-C	-5.65	107.78	113.20
39	m	289	ILE	CA-C-N	5.64	123.78	119.66
39	m	289	ILE	C-N-CA	5.64	123.78	119.66
26	L	58	VAL	N-CA-C	5.62	116.77	108.45
35	1	1371	G	C3'-C2'-O2'	5.62	119.13	110.70
7	b	71	ILE	N-CA-C	5.62	116.25	110.36
3	3	121	THR	N-CA-C	-5.61	104.65	112.45
1	x	189	ARG	CA-C-N	5.61	125.52	119.85
1	x	189	ARG	C-N-CA	5.61	125.52	119.85
36	2	38	U	C4'-C3'-O3'	-5.61	100.99	109.40
37	6	56	U	C4'-C3'-O3'	5.61	117.81	109.40
35	1	1241	U	C4'-C3'-O3'	5.61	117.81	109.40
16	B	341	SER	N-CA-C	5.60	119.94	113.38
17	C	45	ASN	N-CA-C	5.59	117.46	111.36
35	1	228	U	C4'-C3'-O3'	-5.58	104.62	113.00
30	P	10	ASN	CA-C-N	5.58	125.41	119.28
30	P	10	ASN	C-N-CA	5.58	125.41	119.28
35	1	1170	A	C1'-C2'-O2'	5.57	116.75	108.40
35	1	617	G	C4'-C3'-O3'	-5.56	104.66	113.00
35	1	441	U	C4'-C3'-O3'	-5.55	104.68	113.00
29	O	108	ILE	CA-C-N	5.52	126.07	120.38
29	O	108	ILE	C-N-CA	5.52	126.07	120.38
35	1	1433	A	C4'-C3'-O3'	-5.51	101.14	109.40
29	O	27	LEU	N-CA-C	-5.50	104.80	112.45
35	1	644	G	C4'-C3'-O3'	5.49	121.24	113.00
41	o	189	ILE	N-CA-C	5.49	115.94	110.23
35	1	441	U	C2'-C3'-O3'	5.48	121.92	113.70
5	5	287	GLY	N-CA-C	5.48	118.57	110.63
19	E	58	LEU	N-CA-C	5.47	117.83	109.95
35	1	3274	A	C4'-C3'-O3'	5.47	117.61	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	333	VAL	N-CA-C	5.46	115.85	107.77
29	O	110	PRO	O-C-N	5.45	123.82	121.31
35	1	209	A	C4'-C3'-O3'	-5.45	104.82	113.00
35	1	1416	C	C2'-C3'-O3'	-5.44	105.54	113.70
35	1	1344	G	C3'-C2'-O2'	5.42	118.84	110.70
1	x	237	ASP	N-CA-C	-5.42	105.48	113.61
35	1	405	U	C3'-C2'-O2'	5.42	118.83	110.70
35	1	3258	U	C4'-C3'-O3'	-5.42	104.88	113.00
35	1	93	C	C4'-C3'-O3'	5.41	117.52	109.40
35	1	456	U	C2'-C3'-O3'	5.39	121.79	113.70
32	S	23	LYS	N-CA-C	5.38	119.95	112.90
35	1	674	G	C4'-C3'-O3'	-5.38	104.92	113.00
4	4	138	SER	N-CA-C	-5.35	105.53	111.36
35	1	370	U	C2'-C3'-O3'	-5.35	105.68	113.70
17	C	106	TRP	N-CA-C	5.35	118.64	112.97
38	K	114	SER	N-CA-C	-5.34	106.76	113.28
29	O	88	VAL	N-CA-C	-5.33	98.24	109.34
35	1	1302	A	C2'-C3'-O3'	5.33	117.49	109.50
35	1	1394	A	C3'-C2'-O2'	5.33	118.69	110.70
3	3	79	ARG	N-CA-C	5.32	117.40	110.53
28	N	177	GLY	N-CA-C	5.32	117.93	110.38
35	1	649	A	C4'-C3'-O3'	5.32	120.97	113.00
4	4	132	GLN	N-CA-C	-5.31	103.52	110.53
35	1	659	G	C3'-C2'-O2'	5.30	118.66	110.70
43	t	227	ILE	N-CA-C	5.30	120.36	109.34
35	1	1128	U	C2'-C3'-O3'	5.30	117.45	109.50
35	1	218	G	C3'-C2'-O2'	-5.28	106.68	114.60
27	M	9	ALA	CB-CA-C	-5.27	110.52	116.63
17	C	313	LEU	CA-CB-CG	5.25	134.69	116.30
35	1	1392	G	C3'-C2'-O2'	5.25	122.47	114.60
35	1	318	A	C4'-C3'-O3'	-5.24	105.13	113.00
35	1	1393	A	C1'-C2'-O2'	5.24	116.27	108.40
28	N	97	SER	N-CA-C	5.22	117.06	110.33
4	4	227	ASP	N-CA-C	5.21	117.79	110.23
4	4	136	LEU	N-CA-C	-5.19	106.97	113.72
1	x	170	THR	N-CA-C	5.17	116.82	108.34
35	1	1145	G	C1'-C2'-O2'	5.17	116.15	108.40
35	1	693	A	C3'-C2'-O2'	5.16	118.44	110.70
1	x	117	ILE	N-CA-C	5.16	116.24	111.81
17	C	316	ASN	CA-C-N	5.14	126.27	119.84
17	C	316	ASN	C-N-CA	5.14	126.27	119.84
35	1	431	U	C3'-C2'-O2'	5.14	118.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	366	TYR	N-CA-C	5.13	116.68	107.80
20	f	64	ILE	N-CA-C	5.12	114.12	106.85
21	G	134	TYR	N-CA-C	5.11	122.40	114.64
17	C	339	LEU	N-CA-C	5.10	121.66	110.80
35	1	249	U	C2'-C3'-O3'	5.10	117.15	109.50
35	1	360	G	C3'-C2'-O2'	5.09	118.34	110.70
34	Y	33	ALA	CA-C-N	-5.09	115.35	120.85
34	Y	33	ALA	C-N-CA	-5.09	115.35	120.85
3	3	15	CYS	CA-CB-SG	5.07	126.07	114.40
1	x	289	GLU	N-CA-C	5.07	119.17	112.89
4	4	225	VAL	N-CA-C	5.07	115.28	110.42
35	1	1424	C	C4'-C3'-O3'	-5.07	105.40	113.00
35	1	683	U	C1'-C2'-O2'	5.06	116.00	108.40
35	1	12	A	C4'-C3'-O3'	-5.05	105.42	113.00
4	4	95	PHE	CA-C-N	5.05	129.02	120.64
4	4	95	PHE	C-N-CA	5.05	129.02	120.64
13	W	175	ILE	N-CA-C	5.04	115.11	107.75
36	2	84	C	C2'-C3'-O3'	5.04	117.06	109.50
29	O	79	ILE	CB-CA-C	-5.04	103.03	111.29
35	1	20	A	C3'-C2'-O2'	5.03	118.24	110.70
36	2	41	A	C3'-C2'-O2'	5.02	118.24	110.70
35	1	1347	U	C2'-C3'-O3'	5.02	121.22	113.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	118	VAL	Peptide
4	4	135	TYR	Peptide
4	4	136	LEU	Mainchain
4	4	225	VAL	Peptide

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	x	2268	0	2301	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1936	0	2032	37	0
3	3	1434	0	1473	72	0
4	4	1853	0	1887	188	0
5	5	3055	0	3113	49	0
6	A	1211	0	1214	12	0
7	b	3410	0	3463	23	0
8	J	549	0	526	2	0
9	r	628	0	660	11	0
10	s	224	0	259	3	0
11	u	976	0	1008	6	0
12	v	1087	0	1133	27	0
13	W	1870	0	1902	11	0
14	y	1701	0	1697	21	0
15	z	444	0	478	5	0
16	B	2646	0	2726	55	0
17	C	2611	0	2724	82	0
18	e	1009	0	1080	28	0
19	E	1205	0	1291	11	0
20	f	850	0	880	21	0
21	G	1231	0	1284	137	0
22	h	969	0	1078	16	0
23	H	1510	0	1576	21	0
24	i	594	0	641	22	0
25	j	566	0	566	10	0
26	L	864	0	917	32	0
27	M	1041	0	1136	24	0
28	N	1513	0	1564	23	0
29	O	1555	0	1651	12	0
30	P	1062	0	1075	19	0
31	Q	1009	0	1091	25	0
32	S	1432	0	1470	15	0
33	V	936	0	986	11	0
34	Y	984	0	1075	27	0
35	1	38221	0	19213	427	0
36	2	3353	0	1701	60	0
37	6	1370	0	692	24	0
38	K	2073	0	2155	30	0
39	m	1362	0	1347	110	0
40	D	1590	0	1598	16	0
41	o	1107	0	1159	24	0
42	n	2734	0	2777	29	0
43	t	1935	0	2033	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	j	1	0	0	0	0
44	u	1	0	0	0	0
All	All	99980	0	80632	1487	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 8.

