



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:47 AM UTC

PDB ID : 8ZDC / pdb_00008zdc
EMDB ID : EMD-39957
Title : Cryo-EM structure of the human ubiquitylated pre-40S ribosome with R1OK3
Authors : Huang, Z.; Wang, M.; Li, Y.; Beckmann, R.; Cheng, J.
Deposited on : 2024-05-01
Resolution : 3.80 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:

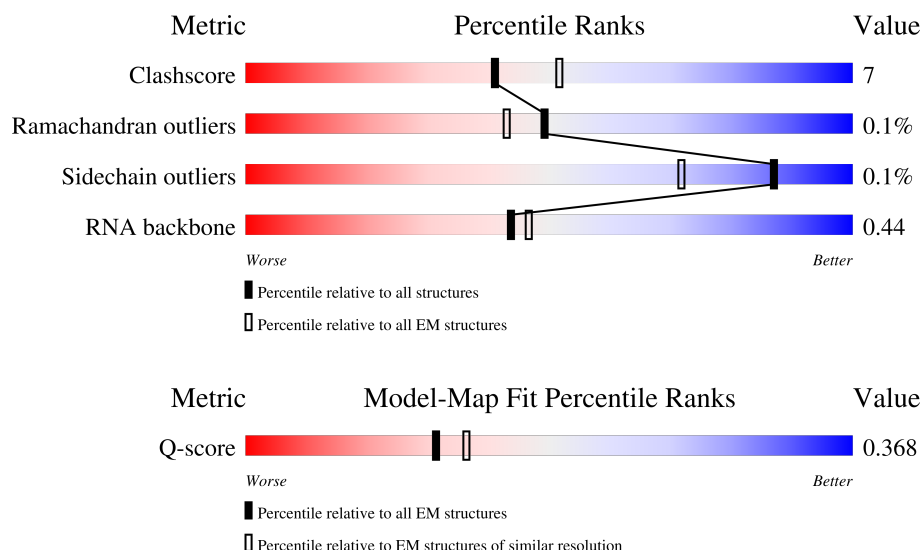
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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.



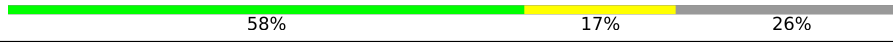
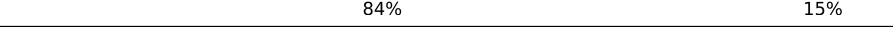
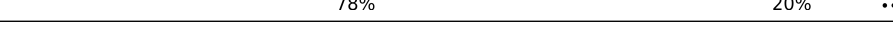
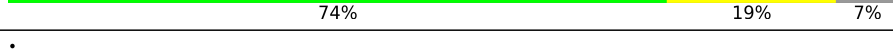
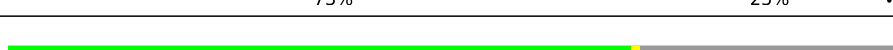
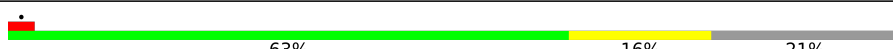
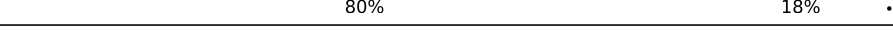
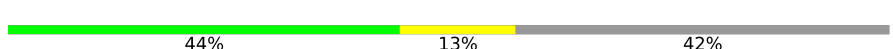
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	2	1873	
2	R	135	
3	A	295	

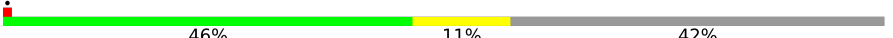
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Mol	Chain	Length	Quality of chain
4	B	264	
5	C	293	
6	E	263	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	L	158	
12	N	151	
13	O	151	
14	V	83	
15	W	130	
16	X	143	
17	Y	133	
18	b	84	
19	x	252	
20	y	412	
21	u	804	
22	t	475	
23	d	56	
24	D	243	
25	F	204	
26	K	165	
27	M	132	
28	P	145	

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Mol	Chain	Length	Quality of chain
29	Q	146	
30	S	152	
31	T	145	
32	U	119	
33	Z	125	
34	c	69	
35	g	317	
36	p	519	
37	i	76	
37	j	76	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 84228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1659	Total	C	N	O	P	0	0
			35427	15813	6366	11590	1658		

- Molecule 2 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	122	Total	C	N	O	S	0	0
			990	621	184	182	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 9 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 11 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 18 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 19 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	x	178	Total	C	N	O	0	0
			880	524	178	178		

- Molecule 20 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	325	Total	C	N	O	S	0	0
			2568	1622	473	463	10		

- Molecule 21 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	615	Total	C	N	O	S	0	0
			4954	3179	885	866	24		

- Molecule 22 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	61	Total	C	N	O		0	0
			517	316	107	94			

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 24 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 25 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 26 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 27 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 29 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 30 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 31 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 32 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 35 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	389	Total	C	N	O	S	0	0
			2419	1468	462	483	6		

- Molecule 37 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	i	73	Total	C	N	O	0	0
			361	215	73	73		
37	j	73	Total	C	N	O	0	0
			361	215	73	73		

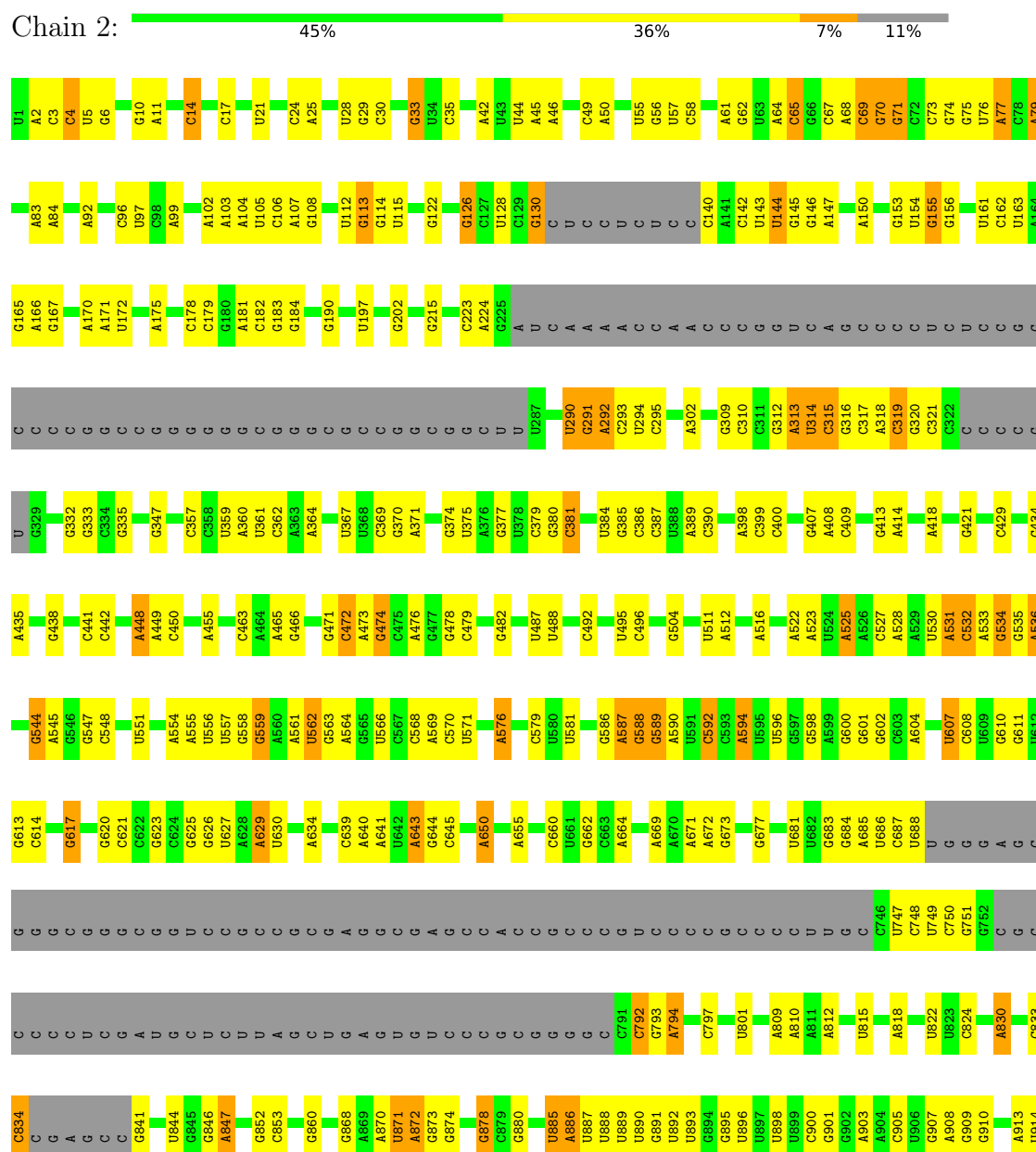
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	y	1	Total	Zn	0
			1	1	
38	d	1	Total	Zn	0
			1	1	

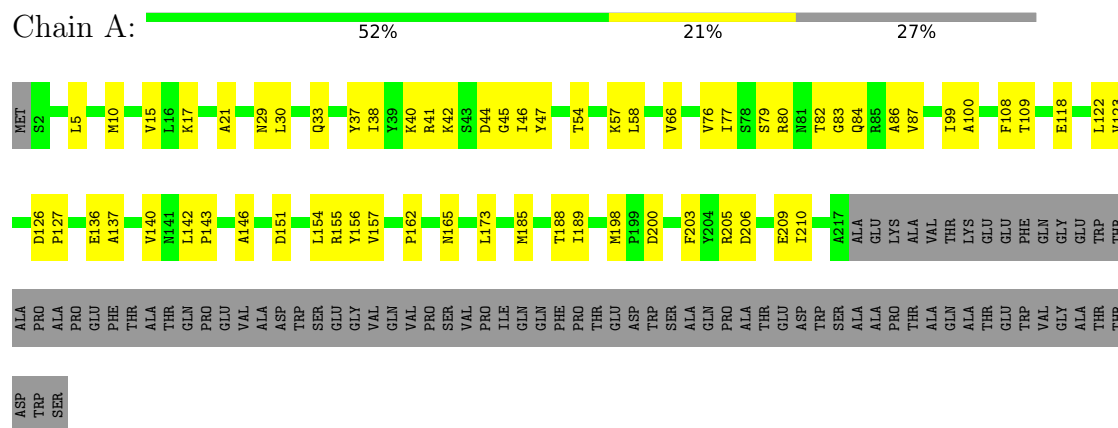
3 Residue-property plots [i](#)

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.

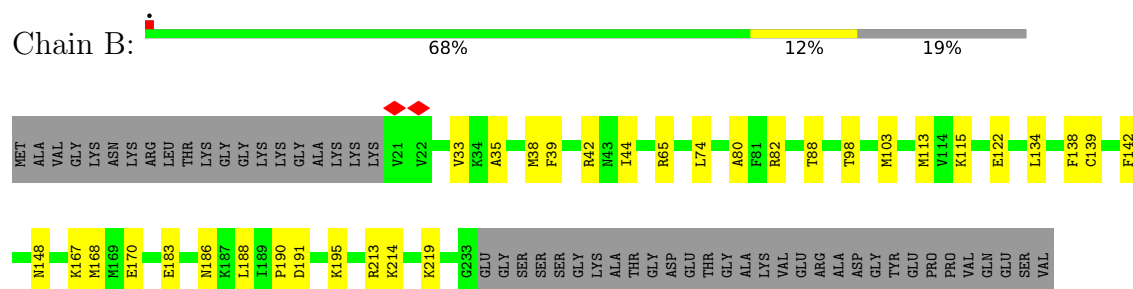
• Molecule 1: 18S rRNA



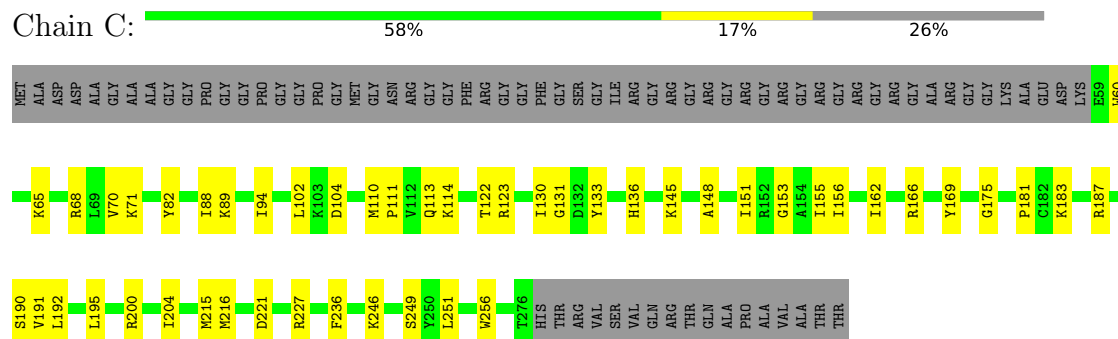




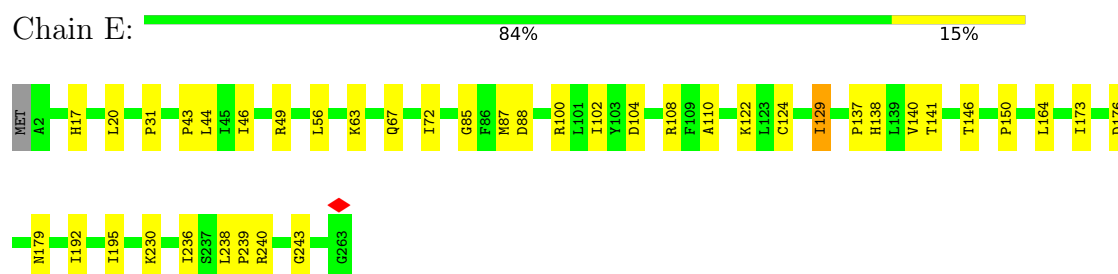
- Molecule 4: Small ribosomal subunit protein eS1



- Molecule 5: Small ribosomal subunit protein uS5

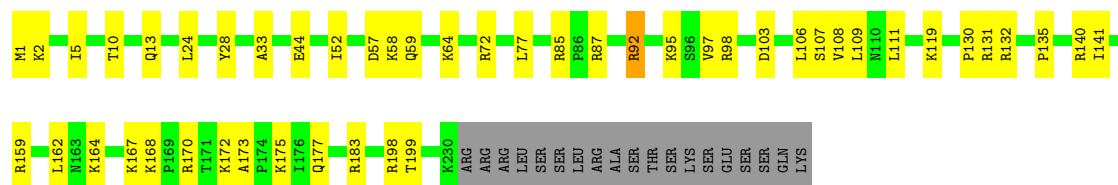


- Molecule 6: Small ribosomal subunit protein eS4, X isoform



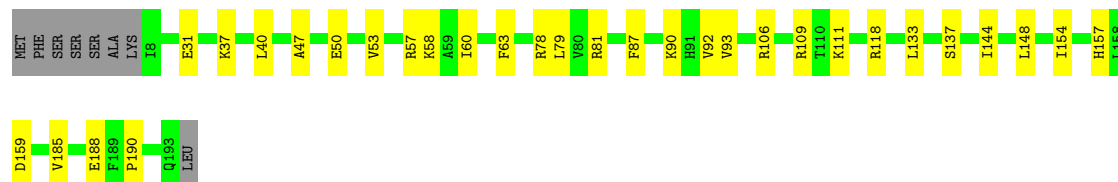
- Molecule 7: Small ribosomal subunit protein eS6





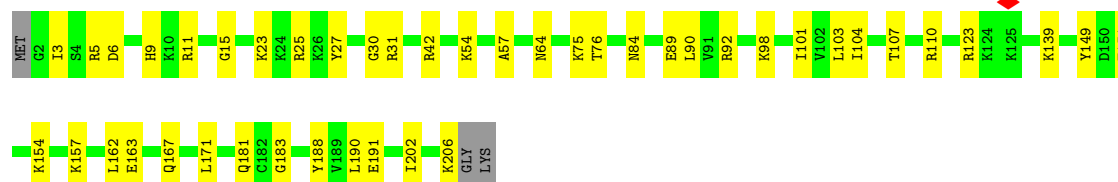
- Molecule 8: Small ribosomal subunit protein eS7

Chain H: 80% 16% .