All (1487) 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)
4:4:54:TRP:HA	4:4:120:LYS:NZ	1.32	1.40
36:2:127:U:H4'	42:n:64:TYR:CE1	1.21	1.32
27:M:8:LYS:CE	35:1:3199:G:OP1	1.76	1.31
4:4:154:LEU:O	4:4:159:LEU:CD2	1.78	1.30
4:4:46:TRP:CH2	4:4:69:LEU:HD21	1.68	1.29
4:4:77:PHE:CD2	4:4:91:ASN:O	1.88	1.27
36:2:127:U:C4'	42:n:64:TYR:CE1	2.00	1.25
4:4:212:THR:HB	4:4:213:PRO:CD	1.67	1.23
36:2:127:U:C4'	42:n:64:TYR:HE1	1.36	1.22
4:4:27:LYS:O	4:4:30:THR:HG23	1.36	1.22
21:G:233:TRP:CG	39:m:240:TYR:HB3	1.77	1.17
21:G:109:LEU:HD12	39:m:275:ARG:CD	1.77	1.15
21:G:172:LYS:HE3	39:m:252:GLU:OE1	1.44	1.15
21:G:70:LYS:HE2	39:m:240:TYR:CE2	1.83	1.13
21:G:221:ASN:OD1	41:o:154:ASN:HB2	1.44	1.13
21:G:105:LYS:HE3	39:m:275:ARG:NH1	1.61	1.12
16:B:41:VAL:HA	16:B:185:GLY:HA3	1.31	1.10
21:G:233:TRP:CE2	39:m:240:TYR:HA	1.85	1.10
35:1:3:U:O2	37:6:232:A:C8	2.05	1.10
3:3:68:GLU:HB2	4:4:57:ASP:HB2	1.33	1.09
21:G:109:LEU:HD12	39:m:275:ARG:HD3	1.09	1.08
21:G:233:TRP:CD2	39:m:240:TYR:HB3	1.88	1.08
21:G:213:LYS:NZ	37:6:54:A:OP1	1.87	1.08
4:4:27:LYS:O	4:4:30:THR:CG2	2.03	1.07
21:G:109:LEU:CD1	39:m:275:ARG:CD	2.33	1.07
4:4:154:LEU:O	4:4:159:LEU:HD21	1.50	1.06
36:2:157:U:O4	43:t:55:PHE:HB3	1.52	1.06
4:4:212:THR:CB	4:4:213:PRO:CD	2.31	1.06
12:v:208:TYR:HA	39:m:267:VAL:HG13	1.33	1.06
4:4:212:THR:HB	4:4:213:PRO:HD3	1.08	1.05
4:4:154:LEU:O	4:4:159:LEU:CG	2.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:127:U:O4'	39:m:323:HIS:NE2	1.94	1.01
23:H:47:LYS:HB2	27:M:7:VAL:CG2	1.89	1.00
4:4:76:TYR:OH	4:4:94:ALA:HB1	1.60	1.00
9:r:5:ASP:HA	35:1:2898:G:H1	1.20	1.00
21:G:233:TRP:CZ3	39:m:240:TYR:HD1	1.78	1.00
36:2:127:U:O4'	39:m:323:HIS:CD2	2.14	0.99
24:i:46:GLU:HB3	39:m:246:TRP:CE2	1.97	0.99
4:4:54:TRP:CA	4:4:120:LYS:NZ	2.25	0.99
31:Q:86:THR:HG22	31:Q:105:ARG:HB2	1.44	0.99
34:Y:80:VAL:HG21	34:Y:104:LEU:HD11	1.41	0.99
4:4:64:ARG:HE	4:4:64:ARG:HA	1.27	0.98
21:G:92:LYS:NZ	37:6:1:C:C2	2.32	0.98
36:2:127:U:OP2	39:m:321:VAL:CG1	2.11	0.97
21:G:233:TRP:CE3	39:m:240:TYR:CD1	2.52	0.97
35:1:973:A:N6	35:1:1108:U:O4	1.98	0.97
4:4:54:TRP:HA	4:4:120:LYS:HZ1	1.20	0.97
27:M:8:LYS:HE2	35:1:3199:G:OP1	1.15	0.96
21:G:105:LYS:HE3	39:m:275:ARG:HH11	1.25	0.95
21:G:109:LEU:CD1	39:m:275:ARG:HD3	1.93	0.95
23:H:47:LYS:HB2	27:M:7:VAL:HG21	1.49	0.95
4:4:154:LEU:O	4:4:159:LEU:HG	1.66	0.94
4:4:54:TRP:HA	4:4:120:LYS:HZ2	1.27	0.94
21:G:233:TRP:CZ2	39:m:240:TYR:HA	2.01	0.94
21:G:105:LYS:CE	39:m:275:ARG:NH1	2.30	0.94
4:4:76:TYR:OH	4:4:94:ALA:C	2.11	0.94
4:4:46:TRP:HH2	4:4:69:LEU:CD2	1.81	0.93
4:4:77:PHE:CE2	4:4:91:ASN:O	2.22	0.92
4:4:46:TRP:HH2	4:4:69:LEU:HD21	1.15	0.92
21:G:109:LEU:CD1	39:m:275:ARG:HD2	1.99	0.92
28:N:172:ARG:HB3	28:N:174:ILE:HD12	1.52	0.92
4:4:53:MET:HE3	4:4:120:LYS:HB3	1.52	0.92
21:G:146:LYS:NZ	21:G:173:MET:O	2.03	0.91
35:1:251:G:H5'	39:m:281:ARG:HH21	1.33	0.91
21:G:233:TRP:CZ3	39:m:240:TYR:CD1	2.58	0.91
21:G:233:TRP:CE2	39:m:240:TYR:CA	2.54	0.91
21:G:233:TRP:CD1	39:m:240:TYR:HB3	2.07	0.90
17:C:150:LEU:HD11	17:C:172:VAL:HG13	1.54	0.90
1:x:170:THR:HG23	1:x:271:GLN:HB2	1.52	0.90
21:G:172:LYS:HE3	39:m:252:GLU:CD	1.96	0.89
35:1:973:A:N1	35:1:1108:U:C5	2.40	0.89
35:1:3121:U:C4	35:1:3123:A:N6	2.40	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y:55:GLU:HB2	34:Y:108:LYS:HB3	1.54	0.89
4:4:32:LYS:HA	4:4:35:LYS:HZ1	1.38	0.89
21:G:70:LYS:CE	39:m:240:TYR:CE2	2.56	0.89
4:4:50:TYR:CE2	4:4:109:GLU:HG2	2.07	0.88
21:G:74:THR:HB	39:m:243:LEU:CD1	2.03	0.88
4:4:29:LEU:O	4:4:32:LYS:HG3	1.73	0.88
4:4:154:LEU:HB2	4:4:220:ILE:HD13	1.54	0.87
28:N:38:ARG:HE	28:N:60:VAL:HG13	1.40	0.87
21:G:233:TRP:NE1	39:m:240:TYR:C	2.33	0.87
35:1:3121:U:N3	35:1:3123:A:N6	2.22	0.86
21:G:114:ALA:HB2	39:m:291:PRO:HD2	1.57	0.86
36:2:157:U:N3	43:t:55:PHE:O	2.07	0.86
21:G:74:THR:HB	39:m:243:LEU:HD13	1.55	0.86
4:4:32:LYS:HA	4:4:35:LYS:NZ	1.91	0.86
4:4:76:TYR:OH	4:4:94:ALA:O	1.93	0.86
4:4:106:MET:HA	4:4:106:MET:HE2	1.57	0.86
4:4:26:LYS:O	4:4:30:THR:HG22	1.75	0.86
9:r:2:PRO:HD2	35:1:3026:G:H4'	1.59	0.85
35:1:808:A:H61	35:1:932:U:H3	1.25	0.85
4:4:225:VAL:HG21	4:4:243:PHE:CE2	2.11	0.85
21:G:172:LYS:CE	39:m:252:GLU:OE1	2.25	0.84
16:B:49:TYR:HE1	16:B:164:THR:HG21	1.43	0.84
21:G:143:ILE:O	21:G:144:GLU:HG2	1.78	0.84
1:x:31:HIS:CD2	35:1:385:A:OP2	2.32	0.83
21:G:231:LYS:HB3	39:m:242:PRO:HB3	1.58	0.82
20:f:67:MET:HE1	20:f:90:PRO:HD3	1.62	0.82
4:4:76:TYR:CZ	4:4:94:ALA:HB1	2.15	0.82
4:4:18:ARG:CZ	4:4:55:PHE:HD1	1.93	0.82
36:2:127:U:OP2	39:m:321:VAL:HG11	1.78	0.82
4:4:76:TYR:OH	4:4:94:ALA:CB	2.26	0.81
16:B:221:THR:HG22	16:B:273:HIS:H	1.45	0.81
2:F:7:LEU:H	4:4:63:GLN:HE22	1.27	0.81
3:3:10:ILE:HB	3:3:15:CYS:HB2	1.60	0.81
35:1:973:A:N1	35:1:1108:U:H5	1.76	0.81
12:v:161:LYS:HZ1	26:L:48:PRO:HB3	1.45	0.81
21:G:70:LYS:CE	39:m:240:TYR:CD2	2.64	0.81
4:4:46:TRP:CZ3	4:4:69:LEU:HD21	2.15	0.81
4:4:225:VAL:HG21	4:4:243:PHE:HE2	1.47	0.80
12:v:208:TYR:HA	39:m:267:VAL:CG1	2.12	0.80
4:4:61:PRO:HD3	35:1:466:G:OP1	1.82	0.80
35:1:3347:A:H61	35:1:3358:U:H3	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:218:ILE:HG22	4:4:222:GLN:HG3	1.64	0.79
35:1:1329:U:O2'	35:1:1330:A:H5''	1.82	0.79
12:v:209:GLN:OE1	40:D:436:ASN:O	1.99	0.79
32:S:13:ARG:HA	32:S:56:GLY:HA2	1.63	0.79
35:1:533:A:N1	35:1:556:U:O4	2.16	0.79
3:3:68:GLU:OE2	4:4:55:PHE:O	1.99	0.79
28:N:110:ALA:HB1	28:N:113:LEU:HD23	1.65	0.78
3:3:97:LEU:HD13	3:3:105:ARG:HA	1.64	0.78
21:G:172:LYS:NZ	39:m:250:HIS:O	2.13	0.78
4:4:153:VAL:O	4:4:158:PRO:HD2	1.84	0.78
34:Y:54:ASP:O	34:Y:70:ILE:HD12	1.83	0.78
3:3:21:ALA:HB2	3:3:27:PHE:HE1	1.47	0.77
21:G:233:TRP:CD2	39:m:240:TYR:CB	2.66	0.77
4:4:65:LEU:HD12	4:4:65:LEU:O	1.83	0.77
21:G:74:THR:N	39:m:243:LEU:HD12	2.00	0.77
4:4:76:TYR:HE2	4:4:95:PHE:HA	1.50	0.76
19:E:54:TYR:HA	19:E:65:ILE:HG22	1.67	0.76
35:1:458:U:H3	35:1:472:A:H61	1.31	0.76
12:v:14:VAL:HG21	25:j:68:LYS:HD3	1.68	0.76
37:6:38:U:O2	37:6:42:G:N1	2.17	0.76
34:Y:31:LEU:HB3	34:Y:101:PRO:HG3	1.67	0.76
35:1:428:A:H2'	35:1:429:U:C6	2.21	0.76
43:t:144:ILE:HG13	43:t:196:ILE:HG22	1.68	0.75
4:4:212:THR:CB	4:4:213:PRO:HD2	2.17	0.75
21:G:221:ASN:CG	41:o:154:ASN:HB2	2.11	0.75
21:G:231:LYS:CB	39:m:242:PRO:HB3	2.15	0.75
4:4:154:LEU:O	4:4:159:LEU:HD23	1.85	0.75
35:1:3293:U:HO2'	35:1:3294:A:H8	1.35	0.75
35:1:696:C:HO2'	35:1:697:A:H8	1.34	0.74
36:2:147:U:P	42:n:88:ARG:NH1	2.60	0.74
1:x:269:ARG:O	1:x:270:LEU:HB2	1.88	0.74
4:4:27:LYS:C	4:4:30:THR:CG2	2.61	0.74
4:4:66:ALA:CB	4:4:123:LEU:CD1	2.65	0.74
35:1:1278:A:HO2'	35:1:1279:C:H6	1.30	0.73
27:M:8:LYS:HE3	35:1:3199:G:OP1	1.86	0.73
22:h:48:ARG:HA	22:h:51:ILE:HD12	1.71	0.73
7:b:161:PRO:HA	35:1:3027:A:H61	1.52	0.73
16:B:49:TYR:CE1	16:B:164:THR:HG21	2.23	0.73
17:C:150:LEU:CD1	17:C:172:VAL:HG13	2.19	0.73
4:4:139:ARG:HG3	4:4:141:TRP:H	1.54	0.73
4:4:154:LEU:HB2	4:4:220:ILE:CD1	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:6:SER:HB2	5:5:406:PHE:HB3	1.70	0.73
4:4:132:GLN:O	4:4:133:LEU:HB2	1.88	0.72
35:1:1105:A:H2'	35:1:1106:G:C8	2.24	0.72
21:G:92:LYS:NZ	37:6:1:C:N3	2.37	0.72
21:G:233:TRP:CE3	39:m:240:TYR:HD1	1.97	0.72
4:4:76:TYR:OH	4:4:94:ALA:CA	2.38	0.72
34:Y:51:ARG:HH21	36:2:71:A:H2'	1.55	0.72
21:G:233:TRP:NE1	39:m:240:TYR:CA	2.53	0.72
24:i:46:GLU:HA	39:m:246:TRP:HE1	1.54	0.71
24:i:46:GLU:OE2	39:m:248:THR:HG23	1.89	0.71
35:1:428:A:H2'	35:1:429:U:H6	1.54	0.71
34:Y:57:LEU:HD12	34:Y:67:GLU:HB3	1.73	0.71
4:4:154:LEU:C	4:4:159:LEU:HD21	2.15	0.71
4:4:77:PHE:HD2	4:4:91:ASN:O	1.71	0.71
35:1:973:A:C2	35:1:1108:U:H5	2.08	0.71
4:4:61:PRO:HD2	4:4:62:GLN:H	1.53	0.71
4:4:69:LEU:O	4:4:69:LEU:HD23	1.91	0.71
35:1:273:A:N1	35:1:292:U:O4	2.24	0.71
4:4:92:ASP:HB3	4:4:145:LEU:HD11	1.72	0.70
4:4:225:VAL:HG22	4:4:238:ILE:HD12	1.73	0.70
23:H:47:LYS:HB2	27:M:7:VAL:HG23	1.72	0.70
35:1:252:U:OP1	39:m:277:MET:HG3	1.90	0.70
35:1:3121:U:H3	35:1:3123:A:N6	1.88	0.70
12:v:209:GLN:H	39:m:267:VAL:HG22	1.55	0.70
21:G:233:TRP:CE2	39:m:240:TYR:HB3	2.26	0.70
4:4:54:TRP:HA	4:4:120:LYS:HZ3	1.50	0.70
21:G:217:THR:HG21	41:o:156:LEU:HB2	1.71	0.70
35:1:249:U:H3'	35:1:250:U:H5''	1.72	0.70
4:4:153:VAL:O	4:4:158:PRO:CD	2.40	0.69
4:4:58:ARG:HD2	35:1:465:U:H4'	1.73	0.69
21:G:95:ASN:HD22	21:G:98:ARG:HE	1.39	0.69
21:G:158:ASP:HB3	21:G:159:PRO:HD3	1.74	0.69
30:P:30:ARG:HH21	30:P:34:GLN:HG3	1.58	0.69
1:x:14:LYS:HA	35:1:351:A:H62	1.58	0.69
3:3:23:ASN:HD22	3:3:25:GLN:HB2	1.58	0.69
3:3:65:LYS:HD3	3:3:77:TRP:CZ2	2.27	0.69
4:4:12:SER:O	4:4:55:PHE:HE1	1.74	0.69
4:4:54:TRP:CA	4:4:120:LYS:HZ1	1.97	0.69
21:G:74:THR:HG22	39:m:243:LEU:HD11	1.75	0.69
16:B:90:VAL:HG13	16:B:104:THR:HG22	1.74	0.69
21:G:172:LYS:HD3	39:m:248:THR:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:343:PHE:HD1	5:5:351:MET:HE3	1.57	0.68
16:B:129:ALA:O	35:1:3150:A:H5'	1.92	0.68
21:G:105:LYS:CE	39:m:275:ARG:HH12	2.03	0.68
24:i:29:LYS:HB2	35:1:266:A:H61	1.59	0.68
31:Q:86:THR:CG2	31:Q:105:ARG:HB2	2.21	0.68
34:Y:48:LEU:HD22	34:Y:118:LEU:HD23	1.75	0.68
4:4:64:ARG:HA	4:4:64:ARG:NE	2.06	0.68
4:4:153:VAL:HG12	4:4:158:PRO:HG2	1.75	0.68
1:x:131:LYS:HD2	3:3:129:GLU:HB2	1.75	0.68
3:3:30:ASN:C	3:3:32:TYR:H	2.02	0.68
4:4:46:TRP:CH2	4:4:69:LEU:CD2	2.55	0.68
26:L:76:THR:HG23	26:L:101:ARG:HH11	1.57	0.68
18:e:128:LEU:HD11	35:1:439:C:N4	2.09	0.68
35:1:252:U:P	39:m:277:MET:HG3	2.34	0.68
3:3:102:LYS:HA	3:3:105:ARG:HB2	1.76	0.67
21:G:146:LYS:HE2	21:G:173:MET:HE3	1.74	0.67
21:G:233:TRP:CE2	39:m:240:TYR:CB	2.77	0.67
35:1:1278:A:O2'	35:1:1279:C:H6	1.77	0.67
35:1:397:A:O2'	35:1:400:G:OP2	2.12	0.67
21:G:205:ALA:CB	38:K:163:VAL:HG23	2.24	0.67
21:G:113:ALA:CB	39:m:279:ILE:CG2	2.73	0.67
35:1:644:G:H4'	35:1:1116:G:H21	1.60	0.67
3:3:8:GLN:OE1	31:Q:24:VAL:HG21	1.95	0.67
4:4:56:SER:O	4:4:120:LYS:HD3	1.94	0.67
4:4:69:LEU:HD23	4:4:69:LEU:C	2.20	0.67
4:4:170:PRO:HB2	4:4:234:LEU:HD11	1.77	0.67
17:C:283:THR:HG22	17:C:285:ASP:H	1.58	0.66
20:f:16:TYR:HD2	20:f:23:ASN:HD22	1.41	0.66
35:1:808:A:N6	35:1:932:U:H3	1.91	0.66
36:2:147:U:OP1	42:n:88:ARG:NH1	2.28	0.66
3:3:143:ARG:HD2	3:3:147:ASN:HD22	1.60	0.66
3:3:93:ILE:HG22	3:3:97:LEU:HD11	1.77	0.66
4:4:27:LYS:HA	4:4:30:THR:CG2	2.26	0.66
18:e:67:SER:HB2	18:e:68:PRO:HD2	1.77	0.66
35:1:1160:C:OP1	35:1:1332:A:H5''	1.96	0.66
4:4:18:ARG:NH2	4:4:55:PHE:HB2	2.11	0.66
35:1:26:A:C2	35:1:27:C:C2	2.83	0.66
4:4:227:ASP:O	4:4:235:ARG:NH1	2.29	0.66
4:4:53:MET:HA	4:4:65:LEU:HD21	1.78	0.66
31:Q:39:ARG:NH1	35:1:1348:U:OP2	2.29	0.66
37:6:7:C:H5	37:6:21:G:H1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:76:TYR:HH	4:4:94:ALA:C	1.88	0.65
16:B:25:ILE:HD13	35:1:3312:U:H4'	1.78	0.65
36:2:157:U:O4	43:t:55:PHE:CB	2.37	0.65
4:4:66:ALA:HB3	4:4:123:LEU:HD11	1.77	0.65
29:O:60:LYS:HB3	35:1:1307:G:H1	1.62	0.65
35:1:696:C:O2'	35:1:697:A:H8	1.79	0.65
4:4:66:ALA:HB3	4:4:123:LEU:CD1	2.26	0.65
4:4:221:PHE:O	4:4:225:VAL:HG23	1.96	0.65
5:5:375:LEU:HB3	5:5:387:PHE:HB2	1.77	0.65
21:G:147:LYS:NZ	35:1:117:U:O4	2.25	0.65
36:2:54:A:H2'	36:2:55:U:O4'	1.97	0.65
35:1:948:C:H2'	35:1:949:C:H6	1.61	0.65
21:G:113:ALA:HB2	39:m:279:ILE:HB	1.79	0.65
30:P:98:ALA:HA	30:P:101:ASN:ND2	2.11	0.65
3:3:68:GLU:CD	4:4:55:PHE:O	2.40	0.65
5:5:323:PHE:CE2	5:5:325:SER:HB3	2.32	0.65
16:B:48:GLY:HA3	16:B:81:THR:HG22	1.78	0.65
27:M:19:ARG:HB3	27:M:35:ILE:HD12	1.79	0.65
1:x:82:MET:HG3	1:x:88:ASN:HD21	1.61	0.64
16:B:366:GLY:HA2	35:1:3086:A:H4'	1.80	0.64
31:Q:34:THR:HG23	31:Q:49:LEU:HD21	1.79	0.64
35:1:948:C:H2'	35:1:949:C:C6	2.32	0.64
35:1:973:A:C6	35:1:1108:U:O4	2.49	0.64
4:4:223:ASP:O	4:4:226:ALA:CB	2.45	0.64
35:1:972:A:H2'	35:1:973:A:C8	2.33	0.64
17:C:187:LEU:HD22	17:C:193:LYS:HD2	1.78	0.64
35:1:3158:G:C8	35:1:3395:G:H2'	2.33	0.64
27:M:46:ILE:HG12	27:M:58:ILE:HG21	1.78	0.64
34:Y:74:TYR:OH	36:2:75:G:OP2	2.16	0.64
21:G:233:TRP:CH2	39:m:240:TYR:HD1	2.16	0.64
35:1:59:G:H2'	36:2:33:A:H2'	1.78	0.64
3:3:9:VAL:HG11	17:C:134:LEU:HD21	1.78	0.64
4:4:155:ARG:C	4:4:159:LEU:HD11	2.23	0.64
28:N:38:ARG:HH21	28:N:60:VAL:HA	1.63	0.64
35:1:254:A:OP1	39:m:274:LYS:NZ	2.27	0.64
21:G:144:GLU:HA	21:G:173:MET:HG3	1.80	0.63
36:2:106:C:H4'	36:2:107:G:H5''	1.80	0.63
2:F:112:ASN:HB3	2:F:207:LEU:O	1.97	0.63
4:4:61:PRO:HG3	35:1:465:U:H3'	1.81	0.63
17:C:138:ARG:HG3	17:C:138:ARG:HH11	1.63	0.63
4:4:27:LYS:C	4:4:30:THR:HG22	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:221:ASN:N	1:x:222:PRO:HD2	2.13	0.63
35:1:2357:A:H2'	35:1:2358:A:C8	2.34	0.63
24:i:46:GLU:CB	39:m:246:TRP:NE1	2.62	0.63
30:P:98:ALA:HA	30:P:101:ASN:HD22	1.63	0.63
3:3:17:HIS:CE1	3:3:28:CYS:SG	2.92	0.63
4:4:61:PRO:CD	4:4:62:GLN:H	2.12	0.63
5:5:213:LEU:HG	5:5:246:VAL:HG11	1.80	0.63
35:1:973:A:N1	35:1:1108:U:C4	2.67	0.63
21:G:74:THR:CB	39:m:243:LEU:CD1	2.75	0.63
17:C:138:ARG:HH21	17:C:240:PRO:HB2	1.63	0.62
27:M:100:ALA:HA	27:M:103:ILE:HD12	1.80	0.62
3:3:30:ASN:O	3:3:32:TYR:N	2.30	0.62
3:3:114:LYS:HB3	18:e:87:MET:HE1	1.80	0.62
4:4:50:TYR:CZ	4:4:109:GLU:HG2	2.34	0.62
29:O:118:VAL:HG23	32:S:164:SER:O	1.99	0.62
17:C:250:TRP:CZ3	17:C:258:LEU:HD22	2.34	0.62
22:h:118:ILE:HD12	26:L:50:PRO:HG3	1.80	0.62
35:1:977:C:H3'	35:1:978:G:H5''	1.81	0.62
43:t:269:GLN:HB2	43:t:270:PRO:HD3	1.80	0.62
21:G:206:GLU:HB2	38:K:162:THR:O	2.00	0.62
5:5:6:SER:CB	5:5:406:PHE:HB3	2.30	0.62
26:L:59:ARG:HD2	35:1:73:C:H2'	1.80	0.62
5:5:3:LEU:HB2	5:5:16:VAL:HB	1.82	0.62
35:1:208:C:H2'	35:1:209:A:O4'	2.00	0.62
35:1:3314:A:H2'	35:1:3315:G:H8	1.65	0.62
35:1:382:U:H3	35:1:387:A:H61	1.48	0.61
41:o:121:ARG:HB2	41:o:173:ILE:HD11	1.81	0.61
21:G:205:ALA:HB1	38:K:163:VAL:HG23	1.81	0.61
35:1:527:A:H61	35:1:565:U:H3	1.48	0.61
14:y:4:ARG:HG2	14:y:208:LEU:HA	1.80	0.61
18:e:63:THR:HA	18:e:66:LEU:HD12	1.82	0.61
35:1:953:G:H2'	35:1:1116:G:C8	2.35	0.61
4:4:54:TRP:HB2	4:4:121:TYR:OH	2.00	0.61
35:1:3314:A:H2'	35:1:3315:G:C8	2.35	0.61
4:4:32:LYS:CA	4:4:35:LYS:HZ1	2.13	0.61
4:4:136:LEU:HB2	4:4:140:ASN:HA	1.82	0.61
21:G:143:ILE:O	21:G:144:GLU:CG	2.48	0.61
21:G:206:GLU:HB3	38:K:163:VAL:HA	1.81	0.61
17:C:138:ARG:HG2	17:C:245:GLY:O	2.01	0.61
4:4:155:ARG:HA	4:4:159:LEU:HD11	1.82	0.61
37:6:43:A:H2'	37:6:44:G:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:29:LEU:HD23	4:4:35:LYS:HE3	1.81	0.61
35:1:532:A:HO2'	35:1:533:A:H8	1.47	0.61
24:i:46:GLU:HA	39:m:246:TRP:NE1	2.14	0.61
43:t:103:ILE:HD11	43:t:128:LEU:HB3	1.82	0.61
35:1:346:C:N4	35:1:349:A:OP2	2.25	0.60
4:4:93:LYS:O	4:4:96:ILE:HG22	2.01	0.60
35:1:528:U:H3	35:1:564:G:H1	1.47	0.60
35:1:533:A:C6	35:1:556:U:O4	2.53	0.60
43:t:187:LEU:HD11	43:t:196:ILE:HG21	1.83	0.60
4:4:170:PRO:HA	4:4:173:ILE:HD12	1.83	0.60
5:5:364:SER:HA	5:5:379:GLY:HA3	1.83	0.60
3:3:97:LEU:HA	3:3:100:TRP:CE3	2.35	0.60
35:1:397:A:H5'	35:1:398:A:OP1	2.01	0.60
35:1:273:A:N1	35:1:292:U:C4	2.68	0.60
1:x:18:ILE:HG23	1:x:22:ILE:HD12	1.83	0.60
4:4:27:LYS:HA	4:4:30:THR:HG21	1.82	0.60
21:G:147:LYS:NZ	39:m:265:ARG:NH1	2.49	0.60
23:H:20:ILE:HG12	23:H:25:VAL:HG22	1.83	0.60
26:L:91:ARG:HH12	35:1:156:G:H22	1.49	0.60
35:1:458:U:H3	35:1:472:A:N6	1.99	0.60
12:v:185:LEU:HA	12:v:188:LEU:HD12	1.83	0.60
17:C:193:LYS:HE2	36:2:21:C:OP1	2.02	0.60
5:5:59:ILE:HG12	5:5:143:LEU:HD21	1.82	0.60
35:1:251:G:C5'	39:m:281:ARG:HH21	2.12	0.60
36:2:6:U:H2'	36:2:7:U:H6	1.65	0.60
17:C:74:ILE:HD13	17:C:75:PRO:HD2	1.84	0.60
21:G:70:LYS:HE3	39:m:240:TYR:CD2	2.35	0.60
35:1:1187:C:H5	35:1:1319:G:H1	1.49	0.60
2:F:219:LYS:HE2	35:1:1169:A:H4'	1.84	0.59
17:C:296:GLN:HB2	35:1:1349:G:N2	2.16	0.59
21:G:74:THR:H	39:m:243:LEU:HD12	1.67	0.59
35:1:109:A:H8	35:1:109:A:OP1	1.85	0.59
2:F:7:LEU:H	4:4:63:GLN:NE2	1.99	0.59
2:F:44:ILE:HG12	2:F:180:SER:HB3	1.82	0.59
21:G:146:LYS:CB	40:D:479:PHE:HB3	2.32	0.59
37:6:23:U:H3	38:K:96:LYS:HE2	1.67	0.59
18:e:61:LYS:HE3	35:1:1340:G:OP2	2.02	0.59
1:x:257:GLN:HB2	30:P:157:VAL:HG13	1.84	0.59
17:C:206:LEU:HB3	17:C:248:VAL:HG22	1.85	0.59
35:1:953:G:H2'	35:1:1116:G:N7	2.17	0.59
21:G:233:TRP:HE1	39:m:240:TYR:C	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:120:ILE:O	3:3:120:ILE:HG22	2.03	0.59
21:G:146:LYS:HE2	21:G:173:MET:HB3	1.84	0.59
4:4:212:THR:OG1	4:4:213:PRO:HD2	2.02	0.59
21:G:70:LYS:HE2	39:m:240:TYR:CD2	2.28	0.59
27:M:21:VAL:HG12	27:M:65:LEU:HA	1.84	0.59
31:Q:82:VAL:HG22	31:Q:102:ALA:HB3	1.85	0.59
3:3:21:ALA:HB2	3:3:27:PHE:CE1	2.32	0.59
4:4:50:TYR:HE2	4:4:109:GLU:HG2	1.67	0.59
21:G:233:TRP:CD1	39:m:240:TYR:CB	2.86	0.59
35:1:1288:U:H2'	35:1:1289:G:H8	1.67	0.59
35:1:3293:U:O2'	35:1:3294:A:H8	1.84	0.59
4:4:46:TRP:CE2	4:4:102:PHE:HB2	2.38	0.59
36:2:6:U:H2'	36:2:7:U:C6	2.36	0.59
4:4:211:LYS:C	4:4:212:THR:HG23	2.28	0.59
12:v:3:SER:HB3	12:v:6:LYS:HB2	1.84	0.59
2:F:60:ARG:HH22	35:1:516:A:H4'	1.68	0.58
4:4:181:TRP:O	4:4:184:LEU:HB2	2.02	0.58
6:A:93:LYS:O	35:1:284:A:N6	2.36	0.58
25:j:72:ARG:HH12	36:2:94:C:H3'	1.68	0.58
35:1:3205:G:H2'	35:1:3206:C:C5	2.37	0.58
3:3:97:LEU:HD23	3:3:100:TRP:HZ3	1.67	0.58
23:H:41:ILE:HD12	35:1:3123:A:H1'	1.85	0.58
35:1:3348:G:H1	35:1:3357:U:H3	1.51	0.58
4:4:77:PHE:CD2	4:4:91:ASN:C	2.78	0.58
24:i:46:GLU:CB	39:m:246:TRP:CE2	2.80	0.58
27:M:99:TRP:CH2	35:1:3206:C:H2'	2.38	0.58
1:x:283:LYS:H	1:x:286:MET:HE2	1.68	0.58
3:3:15:CYS:O	3:3:17:HIS:N	2.28	0.58
4:4:22:LEU:HD21	4:4:49:LEU:CD2	2.34	0.58
13:W:188:VAL:HG11	13:W:202:ILE:HG21	1.85	0.58
35:1:2880:U:H3	35:1:2944:U:H3	1.49	0.58
20:f:48:ARG:NH1	20:f:68:TRP:HB3	2.18	0.58
35:1:1393:A:C8	35:1:1418:A:C6	2.92	0.58
4:4:103:TRP:CE3	4:4:157:LEU:HG	2.39	0.58
5:5:277:SER:HA	5:5:303:LEU:HD12	1.85	0.58
14:y:66:ASN:HD22	14:y:112:ASP:HA	1.67	0.58
17:C:289:ILE:HG21	31:Q:32:LEU:HD11	1.84	0.58
18:e:55:ILE:HB	35:1:947:G:H5'	1.84	0.58
35:1:631:U:H2'	35:1:632:G:H8	1.69	0.58
37:6:15:C:H4'	37:6:16:U:OP2	2.04	0.58
1:x:167:GLU:HG2	5:5:135:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:86:ARG:NH1	36:2:37:A:OP2	2.36	0.58
35:1:1105:A:H2'	35:1:1106:G:H8	1.65	0.58
31:Q:102:ALA:HA	31:Q:122:ILE:O	2.02	0.58
31:Q:123:THR:H	31:Q:126:GLN:NE2	2.02	0.58
35:1:3347:A:N6	35:1:3358:U:H3	1.98	0.58
36:2:147:U:OP2	42:n:88:ARG:CZ	2.52	0.58
4:4:32:LYS:HE2	4:4:77:PHE:H	1.67	0.58
35:1:355:A:H2'	35:1:356:C:O4'	2.03	0.58
21:G:135:GLY:HA3	35:1:148:G:O6	2.03	0.58
2:F:112:ASN:O	2:F:207:LEU:HB2	2.03	0.57
17:C:99:MET:HE2	17:C:102:PRO:HA	1.86	0.57
21:G:109:LEU:HD13	39:m:275:ARG:CD	2.31	0.57
23:H:129:ARG:O	23:H:132:VAL:HG12	2.03	0.57
25:j:39:TYR:CD1	25:j:40:PRO:HA	2.39	0.57
4:4:32:LYS:CA	4:4:35:LYS:NZ	2.66	0.57
21:G:74:THR:CG2	39:m:243:LEU:HD11	2.34	0.57
21:G:130:TYR:HD2	21:G:204:ARG:HD3	1.69	0.57
28:N:4:TYR:OH	35:1:148:G:OP2	2.23	0.57
38:K:81:ILE:HG23	38:K:246:VAL:HB	1.86	0.57
10:s:10:ARG:HD2	35:1:1308:A:H2'	1.87	0.57
17:C:26:PHE:CE1	17:C:126:ILE:HG22	2.39	0.57
28:N:158:HIS:HB3	28:N:161:ALA:HB3	1.86	0.57
5:5:281:LYS:HB3	5:5:328:PHE:CE2	2.39	0.57
16:B:72:VAL:HG23	33:V:88:ARG:HD2	1.85	0.57
17:C:47:ARG:HH11	17:C:109:TRP:HE3	1.52	0.57
29:O:66:LYS:HD2	35:1:3009:G:H5''	1.87	0.57
39:m:253:VAL:HG12	40:D:480:PRO:HG2	1.87	0.57
4:4:211:LYS:O	4:4:212:THR:CG2	2.52	0.57
17:C:317:PRO:HB3	17:C:324:LEU:HD13	1.86	0.57
38:K:113:ALA:HB3	38:K:253:TRP:CH2	2.40	0.57
23:H:38:LEU:O	23:H:41:ILE:HG22	2.04	0.57
35:1:3211:C:H2'	35:1:3212:C:C6	2.39	0.57
1:x:100:ASN:CG	3:3:132:ARG:HE	2.13	0.57
3:3:140:LYS:HD2	35:1:1392:G:O6	2.04	0.57
4:4:32:LYS:H	4:4:35:LYS:NZ	2.03	0.57
4:4:69:LEU:HD13	4:4:124:LEU:HD11	1.85	0.57
4:4:125:ILE:HD13	4:4:169:ILE:HD11	1.86	0.57
13:W:141:ILE:HG12	13:W:179:LYS:HD2	1.85	0.57
17:C:193:LYS:HE2	35:1:1419:A:H5''	1.86	0.57
34:Y:118:LEU:HD12	34:Y:121:ARG:HH22	1.68	0.57
41:o:113:GLN:HE22	43:t:56:VAL:HB	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:106:MET:HA	4:4:106:MET:CE	2.31	0.57
7:b:164:ASP:H	7:b:217:GLN:HE22	1.51	0.57
21:G:85:ASN:OD1	43:t:59:GLU:OE2	2.22	0.57
23:H:24:ILE:HD11	23:H:39:LYS:HD2	1.87	0.57
34:Y:59:VAL:O	34:Y:64:LYS:HG2	2.05	0.57
43:t:269:GLN:CB	43:t:270:PRO:HD3	2.34	0.57
9:r:7:ILE:HD11	35:1:2898:G:C8	2.40	0.56
35:1:656:A:H2'	35:1:657:A:C8	2.40	0.56
5:5:185:ALA:HB1	5:5:186:PRO:HA	1.87	0.56
12:v:28:ILE:HG21	26:L:41:THR:HG23	1.86	0.56
21:G:77:GLN:HA	21:G:229:VAL:HG22	1.87	0.56
35:1:631:U:H2'	35:1:632:G:C8	2.40	0.56
4:4:28:TYR:OH	4:4:35:LYS:HG2	2.05	0.56
37:6:23:U:H5''	43:t:77:ARG:HH12	1.69	0.56
39:m:340:PRO:HD2	39:m:370:LYS:HD2	1.87	0.56
4:4:12:SER:O	4:4:55:PHE:CE1	2.57	0.56
16:B:41:VAL:HA	16:B:185:GLY:CA	2.22	0.56
4:4:27:LYS:CA	4:4:30:THR:CG2	2.83	0.56
5:5:254:LEU:HD23	5:5:323:PHE:HB3	1.86	0.56
38:K:124:LEU:HD21	38:K:126:ILE:HG13	1.87	0.56
35:1:1205:A:N1	35:1:1299:U:H5	2.04	0.56
35:1:1288:U:H2'	35:1:1289:G:C8	2.40	0.56
16:B:159:ARG:HA	16:B:182:GLN:HA	1.88	0.56
21:G:112:GLU:O	21:G:116:VAL:HG23	2.05	0.56
35:1:950:G:H4'	35:1:970:A:H4'	1.87	0.56
35:1:973:A:N1	35:1:1108:U:O4	2.39	0.56
35:1:1194:G:H2'	35:1:1195:A:C8	2.40	0.56
36:2:68:G:H2'	36:2:69:U:O4'	2.06	0.56
16:B:86:VAL:HA	16:B:162:VAL:HG12	1.87	0.56
24:i:46:GLU:HG2	39:m:247:PHE:HB3	1.88	0.56
21:G:113:ALA:CB	39:m:279:ILE:HG22	2.37	0.55
4:4:224:ILE:O	4:4:224:ILE:HG22	2.06	0.55
6:A:92:ARG:HH11	35:1:304:G:H3'	1.70	0.55
1:x:290:LYS:HE3	35:1:395:A:H5''	1.89	0.55
35:1:230:U:H2'	35:1:231:G:O4'	2.07	0.55
5:5:368:HIS:HB3	5:5:376:LEU:HD12	1.89	0.55
35:1:3045:G:H2'	35:1:3046:A:O4'	2.07	0.55
43:t:215:ILE:HG12	43:t:226:GLU:HG2	1.88	0.55
4:4:50:TYR:CE2	4:4:109:GLU:CG	2.88	0.55
13:W:3:ARG:HB2	35:1:1210:U:H5	1.72	0.55
4:4:29:LEU:HA	4:4:35:LYS:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:113:ALA:HB1	39:m:279:ILE:HG22	1.88	0.55
4:4:66:ALA:CB	4:4:123:LEU:HD13	2.36	0.55
5:5:288:ARG:H	35:1:474:G:P	2.30	0.55
21:G:147:LYS:O	21:G:201:THR:HG23	2.07	0.55
29:O:25:LYS:HE3	35:1:1175:C:H5'	1.89	0.55
9:r:8:GLU:HA	9:r:11:ILE:HD12	1.89	0.55
18:e:74:PHE:CE2	18:e:85:LEU:HD21	2.42	0.55
36:2:93:U:H2'	36:2:94:C:O4'	2.07	0.55
34:Y:60:ARG:HB2	34:Y:103:LYS:HD2	1.88	0.55
35:1:324:A:H2'	35:1:325:A:C8	2.41	0.55
37:6:10:A:H2'	37:6:11:C:O4'	2.07	0.55
17:C:142:VAL:HB	17:C:145:ILE:HG12	1.89	0.54
28:N:12:ARG:HD2	35:1:268:A:C5	2.43	0.54
1:x:239:ILE:HG12	1:x:265:LEU:HB2	1.89	0.54
3:3:68:GLU:CB	4:4:57:ASP:HB2	2.21	0.54
4:4:53:MET:HA	4:4:65:LEU:CD2	2.37	0.54
5:5:343:PHE:CD1	5:5:351:MET:HE3	2.41	0.54
24:i:46:GLU:HB3	39:m:246:TRP:NE1	2.19	0.54
29:O:90:HIS:HE1	35:1:2382:G:OP2	1.90	0.54
35:1:1132:C:H2'	35:1:1133:A:H8	1.72	0.54
21:G:147:LYS:HZ1	39:m:265:ARG:NH1	2.04	0.54
35:1:793:C:H2'	35:1:794:U:O4'	2.08	0.54
35:1:1176:C:H2'	35:1:1177:G:N2	2.23	0.54
1:x:187:HIS:CD2	1:x:187:HIS:O	2.60	0.54
21:G:143:ILE:O	21:G:144:GLU:CB	2.55	0.54
28:N:178:HIS:HB2	28:N:179:LYS:NZ	2.22	0.54
32:S:90:MET:HG2	32:S:91:TYR:N	2.21	0.54
4:4:50:TYR:CD1	4:4:50:TYR:C	2.86	0.54
14:y:219:GLU:HA	14:y:224:LEU:HD23	1.90	0.54
1:x:245:ARG:NH2	30:P:159:LYS:HD3	2.22	0.54