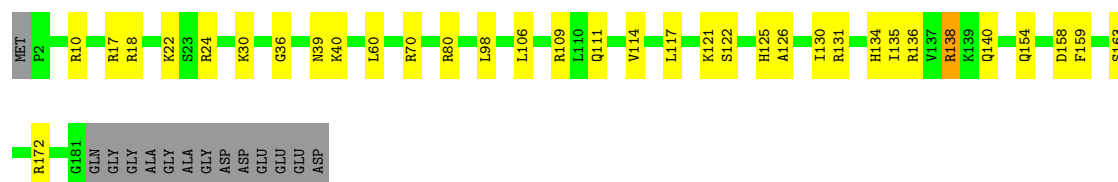
- Molecule 9: Small ribosomal subunit protein eS8

Chain I: 77% 21% .



- Molecule 10: Small ribosomal subunit protein uS4

Chain J: 75% 17% 7% .



- Molecule 11: Small ribosomal subunit protein uS17

Chain L: 80% 15% .



- Molecule 12: Small ribosomal subunit protein uS15

Chain N: 78% 20% ..



- Molecule 13: Small ribosomal subunit protein uS11

Chain O: 74% 16% 11%



- Molecule 14: Small ribosomal subunit protein eS21

Chain V: 82% 17% .



- Molecule 15: Small ribosomal subunit protein uS8

Chain W: 82% 16% ..



- Molecule 16: Small ribosomal subunit protein uS12

Chain X: 78% 20% .



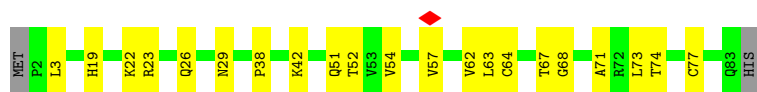
- Molecule 17: Small ribosomal subunit protein eS24

Chain Y: 74% 19% 7%



- Molecule 18: Small ribosomal subunit protein eS27

Chain b: 73% 25% .



- Molecule 19: RNA-binding protein PNO1

Chain x: 70% 29% .



[illegible]

Chain d: 80% 18%

Residue	State
MET	Grey
G2	Green
H10	Yellow
P11	Yellow
R12	Yellow
Q16	Green
R27	Yellow
I31	Yellow
R44	Green
Q45	Green
Y46	Yellow
F52	Yellow
I53	Yellow
K54	Yellow
L55	Green
D56	Yellow

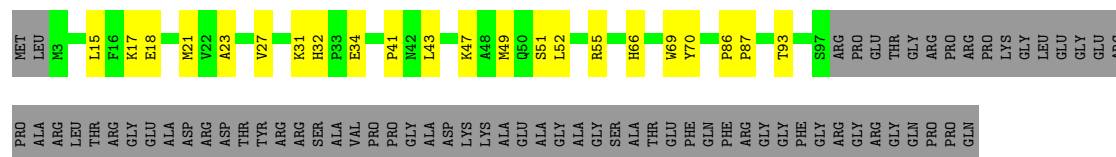
[illegible]

Chain F:



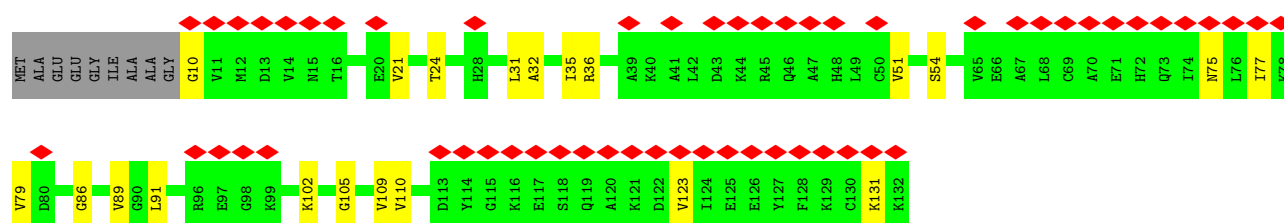
- Molecule 26: Small ribosomal subunit protein eS10

Chain K: 44% 13% 42%



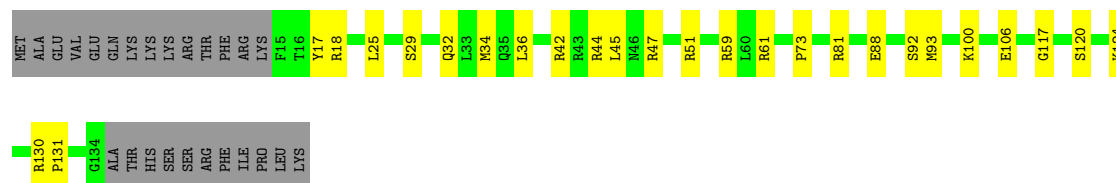
- Molecule 27: Small ribosomal subunit protein eS12

Chain M: 42% 77% 16% 7%



- Molecule 28: Small ribosomal subunit protein uS19

Chain P: 65% 18% 17%



- Molecule 29: Small ribosomal subunit protein uS9

Chain Q: 75% 20% 5%

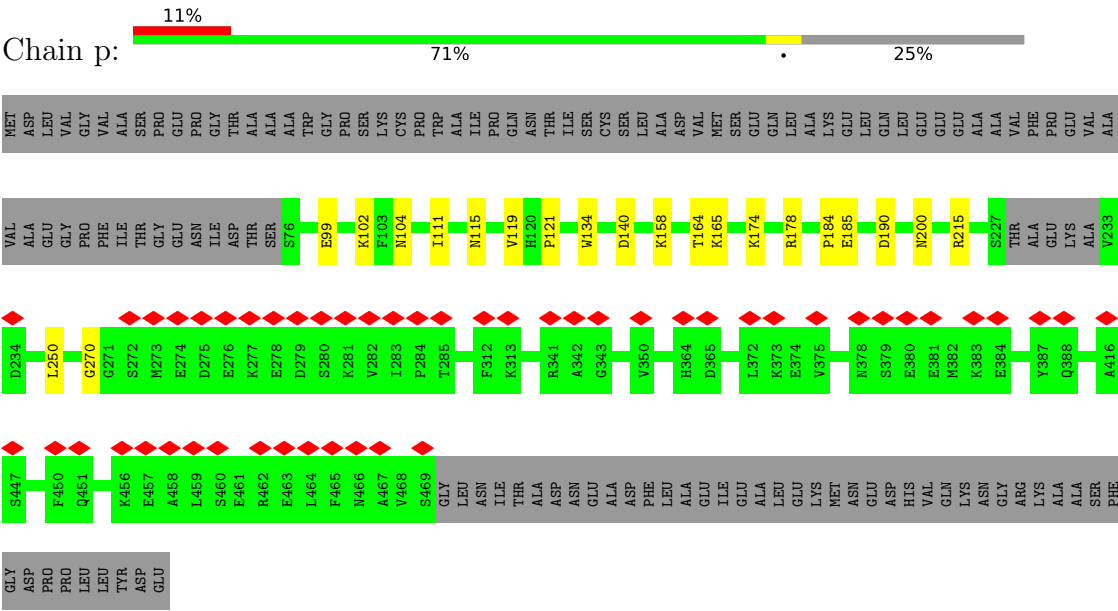


- Molecule 30: Small ribosomal subunit protein uS13

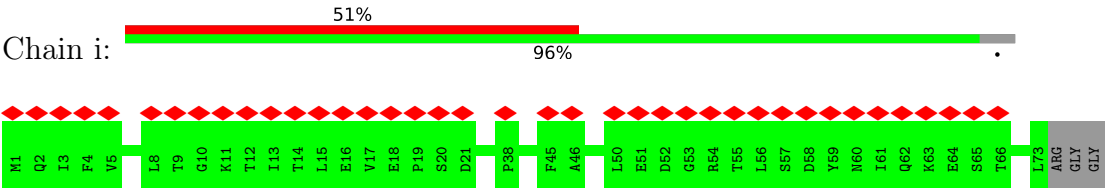
Chain S: 72% 22% 6%



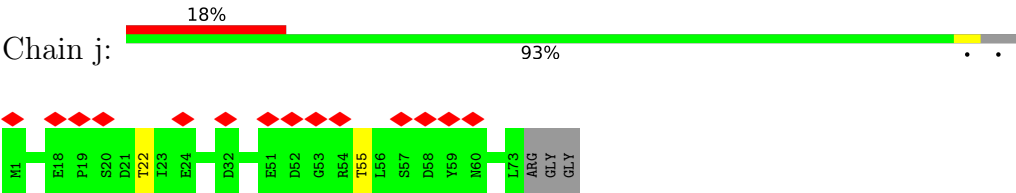
• Molecule 36: Serine/threonine-protein kinase RIO3



• Molecule 37: Ubiquitin



• Molecule 37: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	383.04, 383.04, 383.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.23	0/39613	0.39	1/61728 (0.0%)
2	R	0.30	0/1002	0.69	0/1345
3	A	0.26	0/1742	0.56	0/2367
4	B	0.18	0/1756	0.49	0/2350
5	C	0.30	0/1726	0.66	2/2332 (0.1%)
6	E	0.27	0/2118	0.58	0/2849
7	G	0.21	0/1885	0.53	1/2510 (0.0%)
8	H	0.17	0/1524	0.44	0/2042
9	I	0.26	0/1711	0.58	0/2282
10	J	0.24	0/1524	0.58	0/2035
11	L	0.31	0/1250	0.59	0/1673
12	N	0.24	0/1226	0.56	0/1649
13	O	0.18	0/1022	0.48	0/1372
14	V	0.22	0/631	0.54	0/844
15	W	0.29	0/1051	0.60	0/1406
16	X	0.24	0/1116	0.57	0/1490
17	Y	0.23	0/1031	0.56	1/1370 (0.1%)
18	b	0.19	0/653	0.53	0/876
19	x	0.15	0/879	0.45	0/1223
20	y	0.20	0/2618	0.47	0/3536
21	u	0.18	0/5076	0.50	0/6860
22	t	0.17	0/518	0.47	0/677
23	d	0.22	0/470	0.48	0/623
24	D	0.30	0/1780	0.66	0/2397
25	F	0.21	0/1516	0.62	0/2037
26	K	0.18	0/824	0.55	0/1112
27	M	0.18	0/963	0.56	0/1291
28	P	0.20	0/1003	0.55	0/1341
29	Q	0.25	0/1126	0.64	0/1506
30	S	0.15	0/1202	0.51	0/1610
31	T	0.22	0/1142	0.61	0/1530
32	U	0.26	0/813	0.62	1/1092 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.20	0/580	0.59	0/780
34	c	0.19	0/481	0.58	2/643 (0.3%)
35	g	0.16	0/2497	0.44	0/3399
36	p	0.18	0/2444	0.45	0/3338
37	i	0.11	0/360	0.35	0/500
37	j	0.13	0/360	0.37	0/500
All	All	0.23	0/89233	0.48	8/128515 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	W	0	1
24	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	36	ASP	CA-C-N	6.78	132.04	122.08
34	c	36	ASP	C-N-CA	6.78	132.04	122.08
7	G	10	THR	N-CA-C	-5.82	105.43	113.18
1	2	314	U	C2'-C3'-O3'	5.21	121.52	113.70
5	C	133	TYR	CA-C-N	5.21	131.50	121.54
5	C	133	TYR	C-N-CA	5.21	131.50	121.54
17	Y	42	GLU	N-CA-CB	5.04	118.10	110.28
32	U	57	PRO	N-CA-C	5.01	119.07	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	D	194	PRO	Peptide
15	W	28	ARG	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	2	35427	0	17889	441	0
2	R	990	0	1037	15	0
3	A	1705	0	1706	44	0
4	B	1729	0	1803	19	0
5	C	1690	0	1777	34	0
6	E	2076	0	2177	26	0
7	G	1862	0	2018	35	0
8	H	1501	0	1593	21	0
9	I	1682	0	1769	29	0
10	J	1499	0	1618	26	0
11	L	1229	0	1302	15	0
12	N	1202	0	1289	27	0
13	O	1009	0	1034	18	0
14	V	625	0	628	10	0
15	W	1034	0	1080	17	0
16	X	1098	0	1167	19	0
17	Y	1014	0	1082	18	0
18	b	640	0	665	13	0
19	x	880	0	403	1	0
20	y	2568	0	2624	41	0
21	u	4954	0	5014	74	0
22	t	517	0	566	10	0
23	d	459	0	452	12	0
24	D	1752	0	1848	30	0
25	F	1495	0	1549	24	0
26	K	800	0	818	15	0
27	M	953	0	990	13	0
28	P	984	0	1028	20	0
29	Q	1109	0	1174	19	0
30	S	1184	0	1244	22	0
31	T	1122	0	1153	15	0
32	U	803	0	873	16	0
33	Z	574	0	627	10	0
34	c	479	0	507	15	0
35	g	2440	0	2396	43	0
36	p	2419	0	1696	17	0
37	i	361	0	155	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	j	361	0	155	1	0
38	d	1	0	0	0	0
38	y	1	0	0	0	0
All	All	84228	0	66906	1027	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1027) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:24:C:H42	1:2:650:A:N6	1.58	0.99
1:2:24:C:N4	1:2:650:A:H61	1.59	0.99
1:2:1726:G:H1	1:2:1808:U:H3	1.01	0.97
1:2:1236:G:N2	1:2:1522:A:H62	1.62	0.96
1:2:1091:C:HO2'	15:W:2:VAL:N	1.62	0.96
1:2:944:A:H61	1:2:982:G:H1	0.97	0.95
21:u:258:VAL:HA	21:u:273:LYS:O	1.68	0.93
1:2:1710:C:H42	1:2:1823:A:N6	1.66	0.93
1:2:944:A:N6	1:2:982:G:H1	1.67	0.91
1:2:1236:G:H21	1:2:1522:A:N6	1.68	0.91
6:E:129:ILE:HA	6:E:138:HIS:O	1.71	0.90
29:Q:45:ARG:O	29:Q:48:GLN:HB3	1.71	0.90
1:2:197:U:H3	1:2:202:G:H1	1.22	0.85
1:2:1206:G:H1	1:2:1692:U:H3	0.89	0.84
1:2:1710:C:N4	1:2:1823:A:H61	1.76	0.84
1:2:1236:G:H21	1:2:1522:A:H62	0.84	0.83
1:2:140:C:H42	1:2:313:A:H61	1.27	0.81
32:U:56:MET:HB3	32:U:86:LYS:HB3	1.61	0.79
1:2:1342:U:C2	1:2:1483:A:N6	2.51	0.78
1:2:1342:U:C2	1:2:1483:A:C6	2.73	0.76
1:2:1710:C:N4	1:2:1823:A:N6	2.35	0.74
1:2:925:G:H1	1:2:1017:U:H3	1.37	0.73
29:Q:8:GLN:N	29:Q:99:TYR:HH	1.85	0.73
1:2:1095:C:N3	1:2:1149:A:N1	2.37	0.72
1:2:165:G:H2'	1:2:166:A:H8	1.55	0.72
5:C:123:ARG:HG2	5:C:145:LYS:HA	1.72	0.71
12:N:36:GLN:HG3	12:N:39:LYS:HZ3	1.56	0.71
1:2:1044:G:N7	22:t:427:LYS:NZ	2.39	0.70
1:2:24:C:N3	1:2:650:A:N1	2.40	0.70
1:2:957:A:H3'	1:2:958:G:H21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:723:VAL:HG13	21:u:751:MET:HE3	1.76	0.68
1:2:130:G:N1	1:2:181:A:N6	2.41	0.68
34:c:22:GLY:HA2	34:c:68:LEU:HB2	1.75	0.68
35:g:107:ASP:HB2	35:g:125:ARG:HD2	1.76	0.68
1:2:563:G:N7	1:2:586:G:N2	2.42	0.67
25:F:159:ARG:O	25:F:163:PHE:HB2	1.94	0.67
1:2:496:C:OP1	6:E:49:ARG:NH2	2.28	0.67
1:2:607:U:OP2	36:p:178:ARG:NH1	2.28	0.67
7:G:33:ALA:HA	7:G:52:ILE:O	1.95	0.67
4:B:134:LEU:HB3	4:B:219:LYS:HB2	1.75	0.67
5:C:183:LYS:HA	5:C:195:LEU:O	1.93	0.67
1:2:562:U:H2'	1:2:563:G:H8	1.59	0.67
5:C:192:LEU:HB3	5:C:227:ARG:HB3	1.77	0.67
1:2:1710:C:N3	1:2:1823:A:N1	2.42	0.66
1:2:1283:C:H42	27:M:102:LYS:HD3	1.61	0.66
7:G:162:LEU:HB3	7:G:170:ARG:HB3	1.78	0.66
30:S:39:ARG:NH2	31:T:36:THR:O	2.28	0.66
5:C:113:GLN:HA	5:C:122:THR:HA	1.77	0.66
1:2:1617:G:H3'	28:P:47:ARG:HH22	1.61	0.65
1:2:617:G:H4'	16:X:88:ASP:HB3	1.77	0.65
35:g:87:LEU:HB3	35:g:101:PHE:HB2	1.78	0.65
31:T:44:GLU:HG3	31:T:45:LEU:HG	1.78	0.64
1:2:563:G:C5	1:2:586:G:N2	2.66	0.64
1:2:1206:G:O6	1:2:1692:U:O4	2.15	0.64
1:2:943:U:H2'	1:2:944:A:H8	1.62	0.64
1:2:1123:C:O2'	4:B:148:ASN:O	2.16	0.64
1:2:1343:U:H3	1:2:1484:A:H62	1.44	0.64
21:u:732:ARG:HE	21:u:738:ARG:HH11	1.44	0.64
6:E:238:LEU:HD12	6:E:239:PRO:HD2	1.80	0.64
1:2:1263:U:H4'	23:d:27:ARG:HD2	1.78	0.64
1:2:1363:C:C5	1:2:1375:G:N1	2.63	0.64
8:H:50:GLU:HG2	8:H:58:LYS:HE3	1.78	0.64
21:u:733:THR:HG22	21:u:735:TRP:H	1.62	0.64
1:2:64:A:H2	1:2:83:A:H62	1.44	0.63
1:2:379:C:OP2	9:I:181:GLN:NE2	2.31	0.63
30:S:138:THR:HA	30:S:141:ARG:HH21	1.64	0.63
35:g:31:ILE:HB	35:g:43:TRP:HB2	1.80	0.63
35:g:290:ALA:HB3	35:g:299:PHE:HB2	1.80	0.63
10:J:136:ARG:NH1	10:J:138:ARG:O	2.31	0.63
3:A:79:SER:OG	20:y:345:ARG:NH1	2.31	0.63
12:N:112:LYS:O	12:N:115:LEU:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1017:U:OP1	12:N:62:GLN:NE2	2.32	0.63
28:P:18:ARG:HG3	30:S:93:GLY:HA3	1.80	0.63
1:2:926:A:H61	1:2:1015:U:H3	1.46	0.62
30:S:6:PRO:HB2	30:S:9:PHE:HB2	1.81	0.62
1:2:1396:A:O2'	1:2:1398:G:N7	2.33	0.62
1:2:1679:A:OP1	34:c:20:ARG:NH2	2.33	0.62
17:Y:22:GLN:HE21	17:Y:72:PHE:HZ	1.47	0.62
1:2:1464:C:H4'	2:R:60:ARG:HE	1.64	0.62
3:A:76:VAL:HG12	3:A:123:VAL:HB	1.82	0.62
3:A:108:PHE:HB2	3:A:136:GLU:HB3	1.82	0.62
1:2:1513:C:H2'	1:2:1514:G:H8	1.65	0.62
1:2:1260:A:C2	1:2:1617:G:N2	2.68	0.62
21:u:596:MET:O	21:u:651:VAL:HA	2.00	0.62
1:2:1748:G:H1	1:2:1786:U:H3	1.48	0.62
21:u:298:GLN:NE2	21:u:348:ASP:OD2	2.32	0.62
21:u:705:LYS:HB2	21:u:712:VAL:HB	1.81	0.62
1:2:1619:A:OP1	28:P:44:ARG:NH1	2.33	0.62
3:A:17:LYS:HB3	3:A:173:LEU:HD11	1.82	0.61
1:2:878:G:H1	1:2:908:A:H61	1.47	0.61
1:2:941:C:H2'	1:2:942:G:H8	1.66	0.61
1:2:1091:C:O2'	15:W:2:VAL:N	2.33	0.61
25:F:100:ILE:HA	25:F:178:ILE:HD11	1.81	0.61
1:2:1297:U:OP2	28:P:59:ARG:NH2	2.34	0.61
30:S:3:LEU:N	33:Z:90:GLU:OE2	2.34	0.61
1:2:126:G:OP1	7:G:198:ARG:NH1	2.33	0.61
1:2:830:A:OP2	1:2:846:G:N2	2.33	0.61
1:2:1588:A:H2'	1:2:1589:A:C8	2.35	0.61
3:A:37:TYR:OH	3:A:57:LYS:NZ	2.34	0.61
35:g:36:ARG:HD2	35:g:65:PHE:HB3	1.83	0.61
3:A:38:ILE:HD11	3:A:47:TYR:HB3	1.82	0.61
29:Q:32:ILE:HG23	29:Q:68:ILE:HB	1.83	0.61
1:2:860:G:H21	15:W:107:SER:HB3	1.66	0.60
25:F:75:SER:O	25:F:159:ARG:NH2	2.34	0.60
1:2:170:A:OP2	7:G:140:ARG:NH1	2.34	0.60
1:2:525:A:N6	1:2:589:G:O6	2.33	0.60
1:2:1213:C:H2'	1:2:1214:A:H8	1.66	0.60
16:X:51:VAL:HA	16:X:72:VAL:HG12	1.81	0.60
5:C:200:ARG:HB2	10:J:98:LEU:HD13	1.82	0.60
8:H:154:ILE:HB	8:H:185:VAL:HG22	1.83	0.60
1:2:1275:G:OP2	26:K:47:LYS:NZ	2.35	0.60
1:2:1608:U:O4	1:2:1632:G:N2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:251:ALA:HB3	21:u:583:SER:HB2	1.84	0.60
37:j:22:THR:HA	37:j:55:THR:HA	1.84	0.60
8:H:93:VAL:HG11	8:H:133:LEU:HD12	1.82	0.60
14:V:51:LYS:HD2	14:V:78:ILE:HD11	1.84	0.60
28:P:18:ARG:NH1	28:P:36:LEU:O	2.34	0.59
1:2:1097:G:N2	20:y:325:SER:OG	2.34	0.59
1:2:1722:G:O6	1:2:1812:U:O2	2.20	0.59
35:g:30:MET:HE1	35:g:44:LYS:HG3	1.85	0.59
1:2:1650:A:H5''	29:Q:139:ALA:HB2	1.83	0.59
21:u:262:PRO:HA	21:u:270:GLY:HA3	1.85	0.59
1:2:1606:G:O2'	1:2:1632:G:N2	2.35	0.59
1:2:928:G:H2'	1:2:929:G:C8	2.38	0.59
4:B:190:PRO:O	4:B:195:LYS:NZ	2.36	0.59
1:2:681:U:O2'	1:2:1160:U:OP1	2.20	0.59
3:A:140:VAL:HG13	3:A:142:LEU:HD23	1.83	0.59
17:Y:10:ARG:HG2	17:Y:11:LYS:HG3	1.84	0.59
31:T:9:VAL:O	31:T:11:GLN:NE2	2.36	0.59
1:2:1397:U:O4	29:Q:90:LYS:NZ	2.36	0.58
3:A:40:LYS:NZ	3:A:41:ARG:O	2.31	0.58
1:2:1054:G:H2'	1:2:1055:A:H8	1.66	0.58
4:B:65:ARG:HH22	13:O:51:GLU:HB2	1.67	0.58
6:E:137:PRO:HG2	6:E:150:PRO:HD2	1.83	0.58
21:u:112:HIS:HB2	21:u:123:MET:HB2	1.86	0.58
21:u:600:ARG:NH2	21:u:606:GLU:O	2.36	0.58
1:2:885:U:O2	1:2:901:G:N2	2.32	0.58
35:g:46:THR:H	35:g:53:GLY:HA2	1.69	0.58
11:L:126:VAL:HG12	11:L:145:VAL:HG22	1.85	0.58
9:I:6:ASP:OD1	9:I:9:HIS:ND1	2.36	0.58
10:J:18:ARG:O	10:J:24:ARG:NH1	2.36	0.58
21:u:625:ALA:HB1	21:u:654:VAL:HG21	1.84	0.58
1:2:1658:G:OP2	1:2:1660:C:N4	2.36	0.58
12:N:72:LEU:HA	12:N:75:LEU:HB2	1.86	0.58
21:u:138:ALA:HB1	21:u:146:VAL:HG22	1.86	0.58
1:2:1217:A:O2'	1:2:1684:C:N3	2.34	0.58
8:H:78:ARG:HA	8:H:81:ARG:HG2	1.85	0.58
10:J:114:VAL:HG21	10:J:135:ILE:HD13	1.86	0.58
1:2:1714:U:O2'	22:t:469:ASN:ND2	2.37	0.58
9:I:11:ARG:NH1	9:I:15:GLY:O	2.36	0.58
1:2:384:U:O4	9:I:5:ARG:NH2	2.36	0.58
1:2:594:A:H61	1:2:643:A:H5''	1.68	0.58
1:2:1342:U:O2	1:2:1483:A:C6	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1610:G:N2	30:S:85:ASN:O	2.38	0.57
3:A:42:LYS:NZ	3:A:46:ILE:O	2.37	0.57
1:2:871:U:H3'	1:2:872:A:H4'	1.87	0.57
21:u:139:ARG:NH1	21:u:140:PRO:O	2.38	0.57
35:g:24:THR:HG23	35:g:27:PHE:H	1.69	0.57
1:2:1622:U:H5''	1:2:1623:A:H4'	1.86	0.57
1:2:623:G:O3'	36:p:215:ARG:NH2	2.38	0.57
7:G:33:ALA:CA	7:G:52:ILE:O	2.53	0.57
16:X:135:LYS:HB3	16:X:137:LYS:HZ3	1.68	0.57
35:g:61:GLY:O	35:g:88:ARG:NH1	2.36	0.57
4:B:80:ALA:HB1	13:O:128:ARG:HH12	1.70	0.57
9:I:163:GLU:O	9:I:167:GLN:NE2	2.38	0.57
1:2:1324:G:H1	1:2:1504:U:H3	1.53	0.57
1:2:834:C:O2'	1:2:841:G:N2	2.38	0.57
1:2:1050:A:OP1	1:2:1846:G:N2	2.38	0.57
21:u:617:HIS:HB2	21:u:666:LEU:HB2	1.87	0.57
18:b:64:CYS:HB3	18:b:73:LEU:HD13	1.87	0.57
35:g:107:ASP:OD2	35:g:125:ARG:NH1	2.38	0.57
7:G:159:ARG:HD3	7:G:173:ALA:HB2	1.86	0.56
8:H:47:ALA:HB3	8:H:63:PHE:HB2	1.87	0.56
1:2:975:G:OP1	13:O:98:ARG:NH1	2.38	0.56
6:E:87:MET:HE1	6:E:236:ILE:HD13	1.86	0.56
1:2:77:A:H2	7:G:175:LYS:HG3	1.70	0.56
1:2:166:A:H1'	7:G:13:GLN:HE22	1.70	0.56
1:2:319:C:H2'	1:2:320:G:H8	1.71	0.56
1:2:991:G:N2	20:y:405:ARG:O	2.39	0.56
7:G:57:ASP:HA	7:G:106:LEU:HA	1.88	0.56
9:I:188:TYR:OH	11:L:12:LYS:NZ	2.39	0.56
29:Q:132:PHE:O	29:Q:140:ARG:NH1	2.38	0.56
1:2:511:U:O2'	1:2:576:A:N6	2.38	0.56
1:2:1656:G:O6	1:2:1668:U:O4	2.24	0.56
1:2:1677:U:OP1	25:F:71:ARG:NH2	2.38	0.56
20:y:301:SER:HG	20:y:305:THR:HG1	1.46	0.56
27:M:75:ASN:HD21	27:M:131:LYS:HD3	1.70	0.56
1:2:155:G:H2'	1:2:156:G:H8	1.71	0.56
1:2:566:U:OP1	21:u:199:LYS:NZ	2.38	0.56
1:2:1498:A:OP1	24:D:27:ARG:NH2	2.39	0.56
1:2:61:A:HO2'	1:2:315:C:HO2'	1.52	0.56
1:2:1689:C:H2'	1:2:1690:U:C6	2.40	0.56
11:L:94:HIS:O	11:L:102:PHE:HA	2.06	0.56
13:O:97:LEU:HD11	13:O:112:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:613:G:N1	1:2:629:A:OP1	2.37	0.56
1:2:747:U:O2'	8:H:109:ARG:NE	2.39	0.56
1:2:1601:A:OP2	1:2:1636:G:N2	2.38	0.56
36:p:99:GLU:HA	36:p:102:LYS:HD2	1.87	0.56
1:2:1036:A:N3	1:2:1844:U:O2'	2.39	0.56
1:2:69:C:OP2	7:G:167:LYS:NZ	2.39	0.56
1:2:527:C:H2'	1:2:528:A:H8	1.70	0.56
1:2:996:A:OP1	12:N:114:ARG:NH2	2.39	0.56
15:W:3:ARG:HH12	15:W:28:ARG:HH21	1.53	0.56
21:u:640:LEU:HD22	21:u:773:VAL:HG11	1.87	0.56
1:2:5:U:H2'	1:2:6:G:H8	1.71	0.55
1:2:953:C:O2	13:O:55:ARG:NH1	2.36	0.55
25:F:50:PRO:HG3	25:F:69:VAL:HB	1.88	0.55
26:K:17:LYS:HG3	26:K:18:GLU:HG3	1.87	0.55
8:H:157:HIS:ND1	8:H:188:GLU:OE2	2.39	0.55
9:I:57:ALA:HB2	9:I:183:GLY:HA2	1.88	0.55
20:y:253:LEU:HB3	20:y:259:LEU:HD13	1.87	0.55
24:D:143:ARG:HB3	36:p:184:PRO:HD3	1.88	0.55
30:S:34:LYS:HB2	30:S:100:ALA:HA	1.88	0.55
1:2:1076:G:H5''	12:N:106:ARG:HH22	1.69	0.55
1:2:1581:C:H5'	1:2:1582:C:H5	1.70	0.55
25:F:55:ARG:O	25:F:62:ARG:NH2	2.39	0.55
31:T:18:LEU:HD13	31:T:134:ILE:HD13	1.88	0.55
35:g:17:TRP:HB2	35:g:36:ARG:HG3	1.89	0.55
1:2:1261:C:O2	23:d:10:HIS:NE2	2.40	0.55