9:r:2:PRO:CD	35:1:3026:G:H4'	2.36	0.54
12:v:161:LYS:NZ	26:L:48:PRO:HB3	2.18	0.54
17:C:190:GLY:O	17:C:193:LYS:HG3	2.08	0.54
35:1:273:A:H2'	35:1:274:G:H8	1.72	0.54
35:1:3306:U:H4'	35:1:3309:G:O6	2.08	0.54
21:G:191:ASN:HA	42:n:96:ARG:HH11	1.71	0.54
42:n:132:ILE:HG23	42:n:197:VAL:HG21	1.89	0.54
24:i:68:ARG:HD2	24:i:71:LYS:HD3	1.90	0.54
28:N:48:ALA:O	28:N:53:TYR:HB3	2.08	0.54
32:S:38:LYS:HE2	32:S:61:ILE:HG21	1.89	0.54
35:1:3295:A:H2'	35:1:3296:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:K:250:ASN:HB3	38:K:253:TRP:CD1	2.43	0.54
16:B:209:PHE:HE1	16:B:340:LYS:HB3	1.73	0.54
18:e:76:VAL:HG21	18:e:82:LEU:HB2	1.89	0.54
24:i:54:GLU:HA	24:i:57:LEU:HB2	1.90	0.54
31:Q:71:LEU:HD13	31:Q:99:THR:HG21	1.90	0.54
1:x:110:PHE:HE1	1:x:178:PHE:HE2	1.55	0.54
2:F:86:VAL:HG13	2:F:136:TYR:HB3	1.89	0.54
24:i:40:VAL:HG11	28:N:5:LYS:HG3	1.90	0.54
30:P:82:ARG:HG2	30:P:83:TRP:H	1.72	0.54
34:Y:119:ILE:HG22	34:Y:124:GLY:HA3	1.89	0.54
35:1:632:G:H2'	35:1:633:C:C6	2.43	0.54
1:x:245:ARG:HD2	30:P:157:VAL:HG12	1.90	0.53
16:B:221:THR:CG2	16:B:273:HIS:H	2.17	0.53
35:1:1230:G:H1	35:1:1279:C:H42	1.55	0.53
36:2:26:U:H2'	36:2:27:U:C6	2.43	0.53
37:6:24:A:H1'	38:K:93:LYS:HE2	1.88	0.53
43:t:269:GLN:HB2	43:t:270:PRO:CD	2.37	0.53
3:3:97:LEU:HD23	3:3:100:TRP:CZ3	2.43	0.53
21:G:221:ASN:HD21	41:o:154:ASN:HB3	1.72	0.53
26:L:46:ILE:HG22	26:L:49:ARG:HB2	1.90	0.53
35:1:418:A:H5'	35:1:629:U:O2'	2.08	0.53
35:1:782:U:H2'	35:1:783:A:H4'	1.89	0.53
1:x:235:GLN:NE2	1:x:236:ARG:HE	2.06	0.53
5:5:262:GLU:H	5:5:285:GLN:HE22	1.54	0.53
21:G:105:LYS:HE2	39:m:275:ARG:NH1	2.20	0.53
35:1:3020:U:H3'	35:1:3021:A:H5'	1.90	0.53
35:1:1340:G:H2'	35:1:1341:U:C6	2.44	0.53
36:2:127:U:C1'	39:m:323:HIS:NE2	2.72	0.53
4:4:18:ARG:CZ	4:4:55:PHE:CD1	2.83	0.53
21:G:90:THR:HA	21:G:214:LEU:HD21	1.90	0.53
26:L:53:LEU:HD22	26:L:94:GLY:HA2	1.90	0.53
35:1:1348:U:O4'	35:1:1350:A:H1'	2.08	0.53
4:4:65:LEU:HD12	4:4:65:LEU:C	2.34	0.53
4:4:211:LYS:O	4:4:212:THR:HG23	2.08	0.53
9:r:17:ARG:HB2	9:r:20:HIS:HB2	1.91	0.53
35:1:157:A:H62	35:1:264:G:H21	1.56	0.53
35:1:1255:C:H2'	35:1:1256:G:H8	1.73	0.53
35:1:2363:A:H2'	35:1:2364:G:O4'	2.08	0.53
4:4:93:LYS:O	4:4:93:LYS:HD2	2.08	0.53
7:b:222:PRO:HG2	7:b:239:SER:HB3	1.90	0.53
29:O:87:MET:SD	35:1:1174:G:N2	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y:56:VAL:HG21	34:Y:104:LEU:HD13	1.89	0.53
5:5:51:TRP:HB3	5:5:59:ILE:HG23	1.91	0.53
12:v:55:LEU:HA	22:h:119:LYS:HB2	1.89	0.53
18:e:75:LEU:HD23	18:e:95:GLU:HB3	1.91	0.53
2:F:127:LEU:HD23	2:F:130:ILE:HD11	1.90	0.53
19:E:52:VAL:HG11	19:E:65:ILE:HD13	1.91	0.53
28:N:118:SER:HA	28:N:132:VAL:HA	1.91	0.53
38:K:132:ILE:HG12	38:K:154:ILE:HD12	1.91	0.53
9:r:5:ASP:HA	35:1:2898:G:N1	2.04	0.52
9:r:26:LYS:HG2	35:1:3119:U:H5'	1.90	0.52
21:G:213:LYS:HE3	41:o:160:HIS:HA	1.91	0.52
21:G:72:PRO:HG2	21:G:75:ILE:HD12	1.90	0.52
35:1:1:G:N7	37:6:232:A:C2	2.77	0.52
16:B:122:TRP:CH2	16:B:127:LYS:HG2	2.45	0.52
3:3:11:ASN:HD22	3:3:18:ARG:HH22	1.57	0.52
17:C:299:ILE:HD12	31:Q:39:ARG:HB3	1.91	0.52
35:1:673:U:H2'	35:1:674:G:C8	2.45	0.52
1:x:235:GLN:HE22	1:x:236:ARG:HE	1.58	0.52
4:4:65:LEU:HA	4:4:68:GLU:HG2	1.91	0.52
4:4:225:VAL:HG22	4:4:238:ILE:CD1	2.38	0.52
14:y:57:ARG:HG3	16:B:70:ARG:HH22	1.74	0.52
16:B:32:PHE:CD1	16:B:182:GLN:HG2	2.43	0.52
35:1:664:U:H2'	35:1:665:A:C8	2.45	0.52
14:y:101:LEU:HA	33:V:135:VAL:HG13	1.91	0.52
9:r:2:PRO:HG2	35:1:3026:G:O2'	2.10	0.52
17:C:291:ASN:HD21	35:1:1348:U:H1'	1.75	0.52
35:1:3000:A:H2'	35:1:3001:C:C6	2.45	0.52
5:5:246:VAL:HG12	5:5:248:PRO:HD3	1.91	0.52
12:v:209:GLN:H	39:m:267:VAL:CG2	2.22	0.52
16:B:306:THR:HG21	16:B:316:GLU:HA	1.90	0.52
35:1:278:U:H3	35:1:287:G:H1	1.58	0.52
43:t:77:ARG:HG2	43:t:305:ALA:HB2	1.92	0.52
4:4:234:LEU:O	4:4:238:ILE:HG12	2.09	0.52
17:C:151:VAL:HG22	17:C:250:TRP:HB2	1.91	0.52
35:1:285:A:H1'	35:1:286:U:H5	1.75	0.52
35:1:1255:C:H2'	35:1:1256:G:C8	2.44	0.52
35:1:1416:C:H6	35:1:1416:C:O5'	1.93	0.52
1:x:200:ASN:HB2	1:x:233:HIS:HA	1.92	0.52
29:O:60:LYS:HB3	35:1:1307:G:N1	2.25	0.52
35:1:669:U:H2'	35:1:670:C:O4'	2.10	0.52
38:K:113:ALA:HB3	38:K:253:TRP:HH2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:172:LYS:HG2	42:n:242:LEU:HD11	1.92	0.52
3:3:93:ILE:CG2	3:3:97:LEU:HD11	2.39	0.51
4:4:18:ARG:NE	4:4:55:PHE:HD1	2.08	0.51
6:A:91:ALA:HB1	35:1:284:A:C8	2.45	0.51
16:B:343:TYR:HE1	16:B:345:ASN:HB2	1.75	0.51
35:1:271:C:H2'	35:1:272:G:O4'	2.10	0.51
3:3:141:VAL:C	3:3:143:ARG:H	2.18	0.51
4:4:20:ASN:OD1	4:4:20:ASN:N	2.42	0.51
4:4:223:ASP:O	4:4:226:ALA:HB1	2.09	0.51
7:b:49:LYS:HE2	35:1:2828:G:OP2	2.10	0.51
16:B:288:GLY:HA3	16:B:319:ASN:HA	1.92	0.51
1:x:214:PHE:HA	1:x:217:ILE:HG22	1.90	0.51
31:Q:36:LEU:HD22	31:Q:40:THR:HG23	1.90	0.51
31:Q:36:LEU:HD22	31:Q:40:THR:CG2	2.41	0.51
33:V:136:VAL:HG12	33:V:137:VAL:HG23	1.92	0.51
35:1:669:U:H2'	35:1:670:C:C6	2.45	0.51
42:n:41:ILE:HD12	42:n:71:LEU:HD12	1.93	0.51
42:n:65:ALA:O	42:n:69:GLN:HB2	2.10	0.51
43:t:197:GLY:HA2	43:t:311:GLU:HG3	1.92	0.51
4:4:29:LEU:HA	4:4:35:LYS:HE3	1.91	0.51
5:5:279:LEU:HB2	5:5:296:LEU:HD11	1.91	0.51
29:O:94:ARG:HG2	35:1:3172:A:N1	2.25	0.51
36:2:127:U:OP2	39:m:321:VAL:HG12	2.04	0.51
43:t:146:ARG:HG2	43:t:171:THR:HA	1.92	0.51
18:e:97:ALA:O	18:e:100:ILE:HG12	2.10	0.51
26:L:101:ARG:HH22	26:L:112:ASN:ND2	2.09	0.51
35:1:644:G:OP2	35:1:1116:G:O2'	2.28	0.51
4:4:76:TYR:CZ	4:4:94:ALA:CB	2.90	0.51
5:5:245:PRO:HB2	5:5:276:TRP:CD1	2.46	0.51
12:v:203:LYS:NZ	40:D:311:TYR:OH	2.28	0.51
21:G:233:TRP:CD2	39:m:240:TYR:CD1	2.97	0.51
26:L:58:VAL:HG22	35:1:75:G:OP1	2.10	0.51
35:1:63:A:C6	35:1:64:G:C6	2.98	0.51
38:K:68:GLU:HA	40:D:286:ARG:HH12	1.73	0.51
38:K:86:LYS:HE3	38:K:301:LEU:HB2	1.93	0.51
15:z:6:ARG:HH22	35:1:3131:U:P	2.34	0.51
17:C:148:ILE:HG12	17:C:149:PRO:HA	1.91	0.51
17:C:286:VAL:HG23	31:Q:28:LEU:HD13	1.93	0.51
21:G:186:LEU:O	21:G:189:LEU:HG	2.11	0.51
22:h:47:VAL:O	22:h:51:ILE:HG13	2.10	0.51
28:N:201:ARG:NH2	35:1:692:A:OP1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y:85:VAL:HG11	34:Y:99:LEU:HD11	1.91	0.51
35:1:1108:U:O2	35:1:1108:U:O4'	2.29	0.51
3:3:2:SER:OG	3:3:3:ASP:N	2.30	0.51
7:b:150:LEU:HA	7:b:153:VAL:HG12	1.91	0.51
34:Y:104:LEU:O	34:Y:105:VAL:HG23	2.11	0.51
35:1:625:G:H2'	35:1:626:U:C6	2.46	0.51
6:A:154:GLU:HG2	8:J:209:GLN:HG2	1.92	0.51
23:H:161:LEU:HD23	23:H:179:ILE:HD13	1.92	0.51
26:L:43:ALA:HB2	26:L:51:LEU:HD21	1.93	0.51
1:x:154:LYS:C	1:x:156:LYS:H	2.19	0.51
3:3:41:GLN:CD	35:1:1351:U:C5	2.89	0.51
34:Y:32:SER:O	35:1:225:C:H4'	2.11	0.51
35:1:226:C:H2'	35:1:227:G:O4'	2.10	0.51
36:2:127:U:C4'	39:m:323:HIS:CD2	2.94	0.51
38:K:124:LEU:HD22	38:K:180:ILE:HG23	1.93	0.51
4:4:92:ASP:OD1	4:4:92:ASP:N	2.35	0.50
6:A:46:ARG:HD2	35:1:285:A:H2	1.76	0.50
26:L:70:ARG:NH2	35:1:76:G:OP1	2.44	0.50
35:1:31:C:H2'	35:1:32:U:C6	2.46	0.50
35:1:1114:U:H3'	35:1:1115:G:H21	1.76	0.50
43:t:205:ARG:HG3	43:t:251:ILE:HG21	1.92	0.50
12:v:207:ILE:CG2	39:m:268:PRO:HG2	2.40	0.50
35:1:1117:G:H2'	35:1:1118:C:C6	2.46	0.50
38:K:101:ASN:HB2	38:K:269:GLN:HE22	1.75	0.50
1:x:60:ILE:HG21	1:x:236:ARG:CZ	2.42	0.50
14:y:18:LYS:HB3	14:y:25:LEU:HD12	1.93	0.50
17:C:205:PRO:HB3	17:C:247:PHE:CE2	2.47	0.50
21:G:205:ALA:HB3	38:K:163:VAL:HG23	1.93	0.50
35:1:50:U:H2'	35:1:51:A:H8	1.76	0.50
35:1:107:A:H2'	35:1:108:A:O4'	2.12	0.50
35:1:197:G:H2'	35:1:198:A:C8	2.46	0.50
4:4:15:ARG:HA	4:4:18:ARG:NH1	2.27	0.50
4:4:114:ASP:HA	17:C:288:ARG:HD3	1.93	0.50
21:G:186:LEU:HD23	21:G:189:LEU:HD21	1.93	0.50
31:Q:107:THR:O	31:Q:108:ALA:C	2.54	0.50
35:1:347:G:H2'	35:1:348:A:C8	2.46	0.50
42:n:116:HIS:HA	42:n:119:LYS:HD3	1.94	0.50
42:n:206:PRO:HB2	43:t:228:VAL:HG13	1.92	0.50
3:3:64:MET:HE2	3:3:100:TRP:CZ2	2.45	0.50
35:1:258:G:H2'	35:1:259:C:C6	2.46	0.50
4:4:166:TYR:O	4:4:169:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:224:ILE:C	4:4:226:ALA:HB3	2.37	0.50
15:z:43:LYS:HA	15:z:46:LEU:HD12	1.94	0.50
17:C:150:LEU:CD1	17:C:172:VAL:CG1	2.89	0.50
4:4:29:LEU:O	4:4:32:LYS:CG	2.55	0.50
12:v:208:TYR:CA	39:m:267:VAL:HG13	2.24	0.50
17:C:328:ASN:OD1	17:C:330:TYR:HB3	2.12	0.50
16:B:123:TYR:CE2	16:B:124:LYS:HG3	2.47	0.50
36:2:75:G:H2'	36:2:76:C:C6	2.47	0.50
4:4:18:ARG:NH2	4:4:55:PHE:CB	2.74	0.50
4:4:223:ASP:C	4:4:226:ALA:HB3	2.37	0.50
34:Y:45:ILE:HD11	34:Y:122:LYS:HD3	1.93	0.50
35:1:661:G:H2'	35:1:661:G:N3	2.25	0.50
3:3:34:VAL:HG22	3:3:52:THR:HG23	1.93	0.49
4:4:155:ARG:CA	4:4:159:LEU:HD11	2.42	0.49
15:z:37:LEU:HD13	16:B:203:VAL:HA	1.93	0.49
21:G:140:VAL:HA	21:G:143:ILE:HD12	1.93	0.49
24:i:46:GLU:CA	39:m:246:TRP:NE1	2.74	0.49
35:1:586:C:H4'	35:1:1165:A:H5'	1.94	0.49
35:1:2357:A:H2'	35:1:2358:A:H8	1.76	0.49
36:2:37:A:C8	36:2:39:G:N2	2.80	0.49
38:K:110:TRP:O	38:K:114:SER:HB2	2.12	0.49
3:3:143:ARG:HD2	3:3:147:ASN:ND2	2.27	0.49
9:r:36:SER:OG	35:1:1207:G:O2'	2.29	0.49
20:f:26:ASN:HA	20:f:88:ASN:OD1	2.11	0.49
20:f:76:GLY:HA2	35:1:1327:C:O2'	2.12	0.49
34:Y:51:ARG:HD3	34:Y:52:ARG:H	1.77	0.49
35:1:3020:U:H3'	35:1:3021:A:C5'	2.40	0.49
35:1:3055:U:H3	35:1:3086:A:H62	1.61	0.49
36:2:157:U:C4	43:t:55:PHE:O	2.65	0.49
41:o:109:LYS:HE2	43:t:61:ILE:HD11	1.93	0.49
11:u:78:PRO:HB2	14:y:85:ARG:HB2	1.94	0.49
12:v:207:ILE:HG22	39:m:268:PRO:HG2	1.93	0.49
13:W:220:TYR:HB3	13:W:229:GLU:HB3	1.94	0.49
14:y:85:ARG:HH22	14:y:93:LYS:HA	1.78	0.49
17:C:206:LEU:HA	17:C:226:GLU:O	2.11	0.49
32:S:77:VAL:HG13	32:S:126:VAL:HG22	1.94	0.49
35:1:252:U:OP2	39:m:277:MET:HE2	2.12	0.49
40:D:362:ILE:HG22	40:D:391:LEU:HG	1.93	0.49
3:3:33:ASN:HB3	3:3:44:PRO:HG3	1.93	0.49
12:v:180:ARG:NH2	39:m:277:MET:SD	2.75	0.49
17:C:208:VAL:HG11	17:C:230:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:C:338:LYS:O	17:C:340:GLY:N	2.42	0.49
20:f:27:VAL:HG11	20:f:82:ARG:HD3	1.95	0.49
35:1:3163:A:H2'	35:1:3164:C:O4'	2.13	0.49
3:3:61:TYR:CD1	3:3:79:ARG:HD3	2.48	0.49
35:1:718:G:H1	35:1:750:G:H21	1.60	0.49
35:1:1344:G:H2'	35:1:1345:G:O4'	2.13	0.49
7:b:187:ILE:HD11	7:b:332:ARG:HB2	1.94	0.49
22:h:116:TYR:OH	26:L:94:GLY:HA3	2.13	0.49
35:1:347:G:C6	35:1:348:A:C6	3.01	0.49
35:1:617:G:C6	35:1:618:C:N4	2.81	0.49
5:5:280:THR:HB	5:5:293:GLN:HG2	1.94	0.49
7:b:250:VAL:HG13	7:b:283:VAL:HG13	1.95	0.49
35:1:201:A:H4'	35:1:220:G:C6	2.48	0.49
35:1:1187:C:O2	35:1:1187:C:O4'	2.30	0.49
42:n:249:ASP:HB3	42:n:252:LYS:HB2	1.94	0.49
1:x:208:GLN:O	1:x:212:ARG:HB2	2.13	0.49
3:3:96:HIS:HA	35:1:467:U:H3	1.78	0.49
22:h:58:ILE:HG22	22:h:62:GLN:HE22	1.78	0.49
35:1:251:G:H4'	39:m:277:MET:HB3	1.95	0.49
35:1:1233:G:H1	35:1:1255:C:H5	1.61	0.49
35:1:1426:C:H2'	35:1:1427:U:O4'	2.13	0.49
36:2:154:C:H2'	36:2:155:A:C8	2.48	0.49
5:5:168:LYS:HD2	5:5:178:LEU:HD11	1.94	0.48
35:1:164:A:H61	35:1:257:U:H3	1.61	0.48
35:1:544:C:H2'	35:1:545:U:H2'	1.95	0.48
4:4:150:ILE:O	4:4:154:LEU:HB3	2.12	0.48
4:4:212:THR:HB	4:4:213:PRO:HD2	1.73	0.48
14:y:85:ARG:HD2	14:y:94:ILE:HD12	1.94	0.48
35:1:501:A:H2'	35:1:502:U:C6	2.48	0.48
35:1:2394:G:H2'	35:1:2395:G:C8	2.48	0.48
35:1:3146:G:H2'	35:1:3147:G:H8	1.79	0.48
2:F:151:ARG:HH12	2:F:208:SER:H	1.60	0.48
17:C:193:LYS:HD3	35:1:1420:C:OP2	2.13	0.48
21:G:233:TRP:CD1	39:m:240:TYR:C	2.91	0.48
30:P:116:HIS:CE1	30:P:118:GLN:HB2	2.48	0.48
35:1:622:A:O5'	35:1:622:A:H8	1.96	0.48
35:1:1124:U:O2	35:1:1124:U:O4'	2.31	0.48
40:D:369:ASP:HB3	40:D:372:ASP:HB2	1.96	0.48
35:1:1125:U:H3	35:1:1133:A:H61	1.61	0.48
35:1:1345:G:H1	35:1:1359:C:H42	1.61	0.48
3:3:5:ILE:HA	3:3:8:GLN:HE21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:113:GLU:HB3	16:B:176:ALA:HB2	1.95	0.48
21:G:221:ASN:ND2	41:o:154:ASN:HB3	2.27	0.48
27:M:57:ALA:HB2	32:S:97:VAL:HG21	1.94	0.48
35:1:981:U:O4	35:1:1102:A:N1	2.46	0.48
36:2:116:G:H1	36:2:137:C:H42	1.62	0.48
4:4:125:ILE:CG2	4:4:172:HIS:HD2	2.26	0.48
21:G:128:LYS:HB3	35:1:120:G:C5	2.47	0.48
21:G:146:LYS:CE	21:G:173:MET:HE3	2.42	0.48
35:1:616:G:H2'	35:1:617:G:C8	2.48	0.48
35:1:1299:U:H2'	35:1:1300:G:O4'	2.14	0.48
36:2:67:U:H2'	36:2:68:G:H8	1.79	0.48
37:6:38:U:O2	37:6:42:G:C2	2.65	0.48
37:6:230:A:H4'	37:6:231:A:C2	2.49	0.48
42:n:248:LEU:HB3	42:n:262:TYR:HD1	1.79	0.48
1:x:241:PHE:HD2	1:x:263:PHE:CD2	2.32	0.48
2:F:85:PHE:HB2	2:F:139:PRO:HG3	1.95	0.48
4:4:60:ARG:HA	4:4:63:GLN:HB2	1.95	0.48
4:4:141:TRP:CZ2	4:4:212:THR:HA	2.47	0.48
11:u:56:ARG:HH11	11:u:62:GLU:HG3	1.78	0.48
14:y:12:GLU:HB3	14:y:15:VAL:HG23	1.96	0.48
16:B:117:ARG:HG2	16:B:178:LEU:HD23	1.95	0.48
17:C:181:VAL:HG12	17:C:182:LEU:H	1.79	0.48
19:E:40:LEU:HD23	19:E:86:ALA:HA	1.95	0.48
35:1:972:A:H2'	35:1:973:A:H8	1.74	0.48
1:x:235:GLN:HG2	3:3:156:ALA:HB2	1.96	0.48
4:4:69:LEU:CD2	4:4:69:LEU:C	2.86	0.48
5:5:279:LEU:HB3	5:5:296:LEU:HD21	1.96	0.48
42:n:92:ARG:HH21	42:n:96:ARG:HD2	1.78	0.48
5:5:307:GLU:O	5:5:333:VAL:HA	2.13	0.48
21:G:74:THR:N	39:m:243:LEU:CD1	2.76	0.48
31:Q:35:PHE:CD1	31:Q:35:PHE:C	2.92	0.48
35:1:3119:U:H2'	35:1:3121:U:OP1	2.14	0.48
35:1:3183:A:H2'	35:1:3184:A:H8	1.78	0.48
36:2:154:C:H2'	36:2:155:A:H8	1.78	0.48
38:K:80:LEU:HD22	38:K:245:ASN:HD22	1.79	0.48
5:5:287:GLY:HA3	35:1:473:G:H5''	1.95	0.48
27:M:8:LYS:HE3	35:1:3200:G:OP2	2.14	0.48
27:M:109:ARG:HH21	29:O:199:TYR:HA	1.79	0.48
32:S:8:GLN:HB2	32:S:64:ILE:HD11	1.95	0.48
33:V:54:LEU:HD21	33:V:119:GLY:HA3	1.96	0.48
33:V:80:ARG:HA	33:V:95:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1341:U:H2'	35:1:1342:C:C6	2.49	0.48
27:M:20:VAL:HG13	27:M:66:THR:OG1	2.14	0.47
35:1:506:U:H2'	35:1:507:U:O4'	2.14	0.47
40:D:299:CYS:HB2	40:D:320:HIS:HB2	1.95	0.47
1:x:235:GLN:HE21	3:3:152:ALA:HA	1.79	0.47
3:3:29:ARG:NH1	3:3:29:ARG:HG2	2.28	0.47
4:4:61:PRO:CD	4:4:62:GLN:N	2.76	0.47
4:4:137:GLN:HG3	4:4:139:ARG:H	1.79	0.47
35:1:756:U:H3	35:1:776:U:H3	1.62	0.47
3:3:111:ARG:HD3	18:e:87:MET:HE3	1.96	0.47
6:A:42:ASN:HB3	35:1:285:A:H5''	1.95	0.47
7:b:46:TYR:HB2	7:b:116:LEU:HD21	1.96	0.47
23:H:156:GLN:HE22	35:1:3109:G:H21	1.61	0.47
27:M:60:LEU:HA	27:M:63:VAL:HG12	1.96	0.47
38:K:190:LEU:N	38:K:191:PRO:HD2	2.29	0.47
3:3:124:ARG:CZ	18:e:113:LYS:HG2	2.43	0.47
4:4:154:LEU:HD12	4:4:220:ILE:HD13	1.97	0.47
5:5:22:THR:HB	5:5:396:VAL:HG13	1.97	0.47
24:i:58:ILE:HA	24:i:61:ILE:HD12	1.96	0.47
35:1:3176:G:C6	35:1:3213:A:C2	3.02	0.47
35:1:3199:G:H2'	35:1:3200:G:H8	1.79	0.47
1:x:245:ARG:HD3	30:P:158:ALA:O	2.15	0.47
3:3:106:HIS:HD2	19:E:10:TYR:OH	1.98	0.47
12:v:165:LEU:HD21	26:L:126:PHE:HD1	1.80	0.47
21:G:93:LEU:O	21:G:96:LYS:HB2	2.14	0.47
27:M:99:TRP:CZ2	35:1:3206:C:H2'	2.50	0.47
28:N:53:TYR:CD1	28:N:61:ILE:HD11	2.50	0.47
35:1:3019:U:H5	35:1:3035:A:H61	1.63	0.47
4:4:46:TRP:CD1	4:4:102:PHE:N	2.83	0.47
13:W:6:ARG:HD2	35:1:3117:C:N4	2.29	0.47
18:e:105:ARG:O	18:e:108:ILE:N	2.48	0.47
21:G:92:LYS:NZ	37:6:1:C:O2	2.42	0.47
30:P:39:TRP:HZ3	30:P:47:TYR:CG	2.33	0.47
31:Q:23:ASN:OD1	31:Q:23:ASN:C	2.57	0.47
35:1:3205:G:H2'	35:1:3206:C:H5	1.80	0.47
38:K:67:LEU:HD13	40:D:283:PHE:HZ	1.79	0.47
42:n:35:LEU:HD13	42:n:71:LEU:HD21	1.97	0.47
3:3:40:ARG:HH11	3:3:40:ARG:HG2	1.80	0.47
4:4:154:LEU:HD23	4:4:155:ARG:HG2	1.97	0.47
18:e:47:ARG:HE	18:e:47:ARG:HB3	1.52	0.47
18:e:128:LEU:HA	18:e:128:LEU:HD13	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:74:THR:H	39:m:243:LEU:CD1	2.27	0.47
24:i:58:ILE:HG22	24:i:94:ILE:HD11	1.97	0.47
28:N:68:ARG:HB3	35:1:291:C:OP1	2.14	0.47
28:N:120:TRP:HA	28:N:130:PHE:HD1	1.80	0.47
35:1:283:G:H5'	35:1:284:A:H5'	1.97	0.47
35:1:527:A:N6	35:1:565:U:H3	2.11	0.47
43:t:277:VAL:HG21	43:t:287:ARG:HB3	1.97	0.47
1:x:289:GLU:C	1:x:291:LYS:H	2.23	0.47
2:F:90:LYS:HB2	2:F:220:PHE:CE1	2.49	0.47
3:3:35:THR:HG22	3:3:37:LEU:HB2	1.96	0.47
7:b:46:TYR:HD1	7:b:129:LYS:HG3	1.80	0.47
25:j:75:LYS:HE3	36:2:94:C:OP1	2.14	0.47
35:1:720:A:H3'	35:1:784:A:N6	2.30	0.47
35:1:976:U:C4	35:1:1105:A:N1	2.83	0.47
2:F:178:ILE:HG23	2:F:183:ASP:HB3	1.95	0.47
17:C:58:HIS:CE1	17:C:98:ARG:HD3	2.49	0.47
21:G:221:ASN:ND2	41:o:154:ASN:CB	2.78	0.47
40:D:348:VAL:HG12	40:D:351:ARG:HH22	1.79	0.47
41:o:153:ASN:HA	41:o:164:VAL:HG12	1.97	0.47
1:x:95:ILE:HG23	1:x:121:VAL:HG13	1.96	0.47
2:F:98:LYS:HB3	2:F:99:PRO:HD3	1.95	0.47
3:3:29:ARG:HG2	3:3:29:ARG:HH11	1.79	0.47
4:4:223:ASP:O	4:4:226:ALA:HB3	2.14	0.47
17:C:157:GLU:HA	17:C:215:ILE:HB	1.97	0.47
32:S:141:LYS:HA	32:S:144:LEU:HD12	1.97	0.47
35:1:201:A:H2'	35:1:202:G:C8	2.50	0.47
4:4:228:TYR:O	4:4:229:ASN:CB	2.63	0.46
12:v:12:SER:HB2	12:v:14:VAL:HG23	1.97	0.46
20:f:67:MET:HE1	20:f:90:PRO:CD	2.39	0.46
21:G:101:THR:HG23	21:G:104:GLU:H	1.80	0.46
21:G:136:LEU:HB2	35:1:147:U:OP2	2.14	0.46
28:N:124:ASP:CG	28:N:125:SER:N	2.73	0.46
32:S:30:PHE:CD1	32:S:103:VAL:HG11	2.50	0.46
35:1:201:A:H4'	35:1:220:G:C5	2.49	0.46
35:1:673:U:H2'	35:1:674:G:H8	1.79	0.46
36:2:103:G:C6	36:2:105:A:C6	3.03	0.46
36:2:127:U:H4'	42:n:64:TYR:HE1	0.56	0.46
1:x:110:PHE:CE1	1:x:178:PHE:HE2	2.33	0.46
7:b:161:PRO:HB3	35:1:3027:A:N1	2.30	0.46
35:1:411:U:H2'	35:1:412:G:C8	2.50	0.46
35:1:3328:G:H1	35:1:3378:C:H42	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:6:43:A:H2'	37:6:44:G:H8	1.79	0.46
43:t:244:ILE:HD11	43:t:253:GLU:HG3	1.96	0.46
2:F:88:ARG:HE	2:F:103:LEU:HD13	1.80	0.46
17:C:280:ILE:HD12	31:Q:104:LEU:HD22	1.98	0.46
21:G:206:GLU:CB	38:K:162:THR:O	2.63	0.46
22:h:117:ALA:C	22:h:118:ILE:HG13	2.40	0.46
28:N:203:ARG:HD2	35:1:665:A:OP1	2.15	0.46
31:Q:89:ASP:HB2	31:Q:110:ALA:N	2.30	0.46
34:Y:50:ILE:HD13	34:Y:80:VAL:HG11	1.97	0.46
35:1:1187:C:H5	35:1:1319:G:H22	1.63	0.46
35:1:3187:A:H2	35:1:3205:G:H22	1.63	0.46
38:K:170:ARG:HD2	38:K:194:MET:HA	1.98	0.46
12:v:180:ARG:HH21	39:m:277:MET:CE	2.28	0.46
16:B:218:ILE:HG13	16:B:337:THR:O	2.15	0.46
21:G:233:TRP:HE1	39:m:241:GLU:N	2.13	0.46
22:h:85:THR:O	22:h:86:ARG:C	2.59	0.46
34:Y:12:ARG:NH1	35:1:215:G:OP1	2.45	0.46
2:F:18:ALA:HB3	35:1:1349:G:O6	2.15	0.46
5:5:343:PHE:CE1	5:5:354:LYS:HE2	2.51	0.46
21:G:159:PRO:O	21:G:162:LEU:HB2	2.15	0.46
29:O:56:ASP:HB3	35:1:1192:C:N3	2.31	0.46
35:1:589:A:H1'	35:1:1337:A:H5''	1.97	0.46
37:6:32:A:C5	38:K:285:ARG:NH2	2.83	0.46
16:B:286:GLY:HA3	16:B:321:PHE:CE2	2.50	0.46
17:C:45:ASN:O	17:C:110:ASN:ND2	2.49	0.46
17:C:334:PHE:HD2	35:1:578:A:H2'	1.80	0.46
35:1:62:A:H2'	35:1:63:A:O4'	2.16	0.46
35:1:401:U:OP1	35:1:402:A:H8	1.97	0.46
35:1:653:A:C2	35:1:1443:G:C5	3.03	0.46
3:3:76:LEU:HA	3:3:76:LEU:HD23	1.73	0.46
4:4:27:LYS:CA	4:4:30:THR:HG22	2.46	0.46
4:4:32:LYS:N	4:4:35:LYS:NZ	2.63	0.46
4:4:211:LYS:C	4:4:212:THR:CG2	2.89	0.46
14:y:198:VAL:HG23	14:y:205:VAL:HB	1.98	0.46
16:B:93:VAL:HG13	16:B:102:LEU:HD22	1.96	0.46
21:G:149:LYS:O	21:G:176:PRO:HD2	2.16	0.46
26:L:118:GLU:O	26:L:122:LYS:HG2	2.16	0.46
35:1:341:G:H4'	35:1:342:A:H5'	1.97	0.46
35:1:964:G:H2'	35:1:965:A:H8	1.80	0.46
1:x:14:LYS:HA	35:1:351:A:N6	2.26	0.46
1:x:98:THR:HG23	1:x:149:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:243:ARG:HE	1:x:260:GLY:HA3	1.80	0.46
3:3:62:LEU:HD13	3:3:62:LEU:O	2.16	0.46
4:4:50:TYR:HE2	4:4:109:GLU:CD	2.23	0.46
5:5:331:LEU:HD11	5:5:333:VAL:HG13	1.98	0.46
9:r:18:LEU:HD12	23:H:180:TYR:HD2	1.81	0.46
17:C:25:VAL:HA	17:C:276:LEU:HD11	1.96	0.46
20:f:16:TYR:HD2	20:f:23:ASN:ND2	2.13	0.46
35:1:759:U:H3	35:1:772:U:H3	1.64	0.46
41:o:189:ILE:O	41:o:191:LYS:N	2.49	0.46
16:B:283:TYR:HD1	16:B:354:VAL:HG21	1.81	0.46
16:B:294:GLY:HA2	16:B:359:ILE:HD12	1.97	0.46
24:i:43:LEU:HA	39:m:247:PHE:HD2	1.80	0.46
32:S:129:ILE:HG21	32:S:134:ASP:HB2	1.96	0.46
35:1:805:G:H2'	35:1:936:A:H61	1.81	0.46
35:1:1216:C:H42	35:1:1289:G:H1	1.63	0.46
1:x:85:PHE:HB3	1:x:169:PRO:HG3	1.97	0.46
4:4:142:ASP:HB3	4:4:145:LEU:HB2	1.97	0.46
7:b:12:ALA:HB3	7:b:17:LEU:HD23	1.98	0.46
12:v:186:GLU:HG2	12:v:222:TRP:CZ2	2.51	0.46
17:C:106:TRP:HB3	26:L:24:VAL:HG21	1.98	0.46
21:G:132:VAL:HG12	21:G:200:LEU:HG	1.97	0.46
21:G:146:LYS:HB2	40:D:479:PHE:HB3	1.98	0.46
22:h:55:LEU:HA	22:h:58:ILE:HD12	1.98	0.46
24:i:46:GLU:HB3	39:m:246:TRP:CZ2	2.47	0.46
35:1:743:C:H2'	35:1:744:A:C8	2.51	0.46
42:n:132:ILE:HA	42:n:135:ALA:HB3	1.98	0.46
1:x:60:ILE:HG13	1:x:291:LYS:HE3	1.99	0.45
6:A:107:GLY:HA2	6:A:108:PRO:HD3	1.84	0.45
15:z:22:PHE:CE1	16:B:351:LEU:HA	2.51	0.45
17:C:125:ALA:O	17:C:129:THR:HG23	2.16	0.45
20:f:89:LEU:HA	20:f:90:PRO:HD3	1.61	0.45
21:G:105:LYS:HE2	39:m:275:ARG:HH12	1.77	0.45
27:M:112:LEU:HD13	27:M:117:ARG:HA	1.98	0.45
17:C:22:LEU:HD22	17:C:26:PHE:HD2	1.80	0.45
17:C:193:LYS:HB2	17:C:193:LYS:HE3	1.83	0.45
20:f:20:LYS:NZ	35:1:1177:G:N7	2.54	0.45
20:f:52:VAL:HG22	20:f:66:VAL:HG13	1.97	0.45
22:h:23:ASP:O	22:h:27:GLU:HB2	2.16	0.45
28:N:116:LEU:HD23	28:N:133:ILE:HD11	1.97	0.45
38:K:32:ILE:HD11	38:K:264:GLU:HA	1.99	0.45
1:x:245:ARG:HH21	30:P:159:LYS:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:W:168:LYS:HE3	13:W:201:LEU:HD13	1.99	0.45
26:L:116:LEU:O	26:L:119:TYR:HB3	2.16	0.45
35:1:335:G:N2	36:2:29:U:C2	2.85	0.45
2:F:159:GLN:O	2:F:161:VAL:HG23	2.17	0.45
4:4:153:VAL:O	4:4:158:PRO:HD3	2.16	0.45
6:A:166:ALA:HB3	6:A:169:SER:HB2	1.98	0.45
35:1:1146:C:H2'	35:1:1147:G:H8	1.82	0.45
35:1:3044:G:H2'	35:1:3045:G:H8	1.82	0.45
2:F:47:ARG:O	2:F:50:ALA:HB3	2.17	0.45
7:b:437:ASP:H	16:B:301:THR:HG21	1.82	0.45
35:1:976:U:O4	35:1:1105:A:N1	2.49	0.45
41:o:98:LEU:HD13	41:o:134:TYR:HA	1.97	0.45
1:x:285:GLU:C	1:x:286:MET:N	2.75	0.45
2:F:144:ILE:HG22	2:F:185:ILE:HG12	1.98	0.45
14:y:107:VAL:HG13	14:y:118:HIS:HB2	1.99	0.45
16:B:18:PRO:HB2	16:B:20:LYS:HD2	1.98	0.45
17:C:304:GLN:NE2	35:1:594:U:H3	2.15	0.45
23:H:31:ARG:HB2	23:H:82:VAL:O	2.16	0.45
30:P:71:ALA:O	30:P:74:LYS:HB2	2.17	0.45
42:n:444:ALA:HA	42:n:447:TYR:HD2	1.82	0.45
1:x:31:HIS:CE1	35:1:383:G:C5	3.04	0.45
17:C:140:HIS:HA	17:C:177:ASP:OD1	2.16	0.45
17:C:189:ALA:HB2	35:1:1420:C:C5	2.51	0.45
32:S:143:PHE:HA	32:S:148:LEU:HD22	1.98	0.45
35:1:257:U:H2'	35:1:258:G:C8	2.52	0.45
35:1:408:A:H2'	35:1:409:A:O4'	2.17	0.45
35:1:1299:U:O2	35:1:1299:U:O4'	2.34	0.45
2:F:166:ASN:OD1	2:F:181:ILE:N	2.43	0.45
3:3:144:ARG:O	3:3:148:ARG:HB2	2.16	0.45
4:4:50:TYR:CD1	4:4:121:TYR:CE1	3.04	0.45
4:4:130:PHE:O	4:4:134:LYS:HB2	2.17	0.45
16:B:212:ASN:OD1	16:B:354:VAL:HG22	2.17	0.45
16:B:293:ASN:HD22	16:B:304:THR:HG23	1.81	0.45
19:E:41:ILE:O	19:E:84:VAL:HA	2.17	0.45
21:G:108:ARG:NH2	21:G:109:LEU:HD21	2.32	0.45
27:M:38:ILE:HG22	27:M:44:VAL:HG12	1.99	0.45
35:1:3146:G:H2'	35:1:3147:G:C8	2.52	0.45
4:4:25:LEU:HD12	4:4:25:LEU:O	2.17	0.45
4:4:50:TYR:HE2	4:4:109:GLU:CG	2.28	0.45
16:B:343:TYR:CE1	16:B:345:ASN:HB2	2.52	0.45
17:C:303:GLY:H	35:1:1347:U:H5''	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:78:PHE:C	21:G:80:TYR:H	2.25	0.45
35:1:1229:G:H1	35:1:1280:C:H42	1.64	0.45
35:1:3181:C:H2'	35:1:3182:G:C8	2.52	0.45
43:t:276:GLU:O	43:t:278:SER:N	2.49	0.45
1:x:235:GLN:NE2	3:3:155:ALA:HB3	2.32	0.45
3:3:143:ARG:HD3	3:3:143:ARG:HA	1.65	0.45