1:2:1262:C:H1'	23:d:12:ARG:HH12	1.72	0.55
1:2:1373:C:O2'	2:R:10:LYS:NZ	2.36	0.55
8:H:157:HIS:HB3	8:H:190:PRO:HG3	1.88	0.55
1:2:1160:U:O4	16:X:2:GLY:N	2.39	0.55
1:2:178:C:H2'	1:2:179:C:C6	2.42	0.55
1:2:1130:G:N2	1:2:1130:G:OP2	2.39	0.55
1:2:1407:U:OP1	29:Q:71:ARG:NH2	2.40	0.55
13:O:44:VAL:HG13	13:O:53:ILE:HB	1.89	0.55
35:g:152:SER:H	35:g:169:GLY:HA2	1.71	0.55
1:2:1541:G:H4'	31:T:15:VAL:HG21	1.89	0.55
2:R:87:GLU:HG2	2:R:88:VAL:HG23	1.88	0.55
21:u:703:PRO:HB3	21:u:713:VAL:HG22	1.89	0.55
1:2:1725:U:H2'	1:2:1726:G:H8	1.72	0.55
3:A:54:THR:OG1	3:A:162:PRO:O	2.22	0.55
11:L:7:GLU:OE1	11:L:11:GLN:NE2	2.39	0.55
34:c:13:ARG:HB2	34:c:33:GLU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:p:104:ASN:HD22	36:p:111:ILE:H	1.55	0.55
1:2:165:G:OP2	1:2:165:G:N2	2.38	0.54
1:2:801:U:O4	8:H:106:ARG:NH2	2.39	0.54
1:2:948:C:H2'	1:2:949:G:H8	1.72	0.54
1:2:1313:A:H4'	1:2:1314:U:H5'	1.88	0.54
1:2:1597:C:OP2	33:Z:85:ARG:NH2	2.40	0.54
21:u:637:LYS:HG3	21:u:692:MET:HG2	1.89	0.54
35:g:258:ILE:O	35:g:267:VAL:N	2.40	0.54
1:2:983:A:OP1	1:2:1073:U:O2'	2.25	0.54
24:D:45:ARG:NH2	24:D:84:VAL:O	2.39	0.54
1:2:561:A:O2'	10:J:134:HIS:NE2	2.28	0.54
1:2:943:U:H2'	1:2:944:A:C8	2.40	0.54
1:2:1277:C:H5''	26:K:55:ARG:HE	1.72	0.54
1:2:1722:G:O6	1:2:1812:U:C2	2.60	0.54
5:C:102:LEU:HD22	5:C:130:ILE:HG12	1.89	0.54
16:X:70:VAL:HG21	16:X:94:ILE:HD13	1.89	0.54
25:F:201:LYS:HD3	25:F:204:ARG:HE	1.72	0.54
26:K:31:LYS:HA	26:K:41:PRO:HA	1.89	0.54
2:R:95:ILE:HD11	2:R:118:GLN:HB2	1.89	0.54
2:R:66:VAL:HB	2:R:69:ILE:HG12	1.88	0.54
6:E:100:ARG:HG2	6:E:102:ILE:HG12	1.90	0.54
35:g:127:LYS:HE2	35:g:149:GLU:HA	1.90	0.54
5:C:246:LYS:HA	5:C:249:SER:HB2	1.89	0.54
19:x:110:ASN:O	19:x:114:ARG:N	2.40	0.54
1:2:1726:G:H2'	1:2:1727:G:H8	1.72	0.54
9:I:202:ILE:HG22	9:I:206:LYS:HE2	1.88	0.54
21:u:735:TRP:NE1	21:u:762:GLN:O	2.40	0.54
1:2:1854:U:H2'	1:2:1855:G:H8	1.71	0.54
1:2:1401:A:H4'	32:U:52:GLY:HA3	1.90	0.54
3:A:126:ASP:OD1	3:A:165:ASN:ND2	2.41	0.54
21:u:261:VAL:HB	21:u:271:THR:HB	1.90	0.54
1:2:171:A:H5''	7:G:177:GLN:HG2	1.90	0.54
1:2:925:G:OP1	12:N:121:ARG:NH1	2.41	0.54
34:c:12:ALA:HB3	34:c:56:LEU:HB3	1.90	0.54
33:Z:68:ILE:HB	33:Z:109:TYR:HB2	1.88	0.53
24:D:167:TYR:OH	24:D:202:LYS:O	2.25	0.53
24:D:32:ASP:OD2	24:D:65:ARG:NH1	2.42	0.53
1:2:1219:C:O2'	34:c:26:GLN:OE1	2.26	0.53
1:2:1562:C:H2'	1:2:1563:G:H8	1.72	0.53
26:K:23:ALA:O	26:K:66:HIS:ND1	2.41	0.53
1:2:145:G:H2'	1:2:146:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:167:G:O3'	7:G:131:ARG:NH1	2.41	0.53
16:X:60:LYS:HE2	16:X:116:PRO:HD3	1.90	0.53
35:g:11:LEU:HB2	35:g:307:VAL:HB	1.91	0.53
1:2:562:U:H2'	1:2:563:G:C8	2.43	0.53
1:2:581:U:H4'	17:Y:66:GLY:HA2	1.91	0.53
1:2:1095:C:O2	1:2:1149:A:N6	2.40	0.53
4:B:183:GLU:HA	4:B:186:ASN:HB2	1.90	0.53
8:H:144:ILE:HB	15:W:52:ILE:HB	1.90	0.53
13:O:35:ALA:HB2	13:O:112:ALA:HB2	1.91	0.53
17:Y:25:ILE:HG21	17:Y:40:ILE:HD11	1.89	0.53
1:2:1203:G:O2'	1:2:1205:C:N4	2.42	0.53
7:G:33:ALA:N	7:G:52:ILE:O	2.42	0.53
9:I:101:ILE:HD12	9:I:190:LEU:HD11	1.89	0.53
36:p:250:LEU:HA	36:p:270:GLY:HA2	1.91	0.53
1:2:686:U:O2	8:H:118:ARG:NH2	2.34	0.53
20:y:119:PRO:HB2	20:y:295:LYS:HB3	1.91	0.53
21:u:503:TYR:HB3	21:u:769:LEU:HB3	1.91	0.53
1:2:1343:U:H3	1:2:1484:A:N6	2.06	0.53
7:G:85:ARG:O	7:G:87:ARG:NH1	2.42	0.53
9:I:103:LEU:HA	9:I:171:LEU:O	2.09	0.53
9:I:154:LYS:O	9:I:157:LYS:NZ	2.42	0.53
31:T:82:ARG:HA	31:T:91:HIS:O	2.09	0.53
1:2:1797:U:H2'	1:2:1798:C:C6	2.43	0.53
11:L:4:ILE:HD11	11:L:54:THR:HG23	1.89	0.53
1:2:380:G:OP1	9:I:31:ARG:NH1	2.35	0.52
1:2:878:G:H1	1:2:908:A:N6	2.06	0.52
1:2:1541:G:N2	31:T:12:GLN:OE1	2.42	0.52
3:A:157:VAL:O	14:V:65:SER:OG	2.26	0.52
3:A:200:ASP:HA	3:A:203:PHE:CD2	2.43	0.52
3:A:127:PRO:HD3	3:A:146:ALA:HB1	1.91	0.52
21:u:675:MET:HE1	21:u:790:LEU:H	1.75	0.52
1:2:33:G:O2'	1:2:564:A:O2'	2.26	0.52
1:2:1872:G:H21	20:y:121:THR:HG22	1.74	0.52
3:A:155:ARG:HG2	3:A:156:TYR:HD2	1.74	0.52
6:E:56:LEU:HD11	17:Y:72:PHE:HE2	1.74	0.52
6:E:140:VAL:HG22	6:E:146:THR:HG22	1.91	0.52
24:D:166:TYR:OH	24:D:202:LYS:NZ	2.37	0.52
27:M:51:VAL:HB	27:M:109:VAL:HB	1.91	0.52
1:2:613:G:N2	1:2:626:G:OP1	2.41	0.52
1:2:1215:C:H42	1:2:1220:A:H61	1.57	0.52
4:B:82:ARG:HH12	4:B:191:ASP:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:118:GLU:HB2	5:C:65:LYS:HE3	1.92	0.52
21:u:260:PHE:HB2	21:u:570:VAL:HG21	1.92	0.52
5:C:169:TYR:OH	5:C:175:GLY:O	2.28	0.52
1:2:317:C:OP2	7:G:183:ARG:NH1	2.33	0.52
1:2:367:U:H4'	1:2:371:A:C8	2.45	0.52
1:2:377:G:H5''	9:I:98:LYS:HB3	1.90	0.52
1:2:495:U:OP1	6:E:49:ARG:NH1	2.42	0.52
1:2:1550:G:H3'	1:2:1579:A:H61	1.75	0.52
1:2:1503:C:H4'	21:u:702:HIS:CE1	2.44	0.52
10:J:117:LEU:HD21	10:J:154:GLN:HE21	1.74	0.52
3:A:33:GLN:HB3	3:A:154:LEU:HD12	1.92	0.52
9:I:163:GLU:HG3	9:I:167:GLN:HE22	1.74	0.52
35:g:172:LYS:HB3	35:g:191:HIS:HB2	1.92	0.52
1:2:833:C:H2'	1:2:834:C:H4'	1.92	0.52
1:2:1301:A:OP1	28:P:51:ARG:NH2	2.43	0.52
1:2:21:U:O2	10:J:17:ARG:NH2	2.43	0.51
1:2:986:G:OP2	1:2:988:C:N4	2.43	0.51
1:2:1531:A:H4'	1:2:1605:G:H4'	1.93	0.51
18:b:62:VAL:HG13	18:b:74:THR:HG21	1.91	0.51
35:g:245:ARG:NH1	35:g:295:GLY:O	2.44	0.51
5:C:60:TRP:HH2	5:C:70:VAL:HG12	1.74	0.51
1:2:815:U:OP1	10:J:10:ARG:NH2	2.42	0.51
1:2:1528:G:O2'	1:2:1666:C:OP1	2.28	0.51
1:2:1600:G:C6	1:2:1602:U:O2	2.63	0.51
23:d:52:PHE:HE2	32:U:63:ILE:HD13	1.76	0.51
35:g:298:LEU:HB2	35:g:310:TRP:HB2	1.93	0.51
17:Y:59:GLY:O	17:Y:71:GLY:CA	2.59	0.51
21:u:594:LEU:HD13	21:u:656:ALA:HB3	1.92	0.51
1:2:1217:A:H2'	1:2:1218:C:H6	1.76	0.51
4:B:35:ALA:HB3	4:B:42:ARG:HA	1.92	0.51
7:G:1:MET:HE1	7:G:109:LEU:HB2	1.93	0.51
11:L:22:ARG:HH21	11:L:27:GLU:HG3	1.75	0.51
16:X:123:VAL:HG12	16:X:124:LYS:HG3	1.93	0.51
36:p:174:LYS:HD3	36:p:178:ARG:HH21	1.74	0.51
1:2:1341:C:H4'	1:2:1342:U:H5'	1.92	0.51
8:H:137:SER:HB2	8:H:159:ASP:HB3	1.93	0.51
21:u:727:LYS:HA	21:u:741:ILE:HD11	1.92	0.51
24:D:212:GLU:O	36:p:115:ASN:ND2	2.42	0.51
1:2:1786:U:H2'	1:2:1787:G:H8	1.75	0.51
20:y:7:VAL:HG21	20:y:24:GLY:HA3	1.92	0.51
1:2:1415:C:O2'	31:T:132:ASP:OD2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1741:U:OP1	9:I:42:ARG:NH1	2.44	0.51
1:2:587:A:OP2	10:J:172:ARG:NH2	2.44	0.51
1:2:610:G:H2'	1:2:611:G:H8	1.75	0.51
1:2:1210:G:H2'	1:2:1211:G:C8	2.46	0.51
1:2:1758:G:C2	1:2:1775:U:O2	2.63	0.51
1:2:105:U:H2'	1:2:106:C:O4'	2.11	0.51
1:2:1338:G:H4'	32:U:74:SER:H	1.76	0.51
1:2:919:A:OP2	12:N:64:ARG:NH1	2.43	0.50
1:2:1368:U:O3'	2:R:2:GLY:N	2.44	0.50
1:2:1391:C:H1'	23:d:56:ASP:HB3	1.93	0.50
1:2:1669:G:OP1	32:U:79:ARG:NH1	2.44	0.50
1:2:1718:G:H21	1:2:1815:A:H62	1.58	0.50
1:2:1779:G:H2'	1:2:1780:G:C8	2.46	0.50
21:u:703:PRO:HA	21:u:713:VAL:HA	1.92	0.50
3:A:83:GLY:O	3:A:86:ALA:HB3	2.11	0.50
13:O:103:ASN:ND2	13:O:141:ARG:O	2.44	0.50
20:y:263:ALA:HB3	20:y:300:VAL:HB	1.94	0.50
22:t:418:ARG:HB3	22:t:430:ARG:HH12	1.77	0.50
1:2:617:G:C6	1:2:625:G:C2	2.99	0.50
8:H:31:GLU:O	8:H:37:LYS:NZ	2.44	0.50
16:X:107:ARG:HD3	16:X:112:VAL:HG22	1.93	0.50
1:2:359:U:OP2	16:X:18:ARG:NH1	2.43	0.50
1:2:1244:U:O4	1:2:1257:G:N2	2.44	0.50
3:A:21:ALA:HB2	3:A:173:LEU:HD13	1.92	0.50
1:2:223:C:H2'	1:2:224:A:C8	2.47	0.50
1:2:1244:U:N3	1:2:1257:G:N1	2.58	0.50
20:y:368:ALA:HA	34:c:66:ARG:HA	1.93	0.50
1:2:1101:U:H2'	1:2:1102:G:H8	1.77	0.50
3:A:188:THR:HG23	3:A:189:ILE:HG13	1.92	0.50
7:G:64:LYS:HB2	7:G:97:VAL:HG11	1.92	0.50
25:F:159:ARG:O	25:F:163:PHE:CB	2.60	0.50
1:2:57:U:OP1	1:2:504:G:O2'	2.29	0.50
1:2:1213:C:H2'	1:2:1214:A:C8	2.44	0.50
20:y:234:CYS:HB3	20:y:236:THR:HG23	1.94	0.50
35:g:199:THR:HG21	35:g:240:CYS:HA	1.92	0.50
1:2:28:U:H2'	1:2:29:G:H8	1.76	0.50
1:2:975:G:H21	13:O:50:LYS:HA	1.76	0.50
8:H:53:VAL:O	8:H:57:ARG:HB3	2.11	0.50
21:u:157:LEU:HD11	21:u:232:LEU:HD21	1.94	0.50
1:2:1013:U:OP1	1:2:1129:G:O2'	2.30	0.50
1:2:1404:U:OP1	32:U:21:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:130:PRO:HG2	7:G:132:ARG:HH12	1.77	0.50
35:g:245:ARG:HH12	35:g:312:VAL:HG21	1.77	0.50
1:2:441:C:H2'	1:2:442:C:C6	2.47	0.49
24:D:28:GLU:OE1	26:K:70:TYR:OH	2.28	0.49
1:2:818:A:OP1	10:J:80:ARG:NH2	2.42	0.49
1:2:941:C:H2'	1:2:942:G:C8	2.47	0.49
4:B:39:PHE:HB3	4:B:74:LEU:HB3	1.94	0.49
12:N:105:ASN:O	12:N:105:ASN:ND2	2.43	0.49
28:P:29:SER:OG	28:P:32:GLN:OE1	2.31	0.49
29:Q:38:PRO:HD2	29:Q:41:MET:HG3	1.94	0.49
32:U:58:THR:HA	32:U:84:ILE:O	2.12	0.49
1:2:5:U:H2'	1:2:6:G:C8	2.47	0.49
1:2:1580:A:H3'	1:2:1581:C:H5''	1.93	0.49
1:2:1726:G:H2'	1:2:1727:G:C8	2.47	0.49
5:C:166:ARG:HD3	5:C:181:PRO:HG2	1.93	0.49
1:2:10:G:O2'	5:C:113:GLN:NE2	2.45	0.49
1:2:223:C:H2'	1:2:224:A:H8	1.76	0.49
2:R:41:ILE:HD11	2:R:46:LEU:HB3	1.94	0.49
3:A:143:PRO:HG3	14:V:32:ILE:HB	1.93	0.49
35:g:9:GLY:HA3	35:g:52:TYR:HB2	1.94	0.49
1:2:162:C:O3'	7:G:95:LYS:NZ	2.46	0.49
1:2:1617:G:H22	1:2:1620:A:H5'	1.77	0.49
3:A:200:ASP:HA	3:A:203:PHE:HD2	1.78	0.49
13:O:98:ARG:HE	13:O:134:PRO:HD3	1.78	0.49
24:D:192:TRP:CG	24:D:193:ASP:H	2.31	0.49
35:g:216:ALA:HB3	35:g:230:LEU:HB2	1.94	0.49
35:g:256:ILE:HB	35:g:270:LEU:HB2	1.93	0.49
3:A:154:LEU:HD22	3:A:157:VAL:HG21	1.95	0.49
21:u:161:ASP:OD1	21:u:161:ASP:N	2.41	0.49
25:F:134:VAL:HB	25:F:136:ARG:HE	1.78	0.49
32:U:68:THR:HG22	32:U:70:CYS:H	1.77	0.49
35:g:133:ASN:HD22	35:g:137:VAL:HB	1.78	0.49
1:2:291:G:N2	11:L:68:ILE:O	2.35	0.49
2:R:17:ILE:HG13	2:R:57:LEU:HD23	1.93	0.49
7:G:44:GLU:HG3	7:G:119:LYS:HE3	1.95	0.49
10:J:121:LYS:H	10:J:125:HIS:HD2	1.61	0.49
20:y:43:ARG:HH21	20:y:46:LEU:HD22	1.78	0.49
1:2:1016:U:O4	12:N:19:ARG:NH2	2.45	0.49
1:2:1126:G:OP1	3:A:41:ARG:NH2	2.45	0.49
20:y:282:ARG:NH1	20:y:284:PHE:O	2.37	0.49
29:Q:97:GLN:HB2	29:Q:105:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:4:C:O2'	10:J:18:ARG:NH2	2.46	0.49
11:L:84:ARG:HD3	11:L:115:PRO:HD3	1.95	0.49
25:F:167:LYS:HE2	25:F:172:CYS:HA	1.94	0.49
7:G:59:GLN:HB2	7:G:72:ARG:HH22	1.78	0.49
17:Y:15:ASN:ND2	17:Y:22:GLN:OE1	2.45	0.49
21:u:258:VAL:CA	21:u:273:LYS:O	2.52	0.49
1:2:1397:U:H3	29:Q:12:VAL:HA	1.78	0.48
1:2:1479:G:OP1	29:Q:138:ARG:NH2	2.46	0.48
9:I:162:LEU:HD11	9:I:191:GLU:HG2	1.95	0.48
24:D:22:ASN:OD1	24:D:34:TYR:OH	2.25	0.48
24:D:148:LYS:HE2	36:p:185:GLU:HG3	1.95	0.48
1:2:641:A:OP1	10:J:40:LYS:NZ	2.45	0.48
1:2:926:A:N6	1:2:1015:U:H3	2.10	0.48
1:2:1337:C:H2'	1:2:1338:G:H8	1.77	0.48
3:A:10:MET:HE2	3:A:15:VAL:HG22	1.96	0.48
5:C:131:GLY:HA3	5:C:216:MET:HB3	1.94	0.48
13:O:142:ARG:HD3	13:O:144:GLY:H	1.78	0.48
21:u:600:ARG:HD3	21:u:646:ALA:HA	1.95	0.48
24:D:194:PRO:HB3	24:D:201:LYS:HA	1.94	0.48
1:2:1462:U:H1'	20:y:350:ARG:HH12	1.78	0.48
1:2:1620:A:OP2	28:P:44:ARG:NH2	2.43	0.48
9:I:107:THR:HB	9:I:110:ARG:HH21	1.78	0.48
21:u:89:PRO:HA	21:u:159:LEU:HB2	1.94	0.48
35:g:89:LEU:HB3	35:g:99:ARG:HB2	1.96	0.48
1:2:748:C:H42	1:2:794:A:H61	1.62	0.48
1:2:1821:U:H2'	1:2:1822:A:C8	2.48	0.48
3:A:205:ARG:HE	3:A:210:ILE:HG12	1.79	0.48
8:H:60:ILE:HB	8:H:92:VAL:HA	1.95	0.48
16:X:46:HIS:CD2	16:X:103:ALA:HB2	2.48	0.48
21:u:600:ARG:HH11	21:u:644:LEU:HD23	1.78	0.48
31:T:13:GLU:OE2	31:T:16:ARG:NH1	2.47	0.48
35:g:213:ASP:OD1	35:g:213:ASP:N	2.46	0.48
35:g:251:ALA:HB2	35:g:289:LEU:HD22	1.94	0.48
1:2:847:A:OP1	6:E:108:ARG:NH2	2.46	0.48
1:2:1598:G:H2'	33:Z:81:GLY:H	1.78	0.48
4:B:103:MET:HG3	4:B:188:LEU:HD21	1.95	0.48
8:H:58:LYS:HB3	8:H:90:LYS:HG3	1.96	0.48
11:L:127:THR:HB	11:L:144:LYS:HG2	1.96	0.48
12:N:115:LEU:HA	12:N:118:ILE:HD12	1.94	0.48
21:u:300:LYS:HG3	21:u:563:SER:HB3	1.95	0.48
24:D:6:SER:O	24:D:10:LYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:73:GLY:O	31:T:76:THR:OG1	2.26	0.48
1:2:126:G:H2'	7:G:199:THR:HG21	1.95	0.48
1:2:1232:U:H2'	1:2:1233:G:H8	1.79	0.48
1:2:1277:C:H2'	1:2:1278:A:H8	1.78	0.48
1:2:1280:G:H2'	1:2:1281:G:H8	1.79	0.48
23:d:46:TYR:OH	24:D:23:GLU:OE1	2.31	0.48
1:2:65:C:H4'	7:G:172:LYS:HD3	1.96	0.48
1:2:381:C:N4	9:I:27:TYR:O	2.33	0.48
1:2:1143:A:OP2	5:C:187:ARG:NH2	2.46	0.48
1:2:1648:G:N2	1:2:1675:A:OP2	2.40	0.48
16:X:41:PHE:O	16:X:76:LYS:NZ	2.44	0.48
18:b:19:HIS:HB3	18:b:22:LYS:HG3	1.96	0.48
21:u:604:ASN:HD22	21:u:679:ILE:HG22	1.78	0.48
1:2:1033:G:H1	1:2:1080:A:HO2'	1.62	0.48
1:2:1153:C:OP2	15:W:71:LYS:NZ	2.36	0.48
1:2:1268:C:H4'	28:P:100:LYS:HG3	1.96	0.48
21:u:144:HIS:HB2	21:u:786:PRO:HD2	1.95	0.48
1:2:1406:G:H2'	1:2:1407:U:C6	2.48	0.48
1:2:1454:A:H2	1:2:1476:A:H1'	1.79	0.47
1:2:1547:C:H1'	1:2:1670:C:H4'	1.96	0.47
35:g:259:TRP:HA	35:g:266:ILE:HA	1.96	0.47
36:p:119:VAL:HG12	36:p:121:PRO:HD3	1.95	0.47
1:2:530:U:H2'	1:2:531:A:H8	1.79	0.47
1:2:924:G:OP2	12:N:3:ARG:NH1	2.47	0.47
1:2:1454:A:H3'	2:R:5:ARG:HH21	1.80	0.47
1:2:1707:U:H3	1:2:1827:U:H3	1.61	0.47
1:2:1726:G:O6	1:2:1808:U:O4	2.32	0.47
24:D:162:ASP:N	24:D:163:PRO:HD2	2.29	0.47
30:S:138:THR:HG23	30:S:139:THR:HG23	1.95	0.47
1:2:588:G:OP2	1:2:588:G:N2	2.41	0.47
1:2:1248:U:H1'	29:Q:146:ARG:HB3	1.95	0.47
1:2:1692:U:H2'	1:2:1693:G:C8	2.48	0.47
1:2:1786:U:H2'	1:2:1787:G:C8	2.50	0.47
6:E:122:LYS:HD2	6:E:164:LEU:HD21	1.96	0.47
13:O:44:VAL:HG23	13:O:93:LEU:HD11	1.94	0.47
22:t:438:ARG:HD3	22:t:438:ARG:HA	1.71	0.47
25:F:27:ASP:OD1	25:F:107:ASN:ND2	2.47	0.47
36:p:164:THR:OG1	36:p:165:LYS:N	2.41	0.47
1:2:30:C:O2'	1:2:596:U:OP1	2.32	0.47
1:2:1279:C:H2'	1:2:1280:G:H8	1.79	0.47
1:2:1567:G:H2'	1:2:1568:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:y:301:SER:OG	20:y:305:THR:OG1	2.28	0.47
34:c:35:MET:SD	34:c:35:MET:N	2.87	0.47
1:2:551:U:OP1	36:p:158:LYS:NZ	2.47	0.47
1:2:641:A:O2'	1:2:645:C:OP1	2.32	0.47
1:2:1379:A:OP1	20:y:333:LYS:NZ	2.47	0.47
1:2:1539:U:H2'	1:2:1540:G:C8	2.49	0.47
7:G:135:PRO:HG2	7:G:141:ILE:HD13	1.97	0.47
15:W:27:ILE:HB	15:W:61:ILE:HB	1.97	0.47
17:Y:41:ARG:NH2	17:Y:52:PRO:O	2.47	0.47
25:F:91:ARG:O	25:F:95:HIS:ND1	2.47	0.47
1:2:885:U:H3	1:2:901:G:H1	1.62	0.47
1:2:1260:A:H61	1:2:1617:G:H1'	1.78	0.47
30:S:14:ARG:HE	30:S:17:ASN:HA	1.78	0.47
1:2:315:C:H2'	1:2:316:G:H8	1.80	0.47
1:2:600:G:H2'	1:2:601:G:C8	2.49	0.47
1:2:1409:A:H2'	1:2:1410:C:C6	2.50	0.47
1:2:1532:C:H3'	1:2:1637:A:H62	1.78	0.47
3:A:41:ARG:HD2	3:A:45:GLY:HA2	1.97	0.47
3:A:80:ARG:NH1	3:A:82:THR:OG1	2.48	0.47
3:A:109:THR:O	5:C:89:LYS:NZ	2.45	0.47
3:A:198:MET:HE1	3:A:200:ASP:HB2	1.96	0.47
7:G:164:LYS:HB3	7:G:167:LYS:HD2	1.96	0.47
13:O:56:VAL:HG13	13:O:60:MET:HG3	1.97	0.47
16:X:71:ARG:NH1	22:t:469:ASN:OD1	2.33	0.47
21:u:685:MET:SD	21:u:686:SER:N	2.88	0.47
24:D:67:ARG:HD2	26:K:93:THR:HA	1.97	0.47
34:c:12:ALA:HB1	34:c:32:VAL:HG13	1.97	0.47
8:H:60:ILE:HD11	8:H:90:LYS:HG2	1.97	0.47
13:O:45:THR:HA	13:O:52:THR:HA	1.97	0.47
25:F:19:LEU:HB3	25:F:23:TRP:HB2	1.96	0.47
25:F:137:GLN:HE22	34:c:66:ARG:HB3	1.80	0.47
30:S:35:GLY:O	30:S:97:GLN:NE2	2.48	0.47
1:2:292:A:O2'	11:L:39:ASN:O	2.28	0.47
1:2:1277:C:OP1	26:K:51:SER:OG	2.31	0.47
1:2:1736:G:H2'	1:2:1737:G:C8	2.50	0.47
17:Y:104:ARG:O	17:Y:108:LYS:HG2	2.15	0.47
20:y:389:ASP:HB2	20:y:392:LEU:HG	1.97	0.47
1:2:1054:G:H2'	1:2:1055:A:C8	2.48	0.47
1:2:1061:U:O4	1:2:1702:G:O2'	2.32	0.47
6:E:87:MET:HE3	6:E:100:ARG:HD3	1.97	0.47
15:W:101:PHE:HA	15:W:113:HIS:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:114:MET:HE3	17:Y:122:LYS:HB3	1.96	0.47
20:y:340:LEU:HG	20:y:341:THR:HG23	1.97	0.47
32:U:26:SER:HB3	32:U:110:VAL:HG13	1.97	0.47
1:2:455:A:O2'	1:2:1735:A:N3	2.46	0.46
1:2:792:C:H2'	1:2:793:G:H8	1.80	0.46
1:2:919:A:H5'	15:W:57:ARG:HD2	1.96	0.46
1:2:1653:U:H3	1:2:1671:G:H1	1.63	0.46
5:C:251:LEU:HD12	14:V:23:ILE:HG13	1.97	0.46
9:I:3:ILE:O	9:I:30:GLY:N	2.47	0.46
12:N:29:THR:HG23	12:N:32:ASP:H	1.80	0.46
21:u:272:LEU:HB2	21:u:565:VAL:HG11	1.98	0.46
1:2:980:A:H2'	1:2:981:A:C8	2.50	0.46
1:2:1617:G:N2	1:2:1620:A:OP2	2.48	0.46
12:N:83:ASP:OD1	12:N:84:LEU:N	2.48	0.46
23:d:52:PHE:HE1	32:U:82:MET:HE3	1.80	0.46
20:y:351:LEU:HD22	20:y:355:ALA:HB1	1.97	0.46
21:u:594:LEU:HD11	21:u:658:ILE:HA	1.98	0.46
28:P:130:ARG:HE	28:P:131:PRO:HD2	1.80	0.46
1:2:1244:U:O2	1:2:1255:G:N2	2.47	0.46
1:2:1363:C:C4	1:2:1375:G:N1	2.74	0.46
8:H:148:LEU:HA	15:W:42:MET:HE2	1.96	0.46
21:u:272:LEU:HD22	21:u:565:VAL:HG21	1.98	0.46
30:S:75:ARG:HH21	30:S:95:TYR:HB2	1.81	0.46
1:2:570:C:O2'	17:Y:34:THR:O	2.27	0.46
1:2:1408:U:H2'	1:2:1409:A:H8	1.81	0.46
3:A:29:ASN:HB3	3:A:151:ASP:HB3	1.98	0.46
16:X:109:GLY:HA2	16:X:119:ARG:HD2	1.97	0.46
25:F:155:CYS:HB3	25:F:159:ARG:HH21	1.81	0.46
35:g:242:SER:HB3	35:g:247:TRP:H	1.81	0.46
1:2:153:G:H2'	1:2:154:U:C6	2.51	0.46
1:2:587:A:H5'	1:2:592:C:H41	1.81	0.46
1:2:607:U:O2'	24:D:143:ARG:NH2	2.49	0.46
1:2:1539:U:H2'	1:2:1540:G:H8	1.80	0.46
1:2:1680:G:OP1	25:F:60:ARG:NH1	2.48	0.46
6:E:124:CYS:HB3	6:E:141:THR:HB	1.98	0.46
30:S:51:ASP:HB3	30:S:54:LYS:HG3	1.98	0.46
35:g:197:THR:OG1	35:g:237:ASN:O	2.31	0.46
4:B:88:THR:HA	4:B:98:THR:HA	1.97	0.46
34:c:16:LYS:HB2	34:c:31:ARG:HG3	1.97	0.46
3:A:5:LEU:HD21	14:V:41:LYS:HA	1.98	0.46
18:b:42:LYS:HE3	18:b:57:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:125:LEU:HD11	21:u:311:LEU:HA	1.97	0.46
21:u:272:LEU:O	21:u:561:HIS:HA	2.16	0.46
31:T:140:ALA:HA	31:T:143:LYS:HG2	1.98	0.46
1:2:374:G:H2'	1:2:375:U:C6	2.51	0.46
6:E:17:HIS:HB2	6:E:108:ARG:HA	1.97	0.46
6:E:20:LEU:HD21	6:E:46:ILE:HD12	1.97	0.46
10:J:22:LYS:HZ1	36:p:200:ASN:H	1.64	0.46
21:u:213:LYS:O	21:u:214:ARG:NH1	2.48	0.46
26:K:15:LEU:HD22	26:K:21:MET:HE2	1.98	0.46
1:2:919:A:H62	12:N:70:LYS:HE2	1.81	0.45
1:2:1536:G:H2'	1:2:1537:A:H8	1.80	0.45
24:D:40:ARG:HG3	24:D:47:GLU:HB2	1.98	0.45
30:S:86:ARG:HD2	30:S:98:VAL:HG21	1.98	0.45
1:2:144:U:H2'	1:2:145:G:H8	1.81	0.45
1:2:178:C:H2'	1:2:179:C:H6	1.79	0.45
1:2:1279:C:H2'	1:2:1280:G:C8	2.51	0.45
1:2:1347:U:O3'	5:C:145:LYS:NZ	2.46	0.45
1:2:1447:G:H2'	1:2:1448:A:H8	1.81	0.45
5:C:68:ARG:HH21	5:C:71:LYS:HG2	1.81	0.45
11:L:20:LYS:HB2	11:L:20:LYS:HE2	1.76	0.45
12:N:136:PRO:HG2	12:N:139:TRP:HB2	1.99	0.45
21:u:780:ASP:N	21:u:780:ASP:OD1	2.49	0.45
1:2:643:A:OP1	10:J:39:ASN:ND2	2.49	0.45
1:2:959:G:OP2	13:O:38:ASN:ND2	2.27	0.45
1:2:1275:G:H22	1:2:1506:A:P	2.40	0.45
10:J:30:LYS:HB2	10:J:30:LYS:HE3	1.76	0.45
17:Y:59:GLY:O	17:Y:71:GLY:HA2	2.17	0.45
29:Q:18:THR:HB	29:Q:75:GLY:HA2	1.99	0.45
1:2:24:C:H42	1:2:650:A:H61	0.75	0.45
1:2:979:C:H2'	1:2:980:A:C8	2.52	0.45
1:2:1100:A:H5'	20:y:320:ARG:HD2	1.97	0.45
2:R:71:ILE:O	2:R:74:GLN:NE2	2.35	0.45
2:R:71:ILE:HG12	2:R:73:LEU:HD23	1.98	0.45
6:E:192:ILE:HG22	6:E:243:GLY:HA3	1.99	0.45
10:J:106:LEU:HD23	10:J:109:ARG:HD2	1.99	0.45
14:V:66:ASP:OD1	14:V:67:ASP:N	2.48	0.45
17:Y:6:THR:HB	17:Y:28:LEU:HB2	1.98	0.45
21:u:141:GLY:N	21:u:173:CYS:SG	2.80	0.45
21:u:261:VAL:O	21:u:271:THR:N	2.47	0.45
1:2:1234:C:H5''	1:2:1246:A:H61	1.82	0.45
1:2:1351:G:O2'	1:2:1378:A:N1	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S:22:GLY:HA2	30:S:56:ALA:HB3	1.97	0.45
35:g:83:TRP:HE1	35:g:109:LEU:HD23	1.82	0.45
35:g:244:ASN:HD21	35:g:295:GLY:HA3	1.81	0.45
1:2:1546:G:H22	1:2:1655:C:H1'	1.81	0.45
3:A:84:GLN:HE22	3:A:100:ALA:HA	1.81	0.45
10:J:122:SER:O	10:J:126:ALA:N	2.46	0.45
20:y:395:GLY:HA2	20:y:398:ARG:HB2	1.98	0.45
22:t:427:LYS:HG3	22:t:430:ARG:HH21	1.82	0.45
6:E:176:ASP:O	6:E:179:ASN:ND2	2.47	0.45
27:M:21:VAL:O	27:M:24:THR:OG1	2.26	0.45
1:2:1598:G:O5'	33:Z:80:ARG:NH2	2.50	0.45
2:R:42:PRO:HB2	2:R:43:SER:H	1.43	0.45
5:C:221:ASP:OD1	5:C:221:ASP:N	2.50	0.45
12:N:75:LEU:HB3	12:N:81:ALA:HB2	1.99	0.45
15:W:87:GLU:HA	15:W:90:GLN:HG2	1.97	0.45
1:2:479:C:O2'	21:u:72:LYS:NZ	2.38	0.45
1:2:951:C:H2'	1:2:952:G:C8	2.52	0.45
1:2:1536:G:H2'	1:2:1537:A:C8	2.52	0.45
1:2:1579:A:H4'	1:2:1581:C:H5	1.82	0.45
24:D:29:LEU:HB3	24:D:32:ASP:HB2	1.99	0.45
1:2:1288:U:O4	1:2:1311:C:N3	2.50	0.45
1:2:1466:G:OP1	2:R:5:ARG:NH1	2.49	0.45
1:2:1785:C:O2'	1:2:1786:U:O4'	2.34	0.45
7:G:58:LYS:HA	7:G:107:SER:HB3	1.98	0.45
24:D:94:ARG:NH2	24:D:104:SER:OG	2.50	0.45
25:F:28:VAL:HG21	25:F:109:LEU:HD22	1.99	0.45
31:T:112:MET:HG3	31:T:127:GLY:HA3	1.99	0.45
35:g:99:ARG:NH1	35:g:135:LEU:O	2.50	0.45
1:2:107:A:H2'	1:2:108:G:C8	2.53	0.44
1:2:472:C:O2'	1:2:474:G:OP1	2.32	0.44
1:2:1256:G:H1	23:d:31:ILE:HG12	1.81	0.44
1:2:1781:A:H2'	1:2:1782:G:C8	2.52	0.44
5:C:114:LYS:HE2	5:C:123:ARG:NH2	2.32	0.44
20:y:351:LEU:HB3	20:y:355:ALA:HB3	1.99	0.44
20:y:377:ASP:OD2	20:y:380:SER:OG	2.30	0.44
25:F:24:SER:O	25:F:107:ASN:ND2	2.35	0.44
33:Z:82:SER:HA	33:Z:85:ARG:HE	1.82	0.44
1:2:1615:U:H2'	1:2:1616:U:H6	1.83	0.44
4:B:113:MET:HB3	4:B:142:PHE:HE2	1.82	0.44
5:C:82:TYR:OH	5:C:162:ILE:O	2.24	0.44
5:C:191:VAL:HG11	5:C:236:PHE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:PHE:HB3	8:H:90:LYS:HE2	1.99	0.44
10:J:159:PHE:O	10:J:163:SER:OG	2.24	0.44
17:Y:37:LYS:HE3	17:Y:60:PHE:HD2	1.82	0.44
23:d:52:PHE:CE1	32:U:82:MET:HE3	2.52	0.44
24:D:141:LYS:HE2	24:D:179:GLN:HB3	1.99	0.44
35:g:7:LEU:HB2	35:g:272:GLN:HE22	1.82	0.44
35:g:110:SER:HB3	35:g:155:ARG:HH12	1.82	0.44
1:2:70:G:H2'	1:2:71:G:H5''	1.99	0.44
1:2:476:A:N3	1:2:488:U:O2'	2.40	0.44
5:C:104:ASP:HB3	5:C:130:ILE:HA	1.99	0.44
16:X:54:LYS:HD3	16:X:91:LEU:HD11	1.98	0.44
33:Z:69:THR:HB	33:Z:72:VAL:HG23	1.99	0.44
1:2:558:G:H2'	1:2:559:G:C8	2.53	0.44
1:2:1606:G:N2	1:2:1632:G:H2'	2.33	0.44
3:A:58:LEU:HD12	3:A:58:LEU:HA	1.81	0.44
4:B:167:LYS:HA	4:B:170:GLU:HG2	1.99	0.44
10:J:60:LEU:HD22	10:J:70:ARG:HA	2.00	0.44
13:O:62:VAL:HG11	13:O:67:ASP:HB2	1.98	0.44
21:u:80:GLY:O	21:u:132:ARG:NH2	2.47	0.44
27:M:10:GLY:HA2	27:M:123:VAL:HG22	2.00	0.44
34:c:13:ARG:NH2	34:c:53:GLY:O	2.51	0.44
1:2:35:C:H5''	1:2:579:C:H5''	1.99	0.44
1:2:1210:G:H2'	1:2:1211:G:H8	1.83	0.44
1:2:1725:U:H2'	1:2:1726:G:C8	2.51	0.44
21:u:73:ARG:NE	21:u:73:ARG:O	2.49	0.44
34:c:16:LYS:H	34:c:31:ARG:HB2	1.82	0.44
36:p:140:ASP:OD1	36:p:140:ASP:N	2.51	0.44
1:2:1351:G:H1	1:2:1360:U:H3	1.65	0.44
1:2:1493:C:H5''	1:2:1494:U:H3'	1.99	0.44
1:2:1808:U:O4	1:2:1809:A:N6	2.50	0.44
25:F:144:LEU:HD23	34:c:49:PRO:HB2	1.99	0.44
1:2:448:A:H5''	9:I:25:ARG:HA	1.99	0.44
1:2:1047:C:OP1	13:O:143:LYS:NZ	2.40	0.44
1:2:1614:A:OP2	28:P:42:ARG:NH2	2.50	0.44
5:C:136:HIS:HB3	5:C:162:ILE:HG23	2.00	0.44
12:N:47:PRO:HG2	12:N:72:LEU:HD23	2.00	0.44
14:V:58:ALA:O	14:V:62:MET:HG3	2.18	0.44
23:d:52:PHE:CE2	32:U:63:ILE:HD13	2.52	0.44
26:K:32:HIS:CD2	26:K:34:GLU:HB2	2.53	0.44
30:S:18:THR:HG21	30:S:33:ILE:HG22	1.99	0.44
35:g:193:GLY:HA3	35:g:212:LYS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:96:C:H2'	1:2:97:U:C6	2.53	0.44
1:2:1070:A:H5'	22:t:434:ILE:HD13	2.00	0.44
1:2:1593:C:H2'	1:2:1594:A:H8	1.83	0.44
28:P:73:PRO:HG2	28:P:92:SER:HA	2.00	0.44
1:2:1239:U:H5''	28:P:124:LYS:HD3	1.98	0.44
1:2:1280:G:H2'	1:2:1281:G:C8	2.53	0.44
1:2:1363:C:N4	1:2:1375:G:C6	2.86	0.44
1:2:1562:C:H2'	1:2:1563:G:C8	2.51	0.44
3:A:122:LEU:HA	3:A:122:LEU:HD12	1.78	0.44
4:B:38:MET:SD	4:B:38:MET:N	2.91	0.44
5:C:88:ILE:HD13	5:C:94:ILE:HD11	1.99	0.44
21:u:147:LEU:O	21:u:151:LYS:NZ	2.37	0.44
24:D:125:PHE:HE2	36:p:134:TRP:H	1.65	0.44
32:U:61:LEU:HB2	32:U:82:MET:HB3	2.00	0.44
35:g:129:ILE:HD11	35:g:151:VAL:HG11	2.00	0.44
1:2:1310:U:OP2	27:M:36:ARG:NH2	2.44	0.43
1:2:1375:G:H2'	1:2:1376:A:H8	1.83	0.43
1:2:1565:C:H41	31:T:101:ARG:NH2	2.16	0.43
5:C:151:ILE:O	5:C:155:ILE:HD12	2.18	0.43
8:H:40:LEU:HD21	8:H:79:LEU:HD21	2.00	0.43
21:u:253:LEU:HB3	21:u:581:ALA:O	2.18	0.43
21:u:588:GLU:HA	21:u:658:ILE:HG23	2.00	0.43
34:c:13:ARG:N	34:c:33:GLU:O	2.51	0.43
1:2:1655:C:H2'	1:2:1656:G:H8	1.82	0.43
7:G:5:ILE:HD13	7:G:111:LEU:HB2	1.99	0.43
16:X:54:LYS:HG2	16:X:70:VAL:HG22	2.00	0.43
27:M:86:GLY:HA3	27:M:105:GLY:HA2	2.00	0.43
1:2:639:C:H2'	1:2:640:A:H8	1.83	0.43
1:2:1232:U:H3	1:2:1526:G:H1	1.65	0.43
1:2:1285:G:H5'	27:M:35:ILE:HB	1.99	0.43
1:2:1652:G:H1	1:2:1672:U:H3	1.66	0.43
1:2:1778:C:H2'	1:2:1779:G:C8	2.53	0.43
2:R:74:GLN:HB3	2:R:78:ARG:HD3	2.00	0.43
6:E:63:LYS:O	6:E:67:GLN:NE2	2.37	0.43
6:E:63:LYS:NZ	17:Y:84:LYS:O	2.34	0.43
14:V:53:TYR:OH	14:V:76:ASP:OD2	2.34	0.43
15:W:36:ARG:HD2	15:W:110:ILE:HD12	2.01	0.43
16:X:72:VAL:HG11	16:X:100:VAL:HG11	2.01	0.43
22:t:453:LYS:HB2	22:t:453:LYS:HE2	1.78	0.43
1:2:1143:A:H5'	5:C:190:SER:HB2	2.00	0.43
1:2:1410:C:H2'	1:2:1411:G:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:122:GLU:OE2	4:B:213:ARG:NH2	2.51	0.43
5:C:190:SER:O	5:C:190:SER:OG	2.26	0.43
7:G:2:LYS:HB2	7:G:108:VAL:HG22	2.00	0.43
9:I:64:ASN:HA	9:I:75:LYS:HA	1.99	0.43
12:N:115:LEU:O	12:N:119:GLU:HG2	2.17	0.43
27:M:54:SER:N	27:M:79:VAL:O	2.49	0.43
1:2:1673:U:H2'	1:2:1674:G:O4'	2.18	0.43
3:A:84:GLN:O	3:A:87:VAL:HG12	2.18	0.43
5:C:204:ILE:HD11	5:C:215:MET:SD	2.58	0.43
7:G:24:LEU:HB3	7:G:28:TYR:CZ	2.53	0.43
10:J:22:LYS:NZ	36:p:200:ASN:H	2.15	0.43
10:J:36:GLY:O	10:J:111:GLN:NE2	2.40	0.43
20:y:60:PRO:HA	20:y:63:VAL:HG22	2.00	0.43
21:u:211:VAL:HG13	21:u:215:PHE:HD2	1.84	0.43
25:F:41:VAL:HB	25:F:45:TYR:HB2	1.99	0.43
1:2:61:A:O2'	1:2:315:C:O2'	2.27	0.43
1:2:435:A:OP1	9:I:23:LYS:NZ	2.45	0.43
1:2:478:G:O4'	21:u:234:ARG:NH2	2.51	0.43
1:2:1605:G:H21	1:2:1634:A:H62	1.66	0.43
6:E:31:PRO:HG3	6:E:43:PRO:HG3	2.01	0.43
11:L:75:GLY:HA3	11:L:88:ILE:HD12	2.00	0.43
12:N:27:LYS:H	12:N:27:LYS:HG2	1.68	0.43