4:4:114:ASP:OD1	4:4:117:ARG:HD2	2.17	0.45
4:4:115:ARG:HG3	17:C:288:ARG:HG3	1.99	0.45
4:4:225:VAL:HG21	4:4:243:PHE:CZ	2.51	0.45
5:5:4:LEU:HG	5:5:410:LEU:HD11	1.98	0.45
14:y:101:LEU:HB3	33:V:135:VAL:HG22	1.99	0.45
17:C:26:PHE:HE2	17:C:255:PHE:CE1	2.35	0.45
17:C:207:VAL:O	17:C:227:THR:HA	2.17	0.45
18:e:44:ARG:HD2	35:1:1144:U:H5'	1.98	0.45
18:e:91:THR:HB	18:e:92:TYR:CD1	2.52	0.45
26:L:73:ARG:NH1	35:1:110:G:OP2	2.50	0.45
35:1:483:G:C6	35:1:484:C:C4	3.05	0.45
36:2:28:C:H2'	36:2:29:U:C6	2.52	0.45
5:5:131:VAL:HG12	5:5:132:LYS:N	2.32	0.44
35:1:665:A:H2'	35:1:666:A:C8	2.52	0.44
1:x:249:LYS:C	1:x:251:ASN:H	2.25	0.44
3:3:97:LEU:HA	3:3:100:TRP:CZ3	2.51	0.44
12:v:31:GLN:HG2	26:L:44:ALA:O	2.18	0.44
20:f:92:LYS:HD2	35:1:3173:G:O6	2.16	0.44
21:G:231:LYS:CG	39:m:242:PRO:HB3	2.47	0.44
26:L:46:ILE:HG22	26:L:46:ILE:O	2.17	0.44
26:L:55:ARG:HD3	26:L:73:ARG:O	2.18	0.44
29:O:93:ALA:CB	35:1:631:U:H5''	2.47	0.44
35:1:340:C:N4	35:1:341:G:O6	2.50	0.44
35:1:436:A:H61	35:1:623:U:H3	1.64	0.44
23:H:27:VAL:HG11	23:H:79:ILE:HA	1.99	0.44
23:H:114:VAL:HB	23:H:124:ARG:HB2	1.98	0.44
32:S:77:VAL:HG22	32:S:126:VAL:HG13	1.97	0.44
4:4:150:ILE:HG12	4:4:220:ILE:HD11	1.99	0.44
5:5:181:LEU:HB3	5:5:226:LEU:HD23	1.98	0.44
16:B:365:PHE:HZ	35:1:3375:A:N7	2.16	0.44
17:C:222:VAL:HG22	17:C:225:VAL:CG2	2.47	0.44
20:f:48:ARG:HH12	20:f:68:TRP:HB3	1.81	0.44
35:1:688:G:O5'	35:1:688:G:H8	2.00	0.44
36:2:45:C:H2'	36:2:46:G:O4'	2.17	0.44
3:3:111:ARG:HH11	18:e:87:MET:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:339:LYS:O	5:5:340:LYS:HB3	2.17	0.44
7:b:436:LEU:HD11	11:u:90:LEU:HD23	1.99	0.44
18:e:25:TYR:HB3	18:e:27:ARG:HD3	1.98	0.44
25:j:18:LEU:HD23	25:j:25:ARG:HG3	1.98	0.44
34:Y:54:ASP:OD1	34:Y:54:ASP:N	2.51	0.44
35:1:977:C:H3'	35:1:978:G:C5'	2.46	0.44
35:1:1220:U:H5''	35:1:1221:A:H5'	2.00	0.44
35:1:1301:A:N6	35:1:2827:U:O2'	2.51	0.44
36:2:15:G:C6	36:2:16:G:N1	2.86	0.44
1:x:14:LYS:HB2	35:1:351:A:N7	2.33	0.44
4:4:60:ARG:N	4:4:61:PRO:HD3	2.33	0.44
20:f:8:TYR:HB2	20:f:100:ILE:O	2.18	0.44
21:G:221:ASN:HD21	41:o:154:ASN:CB	2.30	0.44
25:j:22:CYS:O	36:2:43:A:H4'	2.18	0.44
32:S:10:ILE:HG13	32:S:59:VAL:HB	1.99	0.44
2:F:178:ILE:HD11	2:F:187:GLU:HG3	1.99	0.44
7:b:441:VAL:HG22	11:u:93:MET:HE1	1.98	0.44
12:v:162:LEU:HA	12:v:165:LEU:HD12	2.00	0.44
20:f:38:PRO:HD3	20:f:77:ASN:O	2.17	0.44
21:G:158:ASP:CB	21:G:159:PRO:HD3	2.45	0.44
23:H:86:TYR:CE2	23:H:151:VAL:HG22	2.53	0.44
24:i:29:LYS:HB2	35:1:266:A:N6	2.29	0.44
25:j:67:LEU:HD22	25:j:67:LEU:HA	1.72	0.44
33:V:80:ARG:HD3	33:V:117:PRO:HD2	2.00	0.44
35:1:109:A:H4'	35:1:110:G:OP1	2.17	0.44
35:1:638:C:H42	35:1:651:G:H1	1.63	0.44
35:1:1132:C:H2'	35:1:1133:A:C8	2.51	0.44
40:D:433:ILE:HG23	40:D:434:LYS:HG3	1.99	0.44
6:A:33:THR:HA	6:A:85:ASN:HB2	2.00	0.44
22:h:66:VAL:HA	22:h:69:LEU:HD23	2.00	0.44
26:L:120:GLN:HA	26:L:123:ILE:HG12	1.99	0.44
31:Q:80:THR:HG22	31:Q:100:THR:HB	1.98	0.44
31:Q:96:PHE:HA	31:Q:97:PRO:HD3	1.86	0.44
35:1:201:A:H2'	35:1:202:G:H8	1.83	0.44
35:1:743:C:H2'	35:1:744:A:H8	1.82	0.44
35:1:2917:G:H22	35:1:2929:C:H5	1.65	0.44
35:1:3123:A:C2	35:1:3124:G:H1'	2.52	0.44
37:6:4:U:H3'	37:6:5:C:H5'	1.99	0.44
42:n:186:VAL:HG21	42:n:375:ILE:HG12	1.99	0.44
43:t:213:ARG:HH11	43:t:228:VAL:HG22	1.82	0.44
1:x:59:THR:HG22	35:1:391:A:H4'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:254:LEU:HD22	5:5:323:PHE:HD2	1.82	0.44
5:5:267:ASN:HA	5:5:285:GLN:HG2	2.00	0.44
14:y:18:LYS:HB2	14:y:60:GLY:HA2	1.99	0.44
17:C:6:VAL:N	17:C:20:LEU:O	2.49	0.44
21:G:134:TYR:CB	21:G:190:VAL:HG21	2.48	0.44
22:h:117:ALA:HB3	26:L:124:ILE:HD11	1.99	0.44
30:P:56:ARG:HD3	30:P:75:GLU:OE1	2.18	0.44
35:1:1368:U:H2'	35:1:1369:A:H8	1.82	0.44
35:1:3016:A:H2'	35:1:3017:A:H8	1.83	0.44
38:K:83:VAL:HG21	38:K:270:LEU:HD13	1.99	0.44
40:D:268:TYR:HA	40:D:392:MET:H	1.83	0.44
2:F:84:VAL:HG21	2:F:127:LEU:HD11	2.00	0.43
5:5:281:LYS:HE3	5:5:292:ALA:HB3	1.99	0.43
16:B:171:LEU:HD21	16:B:333:LYS:HG2	2.00	0.43
16:B:216:ASP:HB2	16:B:277:SER:O	2.18	0.43
17:C:20:LEU:HA	17:C:21:PRO:HD2	1.74	0.43
17:C:183:LYS:HE3	35:1:1386:A:N7	2.33	0.43
19:E:40:LEU:HB3	19:E:84:VAL:HG13	2.00	0.43
32:S:90:MET:HG2	32:S:91:TYR:H	1.80	0.43
35:1:3:U:O2	37:6:232:A:N7	2.47	0.43
35:1:101:G:H2'	35:1:102:C:O4'	2.17	0.43
41:o:97:ARG:HD2	41:o:161:LEU:O	2.17	0.43
42:n:365:PHE:CD1	42:n:409:HIS:HB2	2.53	0.43
3:3:15:CYS:SG	3:3:17:HIS:NE2	2.89	0.43
3:3:65:LYS:HB2	3:3:77:TRP:NE1	2.33	0.43
3:3:97:LEU:O	3:3:98:LEU:C	2.61	0.43
17:C:40:THR:HG22	35:1:1426:C:H4'	2.00	0.43
21:G:220:ALA:HB1	41:o:154:ASN:ND2	2.33	0.43
23:H:6:THR:O	23:H:56:ALA:HA	2.18	0.43
35:1:26:A:C6	35:1:27:C:C4	3.06	0.43
35:1:157:A:H2'	35:1:158:G:O4'	2.18	0.43
35:1:533:A:C2	35:1:560:G:N2	2.86	0.43
35:1:3128:G:O5'	35:1:3128:G:H8	2.02	0.43
4:4:28:TYR:CZ	4:4:35:LYS:HG2	2.53	0.43
7:b:160:LEU:HA	7:b:161:PRO:HD2	1.88	0.43
21:G:85:ASN:CG	41:o:155:TYR:CZ	2.97	0.43
23:H:23:ARG:NH2	35:1:3187:A:OP1	2.51	0.43
30:P:148:LEU:HD12	30:P:148:LEU:C	2.43	0.43
33:V:126:TRP:HA	33:V:127:PRO:HD3	1.83	0.43
35:1:19:U:H2'	35:1:20:A:C8	2.52	0.43
35:1:677:A:C8	35:1:786:A:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:757:C:H42	35:1:774:G:H1	1.65	0.43
35:1:1407:A:C8	35:1:1408:G:H1'	2.53	0.43
3:3:116:THR:C	3:3:118:VAL:H	2.26	0.43
3:3:158:ILE:H	3:3:158:ILE:HG13	1.29	0.43
16:B:173:GLN:O	16:B:175:LYS:N	2.50	0.43
27:M:77:ARG:HB3	35:1:525:C:OP1	2.19	0.43
28:N:183:THR:HB	35:1:49:A:H61	1.84	0.43
35:1:808:A:N1	35:1:932:U:O4	2.52	0.43
37:6:54:A:OP2	41:o:97:ARG:HG3	2.18	0.43
43:t:58:ALA:O	43:t:62:VAL:HG23	2.18	0.43
43:t:261:PHE:O	43:t:265:ASN:HB2	2.18	0.43
1:x:278:THR:O	5:5:380:LEU:HD12	2.17	0.43
12:v:208:TYR:O	12:v:210:GLN:N	2.51	0.43
16:B:370:PHE:HB3	16:B:375:GLU:HB3	2.01	0.43
18:e:27:ARG:HG2	18:e:28:VAL:N	2.32	0.43
26:L:27:ASP:O	26:L:28:GLN:C	2.61	0.43
30:P:82:ARG:HG2	30:P:83:TRP:N	2.34	0.43
35:1:584:G:H2'	35:1:585:A:C8	2.53	0.43
35:1:3044:G:H2'	35:1:3045:G:C8	2.53	0.43
42:n:256:ILE:HG23	42:n:258:GLY:H	1.83	0.43
2:F:88:ARG:HH21	2:F:103:LEU:HD13	1.83	0.43
2:F:185:ILE:O	2:F:189:ILE:HG22	2.17	0.43
3:3:8:GLN:C	3:3:8:GLN:CD	2.86	0.43
3:3:12:GLN:O	3:3:13:SER:CB	2.66	0.43
16:B:348:ARG:HG3	35:1:3037:U:H5'	2.00	0.43
23:H:5:GLN:HG2	23:H:58:HIS:HD2	1.84	0.43
35:1:675:C:O2'	35:1:679:U:OP1	2.33	0.43
35:1:1379:G:C6	35:1:1428:A:C2	3.06	0.43
35:1:1390:A:H4'	35:1:1391:C:H5''	2.00	0.43
35:1:2986:U:H4'	35:1:2987:A:OP1	2.17	0.43
35:1:3234:A:H61	35:1:3253:G:H1	1.67	0.43
36:2:67:U:H2'	36:2:68:G:C8	2.54	0.43
7:b:449:ILE:HD11	11:u:89:THR:HG22	2.01	0.43
10:s:13:THR:HG21	35:1:1152:G:N7	2.33	0.43
13:W:70:ARG:HE	13:W:97:SER:HA	1.83	0.43
14:y:7:PHE:HB2	14:y:34:PHE:CD1	2.54	0.43
16:B:188:ILE:H	16:B:188:ILE:HG13	1.59	0.43
21:G:147:LYS:HZ1	39:m:265:ARG:HH11	1.66	0.43
34:Y:126:LEU:H	34:Y:126:LEU:HG	1.56	0.43
35:1:187:A:C5	35:1:211:A:C2	3.07	0.43
35:1:303:G:N2	35:1:313:A:C4	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:655:C:H2'	35:1:656:A:C8	2.54	0.43
2:F:84:VAL:HG22	2:F:119:VAL:HG22	2.01	0.43
3:3:35:THR:C	3:3:37:LEU:H	2.27	0.43
17:C:29:PRO:HD2	17:C:277:PRO:HG2	2.01	0.43
21:G:78:PHE:HA	21:G:179:ILE:HD13	2.01	0.43
35:1:618:C:H1'	35:1:621:A:H8	1.83	0.43
35:1:1326:A:H2'	35:1:1327:C:O4'	2.18	0.43
36:2:59:A:H5''	36:2:61:A:C8	2.53	0.43
1:x:65:VAL:HG22	1:x:292:LYS:H	1.84	0.43
1:x:171:PHE:N	1:x:171:PHE:CD1	2.86	0.43
2:F:120:THR:O	2:F:124:LEU:HB2	2.19	0.43
2:F:222:HIS:ND1	2:F:224:ILE:HG12	2.34	0.43
3:3:29:ARG:HH11	3:3:29:ARG:CG	2.32	0.43
17:C:304:GLN:HE22	35:1:594:U:H3	1.66	0.43
35:1:976:U:C5	35:1:1105:A:N1	2.87	0.43
41:o:88:GLU:HB2	41:o:169:LYS:HE3	2.01	0.43
1:x:18:ILE:C	1:x:20:ALA:H	2.27	0.43
1:x:128:PHE:CE2	35:1:441:U:H2'	2.54	0.43
4:4:95:PHE:CD2	4:4:95:PHE:C	2.97	0.43
16:B:123:TYR:HE2	35:1:3389:U:H3	1.66	0.43
17:C:222:VAL:HG22	17:C:225:VAL:HG21	2.01	0.43
19:E:170:LYS:HD3	20:f:34:GLY:HA3	2.00	0.43
35:1:252:U:OP1	39:m:277:MET:CG	2.63	0.43
35:1:372:A:H2'	35:1:373:A:C8	2.53	0.43
35:1:427:C:N4	35:1:428:A:N6	2.67	0.43
35:1:1295:G:H2'	35:1:1296:C:C6	2.54	0.43
41:o:203:LYS:O	41:o:207:ARG:HB2	2.19	0.43
4:4:212:THR:OG1	4:4:213:PRO:CD	2.63	0.42
17:C:107:ARG:O	17:C:109:TRP:CD1	2.72	0.42
17:C:195:ARG:NH2	35:1:340:C:C5	2.87	0.42
18:e:64:LYS:HD3	18:e:65:PHE:CE2	2.54	0.42
28:N:58:GLY:HA3	28:N:142:ILE:HD11	2.00	0.42
30:P:69:ARG:HH21	35:1:2992:U:H1'	1.84	0.42
35:1:325:A:H5''	35:1:326:U:OP2	2.19	0.42
37:6:23:U:H1'	38:K:191:PRO:HG3	2.00	0.42
39:m:291:PRO:HA	39:m:294:LEU:HD12	2.00	0.42
1:x:131:LYS:HA	1:x:131:LYS:HD3	1.78	0.42
2:F:37:ASN:HA	2:F:40:LYS:HB3	2.01	0.42
4:4:137:GLN:HG3	4:4:139:ARG:HG2	2.01	0.42
7:b:157:ILE:HA	7:b:160:LEU:HD12	2.00	0.42
17:C:322:GLN:HB3	35:1:608:A:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:157:VAL:HG13	35:1:147:U:C4	2.54	0.42
26:L:46:ILE:CG2	26:L:49:ARG:HB2	2.49	0.42
35:1:432:G:H2'	35:1:433:A:C8	2.53	0.42
35:1:1361:U:H2'	35:1:1362:G:C8	2.54	0.42
1:x:254:VAL:HG13	3:3:163:GLU:HG2	2.00	0.42
1:x:274:ILE:H	1:x:274:ILE:HG13	1.56	0.42
5:5:370:HIS:C	5:5:372:GLY:H	2.27	0.42
16:B:90:VAL:CG1	16:B:104:THR:HG22	2.47	0.42
19:E:80:ASN:HB3	19:E:83:TYR:HD2	1.83	0.42
21:G:108:ARG:HH21	21:G:109:LEU:HD21	1.84	0.42
26:L:93:ILE:HG22	26:L:93:ILE:O	2.17	0.42
27:M:44:VAL:HG13	27:M:60:LEU:HD11	2.00	0.42
32:S:155:ARG:N	32:S:170:THR:OG1	2.52	0.42
34:Y:27:ARG:NH1	34:Y:76:LEU:HA	2.34	0.42
40:D:472:LYS:HB2	40:D:477:TYR:HB2	2.00	0.42
43:t:223:GLU:N	43:t:224:PRO:HD3	2.34	0.42
1:x:12:LYS:HE2	35:1:369:A:OP2	2.20	0.42
3:3:26:ASN:HB2	35:1:1354:G:N7	2.35	0.42
4:4:61:PRO:O	4:4:65:LEU:N	2.40	0.42
6:A:138:SER:O	6:A:179:PHE:HB2	2.19	0.42
7:b:104:LEU:O	7:b:108:VAL:HG23	2.19	0.42
17:C:114:ASN:HD22	35:1:680:G:H5''	1.84	0.42
34:Y:3:LYS:HD2	34:Y:8:VAL:O	2.19	0.42
34:Y:50:ILE:HD11	34:Y:70:ILE:HG12	2.00	0.42
43:t:64:LYS:HE2	43:t:154:ASN:HD21	1.85	0.42
1:x:18:ILE:HG22	1:x:19:PHE:N	2.35	0.42
3:3:17:HIS:HE1	3:3:28:CYS:SG	2.42	0.42
5:5:248:PRO:HA	5:5:274:THR:HA	2.01	0.42
5:5:317:VAL:HG12	5:5:323:PHE:HA	2.01	0.42
7:b:164:ASP:HA	7:b:165:PRO:HD3	1.90	0.42
13:W:53:LEU:HA	13:W:56:ILE:HD12	2.00	0.42
17:C:47:ARG:HG2	35:1:338:A:OP1	2.20	0.42
18:e:11:LYS:HD2	18:e:11:LYS:HA	1.48	0.42
31:Q:62:VAL:O	31:Q:87:VAL:HA	2.19	0.42
35:1:210:U:H2'	35:1:210:U:OP1	2.19	0.42
35:1:293:C:H2'	35:1:294:U:O4'	2.19	0.42
35:1:625:G:H2'	35:1:626:U:H6	1.83	0.42
35:1:3326:G:H1	35:1:3380:U:H3	1.67	0.42
41:o:108:SER:O	41:o:112:ALA:HB2	2.19	0.42
1:x:240:PHE:CD1	1:x:264:THR:HG22	2.55	0.42
4:4:13:ASN:HB2	17:C:7:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:35:LYS:HB2	4:4:35:LYS:HE2	1.72	0.42
5:5:142:THR:HG22	5:5:158:ALA:HB3	2.00	0.42
5:5:193:TYR:OH	5:5:256:PRO:HG3	2.18	0.42
12:v:192:HIS:HB2	12:v:199:MET:HE2	2.01	0.42
17:C:154:THR:OG1	17:C:252:GLU:HB3	2.19	0.42
23:H:21:LYS:HB2	35:1:3198:U:H1'	2.01	0.42
29:O:87:MET:HB3	35:1:1175:C:O2	2.19	0.42
35:1:660:A:C2	35:1:1435:A:C2	3.08	0.42
35:1:3064:U:H2'	35:1:3065:G:H8	1.84	0.42
2:F:136:TYR:O	2:F:231:ASN:HA	2.19	0.42
10:s:10:ARG:HG2	35:1:1310:G:H5''	2.01	0.42
17:C:11:LEU:HD13	17:C:159:ILE:HD11	2.02	0.42
21:G:105:LYS:HE3	39:m:275:ARG:HH12	1.59	0.42
28:N:120:TRP:HA	28:N:130:PHE:CD1	2.54	0.42
35:1:497:C:H2'	35:1:498:A:O4'	2.20	0.42
35:1:561:C:H2'	35:1:562:C:C6	2.55	0.42
42:n:64:TYR:CE2	42:n:66:LYS:HB3	2.55	0.42
1:x:241:PHE:HD2	1:x:263:PHE:CG	2.38	0.42
7:b:382:VAL:HG11	14:y:202:TYR:CE1	2.55	0.42
17:C:326:ARG:NH1	35:1:608:A:O3'	2.52	0.42
21:G:191:ASN:HA	42:n:96:ARG:NH1	2.34	0.42
26:L:55:ARG:HB3	26:L:56:PRO:HD2	2.02	0.42
34:Y:95:VAL:HA	34:Y:96:PRO:HD3	1.91	0.42
35:1:242:C:O2'	35:1:243:G:H8	2.03	0.42
35:1:1256:G:H2'	35:1:1257:C:C6	2.55	0.42
38:K:86:LYS:HD2	38:K:301:LEU:HD13	2.02	0.42
41:o:99:PRO:HA	41:o:160:HIS:NE2	2.35	0.42
3:3:89:ALA:O	3:3:92:GLN:HB3	2.20	0.42
5:5:240:LEU:C	5:5:242:MET:H	2.28	0.42
5:5:369:VAL:HG12	5:5:372:GLY:HA2	2.02	0.42
11:u:82:ASN:HB3	11:u:85:LEU:HB2	2.02	0.42
12:v:209:GLN:O	39:m:263:LYS:HE3	2.20	0.42
14:y:153:SER:HB2	14:y:194:GLY:HA2	2.01	0.42
16:B:95:THR:HG22	35:1:3243:A:H4'	2.02	0.42
21:G:113:ALA:CB	39:m:279:ILE:HB	2.49	0.42
30:P:120:ASN:OD1	30:P:120:ASN:N	2.52	0.42
35:1:1257:C:H42	35:1:1261:G:H22	1.67	0.42
1:x:110:PHE:CE1	1:x:178:PHE:CE2	3.08	0.42
8:J:205:LEU:HA	8:J:209:GLN:HG3	2.02	0.42
13:W:70:ARG:NH1	13:W:71:LYS:HE3	2.35	0.42
17:C:74:ILE:HA	17:C:75:PRO:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:17:ALA:O	35:1:591:G:O2'	2.37	0.42
35:1:11:A:H1'	36:2:148:G:N2	2.35	0.42
35:1:172:G:H1	35:1:246:U:H3	1.68	0.42
35:1:1229:G:H2'	35:1:1230:G:C8	2.55	0.42
35:1:3182:G:H2'	35:1:3183:A:C8	2.55	0.42
35:1:3200:G:H2'	35:1:3201:C:C6	2.55	0.42
1:x:207:GLY:C	1:x:209:THR:H	2.27	0.41
2:F:214:TRP:CD2	2:F:219:LYS:HD3	2.55	0.41
14:y:38:PHE:HE1	14:y:205:VAL:HG21	1.85	0.41
16:B:139:GLN:HG3	16:B:141:GLY:H	1.84	0.41
16:B:284:ARG:HE	16:B:356:LEU:HD13	1.84	0.41
21:G:134:TYR:CG	21:G:190:VAL:HG21	2.55	0.41
24:i:36:ARG:O	24:i:40:VAL:HG23	2.20	0.41
26:L:50:PRO:O	26:L:52:ASP:N	2.40	0.41
34:Y:118:LEU:HD12	34:Y:121:ARG:HH12	1.85	0.41
35:1:657:A:H4'	36:2:18:U:OP1	2.20	0.41
35:1:947:G:H2'	35:1:948:C:C6	2.55	0.41
35:1:1439:U:C2	35:1:1440:G:C8	3.08	0.41
35:1:3139:A:H2'	35:1:3140:G:O4'	2.20	0.41
43:t:223:GLU:H	43:t:224:PRO:HD3	1.85	0.41
1:x:221:ASN:N	1:x:222:PRO:CD	2.82	0.41
4:4:140:ASN:OD1	4:4:140:ASN:N	2.44	0.41
17:C:217:LYS:HG2	17:C:220:ARG:NH2	2.35	0.41
19:E:66:SER:HB3	19:E:76:LEU:HD23	2.02	0.41
21:G:221:ASN:CG	41:o:154:ASN:CB	2.86	0.41
31:Q:36:LEU:HD23	31:Q:36:LEU:HA	1.70	0.41
33:V:81:GLN:H	33:V:95:PHE:HD2	1.68	0.41
35:1:744:A:C6	35:1:745:C:C2	3.08	0.41
42:n:64:TYR:HB3	42:n:67:ASP:HB2	2.01	0.41
2:F:90:LYS:HB2	2:F:220:PHE:HE1	1.84	0.41
2:F:138:TYR:HA	2:F:139:PRO:HD3	1.81	0.41
15:z:18:ARG:HD3	16:B:344:THR:HB	2.02	0.41
16:B:328:ILE:HG21	16:B:336:VAL:HG11	2.03	0.41
18:e:128:LEU:HD21	35:1:439:C:C5	2.56	0.41
27:M:20:VAL:CG1	27:M:68:LEU:HB2	2.50	0.41
35:1:340:C:H2'	35:1:341:G:C8	2.55	0.41
35:1:1151:U:H3'	35:1:1152:G:N2	2.35	0.41
35:1:1200:A:O2'	35:1:1201:C:O2	2.36	0.41
35:1:1338:C:H2'	35:1:1339:C:H6	1.85	0.41
35:1:1449:A:C2	35:1:2356:A:C4	3.09	0.41
35:1:3183:A:H2'	35:1:3184:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:60:ARG:H	4:4:61:PRO:HD3	1.84	0.41
4:4:73:HIS:CE1	4:4:132:GLN:HE21	2.39	0.41
4:4:155:ARG:HA	4:4:159:LEU:HD21	2.02	0.41
14:y:83:HIS:HA	14:y:86:ASN:HD22	1.86	0.41
17:C:188:ARG:HG3	17:C:190:GLY:H	1.85	0.41
20:f:53:TYR:N	20:f:53:TYR:CD1	2.88	0.41
20:f:71:VAL:HG13	20:f:81:VAL:HG13	2.02	0.41
21:G:144:GLU:HA	21:G:173:MET:HE2	2.02	0.41
31:Q:72:LYS:HB3	35:1:719:U:H1'	2.02	0.41
36:2:53:A:H2'	36:2:54:A:O4'	2.20	0.41
37:6:8:A:H2'	37:6:9:A:C8	2.56	0.41
38:K:125:LEU:HD13	38:K:151:VAL:HG13	2.02	0.41
4:4:50:TYR:CE1	4:4:121:TYR:CZ	3.09	0.41
4:4:58:ARG:HD2	35:1:465:U:C4'	2.47	0.41
7:b:392:ASP:HA	7:b:393:PRO:HD3	1.95	0.41
27:M:32:LEU:HD11	27:M:94:TRP:CD2	2.56	0.41
35:1:678:G:C5	35:1:703:G:C2	3.08	0.41
2:F:155:LYS:O	2:F:156:ILE:HG13	2.20	0.41
4:4:77:PHE:CD1	4:4:91:ASN:HA	2.55	0.41
5:5:382:ARG:HG2	5:5:403:ARG:HA	2.03	0.41
6:A:136:VAL:HB	6:A:176:VAL:HG12	2.02	0.41
17:C:296:GLN:HB2	35:1:1349:G:C2	2.54	0.41
21:G:147:LYS:HZ2	39:m:265:ARG:NH1	2.18	0.41
24:i:47:ILE:HA	24:i:47:ILE:HD13	1.74	0.41
28:N:178:HIS:HB2	28:N:179:LYS:HZ2	1.83	0.41
35:1:410:U:H2'	35:1:411:U:H6	1.86	0.41
35:1:1338:C:H2'	35:1:1339:C:C6	2.55	0.41
36:2:39:G:H4'	36:2:40:A:H5'	2.02	0.41
36:2:118:C:H2'	36:2:119:C:C6	2.56	0.41
4:4:58:ARG:HD2	35:1:465:U:C5'	2.50	0.41
4:4:67:ASN:O	4:4:71:GLU:HB2	2.21	0.41
5:5:133:ARG:HB3	5:5:136:LEU:HG	2.02	0.41
14:y:133:LEU:HB2	14:y:135:VAL:HG22	2.01	0.41
24:i:45:ARG:HB3	39:m:246:TRP:CZ2	2.56	0.41
25:j:55:ARG:HE	25:j:55:ARG:HB2	1.63	0.41
28:N:30:TYR:CD2	28:N:63:ARG:HD3	2.56	0.41
30:P:16:SER:HB2	30:P:149:VAL:HG22	2.03	0.41
35:1:31:C:H2'	35:1:32:U:H6	1.85	0.41
35:1:504:A:H2'	35:1:505:G:H8	1.85	0.41
35:1:590:G:C6	35:1:591:G:N1	2.89	0.41
35:1:676:G:N2	35:1:787:G:C5	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:697:A:H2'	35:1:698:U:O4'	2.21	0.41
35:1:785:G:N3	35:1:785:G:H2'	2.36	0.41
35:1:786:A:H4'	35:1:787:G:H5'	2.03	0.41
35:1:1407:A:N7	35:1:1408:G:H1'	2.36	0.41
35:1:2909:U:H2'	35:1:2910:A:O4'	2.20	0.41
1:x:97:LEU:HD13	1:x:148:VAL:HG13	2.02	0.41
3:3:73:PRO:HD2	17:C:147:GLU:HA	2.02	0.41
5:5:219:ILE:H	5:5:219:ILE:HG13	1.76	0.41
6:A:96:ASP:O	35:1:284:A:N1	2.54	0.41
16:B:45:SER:HB3	16:B:339:ARG:HA	2.03	0.41
23:H:16:VAL:HG21	23:H:79:ILE:HG23	2.02	0.41
24:i:51:SER:HB2	24:i:52:PRO:HD2	2.03	0.41
33:V:102:ILE:H	33:V:102:ILE:HG13	1.72	0.41
35:1:392:G:C2	35:1:393:U:C5	3.08	0.41
35:1:619:A:H5'	35:1:621:A:H1'	2.03	0.41
35:1:980:A:H1'	35:1:981:U:H5	1.85	0.41
35:1:1341:U:H2'	35:1:1342:C:H6	1.85	0.41
3:3:65:LYS:HD3	3:3:77:TRP:CE2	2.56	0.41
7:b:76:PRO:HB2	7:b:245:HIS:HD2	1.85	0.41
13:W:70:ARG:O	13:W:74:GLN:HG2	2.21	0.41
17:C:122:THR:HG22	17:C:238:LEU:HD12	2.03	0.41
18:e:26:HIS:HB3	35:1:655:C:H5''	2.03	0.41
18:e:119:VAL:HG12	18:e:121:ASN:H	1.84	0.41
20:f:16:TYR:CG	20:f:25:PRO:HA	2.56	0.41
23:H:128:VAL:HA	23:H:157:ASN:HD21	1.86	0.41
26:L:54:LEU:HD13	26:L:75:PHE:CE1	2.55	0.41
33:V:17:LEU:HG	33:V:98:ASN:HD22	1.85	0.41
35:1:107:A:O2'	35:1:324:A:N3	2.49	0.41
35:1:744:A:H2'	35:1:745:C:O4'	2.20	0.41
35:1:751:A:H2'	35:1:752:C:C6	2.56	0.41
35:1:3007:U:H2'	35:1:3008:A:C8	2.56	0.41
35:1:3110:C:H2'	35:1:3111:U:C6	2.56	0.41
36:2:28:C:H2'	36:2:29:U:H6	1.86	0.41
36:2:36:G:O2'	36:2:104:A:N1	2.46	0.41
36:2:143:U:H2'	36:2:144:G:O4'	2.21	0.41
1:x:267:LEU:HD21	1:x:270:LEU:HD23	2.03	0.41
3:3:27:PHE:HA	3:3:37:LEU:HA	2.02	0.41
4:4:50:TYR:HE1	4:4:121:TYR:CZ	2.39	0.41
18:e:100:ILE:N	18:e:100:ILE:HD13	2.34	0.41
26:L:104:ARG:HH11	35:1:74:G:H5''	1.85	0.41
35:1:386:A:O5'	35:1:386:A:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:393:U:H2'	35:1:394:G:C8	2.55	0.41
35:1:411:U:H2'	35:1:412:G:H8	1.85	0.41
37:6:36:U:H2'	37:6:37:C:C6	2.56	0.41
2:F:106:LEU:O	2:F:107:ARG:HB2	2.20	0.40
5:5:377:GLN:C	5:5:377:GLN:CD	2.88	0.40
7:b:12:ALA:HA	7:b:13:PRO:HD3	1.87	0.40
17:C:135:VAL:HG12	17:C:142:VAL:HG21	2.03	0.40
17:C:193:LYS:CE	36:2:21:C:OP1	2.68	0.40
17:C:334:PHE:CD2	35:1:578:A:H2'	2.56	0.40
27:M:21:VAL:HB	27:M:63:VAL:CG2	2.50	0.40
30:P:122:ALA:HB1	30:P:123:PRO:HD2	2.02	0.40
35:1:430:U:H2'	35:1:431:U:C6	2.55	0.40
36:2:103:G:C6	36:2:105:A:N6	2.89	0.40
36:2:147:U:P	42:n:88:ARG:CZ	3.09	0.40
2:F:11:SER:HB2	35:1:1349:G:H2'	2.03	0.40
2:F:67:ARG:HD3	35:1:520:U:C4	2.56	0.40
4:4:25:LEU:HD11	4:4:29:LEU:CD1	2.52	0.40
4:4:60:ARG:N	4:4:61:PRO:CD	2.84	0.40
14:y:61:ARG:HD2	14:y:195:ALA:HB2	2.02	0.40
16:B:79:VAL:HG22	16:B:81:THR:HG23	2.02	0.40
16:B:123:TYR:CD2	35:1:3389:U:O4	2.75	0.40
17:C:26:PHE:HE1	17:C:126:ILE:HG22	1.84	0.40
21:G:130:TYR:CE1	21:G:202:GLU:HB3	2.56	0.40
22:h:51:ILE:HG22	22:h:55:LEU:HD12	2.03	0.40
31:Q:62:VAL:HB	31:Q:83:VAL:HG11	2.01	0.40
2:F:218:ARG:HA	35:1:1170:A:OP1	2.22	0.40
3:3:6:VAL:O	3:3:9:VAL:HG12	2.21	0.40
13:W:6:ARG:NH1	35:1:3117:C:N3	2.68	0.40
16:B:119:TYR:CE1	35:1:3295:A:H5''	2.56	0.40
19:E:38:THR:H	19:E:54:TYR:HB3	1.87	0.40
20:f:24:ASN:HA	20:f:25:PRO:HD3	1.88	0.40
21:G:70:LYS:HE3	39:m:240:TYR:CG	2.56	0.40
21:G:73:PRO:HG2	39:m:243:LEU:H	1.86	0.40
21:G:134:TYR:HB3	21:G:190:VAL:HG21	2.02	0.40
21:G:206:GLU:CB	38:K:163:VAL:HA	2.50	0.40
25:j:27:PHE:HA	25:j:34:CYS:HA	2.03	0.40
26:L:105:ASN:HD22	26:L:108:ILE:HG12	1.86	0.40
35:1:382:U:H3	35:1:387:A:N6	2.15	0.40
36:2:127:U:O4'	39:m:323:HIS:HD2	1.92	0.40
40:D:300:ASN:HA	40:D:303:LYS:HE3	2.04	0.40
42:n:30:ALA:O	42:n:34:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v:55:LEU:H	12:v:55:LEU:HG	1.45	0.40
16:B:159:ARG:HG2	16:B:182:GLN:CB	2.52	0.40
18:e:21:HIS:C	18:e:23:ASP:H	2.28	0.40
18:e:128:LEU:HD11	35:1:439:C:C4	2.55	0.40
20:f:47:LYS:HA	20:f:104:PRO:HD2	2.01	0.40
21:G:145:ASN:HA	39:m:255:PRO:HB3	2.02	0.40
35:1:358:G:N2	35:1:361:A:OP2	2.47	0.40
35:1:655:C:H2'	35:1:656:A:H8	1.87	0.40
35:1:1226:G:H1	35:1:1283:C:H42	1.68	0.40
36:2:127:U:C3'	42:n:64:TYR:HE1	2.20	0.40
4:4:114:ASP:HA	17:C:288:ARG:CD	2.52	0.40
4:4:154:LEU:HD12	4:4:220:ILE:CD1	2.51	0.40
17:C:195:ARG:NH2	35:1:340:C:C6	2.90	0.40
17:C:283:THR:C	17:C:285:ASP:H	2.28	0.40
21:G:128:LYS:HA	21:G:129:PRO:HD3	1.78	0.40
21:G:146:LYS:HB3	40:D:479:PHE:HB3	2.02	0.40
22:h:53:CYS:O	22:h:57:VAL:HG23	2.22	0.40
22:h:77:PRO:HD2	22:h:80:LEU:HD12	2.04	0.40
25:j:72:ARG:NH1	36:2:94:C:H3'	2.34	0.40
35:1:288:C:H2'	35:1:289:A:C8	2.56	0.40
41:o:120:VAL:HG23	41:o:137:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	259/295 (88%)	203 (78%)	44 (17%)	12 (5%)	2	17
2	F	239/244 (98%)	212 (89%)	23 (10%)	4 (2%)	7	35
3	3	171/306 (56%)	122 (71%)	38 (22%)	11 (6%)	1	12
4	4	209/278 (75%)	173 (83%)	26 (12%)	10 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	377/463 (81%)	338 (90%)	33 (9%)	6 (2%)	7	36
6	A	139/291 (48%)	122 (88%)	12 (9%)	5 (4%)	2	22
7	b	413/647 (64%)	381 (92%)	27 (6%)	5 (1%)	10	41
8	J	64/427 (15%)	58 (91%)	4 (6%)	2 (3%)	3	25
9	r	71/261 (27%)	65 (92%)	4 (6%)	2 (3%)	4	26
10	s	25/520 (5%)	25 (100%)	0	0	100	100
11	u	114/199 (57%)	109 (96%)	4 (4%)	1 (1%)	14	46
12	v	124/231 (54%)	115 (93%)	9 (7%)	0	100	100
13	W	230/236 (98%)	213 (93%)	15 (6%)	2 (1%)	14	46
14	y	223/245 (91%)	210 (94%)	13 (6%)	0	100	100
15	z	53/106 (50%)	49 (92%)	4 (8%)	0	100	100
16	B	329/387 (85%)	289 (88%)	30 (9%)	10 (3%)	3	25
17	C	341/362 (94%)	295 (86%)	30 (9%)	16 (5%)	2	17
18	e	123/130 (95%)	113 (92%)	9 (7%)	1 (1%)	16	49
19	E	147/176 (84%)	131 (89%)	16 (11%)	0	100	100
20	f	104/107 (97%)	98 (94%)	4 (4%)	2 (2%)	6	33
21	G	155/256 (60%)	134 (86%)	17 (11%)	4 (3%)	4	27
22	h	117/120 (98%)	104 (89%)	8 (7%)	5 (4%)	2	18
23	H	188/191 (98%)	167 (89%)	20 (11%)	1 (0%)	24	57
24	i	72/100 (72%)	66 (92%)	4 (6%)	2 (3%)	4	26
25	j	69/88 (78%)	62 (90%)	5 (7%)	2 (3%)	3	26
26	L	106/199 (53%)	97 (92%)	7 (7%)	2 (2%)	6	33
27	M	132/138 (96%)	121 (92%)	9 (7%)	2 (2%)	8	37
28	N	173/204 (85%)	150 (87%)	22 (13%)	1 (1%)	21	54
29	O	195/199 (98%)	66 (34%)	44 (23%)	85 (44%)	0	0
30	P	133/184 (72%)	118 (89%)	13 (10%)	2 (2%)	8	37
31	Q	129/186 (69%)	117 (91%)	12 (9%)	0	100	100
32	S	168/172 (98%)	143 (85%)	18 (11%)	7 (4%)	2	19
33	V	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
34	Y	123/127 (97%)	110 (89%)	11 (9%)	2 (2%)	7	36
38	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	m	159/807 (20%)	144 (91%)	14 (9%)	1 (1%)	21	54
40	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
41	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	16	49
42	n	326/605 (54%)	302 (93%)	22 (7%)	2 (1%)	21	54
43	t	240/322 (74%)	214 (89%)	20 (8%)	6 (2%)	4	28
All	All	6936/11047 (63%)	6068 (88%)	652 (9%)	216 (3%)	5	25

All (216) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	x	119	PRO
1	x	128	PHE
1	x	222	PRO
2	F	160	ARG
2	F	164	SER
3	3	13	SER
3	3	31	GLU
3	3	133	HIS
4	4	137	GLN
4	4	212	THR
5	5	340	LYS
6	A	43	TYR
7	b	198	ALA
16	B	34	LYS
17	C	339	LEU
25	j	68	LYS
27	M	29	ALA
29	O	9	ILE
29	O	16	VAL
29	O	17	GLY
29	O	18	ARG
29	O	20	ALA
29	O	21	SER
29	O	43	ILE
29	O	46	GLU
29	O	48	PHE
29	O	53	LYS
29	O	60	LYS
29	O	64	PHE
29	O	76	PRO

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Mol	Chain	Res	Type
29	O	77	SER
29	O	81	TYR
29	O	82	LYS
29	O	83	ALA
29	O	85	ARG
29	O	93	ALA
29	O	99	LEU
29	O	118	VAL
29	O	121	PRO
29	O	122	GLN
29	O	126	VAL
29	O	127	LEU
29	O	138	LEU
29	O	139	GLY
29	O	142	SER
29	O	143	THR
29	O	144	SER
29	O	149	TYR
29	O	150	GLU
29	O	153	VAL
29	O	154	ALA
29	O	156	LEU
29	O	158	ALA
29	O	162	VAL
29	O	163	SER
29	O	168	TYR
29	O	169	ALA
29	O	170	LYS
29	O	175	THR
29	O	176	LYS
29	O	179	ALA
29	O	189	ASP
29	O	190	VAL
29	O	191	ALA
29	O	192	LYS
41	o	190	THR
43	t	227	ILE
43	t	269	GLN
2	F	157	ASN
2	F	159	GLN
3	3	86	TYR
6	A	63	PRO