20:y:110:VAL:HG12	20:y:306:LEU:HD23	1.99	0.43
30:S:73:ASN:HB2	30:S:76:GLN:HE22	1.84	0.43
1:2:73:C:N4	7:G:168:LYS:HD3	2.34	0.43
1:2:1024:A:OP2	12:N:124:ARG:NH2	2.44	0.43
1:2:1337:C:H2'	1:2:1338:G:C8	2.53	0.43
3:A:57:LYS:HD2	3:A:57:LYS:HA	1.78	0.43
12:N:55:ARG:HH22	18:b:51:GLN:CD	2.26	0.43
20:y:28:TYR:HB3	20:y:89:LEU:HD21	2.01	0.43
28:P:34:MET:HB2	28:P:45:LEU:HD22	2.00	0.43
28:P:61:ARG:HH12	28:P:88:GLU:HB3	1.84	0.43
1:2:522:A:H4'	10:J:131:ARG:NH2	2.34	0.43
1:2:1023:A:OP2	12:N:124:ARG:NE	2.52	0.43
1:2:1326:U:H4'	1:2:1327:G:H5''	2.00	0.43
4:B:33:VAL:HG23	4:B:44:ILE:HG13	2.01	0.43
30:S:124:ARG:HB3	30:S:131:VAL:HG12	2.01	0.43
1:2:1748:G:H2'	1:2:1749:G:H8	1.82	0.43
5:C:110:MET:HA	5:C:111:PRO:HD3	1.88	0.43
24:D:53:THR:HG23	24:D:94:ARG:HG3	2.00	0.43
1:2:1010:G:H2'	1:2:1011:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1138:C:C2	14:V:61:ARG:HD3	2.54	0.42
1:2:1845:A:H2'	1:2:1846:G:C8	2.54	0.42
11:L:61:PRO:HD3	11:L:141:ASN:HD21	1.83	0.42
12:N:56:ASP:OD2	18:b:52:THR:OG1	2.25	0.42
35:g:253:GLY:O	35:g:286:CYS:N	2.45	0.42
1:2:28:U:H2'	1:2:29:G:C8	2.52	0.42
1:2:929:G:H2'	1:2:930:C:O4'	2.19	0.42
1:2:952:G:O2'	13:O:51:GLU:OE2	2.36	0.42
1:2:1648:G:H4'	1:2:1649:U:O5'	2.19	0.42
18:b:23:ARG:NH2	18:b:29:ASN:OD1	2.50	0.42
35:g:83:TRP:CD1	35:g:107:ASP:HB3	2.54	0.42
1:2:928:G:H21	18:b:68:GLY:HA2	1.83	0.42
1:2:952:G:H2'	1:2:953:C:C6	2.54	0.42
1:2:1677:U:H2'	1:2:1678:A:C8	2.54	0.42
21:u:125:LEU:HD12	21:u:132:ARG:HG2	2.01	0.42
21:u:166:TRP:HZ3	21:u:171:ASP:HB2	1.84	0.42
1:2:640:A:H2'	1:2:641:A:C8	2.54	0.42
1:2:1328:G:H4'	21:u:706:ILE:HB	2.01	0.42
6:E:44:LEU:HD13	6:E:72:ILE:HD11	2.01	0.42
20:y:14:PHE:O	20:y:45:ARG:NH2	2.52	0.42
20:y:16:ARG:HH21	20:y:255:VAL:HB	1.85	0.42
21:u:254:PHE:O	21:u:276:GLY:HA3	2.19	0.42
24:D:138:VAL:HA	24:D:183:GLY:O	2.18	0.42
1:2:527:C:H2'	1:2:528:A:C8	2.52	0.42
1:2:610:G:H2'	1:2:611:G:C8	2.54	0.42
1:2:944:A:N1	1:2:982:G:N2	2.54	0.42
1:2:1049:A:H61	22:t:438:ARG:HH21	1.67	0.42
5:C:153:GLY:HA2	5:C:156:ILE:HG12	2.01	0.42
28:P:93:MET:HE1	28:P:106:GLU:HA	2.01	0.42
35:g:290:ALA:N	35:g:299:PHE:O	2.50	0.42
1:2:29:G:H4'	16:X:129:SER:HB3	2.01	0.42
1:2:948:C:H2'	1:2:949:G:C8	2.53	0.42
1:2:979:C:H2'	1:2:980:A:H8	1.83	0.42
1:2:1284:A:C6	27:M:91:LEU:HD22	2.55	0.42
1:2:1406:G:H2'	1:2:1407:U:H6	1.83	0.42
1:2:1447:G:O4'	32:U:55:ARG:NH1	2.53	0.42
3:A:42:LYS:HG3	3:A:44:ASP:H	1.83	0.42
4:B:139:CYS:HB3	4:B:168:MET:HE2	2.01	0.42
9:I:84:ASN:HD22	9:I:90:LEU:HB2	1.83	0.42
16:X:40:PRO:HA	16:X:79:LYS:HD3	2.01	0.42
21:u:178:PHE:HE1	21:u:182:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:515:ASP:HB2	21:u:518:GLU:HB2	2.00	0.42
29:Q:73:LYS:HD2	29:Q:73:LYS:HA	1.86	0.42
1:2:70:G:H1	1:2:79:A:H61	1.67	0.42
1:2:909:G:H2'	1:2:910:G:C8	2.55	0.42
1:2:1125:C:OP2	20:y:320:ARG:NH2	2.42	0.42
1:2:1230:C:H2'	1:2:1231:C:H6	1.85	0.42
3:A:30:LEU:HB2	3:A:47:TYR:HE2	1.85	0.42
9:I:110:ARG:HD2	9:I:123:ARG:HH12	1.84	0.42
10:J:140:GLN:NE2	17:Y:64:PHE:O	2.42	0.42
27:M:31:LEU:HD13	27:M:89:VAL:HG13	2.01	0.42
1:2:533:A:H2'	1:2:534:G:C8	2.54	0.42
1:2:568:C:H2'	1:2:569:A:C8	2.55	0.42
1:2:1232:U:H2'	1:2:1233:G:C8	2.54	0.42
33:Z:111:ARG:NH1	33:Z:113:THR:O	2.52	0.42
1:2:130:G:O6	1:2:181:A:N1	2.53	0.42
1:2:639:C:H2'	1:2:640:A:C8	2.54	0.42
1:2:1152:U:O2'	15:W:16:ASN:OD1	2.26	0.42
1:2:1281:G:H2'	1:2:1282:A:H8	1.83	0.42
1:2:1288:U:N3	1:2:1311:C:O2	2.53	0.42
1:2:1568:C:O2	1:2:1627:C:O2'	2.32	0.42
7:G:98:ARG:HH22	7:G:103:ASP:HB2	1.85	0.42
12:N:4:MET:SD	12:N:124:ARG:NH1	2.92	0.42
12:N:69:ASN:OD1	12:N:70:LYS:N	2.52	0.42
20:y:285:CYS:HB3	20:y:293:LEU:HD11	2.02	0.42
20:y:312:ARG:HD2	20:y:312:ARG:HA	1.88	0.42
1:2:535:G:H2'	1:2:536:A:C8	2.54	0.42
1:2:1634:A:H4'	30:S:142:ARG:HH22	1.84	0.42
3:A:66:VAL:HG21	3:A:185:MET:HB3	2.01	0.42
5:C:148:ALA:HB3	36:p:190:ASP:H	1.84	0.42
20:y:326:LEU:HA	20:y:327:PRO:HD3	1.93	0.42
21:u:675:MET:HE1	21:u:789:TRP:HA	2.01	0.42
28:P:17:TYR:HB3	28:P:25:LEU:HD11	2.02	0.42
30:S:5:ILE:HG12	33:Z:50:PHE:HB2	2.01	0.42
1:2:130:G:H1	1:2:181:A:N6	2.17	0.41
1:2:389:A:H2'	1:2:390:C:C6	2.55	0.41
1:2:677:G:N1	1:2:1027:A:OP2	2.35	0.41
1:2:886:A:H1'	1:2:900:C:H42	1.85	0.41
1:2:1559:C:H2'	1:2:1560:U:O4'	2.20	0.41
20:y:359:THR:HB	20:y:374:VAL:HG23	2.02	0.41
26:K:27:VAL:HG13	26:K:43:LEU:HD22	2.02	0.41
1:2:1025:U:OP1	1:2:1090:C:O2'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1523:C:H3'	30:S:141:ARG:HH11	1.85	0.41
3:A:77:ILE:HG13	3:A:99:ILE:HB	2.02	0.41
3:A:122:LEU:HD22	3:A:137:ALA:HB2	2.02	0.41
15:W:57:ARG:HH22	18:b:26:GLN:HB2	1.84	0.41
20:y:277:THR:HG21	20:y:282:ARG:HD2	2.02	0.41
29:Q:50:LYS:O	29:Q:53:GLU:HG2	2.20	0.41
1:2:1215:C:H42	1:2:1220:A:N6	2.18	0.41
1:2:1249:C:OP2	1:2:1250:A:O2'	2.33	0.41
1:2:1375:G:H2'	1:2:1376:A:C8	2.56	0.41
1:2:1400:U:O4	1:2:1401:A:N6	2.53	0.41
15:W:22:LYS:HD3	18:b:3:LEU:HD23	2.02	0.41
21:u:272:LEU:HD22	21:u:565:VAL:HG11	2.03	0.41
28:P:81:ARG:NH2	28:P:117:GLY:O	2.53	0.41
30:S:110:ASP:OD1	30:S:113:ARG:NH1	2.49	0.41
35:g:257:LYS:HB3	35:g:259:TRP:HE1	1.86	0.41
1:2:1620:A:P	28:P:44:ARG:HH21	2.43	0.41
12:N:4:MET:HE2	12:N:4:MET:HB3	1.86	0.41
20:y:219:GLN:HG3	20:y:220:GLU:H	1.85	0.41
23:d:54:LYS:HB2	23:d:54:LYS:HE3	1.88	0.41
1:2:126:G:H8	7:G:199:THR:HG21	1.86	0.41
1:2:980:A:H2'	1:2:981:A:H8	1.85	0.41
1:2:1069:U:H2'	1:2:1070:A:H8	1.86	0.41
1:2:1172:U:H2'	1:2:1173:A:H8	1.86	0.41
1:2:1727:G:H2'	1:2:1728:U:C6	2.55	0.41
3:A:206:ASP:O	3:A:209:GLU:N	2.50	0.41
15:W:47:ILE:HD11	15:W:63:VAL:HG11	2.02	0.41
21:u:146:VAL:O	21:u:150:ALA:CB	2.69	0.41
21:u:223:LEU:HD11	21:u:232:LEU:HD22	2.02	0.41
24:D:8:LYS:HG2	32:U:61:LEU:HD21	2.03	0.41
24:D:142:LEU:HD13	24:D:150:MET:HE2	2.03	0.41
25:F:17:ILE:HA	25:F:48:TYR:HE1	1.85	0.41
29:Q:13:PHE:H	29:Q:90:LYS:HZ1	1.68	0.41
35:g:239:LEU:HD23	35:g:250:ALA:HA	2.02	0.41
1:2:1004:U:H2'	1:2:1005:G:H8	1.85	0.41
1:2:1407:U:H2'	1:2:1408:U:C6	2.56	0.41
1:2:1463:U:O4	20:y:38:ARG:NH1	2.54	0.41
1:2:1538:C:H4'	31:T:45:LEU:HD12	2.02	0.41
1:2:1633:A:H2'	1:2:1634:A:H8	1.86	0.41
4:B:115:LYS:HD2	4:B:115:LYS:HA	1.83	0.41
9:I:139:LYS:HD2	9:I:149:TYR:HE2	1.85	0.41
9:I:151:GLU:HA	9:I:154:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:121:ASN:OD1	21:u:121:ASN:N	2.50	0.41
24:D:135:GLU:OE1	24:D:151:LYS:NZ	2.48	0.41
24:D:136:VAL:HA	24:D:185:LYS:O	2.21	0.41
25:F:101:HIS:ND1	25:F:106:GLU:O	2.53	0.41
28:P:81:ARG:NH2	28:P:120:SER:O	2.53	0.41
29:Q:66:VAL:HG22	29:Q:95:TYR:HE2	1.85	0.41
1:2:61:A:N1	1:2:335:G:O2'	2.51	0.41
1:2:112:U:H5''	1:2:113:G:H2'	2.03	0.41
1:2:571:U:OP1	17:Y:37:LYS:HG2	2.21	0.41
1:2:792:C:H2'	1:2:793:G:C8	2.55	0.41
1:2:1256:G:H21	1:2:1659:U:H5'	1.86	0.41
1:2:1363:C:N4	1:2:1375:G:H1	2.16	0.41
1:2:1373:C:OP1	2:R:7:LYS:HB2	2.21	0.41
1:2:1474:A:H2'	1:2:1475:G:C8	2.56	0.41
5:C:256:TRP:CD2	15:W:68:ARG:HD3	2.56	0.41
18:b:54:VAL:HG13	18:b:63:LEU:HB2	2.03	0.41
24:D:136:VAL:HG22	24:D:186:VAL:HG22	2.03	0.41
26:K:86:PRO:HA	26:K:87:PRO:HD3	1.90	0.41
1:2:398:A:OP1	1:2:399:C:O2'	2.23	0.41
4:B:138:PHE:HB2	4:B:214:LYS:H	1.85	0.41
6:E:179:ASN:HB2	6:E:195:ILE:HD12	2.03	0.41
9:I:54:LYS:HE2	9:I:181:GLN:HG2	2.02	0.41
17:Y:7:ILE:HG23	17:Y:25:ILE:HG23	2.03	0.41
33:Z:99:LEU:HD21	33:Z:102:LYS:HB3	2.03	0.41
1:2:531:A:H2'	1:2:532:C:C6	2.56	0.41
1:2:1084:A:OP1	1:2:1858:G:O2'	2.32	0.41
1:2:1231:C:O2'	1:2:1253:A:N6	2.53	0.41
1:2:1336:C:O2'	23:d:44:ARG:NH1	2.53	0.41
1:2:1367:U:O2	1:2:1373:C:N3	2.54	0.41
1:2:1570:G:O2'	1:2:1614:A:O2'	2.34	0.41
7:G:77:LEU:O	7:G:92:ARG:HA	2.21	0.41
7:G:109:LEU:HD12	7:G:109:LEU:HA	1.96	0.41
18:b:38:PRO:HD3	18:b:77:CYS:HA	2.03	0.41
21:u:294:TYR:OH	21:u:572:CYS:SG	2.63	0.41
21:u:303:ASP:HA	21:u:344:LEU:HA	2.03	0.41
25:F:101:HIS:HD1	25:F:108:PRO:HD3	1.86	0.41
26:K:21:MET:HG2	26:K:69:TRP:HE3	1.86	0.41
26:K:49:MET:HE3	26:K:49:MET:O	2.20	0.41
27:M:51:VAL:HG22	27:M:77:ILE:HB	2.02	0.41
1:2:1372:C:OP1	1:2:1385:G:N2	2.42	0.41
6:E:173:ILE:HG23	6:E:230:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:101:ARG:HB3	16:X:10:ALA:HB2	2.03	0.41
20:y:20:LEU:HD11	20:y:255:VAL:HA	2.03	0.41
20:y:246:LEU:HD11	20:y:302:ASP:HA	2.03	0.41
29:Q:70:VAL:HG11	29:Q:84:ILE:HG23	2.03	0.41
30:S:84:LEU:HD22	30:S:97:GLN:HB2	2.02	0.41
1:2:84:A:N3	1:2:150:A:O2'	2.51	0.40
1:2:290:U:N3	1:2:293:C:OP2	2.48	0.40
1:2:544:G:H2'	1:2:545:A:H8	1.86	0.40
1:2:844:U:OP1	6:E:240:ARG:NH2	2.54	0.40
1:2:960:U:H5'	1:2:1065:G:H5'	2.02	0.40
1:2:1284:A:H5''	1:2:1285:G:H3'	2.02	0.40
10:J:126:ALA:O	10:J:130:ILE:HG12	2.21	0.40
18:b:67:THR:HG22	18:b:71:ALA:HA	2.03	0.40
25:F:33:ILE:HA	25:F:36:GLN:HG2	2.03	0.40
1:2:1408:U:H2'	1:2:1409:A:C8	2.56	0.40
6:E:85:GLY:N	6:E:88:ASP:OD2	2.53	0.40
6:E:104:ASP:HB2	6:E:110:ALA:HB2	2.03	0.40
9:I:76:THR:HG21	9:I:104:ILE:HD12	2.02	0.40
9:I:89:GLU:O	9:I:92:ARG:HG3	2.21	0.40
24:D:199:GLY:HA2	24:D:200:PRO:HD3	1.92	0.40
35:g:87:LEU:HD11	35:g:111:VAL:HG11	2.04	0.40
1:2:951:C:H2'	1:2:952:G:H8	1.87	0.40
1:2:1272:C:H2'	1:2:1273:C:C6	2.56	0.40
1:2:1491:G:H2'	1:2:1492:U:C6	2.57	0.40
7:G:130:PRO:HB2	7:G:132:ARG:HH22	1.87	0.40
8:H:109:ARG:HD3	8:H:111:LYS:HG3	2.02	0.40
20:y:269:ARG:HG3	20:y:276:THR:HG22	2.02	0.40
20:y:360:ASN:HD21	20:y:363:ALA:HB2	1.87	0.40
20:y:381:ARG:HH21	20:y:385:LEU:HD11	1.87	0.40
22:t:469:ASN:OD1	22:t:470:VAL:N	2.55	0.40
26:K:52:LEU:HD23	26:K:55:ARG:HD2	2.03	0.40
32:U:51:LYS:HB2	32:U:90:ASP:HB2	2.03	0.40
1:2:14:C:OP1	5:C:190:SER:HB3	2.22	0.40
1:2:144:U:H2'	1:2:145:G:C8	2.56	0.40
1:2:602:G:N2	1:2:620:G:N7	2.62	0.40
1:2:981:A:H2'	1:2:982:G:C8	2.57	0.40
1:2:1212:G:H2'	1:2:1213:C:C6	2.57	0.40
3:A:205:ARG:HD2	3:A:205:ARG:HA	1.77	0.40
10:J:136:ARG:NH2	10:J:158:ASP:OD2	2.55	0.40
21:u:62:LYS:HB2	21:u:62:LYS:HE2	1.92	0.40
27:M:32:ALA:HB3	27:M:110:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:18:LEU:HD12	31:T:21:PHE:HB3	2.04	0.40
34:c:14:VAL:HB	34:c:54:ASP:H	1.87	0.40
1:2:532:C:H2'	1:2:533:A:H8	1.87	0.40
1:2:1290:G:N2	1:2:1310:U:H1'	2.37	0.40
1:2:1712:A:N1	1:2:1822:A:N6	2.69	0.40
11:L:68:ILE:HG13	11:L:143:LEU:HD21	2.02	0.40
14:V:81:LYS:HD3	14:V:81:LYS:HA	1.80	0.40
21:u:84:GLN:OE1	21:u:279:ARG:NH1	2.53	0.40
21:u:144:HIS:HA	21:u:622:ARG:HH12	1.86	0.40
21:u:275:SER:HB3	21:u:559:THR:HG23	2.03	0.40
21:u:594:LEU:HA	21:u:687:VAL:HG23	2.04	0.40
21:u:671:LYS:HB3	21:u:675:MET:HB3	2.03	0.40
29:Q:53:GLU:OE2	29:Q:85:ARG:NE	2.55	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	
2	R	120/135 (89%)	110 (92%)	9 (8%)	1 (1%)	16	48
3	A	214/295 (72%)	204 (95%)	10 (5%)	0	100	100
4	B	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
5	C	216/293 (74%)	206 (95%)	10 (5%)	0	100	100
6	E	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
7	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
8	H	184/194 (95%)	181 (98%)	3 (2%)	0	100	100
9	I	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
10	J	178/194 (92%)	167 (94%)	10 (6%)	1 (1%)	21	54
11	L	149/158 (94%)	139 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
13	O	133/151 (88%)	126 (95%)	7 (5%)	0	100	100
14	V	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
15	W	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	48
16	X	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
17	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
18	b	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
19	x	176/252 (70%)	172 (98%)	4 (2%)	0	100	100
20	y	319/412 (77%)	305 (96%)	14 (4%)	0	100	100
21	u	607/804 (76%)	575 (95%)	32 (5%)	0	100	100
22	t	59/475 (12%)	56 (95%)	2 (3%)	1 (2%)	7	34
23	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
24	D	223/243 (92%)	207 (93%)	15 (7%)	1 (0%)	30	62
25	F	187/204 (92%)	177 (95%)	10 (5%)	0	100	100
26	K	93/165 (56%)	90 (97%)	3 (3%)	0	100	100
27	M	121/132 (92%)	117 (97%)	4 (3%)	0	100	100
28	P	118/145 (81%)	117 (99%)	1 (1%)	0	100	100
29	Q	137/146 (94%)	125 (91%)	12 (9%)	0	100	100
30	S	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
31	T	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
32	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
33	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
34	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
35	g	312/317 (98%)	297 (95%)	15 (5%)	0	100	100
36	p	385/519 (74%)	367 (95%)	18 (5%)	0	100	100
37	i	71/76 (93%)	71 (100%)	0	0	100	100
37	j	71/76 (93%)	71 (100%)	0	0	100	100
All	All	6234/7760 (80%)	5945 (95%)	284 (5%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	42	PRO