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Mol	Chain	Res	Type
9	r	3	GLN
16	B	142	ALA
16	B	155	ALA
16	B	174	LYS
16	B	187	SER
17	C	90	PHE
17	C	140	HIS
17	C	141	ARG
17	C	268	ALA
18	e	86	THR
22	h	86	ARG
24	i	31	GLY
26	L	50	PRO
29	O	8	VAL
29	O	10	ASP
29	O	12	LYS
29	O	63	ALA
29	O	88	VAL
29	O	89	SER
29	O	91	LYS
29	O	125	ARG
29	O	152	VAL
29	O	155	LYS
29	O	167	TYR
29	O	178	VAL
29	O	185	ALA
29	O	187	GLU
29	O	193	GLN
30	P	156	ALA
34	Y	52	ARG
39	m	328	LYS
43	t	277	VAL
1	x	132	LEU
1	x	155	LYS
1	x	281	GLU
1	x	290	LYS
4	4	82	ASN
4	4	157	LEU
5	5	305	GLN
6	A	94	HIS
6	A	105	PRO
7	b	14	ALA

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Mol	Chain	Res	Type
7	b	432	MET
13	W	4	SER
16	B	279	ASN
17	C	3	ARG
17	C	174	ALA
17	C	311	HIS
17	C	320	ASN
21	G	79	GLN
21	G	232	HIS
22	h	42	PRO
22	h	91	ALA
24	i	34	SER
25	j	55	ARG
29	O	19	LEU
29	O	25	LYS
29	O	34	VAL
29	O	61	ALA
29	O	90	HIS
29	O	116	LYS
29	O	123	ALA
29	O	165	ALA
29	O	174	PHE
29	O	194	LEU
32	S	13	ARG
32	S	14	LEU
32	S	22	PRO
1	x	167	GLU
3	3	3	ASP
3	3	16	SER
3	3	17	HIS
3	3	42	SER
3	3	157	LYS
4	4	61	PRO
4	4	87	GLU
4	4	213	PRO
5	5	129	LYS
5	5	211	GLU
8	J	235	ASP
9	r	41	LYS
11	u	81	TYR
16	B	139	GLN
16	B	300	ARG

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Mol	Chain	Res	Type
16	B	333	LYS
17	C	4	PRO
17	C	232	SER
20	f	86	ARG
23	H	110	LYS
29	O	59	ARG
29	O	70	PRO
29	O	128	ARG
32	S	24	LEU
32	S	115	ARG
38	K	284	ASN
43	t	240	GLY
43	t	270	PRO
1	x	201	ASN
1	x	292	LYS
3	3	128	ARG
4	4	77	PHE
7	b	74	VAL
17	C	233	LEU
17	C	269	SER
17	C	317	PRO
17	C	328	ASN
21	G	137	ASN
22	h	85	THR
29	O	37	ARG
29	O	159	LYS
29	O	160	ARG
30	P	84	PRO
38	K	256	PRO
42	n	196	GLU
42	n	456	HIS
43	t	151	LEU
1	x	270	LEU
3	3	73	PRO
5	5	116	ASP
7	b	434	GLU
8	J	227	THR
16	B	108	GLU
22	h	84	LYS
26	L	56	PRO
29	O	50	ASN
29	O	56	ASP

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Mol	Chain	Res	Type
29	O	95	GLY
32	S	167	ARG
17	C	181	VAL
20	f	80	VAL
29	O	145	VAL
4	4	60	ARG
6	A	104	PRO
27	M	39	ILE
29	O	132	GLY
34	Y	59	VAL
1	x	101	VAL
5	5	131	VAL
32	S	21	GLU
13	W	101	GLY
29	O	30	GLY
4	4	153	VAL
21	G	159	PRO
28	N	186	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	252/276 (91%)	202 (80%)	50 (20%)	1	8
2	F	204/205 (100%)	189 (93%)	15 (7%)	13	39
3	3	155/274 (57%)	129 (83%)	26 (17%)	2	13
4	4	203/257 (79%)	172 (85%)	31 (15%)	3	16
5	5	343/410 (84%)	319 (93%)	24 (7%)	14	41
6	A	137/263 (52%)	131 (96%)	6 (4%)	25	52
7	b	377/573 (66%)	347 (92%)	30 (8%)	11	37
8	J	61/383 (16%)	60 (98%)	1 (2%)	55	69
9	r	65/229 (28%)	60 (92%)	5 (8%)	12	38
10	s	24/445 (5%)	22 (92%)	2 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	u	101/180 (56%)	97 (96%)	4 (4%)	28	54
12	v	116/205 (57%)	106 (91%)	10 (9%)	10	34
13	W	209/213 (98%)	200 (96%)	9 (4%)	26	52
14	y	193/211 (92%)	182 (94%)	11 (6%)	18	46
15	z	48/95 (50%)	48 (100%)	0	100	100
16	B	280/323 (87%)	255 (91%)	25 (9%)	9	33
17	C	273/289 (94%)	230 (84%)	43 (16%)	2	15
18	e	108/111 (97%)	91 (84%)	17 (16%)	2	15
19	E	131/153 (86%)	120 (92%)	11 (8%)	10	35
20	f	90/91 (99%)	76 (84%)	14 (16%)	2	16
21	G	128/208 (62%)	111 (87%)	17 (13%)	4	21
22	h	104/105 (99%)	96 (92%)	8 (8%)	12	38
23	H	170/171 (99%)	151 (89%)	19 (11%)	6	27
24	i	61/81 (75%)	52 (85%)	9 (15%)	3	17
25	j	59/71 (83%)	50 (85%)	9 (15%)	3	16
26	L	87/159 (55%)	77 (88%)	10 (12%)	5	25
27	M	106/109 (97%)	99 (93%)	7 (7%)	15	43
28	N	153/176 (87%)	128 (84%)	25 (16%)	2	15
29	O	160/162 (99%)	115 (72%)	45 (28%)	0	3
30	P	109/146 (75%)	94 (86%)	15 (14%)	3	20
31	Q	107/151 (71%)	95 (89%)	12 (11%)	6	27
32	S	155/156 (99%)	142 (92%)	13 (8%)	10	35
33	V	98/105 (93%)	94 (96%)	4 (4%)	27	53
34	Y	108/110 (98%)	93 (86%)	15 (14%)	3	19
38	K	238/346 (69%)	235 (99%)	3 (1%)	61	72
39	m	150/723 (21%)	145 (97%)	5 (3%)	33	58
40	D	175/440 (40%)	168 (96%)	7 (4%)	28	54
41	o	118/199 (59%)	114 (97%)	4 (3%)	32	57
42	n	302/548 (55%)	289 (96%)	13 (4%)	26	52
43	t	216/287 (75%)	209 (97%)	7 (3%)	34	58
All	All	6174/9639 (64%)	5593 (91%)	581 (9%)	10	32

All (581) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	15	ARG
1	x	18	ILE
1	x	22	ILE
1	x	50	GLN
1	x	56	VAL
1	x	60	ILE
1	x	79	ASP
1	x	81	LEU
1	x	87	SER
1	x	88	ASN
1	x	95	ILE
1	x	99	THR
1	x	100	ASN
1	x	101	VAL
1	x	104	LYS
1	x	113	ILE
1	x	115	ILE
1	x	121	VAL
1	x	124	VAL
1	x	125	LYS
1	x	126	ARG
1	x	132	LEU
1	x	138	ILE
1	x	149	ILE
1	x	150	ILE
1	x	154	LYS
1	x	161	THR
1	x	163	ILE
1	x	165	LEU
1	x	170	THR
1	x	176	SER
1	x	179	VAL
1	x	191	THR
1	x	197	LEU
1	x	204	THR
1	x	209	THR
1	x	217	ILE
1	x	223	ASP
1	x	230	ILE
1	x	232	LEU
1	x	235	GLN
1	x	239	ILE

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Mol	Chain	Res	Type
1	x	242	ARG
1	x	247	VAL
1	x	263	PHE
1	x	266	LYS
1	x	270	LEU
1	x	274	ILE
1	x	279	GLU
1	x	290	LYS
2	F	6	ILE
2	F	8	THR
2	F	13	LEU
2	F	22	THR
2	F	86	VAL
2	F	89	ILE
2	F	93	ASN
2	F	111	ILE
2	F	119	VAL
2	F	124	LEU
2	F	129	LEU
2	F	148	VAL
2	F	168	ILE
2	F	179	LEU
2	F	244	ASN
3	3	5	ILE
3	3	8	GLN
3	3	16	SER
3	3	28	CYS
3	3	29	ARG
3	3	33	ASN
3	3	39	THR
3	3	40	ARG
3	3	52	THR
3	3	62	LEU
3	3	66	THR
3	3	71	HIS
3	3	75	LYS
3	3	76	LEU
3	3	78	GLU
3	3	79	ARG
3	3	87	THR
3	3	97	LEU
3	3	106	HIS

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Mol	Chain	Res	Type
3	3	107	LYS
3	3	109	LYS
3	3	111	ARG
3	3	118	VAL
3	3	144	ARG
3	3	153	LEU
3	3	158	ILE
4	4	5	ASN
4	4	15	ARG
4	4	19	VAL
4	4	20	ASN
4	4	30	THR
4	4	35	LYS
4	4	45	LEU
4	4	50	TYR
4	4	57	ASP
4	4	64	ARG
4	4	75	LEU
4	4	92	ASP
4	4	97	LYS
4	4	99	SER
4	4	109	GLU
4	4	111	PHE
4	4	118	LEU
4	4	123	LEU
4	4	125	ILE
4	4	132	GLN
4	4	144	LYS
4	4	150	ILE
4	4	157	LEU
4	4	171	ILE
4	4	177	LEU
4	4	179	ASP
4	4	229	ASN
4	4	234	LEU
4	4	237	LYS
4	4	239	LYS
4	4	242	LEU
5	5	6	SER
5	5	53	ILE
5	5	57	GLU
5	5	63	ASN

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Mol	Chain	Res	Type
5	5	105	ILE
5	5	126	LEU
5	5	134	THR
5	5	136	LEU
5	5	137	VAL
5	5	147	LYS
5	5	190	LEU
5	5	204	ILE
5	5	213	LEU
5	5	219	ILE
5	5	251	LEU
5	5	280	THR
5	5	293	GLN
5	5	299	ASN
5	5	337	ASP
5	5	340	LYS
5	5	351	MET
5	5	352	LEU
5	5	376	LEU
5	5	408	VAL
6	A	51	ASP
6	A	65	LEU
6	A	84	ASN
6	A	87	LEU
6	A	101	LEU
6	A	106	ASN
7	b	8	ILE
7	b	17	LEU
7	b	22	LEU
7	b	31	THR
7	b	32	VAL
7	b	51	LYS
7	b	53	THR
7	b	55	GLU
7	b	70	ASN
7	b	86	TYR
7	b	87	GLU
7	b	94	SER
7	b	116	LEU
7	b	125	CYS
7	b	159	ARG
7	b	160	LEU

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Mol	Chain	Res	Type
7	b	162	SER
7	b	170	LEU
7	b	180	LYS
7	b	184	LEU
7	b	189	LYS
7	b	221	THR
7	b	270	LEU
7	b	275	LYS
7	b	277	LEU
7	b	305	LEU
7	b	324	LEU
7	b	436	LEU
7	b	448	GLU
7	b	456	LEU
8	J	241	GLU
9	r	2	PRO
9	r	3	GLN
9	r	8	GLU
9	r	37	GLU
9	r	72	LYS
10	s	14	LYS
10	s	15	LEU
11	u	27	LYS
11	u	76	ASN
11	u	79	VAL
11	u	85	LEU
12	v	5	ARG
12	v	28	ILE
12	v	30	ILE
12	v	36	ILE
12	v	55	LEU
12	v	164	GLU
12	v	178	SER
12	v	191	LYS
12	v	207	ILE
12	v	218	ARG
13	W	15	THR
13	W	40	VAL
13	W	45	LEU
13	W	47	ASP
13	W	48	VAL
13	W	55	GLU

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Mol	Chain	Res	Type
13	W	57	ARG
13	W	128	ASN
13	W	174	LYS
14	y	3	THR
14	y	88	LEU
14	y	137	VAL
14	y	145	ASN
14	y	146	ILE
14	y	154	LEU
14	y	161	VAL
14	y	173	LEU
14	y	192	VAL
14	y	198	VAL
14	y	203	LEU
16	B	17	LEU
16	B	19	ARG
16	B	24	SER
16	B	25	ILE
16	B	28	ARG
16	B	29	VAL
16	B	37	ARG
16	B	45	SER
16	B	55	THR
16	B	56	ILE
16	B	79	VAL
16	B	85	VAL
16	B	93	VAL
16	B	102	LEU
16	B	114	VAL
16	B	136	LYS
16	B	152	LYS
16	B	164	THR
16	B	184	ASN
16	B	188	ILE
16	B	278	ILE
16	B	305	ILE
16	B	306	THR
16	B	337	THR
16	B	351	LEU
17	C	22	LEU
17	C	25	VAL
17	C	35	VAL

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Mol	Chain	Res	Type
17	C	40	THR
17	C	47	ARG
17	C	52	VAL
17	C	60	THR
17	C	61	SER
17	C	74	ILE
17	C	92	ASN
17	C	105	THR
17	C	111	VAL
17	C	122	THR
17	C	124	SER
17	C	134	LEU
17	C	135	VAL
17	C	136	LEU
17	C	138	ARG
17	C	144	LYS
17	C	147	GLU
17	C	148	ILE
17	C	163	LYS
17	C	172	VAL
17	C	179	LEU
17	C	182	LEU
17	C	187	LEU
17	C	193	LYS
17	C	196	ASN
17	C	220	ARG
17	C	222	VAL
17	C	230	VAL
17	C	275	THR
17	C	278	SER
17	C	280	ILE
17	C	286	VAL
17	C	289	ILE
17	C	295	ILE
17	C	299	ILE
17	C	306	THR
17	C	313	LEU
17	C	322	GLN
17	C	326	ARG
17	C	339	LEU
18	e	11	LYS
18	e	21	HIS

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Mol	Chain	Res	Type
18	e	27	ARG
18	e	34	LYS
18	e	50	ILE
18	e	52	GLN
18	e	73	THR
18	e	80	LYS
18	e	82	LEU
18	e	90	LYS
18	e	91	THR
18	e	100	ILE
18	e	105	ARG
18	e	106	VAL
18	e	120	THR
18	e	126	LEU
18	e	128	LEU
19	E	15	VAL
19	E	22	ARG
19	E	26	ARG
19	E	29	LYS
19	E	31	ARG
19	E	63	LEU
19	E	64	LEU
19	E	79	VAL
19	E	98	VAL
19	E	101	PHE
19	E	155	LEU
20	f	3	GLU
20	f	9	VAL
20	f	10	LYS
20	f	14	LEU
20	f	31	LYS
20	f	49	ILE
20	f	53	TYR
20	f	66	VAL
20	f	81	VAL
20	f	86	ARG
20	f	97	SER
20	f	98	VAL
20	f	100	ILE
20	f	102	LEU
21	G	71	VAL
21	G	111	LYS

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Mol	Chain	Res	Type
21	G	136	LEU
21	G	142	LEU
21	G	143	ILE
21	G	145	ASN
21	G	146	LYS
21	G	150	LEU
21	G	162	LEU
21	G	163	VAL
21	G	166	LEU
21	G	180	VAL
21	G	197	VAL
21	G	200	LEU
21	G	204	ARG
21	G	214	LEU
21	G	229	VAL
22	h	28	LEU
22	h	36	LEU
22	h	48	ARG
22	h	69	LEU
22	h	83	LYS
22	h	102	GLU
22	h	107	LYS
22	h	119	LYS
23	H	1	MET
23	H	5	GLN
23	H	6	THR
23	H	23	ARG
23	H	41	ILE
23	H	48	VAL
23	H	55	VAL
23	H	57	VAL
23	H	59	ASN
23	H	62	ARG
23	H	65	VAL
23	H	68	LEU
23	H	103	ILE
23	H	118	LEU
23	H	134	ILE
23	H	138	THR
23	H	151	VAL
23	H	161	LEU
23	H	167	VAL

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Mol	Chain	Res	Type
24	i	43	LEU
24	i	46	GLU
24	i	47	ILE
24	i	53	TYR
24	i	57	LEU
24	i	58	ILE
24	i	60	LEU
24	i	74	LYS
24	i	84	LYS
25	j	17	THR
25	j	21	ARG
25	j	29	VAL
25	j	36	SER
25	j	58	THR
25	j	61	THR
25	j	67	LEU
25	j	68	LYS
25	j	75	LYS
26	L	41	THR
26	L	45	LYS
26	L	58	VAL
26	L	63	VAL
26	L	69	VAL
26	L	70	ARG
26	L	100	ARG
26	L	101	ARG
26	L	108	ILE
26	L	123	ILE
27	M	15	VAL
27	M	23	ILE
27	M	53	VAL
27	M	69	THR
27	M	80	THR
27	M	122	VAL
27	M	125	LYS
28	N	7	LEU
28	N	19	LEU
28	N	22	LEU
28	N	29	GLU
28	N	38	ARG
28	N	46	ASP
28	N	49	ARG

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Mol	Chain	Res	Type
28	N	66	VAL
28	N	106	VAL
28	N	108	ARG
28	N	116	LEU
28	N	121	VAL
28	N	126	THR
28	N	132	VAL
28	N	133	ILE
28	N	142	ILE
28	N	144	ARG
28	N	145	ASP
28	N	153	ASP
28	N	155	VAL
28	N	167	THR
28	N	171	SER
28	N	174	ILE
28	N	179	LYS
28	N	182	ASN
29	O	7	VAL
29	O	9	ILE
29	O	10	ASP
29	O	12	LYS
29	O	15	LEU
29	O	16	VAL
29	O	22	VAL
29	O	27	LEU
29	O	28	LEU
29	O	31	GLN
29	O	32	LYS
29	O	34	VAL
29	O	35	VAL
29	O	39	GLU
29	O	42	ASN
29	O	46	GLU
29	O	48	PHE
29	O	49	ARG
29	O	50	ASN
29	O	56	ASP
29	O	62	THR
29	O	64	PHE
29	O	74	ARG
29	O	79	ILE

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Mol	Chain	Res	Type
29	O	80	PHE
29	O	82	LYS
29	O	84	LEU
29	O	87	MET
29	O	89	SER
29	O	94	ARG
29	O	99	LEU
29	O	105	PHE
29	O	118	VAL
29	O	124	LEU
29	O	134	LYS
29	O	138	LEU
29	O	140	LYS
29	O	142	SER
29	O	151	ASP
29	O	153	VAL
29	O	156	LEU
29	O	157	GLU
29	O	166	GLU
29	O	184	THR
29	O	189	ASP
30	P	16	SER
30	P	24	VAL
30	P	29	THR
30	P	30	ARG
30	P	41	LEU
30	P	42	THR
30	P	52	LEU
30	P	74	LYS
30	P	78	VAL
30	P	87	SER
30	P	114	VAL
30	P	119	VAL
30	P	120	ASN
30	P	157	VAL
30	P	159	LYS
31	Q	24	VAL
31	Q	28	LEU
31	Q	31	LYS
31	Q	49	LEU
31	Q	55	SER
31	Q	56	LYS

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Mol	Chain	Res	Type
31	Q	57	ILE
31	Q	62	VAL
31	Q	64	VAL
31	Q	69	ARG
31	Q	129	VAL
31	Q	136	ASN
32	S	32	SER
32	S	60	SER
32	S	71	LYS
32	S	94	ILE
32	S	96	ASP
32	S	106	LEU
32	S	115	ARG
32	S	125	LYS
32	S	129	ILE
32	S	134	ASP
32	S	154	HIS
32	S	158	LYS
32	S	169	SER
33	V	22	ILE
33	V	37	ILE
33	V	54	LEU
33	V	102	ILE
34	Y	5	SER
34	Y	17	LYS
34	Y	37	LYS
34	Y	51	ARG
34	Y	54	ASP
34	Y	56	VAL
34	Y	57	LEU
34	Y	59	VAL
34	Y	64	LYS
34	Y	87	LYS
34	Y	95	VAL
34	Y	105	VAL
34	Y	107	THR
34	Y	119	ILE
34	Y	126	LEU
38	K	112	GLU
38	K	163	VAL
38	K	248	LEU
39	m	253	VAL

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Mol	Chain	Res	Type
39	m	263	LYS
39	m	323	HIS
39	m	324	LEU
39	m	329	LEU
40	D	294	VAL
40	D	312	ILE
40	D	394	LEU
40	D	422	ILE
40	D	429	LEU
40	D	451	LEU
40	D	473	VAL
41	o	93	ILE
41	o	109	LYS
41	o	156	LEU
41	o	211	LEU
42	n	36	CYS
42	n	69	GLN
42	n	92	ARG
42	n	103	LYS
42	n	117	ILE
42	n	139	LEU
42	n	145	LEU
42	n	183	ILE
42	n	208	ASN
42	n	376	LEU
42	n	417	LEU
42	n	419	ASN
42	n	427	ILE
43	t	66	LEU
43	t	141	LEU
43	t	144	ILE
43	t	151	LEU
43	t	157	ASN
43	t	187	LEU
43	t	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	31	HIS
1	x	88	ASN
1	x	90	ASN

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Mol	Chain	Res	Type
1	x	102	ASN
1	x	187	HIS
1	x	193	HIS
1	x	228	GLN
1	x	235	GLN
1	x	244	HIS
1	x	262	GLN
2	F	12	GLN
2	F	52	GLN
2	F	200	ASN
3	3	11	ASN
3	3	41	GLN
3	3	147	ASN
4	4	5	ASN
4	4	43	ASN
4	4	63	GLN
4	4	73	HIS
4	4	172	HIS
5	5	75	HIS
5	5	191	GLN
5	5	269	GLN
5	5	285	GLN
5	5	305	GLN
5	5	405	ASN
6	A	95	GLN
6	A	148	HIS
6	A	158	HIS
7	b	23	ASN
7	b	26	GLN
7	b	107	GLN
7	b	124	GLN
7	b	217	GLN
7	b	238	GLN
7	b	245	HIS
7	b	267	GLN
7	b	327	ASN
7	b	406	ASN
8	J	215	HIS
8	J	228	ASN
9	r	3	GLN
9	r	4	ASN
11	u	24	ASN

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Mol	Chain	Res	Type
11	u	76	ASN
11	u	82	ASN
12	v	33	ASN
13	W	14	GLN
13	W	91	GLN
13	W	110	ASN
13	W	199	GLN
13	W	223	ASN
13	W	232	ASN
14	y	21	ASN
14	y	33	ASN
14	y	82	GLN
14	y	83	HIS
14	y	86	ASN
14	y	95	GLN
14	y	157	GLN
14	y	178	GLN
15	z	12	ASN
15	z	55	GLN
16	B	184	ASN
16	B	293	ASN
17	C	48	GLN
17	C	58	HIS
17	C	59	GLN
17	C	110	ASN
17	C	114	ASN
17	C	260	GLN
17	C	291	ASN
17	C	304	GLN
18	e	52	GLN
18	e	104	ASN
19	E	138	GLN
20	f	13	HIS
20	f	42	GLN
21	G	95	ASN
21	G	137	ASN
21	G	145	ASN
21	G	221	ASN
22	h	16	GLN
22	h	34	GLN
22	h	59	ASN
22	h	62	GLN

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Mol	Chain	Res	Type
23	H	8	GLN
23	H	58	HIS
23	H	125	ASN
23	H	139	ASN
23	H	157	ASN
24	i	63	ASN
24	i	92	ASN
26	L	37	ASN
28	N	37	HIS
28	N	182	ASN
29	O	31	GLN
29	O	42	ASN
29	O	122	GLN
29	O	182	ASN
30	P	45	GLN
30	P	55	GLN
30	P	97	ASN
30	P	101	ASN
31	Q	45	ASN
31	Q	73	GLN
31	Q	126	GLN
31	Q	136	ASN
32	S	3	HIS
32	S	8	GLN
32	S	62	ASN
32	S	74	ASN
32	S	157	GLN
34	Y	66	GLN
38	K	42	ASN
40	D	310	ASN
40	D	325	GLN
40	D	330	ASN
40	D	337	ASN
40	D	397	ASN
40	D	420	ASN
40	D	440	HIS
41	o	113	GLN
41	o	154	ASN
42	n	69	GLN
42	n	157	ASN
42	n	164	ASN
42	n	189	GLN

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Mol	Chain	Res	Type
42	n	208	ASN
42	n	419	ASN
43	t	225	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	1	1772/3396 (52%)	504 (28%)	49 (2%)
36	2	153/158 (96%)	39 (25%)	6 (3%)
37	6	63/232 (27%)	30 (47%)	2 (3%)
All	All	1988/3786 (52%)	573 (28%)	57 (2%)

All (573) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	1	3	U
35	1	6	A
35	1	7	C
35	1	11	A
35	1	18	G
35	1	26	A
35	1	30	G
35	1	39	A
35	1	40	A
35	1	41	G
35	1	43	A
35	1	48	A
35	1	49	A
35	1	50	U
35	1	57	A
35	1	59	G
35	1	60	A
35	1	65	A
35	1	66	A
35	1	72	C
35	1	74	G
35	1	75	G
35	1	92	G
35	1	94	G
35	1	96	G
35	1	105	C

Continued on next page...

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Mol	Chain	Res	Type
35	1	110	G
35	1	111	C
35	1	116	A
35	1	117	U
35	1	119	U
35	1	120	G
35	1	122	A
35	1	125	C
35	1	134	U
35	1	135	C
35	1	136	G
35	1	143	G
35	1	146	U
35	1	148	G
35	1	155	G
35	1	156	G
35	1	157	A
35	1	161	G
35	1	164	A
35	1	165	A
35	1	166	C
35	1	170	G
35	1	171	G
35	1	173	G
35	1	190	U
35	1	191	U
35	1	200	C
35	1	206	G
35	1	210	U
35	1	211	A
35	1	213	A
35	1	218	G
35	1	219	A
35	1	220	G
35	1	221	A
35	1	240	U
35	1	241	G
35	1	243	G
35	1	249	U
35	1	250	U
35	1	251	G
35	1	265	A

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Mol	Chain	Res	Type
35	1	267	G
35	1	268	A
35	1	269	G
35	1	270	U
35	1	277	G
35	1	281	G
35	1	282	G
35	1	283	G
35	1	284	A
35	1	285	A
35	1	286	U
35	1	287	G
35	1	295	A
35	1	298	U
35	1	299	G
35	1	304	G
35	1	305	U
35	1	311	C
35	1	315	C
35	1	323	A
35	1	324	A
35	1	329	U
35	1	338	A
35	1	346	C
35	1	349	A
35	1	352	A
35	1	354	U
35	1	368	G
35	1	370	U
35	1	374	A
35	1	376	G
35	1	377	A
35	1	383	G
35	1	385	A
35	1	386	A
35	1	387	A
35	1	388	G
35	1	390	G
35	1	395	A
35	1	398	A
35	1	400	G
35	1	401	U

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Mol	Chain	Res	Type
35	1	402	A
35	1	403	C
35	1	421	G
35	1	422	A
35	1	429	U
35	1	436	A
35	1	438	A
35	1	439	C
35	1	440	A
35	1	442	G
35	1	449	U
35	1	452	G
35	1	454	C
35	1	455	C
35	1	457	C
35	1	459	G
35	1	462	C
35	1	463	C
35	1	465	U
35	1	466	G
35	1	467	U
35	1	468	G
35	1	474	G
35	1	478	A
35	1	479	U
35	1	480	C
35	1	481	U
35	1	482	C
35	1	494	G
35	1	495	G
35	1	498	A
35	1	503	C
35	1	510	G
35	1	515	C
35	1	517	G
35	1	518	G
35	1	519	A
35	1	521	A
35	1	523	A
35	1	527	A
35	1	533	A
35	1	535	G

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Mol	Chain	Res	Type
35	1	543	C
35	1	544	C
35	1	546	C
35	1	547	G
35	1	549	U
35	1	551	A
35	1	552	G
35	1	555	U
35	1	556	U
35	1	557	A
35	1	559	A
35	1	569	A
35	1	570	A
35	1	572	A
35	1	578	A
35	1	579	G
35	1	588	G
35	1	589	A
35	1	590	G
35	1	592	A
35	1	597	G
35	1	602	A
35	1	604	G
35	1	611	A
35	1	618	C
35	1	619	A
35	1	629	U
35	1	636	C
35	1	642	U
35	1	644	G
35	1	645	A
35	1	647	A
35	1	648	C
35	1	649	A
35	1	650	C
35	1	660	A
35	1	661	G
35	1	675	C
35	1	677	A
35	1	681	U
35	1	691	A
35	1	695	C

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Mol	Chain	Res	Type
35	1	704	U
35	1	705	A
35	1	720	A
35	1	721	G
35	1	722	G
35	1	742	G
35	1	750	G
35	1	756	U
35	1	757	C
35	1	776	U
35	1	780	A
35	1	781	G
35	1	783	A
35	1	784	A
35	1	785	G
35	1	786	A
35	1	794	U
35	1	799	G
35	1	806	A
35	1	808	A
35	1	813	G
35	1	814	U
35	1	815	G
35	1	933	A
35	1	936	A
35	1	937	G
35	1	938	C
35	1	941	G
35	1	943	U
35	1	944	C
35	1	953	G
35	1	957	C
35	1	959	C
35	1	961	C
35	1	962	A
35	1	978	G
35	1	979	U
35	1	980	A
35	1	984	G
35	1	985	U
35	1	1103	A
35	1	1104	G

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Mol	Chain	Res	Type
35	1	1111	U
35	1	1112	A
35	1	1116	G
35	1	1117	G
35	1	1124	U
35	1	1125	U
35	1	1128	U
35	1	1129	A
35	1	1130	A
35	1	1132	C
35	1	1143	A
35	1	1144	U
35	1	1151	U
35	1	1153	A
35	1	1155	C
35	1	1157	G
35	1	1159	A
35	1	1160	C
35	1	1161	G
35	1	1177	G
35	1	1178	G
35	1	1179	A
35	1	1180	A
35	1	1181	U
35	1	1182	A
35	1	1186	G
35	1	1192	C
35	1	1193	A
35	1	1196	C
35	1	1197	A
35	1	1198	C
35	1	1199	C
35	1	1200	A
35	1	1201	C
35	1	1204	A
35	1	1212	A
35	1	1220	U
35	1	1221	A
35	1	1222	G
35	1	1227	C
35	1	1233	G
35	1	1234	G

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Mol	Chain	Res	Type
35	1	1235	U
35	1	1239	C
35	1	1241	U
35	1	1242	G
35	1	1244	A
35	1	1245	A
35	1	1246	G
35	1	1253	U
35	1	1258	U
35	1	1262	G
35	1	1263	A
35	1	1264	G
35	1	1265	U
35	1	1277	C
35	1	1278	A
35	1	1279	C
35	1	1285	G
35	1	1286	A
35	1	1287	A
35	1	1301	A
35	1	1302	A
35	1	1303	A
35	1	1304	A
35	1	1305	U
35	1	1307	G
35	1	1308	A
35	1	1309	U
35	1	1318	A
35	1	1325	U
35	1	1329	U
35	1	1330	A
35	1	1332	A
35	1	1345	G
35	1	1347	U
35	1	1348	U
35	1	1349	G
35	1	1350	A
35	1	1351	U
35	1	1352	A
35	1	1353	U
35	1	1354	G
35	1	1355	A

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Mol	Chain	Res	Type
35	1	1357	G
35	1	1359	C
35	1	1379	G
35	1	1386	A
35	1	1390	A
35	1	1391	C
35	1	1392	G
35	1	1397	C
35	1	1399	A
35	1	1400	G
35	1	1408	G
35	1	1417	G
35	1	1419	A
35	1	1434	G
35	1	1437	C
35	1	1443	G
35	1	1446	A
35	1	1450	G
35	1	1452	A
35	1	2364	G
35	1	2371	G
35	1	2372	A
35	1	2374	C
35	1	2375	G
35	1	2377	G
35	1	2381	G
35	1	2393	G
35	1	2394	G
35	1	2826	U
35	1	2828	G
35	1	2833	A
35	1	2836	C
35	1	2837	A
35	1	2843	U
35	1	2845	A
35	1	2847	A
35	1	2857	C
35	1	2858	U
35	1	2877	G
35	1	2878	G
35	1	2879	C
35	1	2887	A

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Mol	Chain	Res	Type
35	1	2889	C
35	1	2894	C
35	1	2899	C
35	1	2903	A
35	1	2916	U
35	1	2919	A
35	1	2921	U
35	1	2923	U
35	1	2924	U
35	1	2925	C
35	1	2926	A
35	1	2927	C
35	1	2929	C
35	1	2930	A
35	1	2935	U
35	1	2936	A
35	1	2938	G
35	1	2941	A
35	1	2942	C
35	1	2943	G
35	1	2944	U
35	1	2945	G
35	1	2946	A
35	1	2947	G
35	1	2984	C
35	1	2986	U
35	1	2987	A
35	1	2990	G
35	1	2992	U
35	1	2996	U
35	1	2997	G
35	1	3003	G
35	1	3006	A
35	1	3012	A
35	1	3019	U
35	1	3021	A
35	1	3022	G
35	1	3023	U
35	1	3027	A
35	1	3028	G
35	1	3029	A
35	1	3030	G

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Mol	Chain	Res	Type
35	1	3032	A
35	1	3037	U
35	1	3046	A
35	1	3049	A
35	1	3054	U
35	1	3055	U
35	1	3057	U
35	1	3058	U
35	1	3059	G
35	1	3069	G
35	1	3070	A
35	1	3074	G
35	1	3075	G
35	1	3078	U
35	1	3086	A
35	1	3088	G
35	1	3092	C
35	1	3094	A
35	1	3099	C
35	1	3100	U
35	1	3101	G
35	1	3109	G
35	1	3116	G
35	1	3121	U
35	1	3122	A
35	1	3124	G
35	1	3129	A
35	1	3130	A
35	1	3131	U
35	1	3142	A
35	1	3143	C
35	1	3173	G
35	1	3174	A
35	1	3176	G
35	1	3179	U
35	1	3180	A
35	1	3181	C
35	1	3187	A
35	1	3188	G
35	1	3194	C
35	1	3195	U
35	1	3196	U

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Mol	Chain	Res	Type
35	1	3198	U
35	1	3199	G
35	1	3205	G
35	1	3206	C
35	1	3207	U
35	1	3213	A
35	1	3217	C
35	1	3218	A
35	1	3219	G
35	1	3228	C
35	1	3229	G
35	1	3234	A
35	1	3242	G
35	1	3243	A
35	1	3244	A
35	1	3245	A
35	1	3246	G
35	1	3247	G
35	1	3249	C
35	1	3256	G
35	1	3259	U
35	1	3263	G
35	1	3267	A
35	1	3268	A
35	1	3270	U
35	1	3273	A
35	1	3275	U
35	1	3276	G
35	1	3286	G
35	1	3288	G
35	1	3289	G
35	1	3290	G
35	1	3304	U
35	1	3313	U
35	1	3316	A
35	1	3317	U
35	1	3319	U
35	1	3320	A
35	1	3330	A
35	1	3340	G
35	1	3341	U
35	1	3345	G

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Mol	Chain	Res	Type
35	1	3346	U
35	1	3347	A
35	1	3351	U
35	1	3352	U
35	1	3355	U
35	1	3356	G
35	1	3360	C
35	1	3363	U
35	1	3368	U
35	1	3369	G
35	1	3375	A
35	1	3376	A
35	1	3378	C
35	1	3382	U
35	1	3390	G
35	1	3396	U
36	2	12	A
36	2	13	A
36	2	23	U
36	2	33	A
36	2	34	U
36	2	35	C
36	2	39	G
36	2	40	A
36	2	48	A
36	2	49	G
36	2	52	A
36	2	59	A
36	2	62	C
36	2	63	G
36	2	75	G
36	2	81	U
36	2	82	U
36	2	83	C
36	2	84	C
36	2	85	G
36	2	86	U
36	2	87	G
36	2	90	U
36	2	95	G
36	2	97	A
36	2	100	U

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Mol	Chain	Res	Type
36	2	105	A
36	2	106	C
36	2	107	G
36	2	113	U
36	2	115	C
36	2	116	G
36	2	121	U
36	2	123	G
36	2	129	C
36	2	144	G
36	2	148	G
36	2	152	G
36	2	157	U
37	6	4	U
37	6	5	C
37	6	6	U
37	6	7	C
37	6	8	A
37	6	9	A
37	6	13	U
37	6	14	U
37	6	15	C
37	6	16	U
37	6	17	G
37	6	23	U
37	6	24	A
37	6	34	A
37	6	36	U
37	6	39	U
37	6	40	U
37	6	42	G
37	6	43	A
37	6	47	A
37	6	52	G
37	6	53	A
37	6	54	A
37	6	56	U
37	6	57	U
37	6	58	G
37	6	59	C
37	6	228	U
37	6	231	A

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Mol	Chain	Res	Type
37	6	232	A

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	1	93	C
35	1	133	U
35	1	156	G
35	1	190	U
35	1	239	G
35	1	285	A
35	1	297	G
35	1	398	A
35	1	406	G
35	1	438	A
35	1	456	U
35	1	480	C
35	1	518	G
35	1	533	A
35	1	548	G
35	1	588	G
35	1	607	A
35	1	618	C
35	1	644	G
35	1	649	A
35	1	720	A
35	1	1102	A
35	1	1104	G
35	1	1128	U
35	1	1160	C
35	1	1177	G
35	1	1241	U
35	1	1302	A
35	1	1307	G
35	1	1329	U
35	1	1347	U
35	1	1354	G
35	1	1356	U
35	1	1418	A
35	1	1434	G
35	1	2392	C
35	1	2828	G

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Mol	Chain	Res	Type
35	1	2857	C
35	1	2986	U
35	1	3022	G
35	1	3069	G
35	1	3121	U
35	1	3205	G
35	1	3217	C
35	1	3218	A
35	1	3228	C
35	1	3267	A
35	1	3269	U
35	1	3350	C
36	2	39	G
36	2	48	A
36	2	71	A
36	2	84	C
36	2	85	G
36	2	114	G
37	6	16	U
37	6	56	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	2	6
1	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	124:G	O3'	125:U	P	7.11
1	2	110:C	O3'	111:A	P	6.92
1	2	125:U	O3'	126:A	P	6.42
1	2	113:U	O3'	114:G	P	4.42
1	2	126:A	O3'	127:U	P	3.70
1	2	128:U	O3'	129:C	P	3.37
1	x	285:GLU	C	286:MET	N	2.75

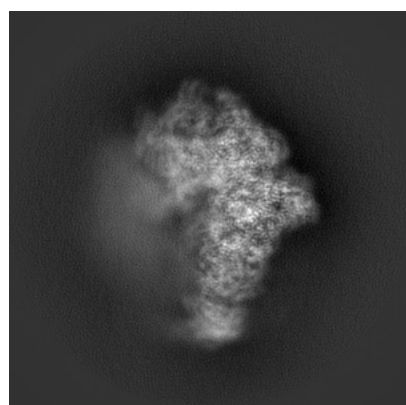
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3893. These allow visual inspection of the internal detail of the map and identification of artifacts.

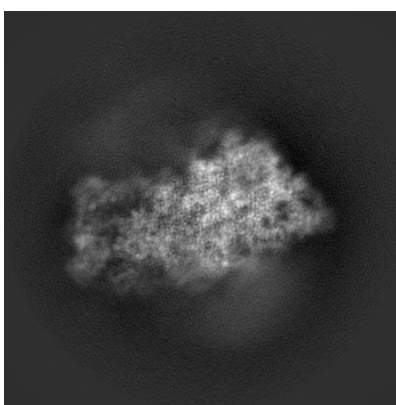
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

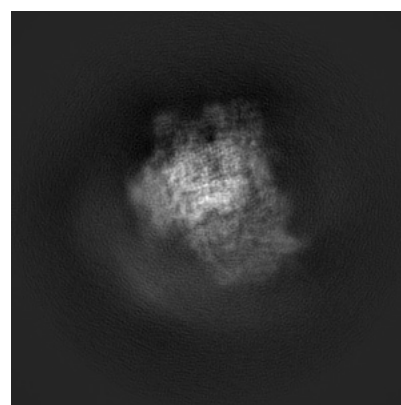
6.1.1 Primary map



X



Y

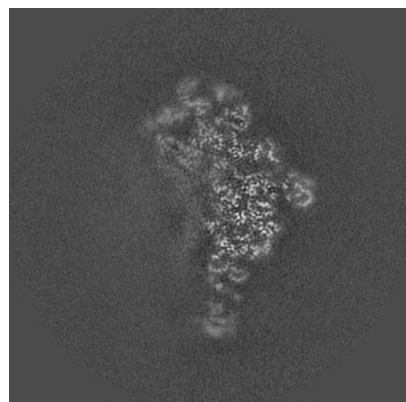


Z

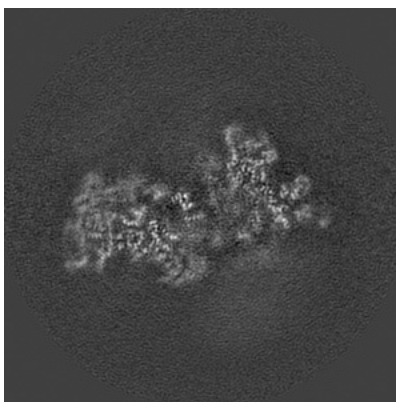
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

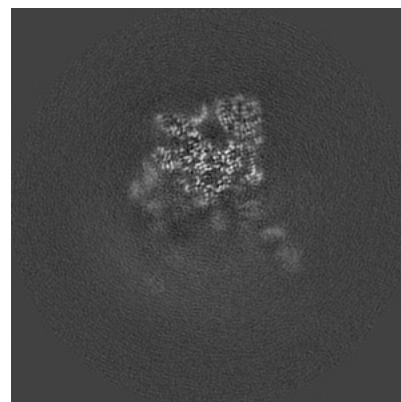
6.2.1 Primary map



X Index: 210



Y Index: 210

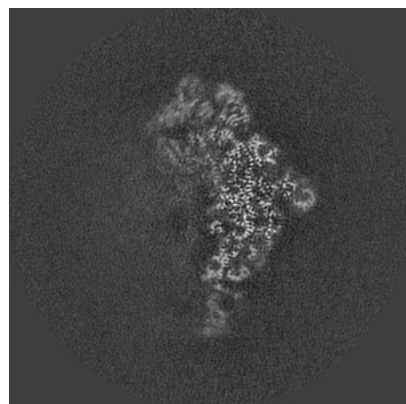


Z Index: 210

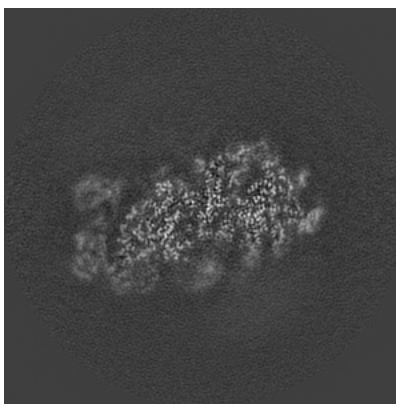
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

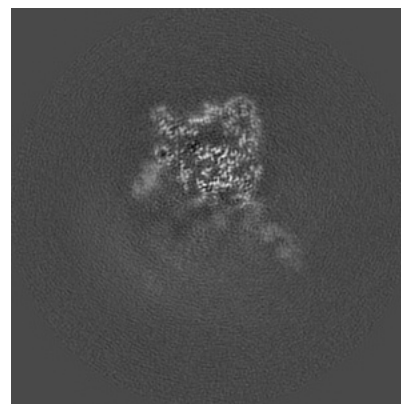
6.3.1 Primary map



X Index: 205



Y Index: 235

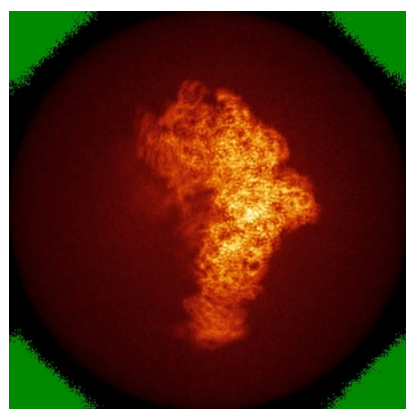


Z Index: 215

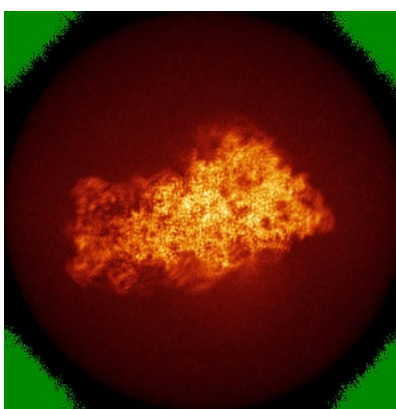
The images above show the largest variance slices of the map in three orthogonal directions.