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Mol	Chain	Res	Type
10	J	138	ARG
24	D	205	PRO
22	t	470	VAL
15	W	29	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	110/122 (90%)	110 (100%)	0	100	100
3	A	180/243 (74%)	180 (100%)	0	100	100
4	B	194/231 (84%)	194 (100%)	0	100	100
5	C	184/225 (82%)	184 (100%)	0	100	100
6	E	224/225 (100%)	223 (100%)	1 (0%)	84	83
7	G	200/218 (92%)	199 (100%)	1 (0%)	81	81
8	H	167/174 (96%)	167 (100%)	0	100	100
9	I	178/180 (99%)	178 (100%)	0	100	100
10	J	160/168 (95%)	160 (100%)	0	100	100
11	L	135/142 (95%)	135 (100%)	0	100	100
12	N	130/131 (99%)	129 (99%)	1 (1%)	73	76
13	O	105/119 (88%)	105 (100%)	0	100	100
14	V	66/67 (98%)	66 (100%)	0	100	100
15	W	112/113 (99%)	112 (100%)	0	100	100
16	X	113/115 (98%)	113 (100%)	0	100	100
17	Y	108/115 (94%)	108 (100%)	0	100	100
18	b	74/76 (97%)	74 (100%)	0	100	100
20	y	285/367 (78%)	285 (100%)	0	100	100
21	u	539/705 (76%)	539 (100%)	0	100	100
22	t	56/434 (13%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	d	48/49 (98%)	47 (98%)	1 (2%)	47	64
24	D	189/202 (94%)	188 (100%)	1 (0%)	81	81
25	F	159/170 (94%)	159 (100%)	0	100	100
26	K	86/136 (63%)	86 (100%)	0	100	100
27	M	104/108 (96%)	104 (100%)	0	100	100
28	P	107/130 (82%)	107 (100%)	0	100	100
29	Q	115/121 (95%)	115 (100%)	0	100	100
30	S	124/132 (94%)	124 (100%)	0	100	100
31	T	114/115 (99%)	114 (100%)	0	100	100
32	U	93/107 (87%)	93 (100%)	0	100	100
33	Z	64/103 (62%)	64 (100%)	0	100	100
34	c	54/62 (87%)	54 (100%)	0	100	100
35	g	272/275 (99%)	272 (100%)	0	100	100
36	p	136/454 (30%)	136 (100%)	0	100	100
All	All	4985/6334 (79%)	4980 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	129	ILE
7	G	92	ARG
12	N	105	ASN
23	d	16	GLN
24	D	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	56	HIS
2	R	116	ASN
3	A	132	GLN
4	B	75	GLN
4	B	76	ASN
6	E	36	HIS
6	E	50	ASN
6	E	161	GLN