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

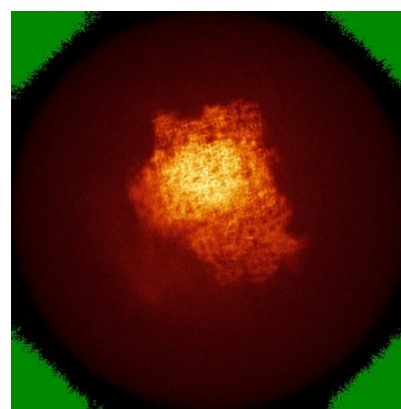
6.4.1 Primary map



X



Y

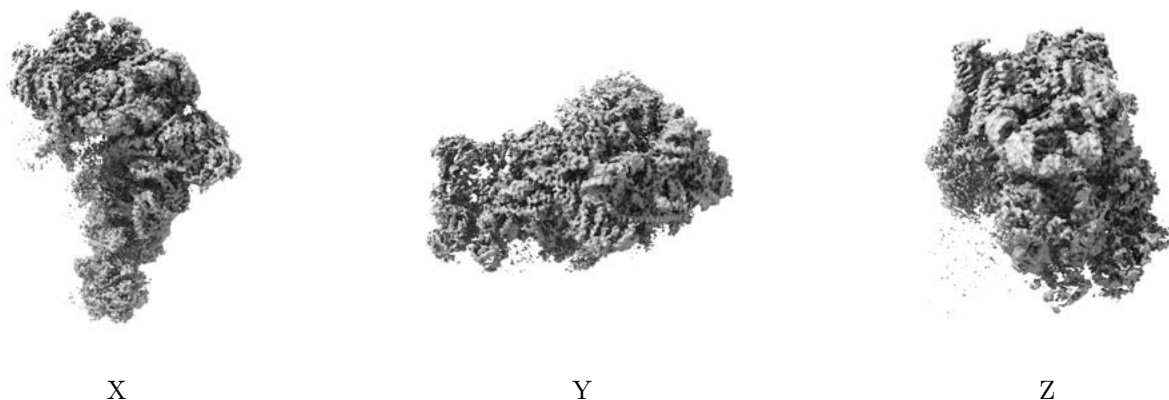


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

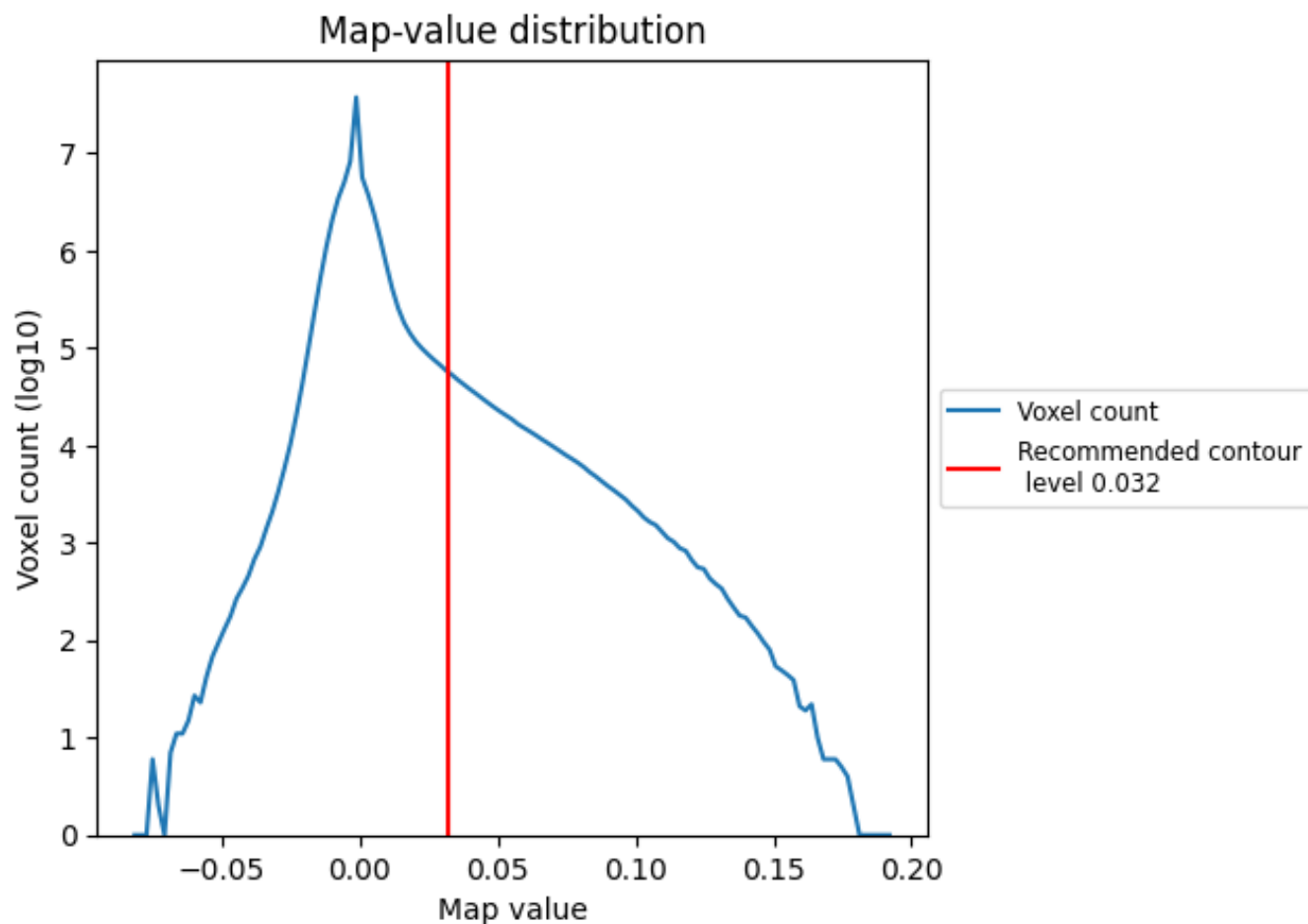
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

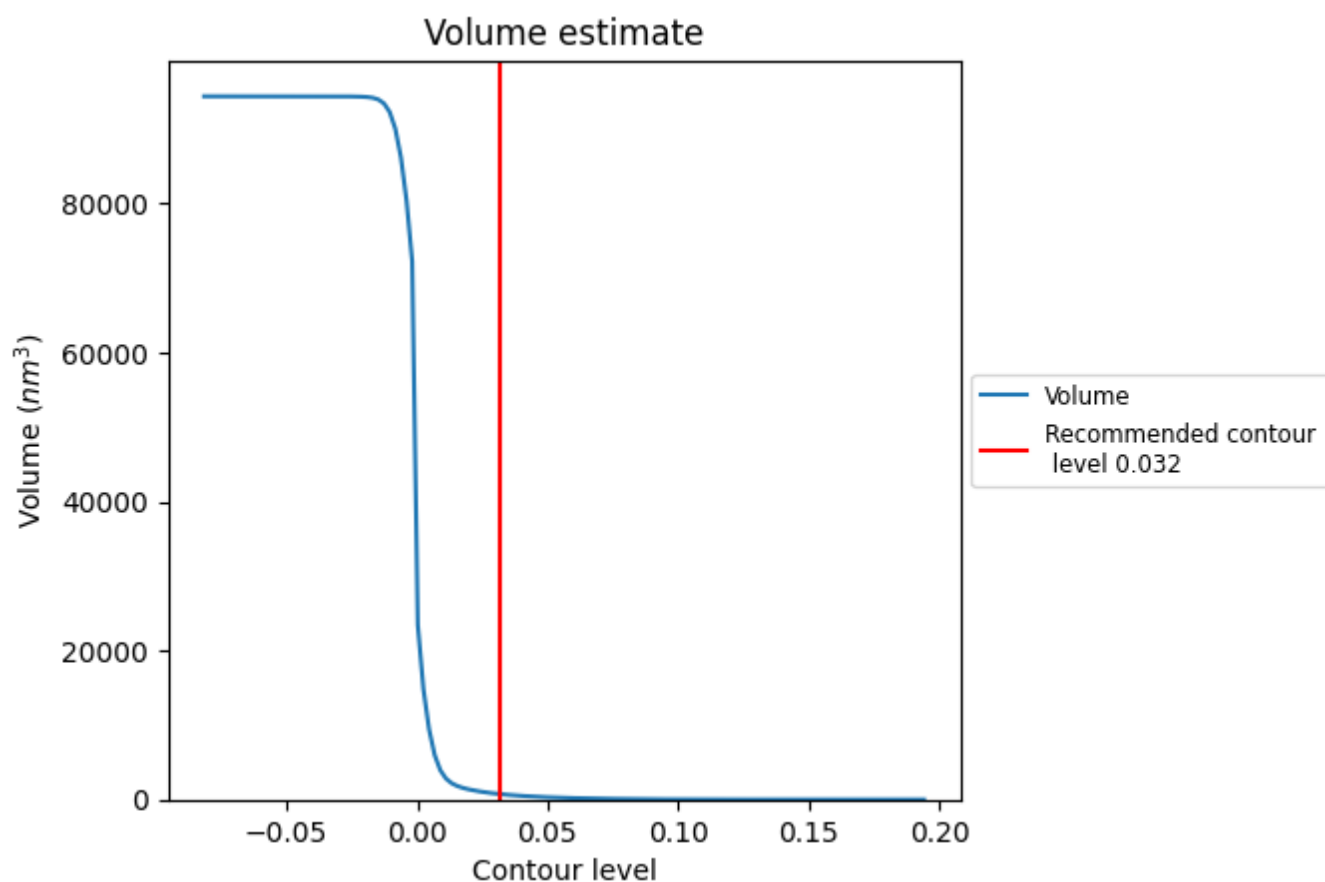
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

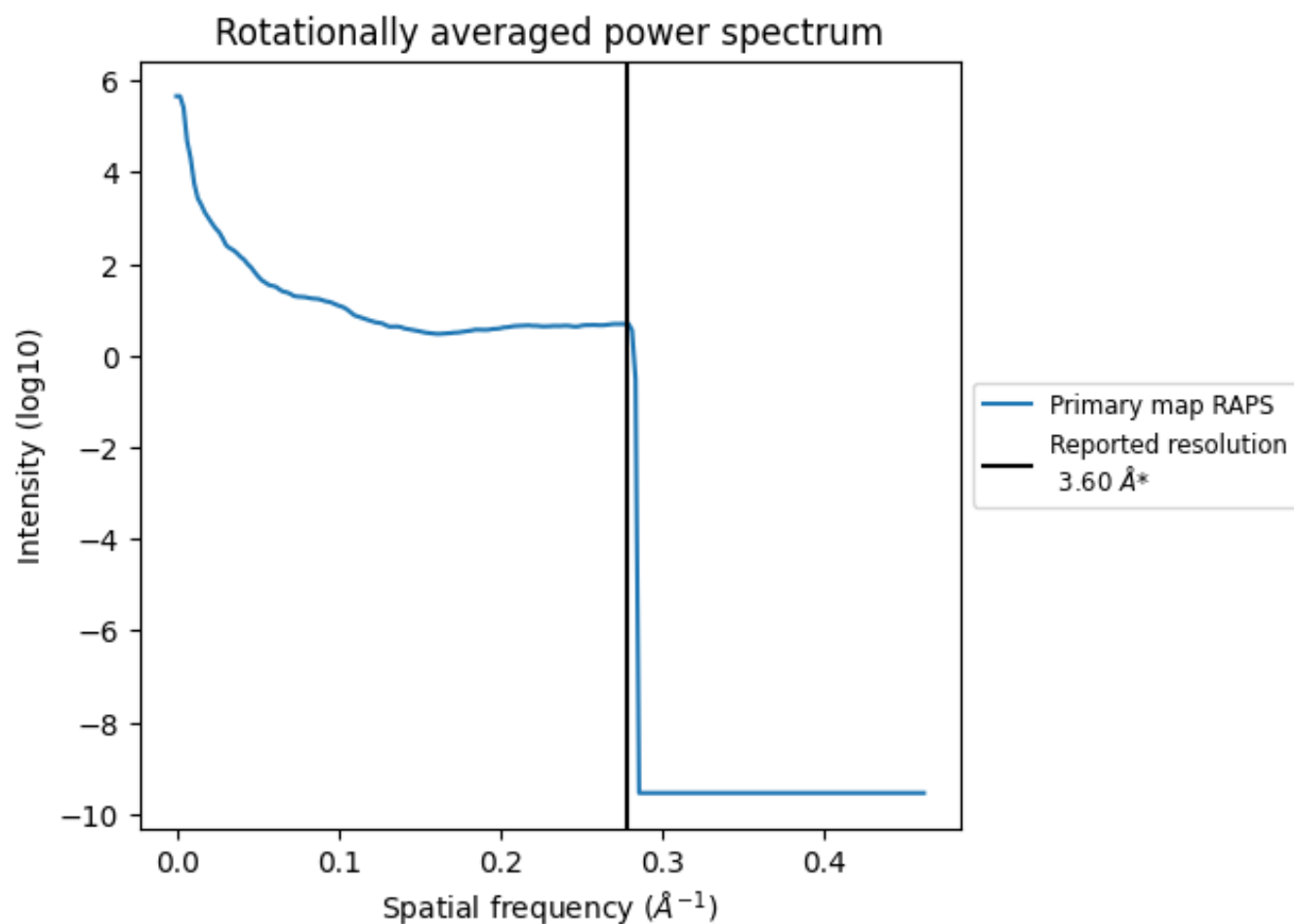
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 657 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 ⓘ

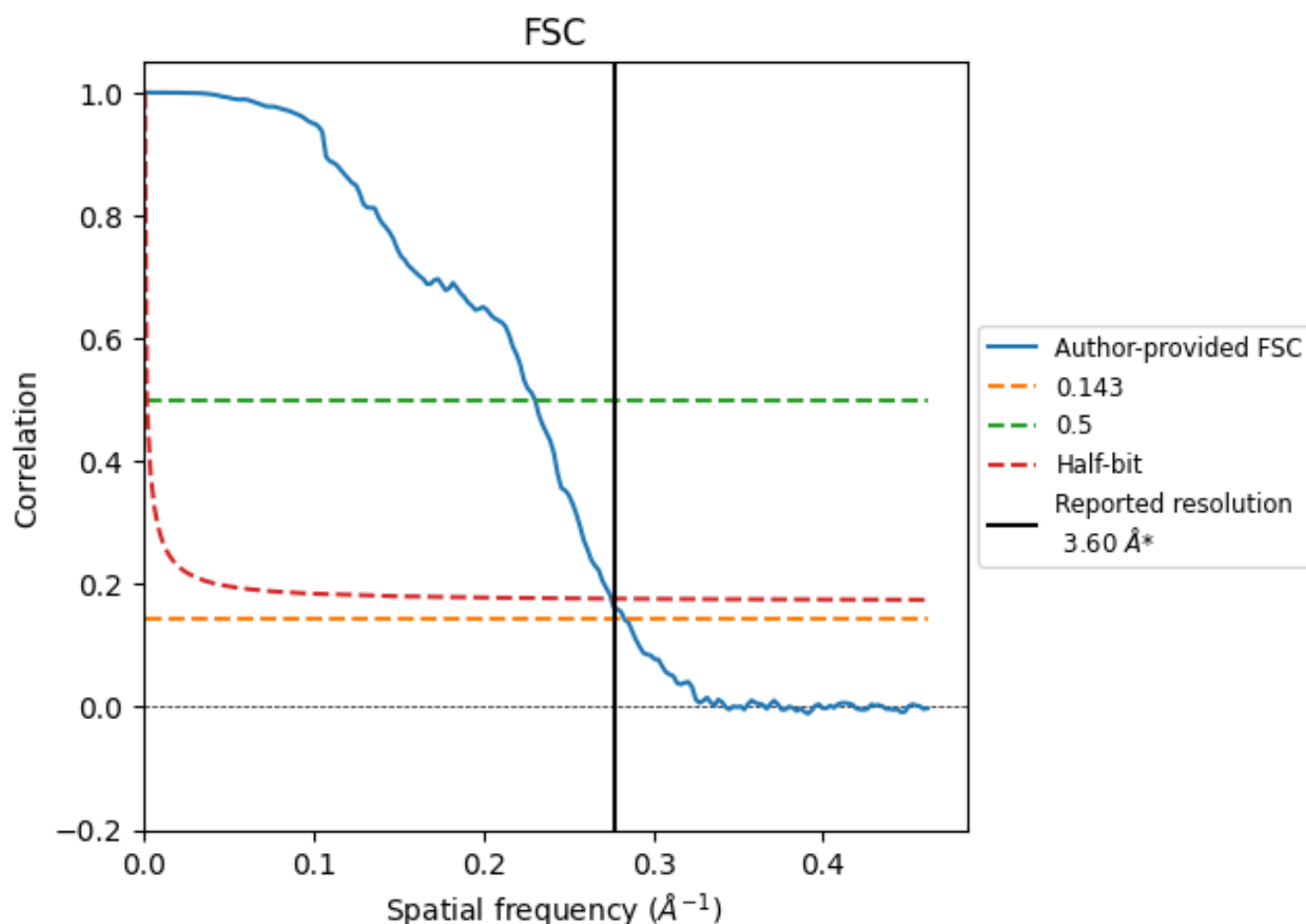


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

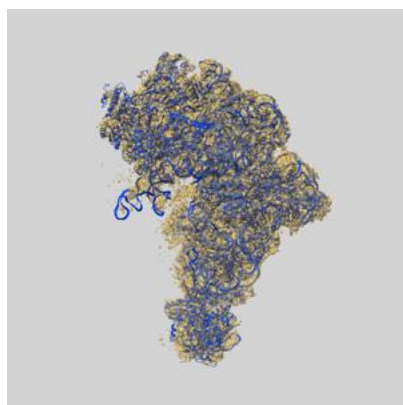
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.34	3.63
Unmasked-calculated*	-	-	-

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

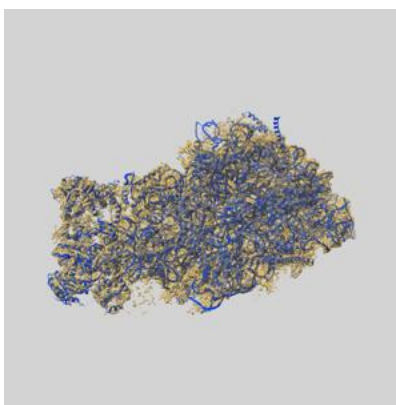
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3893 and PDB model 6EM1. Per-residue inclusion information can be found in section 3 on page 12.

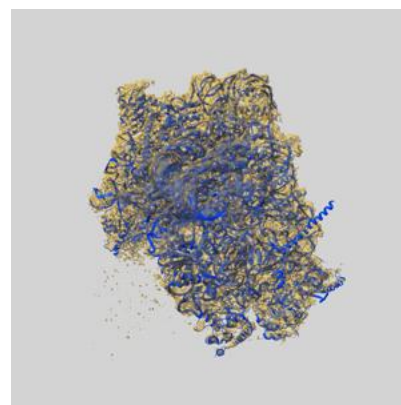
9.1 Map-model overlay [i](#)



X



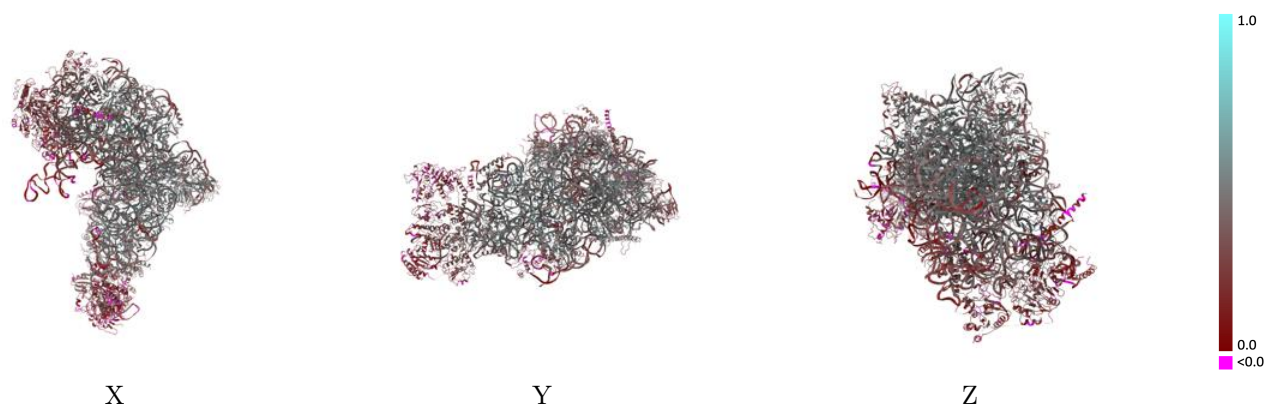
Y



Z

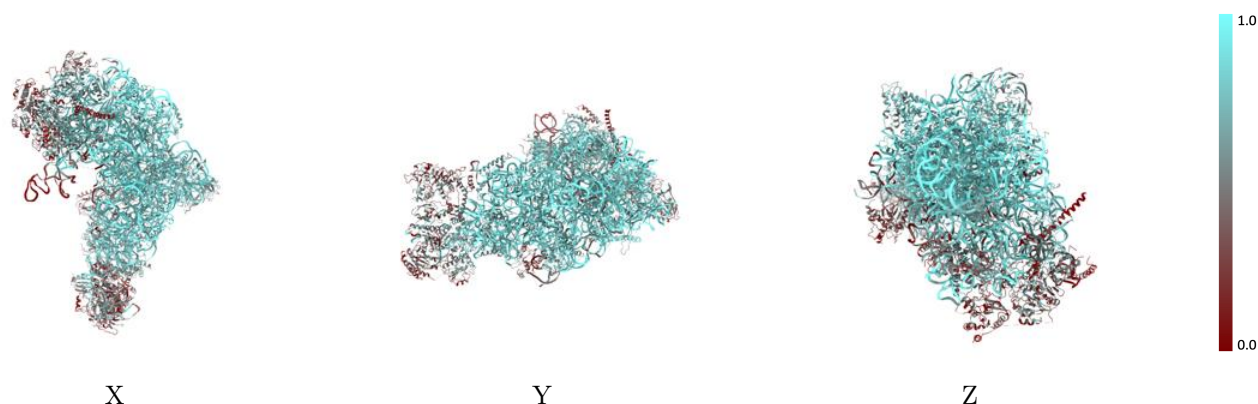
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



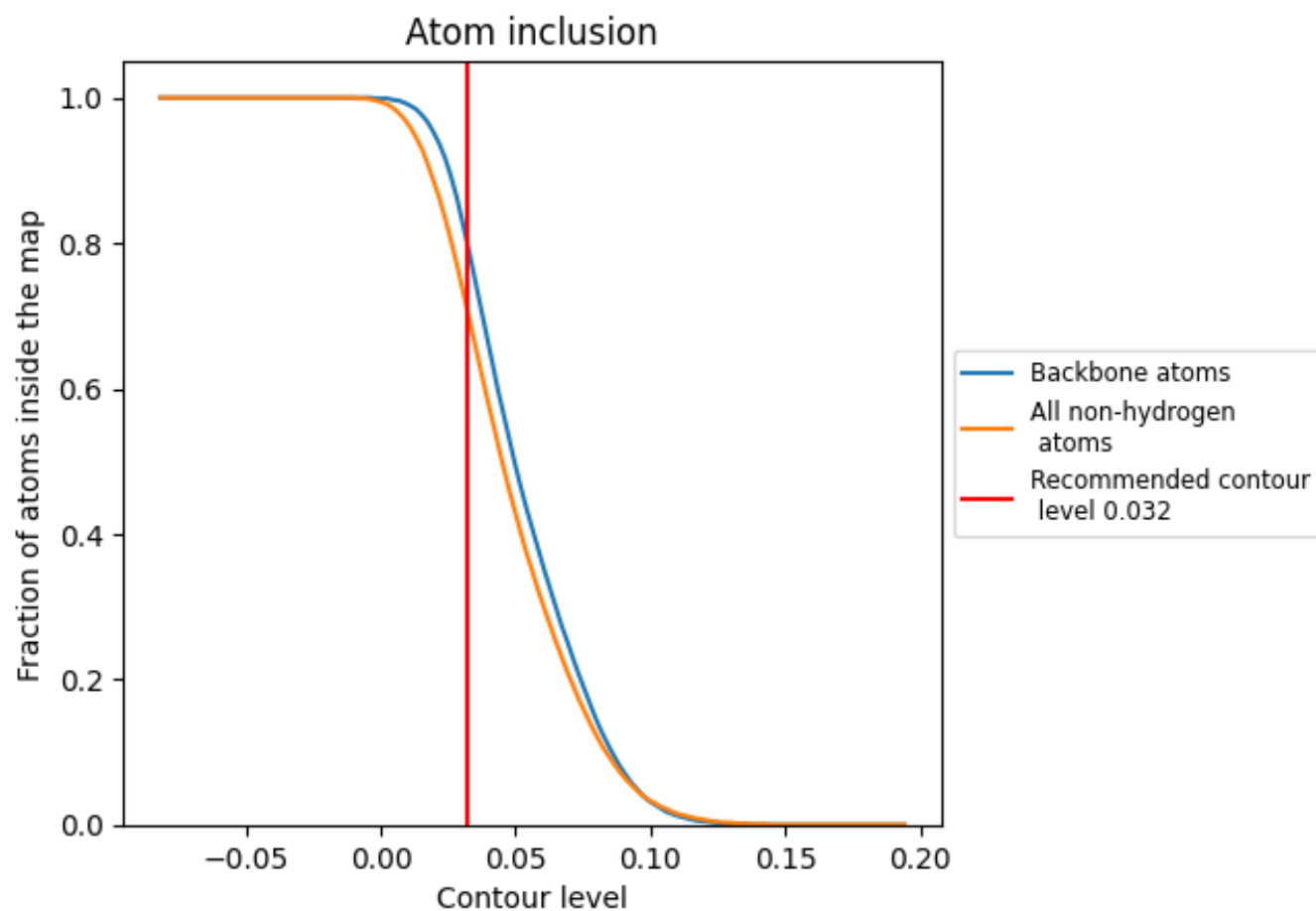
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7100	 0.3710
1	 0.8380	 0.3920
2	 0.8580	 0.3980
3	 0.8310	 0.4580
4	 0.7420	 0.4000
5	 0.7030	 0.4290
6	 0.7170	 0.2680
A	 0.3170	 0.1750
B	 0.7090	 0.3950
C	 0.8090	 0.4990
D	 0.4480	 0.2520
E	 0.7980	 0.4470
F	 0.8270	 0.4720
G	 0.6990	 0.4080
H	 0.6650	 0.4000
J	 0.2350	 0.1530
K	 0.3470	 0.1930
L	 0.8470	 0.4730
M	 0.7990	 0.4490
N	 0.7560	 0.4530
O	 0.8510	 0.5070
P	 0.7880	 0.4650
Q	 0.8170	 0.4720
S	 0.7700	 0.4260
V	 0.3320	 0.2520
W	 0.3570	 0.2620
Y	 0.8500	 0.4930
b	 0.3500	 0.2650
e	 0.7960	 0.5070
f	 0.8310	 0.5010
h	 0.7400	 0.4260
i	 0.6280	 0.3240
j	 0.8450	 0.4920
m	 0.3140	 0.1840
n	 0.3770	 0.1670



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Chain	Atom inclusion	Q-score
o	 0.4420	 0.2170
r	 0.5730	 0.3780
s	 0.4260	 0.3860
t	 0.4690	 0.2110
u	 0.4700	 0.2300
v	 0.7430	 0.4300
x	 0.7760	 0.4350
y	 0.3910	 0.2320
z	 0.1130	 0.1010