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Mol	Chain	Res	Type
6	E	179	ASN
6	E	188	ASN
7	G	13	GLN
7	G	56	ASN
9	I	167	GLN
10	J	154	GLN
11	L	100	ASN
11	L	108	ASN
12	N	101	HIS
12	N	105	ASN
16	X	26	GLN
16	X	46	HIS
20	y	26	ASN
20	y	219	GLN
21	u	59	GLN
21	u	114	ASN
21	u	239	GLN
21	u	683	HIS
22	t	421	ASN
23	d	5	GLN
23	d	45	GLN
24	D	101	GLN
24	D	159	HIS
25	F	137	GLN
31	T	51	ASN
31	T	63	HIS
32	U	92	HIS
36	p	187	GLN
36	p	209	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1646/1873 (87%)	435 (26%)	22 (1%)

All (435) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C

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Mol	Chain	Res	Type
1	2	11	A
1	2	14	C
1	2	17	C
1	2	25	A
1	2	33	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	49	C
1	2	50	A
1	2	55	U
1	2	56	G
1	2	58	C
1	2	62	G
1	2	65	C
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	71	G
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	99	A
1	2	103	A
1	2	104	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	122	G
1	2	126	G
1	2	128	U
1	2	130	G
1	2	142	C
1	2	143	U
1	2	144	U
1	2	147	A
1	2	155	G

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Mol	Chain	Res	Type
1	2	161	U
1	2	163	U
1	2	172	U
1	2	175	A
1	2	182	C
1	2	183	G
1	2	184	G
1	2	190	G
1	2	215	G
1	2	290	U
1	2	291	G
1	2	292	A
1	2	294	U
1	2	295	C
1	2	302	A
1	2	309	G
1	2	310	C
1	2	312	G
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	321	C
1	2	333	G
1	2	347	G
1	2	357	C
1	2	360	A
1	2	361	U
1	2	362	C
1	2	364	A
1	2	369	C
1	2	370	G
1	2	381	C
1	2	385	G
1	2	386	C
1	2	387	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	413	G
1	2	414	A

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Mol	Chain	Res	Type
1	2	418	A
1	2	421	G
1	2	429	C
1	2	434	G
1	2	438	G
1	2	448	A
1	2	449	A
1	2	450	C
1	2	463	C
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	487	U
1	2	492	C
1	2	512	A
1	2	516	A
1	2	523	A
1	2	525	A
1	2	531	A
1	2	532	C
1	2	534	G
1	2	536	A
1	2	544	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	555	A
1	2	556	U
1	2	557	U
1	2	559	G
1	2	562	U
1	2	576	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	592	C
1	2	594	A
1	2	598	G

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Mol	Chain	Res	Type
1	2	604	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	621	C
1	2	627	U
1	2	629	A
1	2	630	U
1	2	634	A
1	2	643	A
1	2	644	G
1	2	650	A
1	2	655	A
1	2	660	C
1	2	662	G
1	2	664	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	684	G
1	2	685	A
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	809	A
1	2	810	A
1	2	812	A
1	2	822	U
1	2	824	C
1	2	830	A
1	2	834	C
1	2	847	A
1	2	852	G
1	2	853	C

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Mol	Chain	Res	Type
1	2	868	G
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	885	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	898	U
1	2	903	A
1	2	905	C
1	2	907	G
1	2	913	A
1	2	914	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	930	C
1	2	933	G
1	2	954	U
1	2	955	A
1	2	956	G
1	2	963	A
1	2	969	U
1	2	970	G
1	2	971	G
1	2	978	G
1	2	981	A
1	2	990	A
1	2	992	A

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Mol	Chain	Res	Type
1	2	1008	A
1	2	1009	A
1	2	1016	U
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1028	A
1	2	1040	G
1	2	1041	G
1	2	1045	U
1	2	1049	A
1	2	1054	G
1	2	1055	A
1	2	1056	U
1	2	1057	C
1	2	1058	A
1	2	1059	G
1	2	1062	A
1	2	1067	C
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1087	A
1	2	1088	U
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1108	G
1	2	1109	C
1	2	1110	G
1	2	1112	U
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1120	U
1	2	1121	G
1	2	1123	C
1	2	1126	G
1	2	1138	C
1	2	1151	G

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Mol	Chain	Res	Type
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1168	G
1	2	1171	G
1	2	1195	A
1	2	1206	G
1	2	1207	G
1	2	1208	A
1	2	1210	G
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1227	G
1	2	1228	A
1	2	1229	G
1	2	1236	G
1	2	1241	A
1	2	1242	U
1	2	1243	U
1	2	1244	U
1	2	1248	U
1	2	1251	A
1	2	1253	A
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1264	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1286	G
1	2	1288	U
1	2	1298	G
1	2	1300	U
1	2	1302	G
1	2	1303	C
1	2	1304	U

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Mol	Chain	Res	Type
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1327	G
1	2	1328	G
1	2	1329	U
1	2	1331	C
1	2	1333	U
1	2	1343	U
1	2	1348	G
1	2	1358	U
1	2	1363	C
1	2	1364	U
1	2	1371	U
1	2	1372	C
1	2	1377	U
1	2	1378	A
1	2	1382	A
1	2	1398	G
1	2	1404	U
1	2	1413	G
1	2	1414	A
1	2	1425	G
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1446	A
1	2	1447	G
1	2	1452	A
1	2	1453	C
1	2	1454	A
1	2	1463	U
1	2	1466	G
1	2	1468	C
1	2	1476	A
1	2	1477	U
1	2	1478	U

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Mol	Chain	Res	Type
1	2	1483	A
1	2	1489	A
1	2	1490	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1501	C
1	2	1502	C
1	2	1503	C
1	2	1505	U
1	2	1518	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1527	C
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1547	C
1	2	1549	U
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1570	G
1	2	1575	G
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1601	A
1	2	1603	G
1	2	1607	A

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Mol	Chain	Res	Type
1	2	1609	C
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1632	G
1	2	1634	A
1	2	1637	A
1	2	1647	A
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1655	C
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1681	U
1	2	1682	C
1	2	1683	C
1	2	1688	C
1	2	1689	C
1	2	1699	A
1	2	1706	G
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1728	U
1	2	1729	U
1	2	1744	G
1	2	1751	C
1	2	1756	C
1	2	1773	C
1	2	1775	U
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1805	G
1	2	1808	U
1	2	1813	A
1	2	1816	G
1	2	1819	A

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Mol	Chain	Res	Type
1	2	1826	G
1	2	1841	C
1	2	1848	U
1	2	1850	A
1	2	1859	A
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A
1	2	1870	A
1	2	1873	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	143	U
1	2	291	G
1	2	314	U
1	2	332	G
1	2	465	A
1	2	472	C
1	2	554	A
1	2	870	A
1	2	980	A
1	2	1308	U
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1430	C
1	2	1494	U
1	2	1534	C
1	2	1558	C
1	2	1647	A
1	2	1648	G
1	2	1726	G

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

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](#)

There are no chain breaks in this entry.

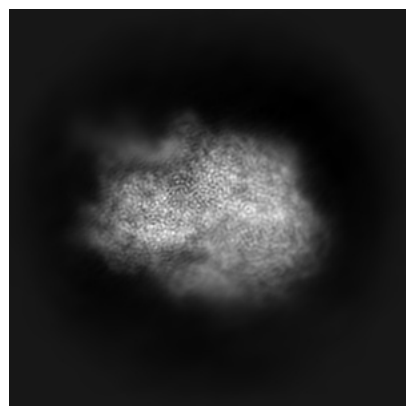
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39957. These allow visual inspection of the internal detail of the map and identification of artifacts.

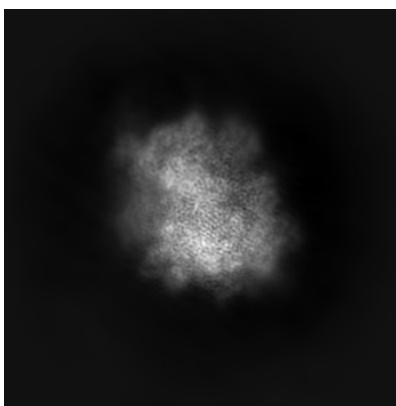
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

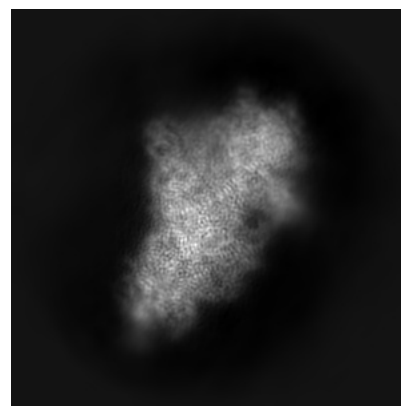
6.1.1 Primary map



X

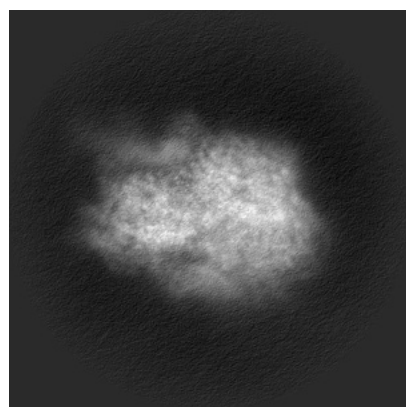


Y

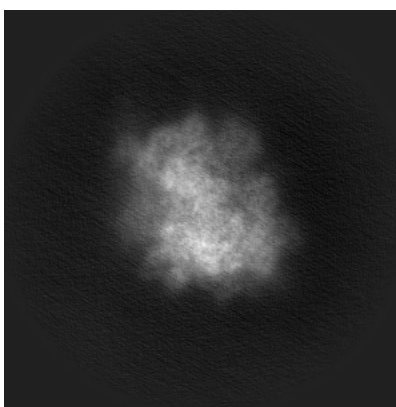


Z

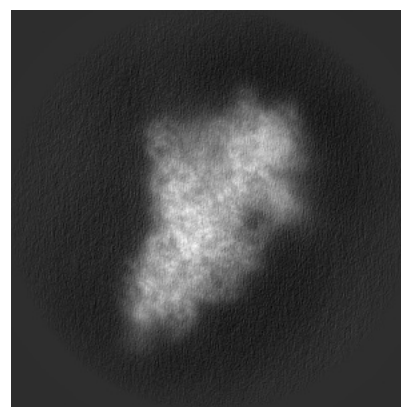
6.1.2 Raw map



X



Y

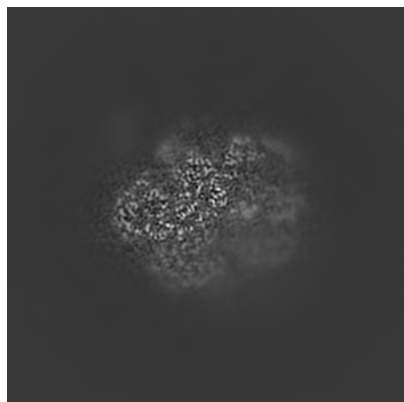


Z

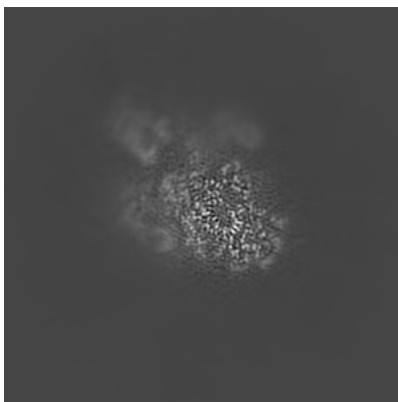
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

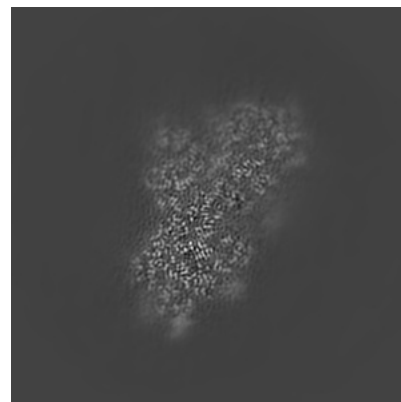
6.2.1 Primary map



X Index: 180

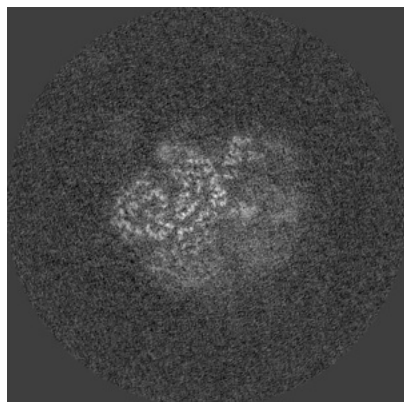


Y Index: 180

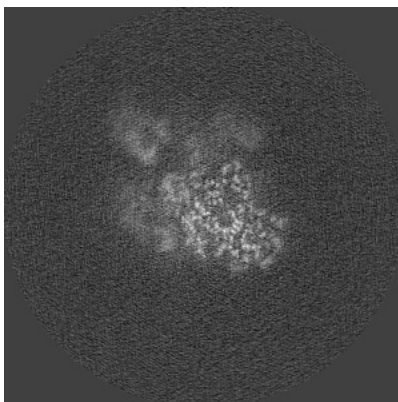


Z Index: 180

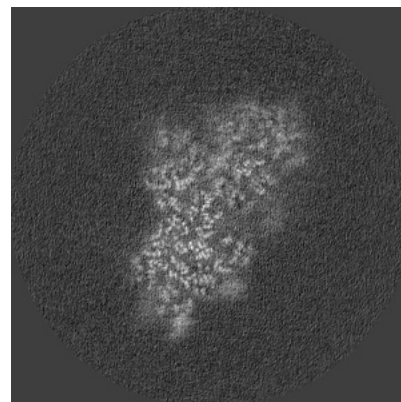
6.2.2 Raw map



X Index: 180



Y Index: 180

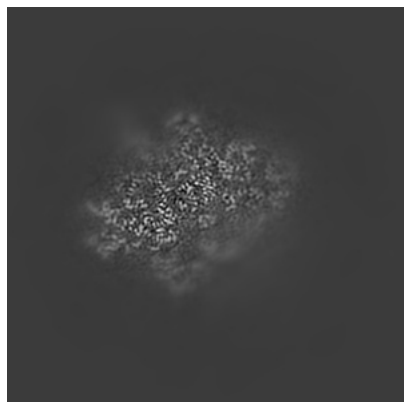


Z Index: 180

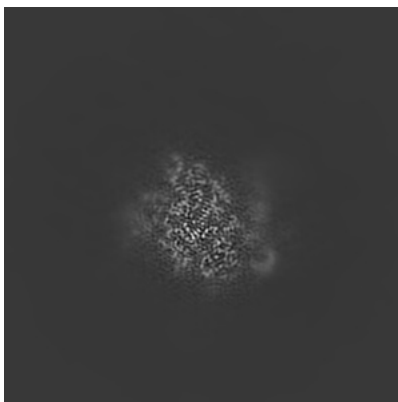
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

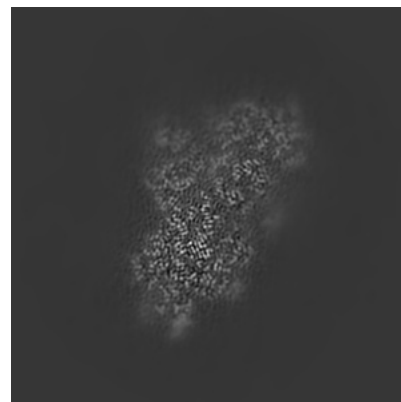
6.3.1 Primary map



X Index: 158

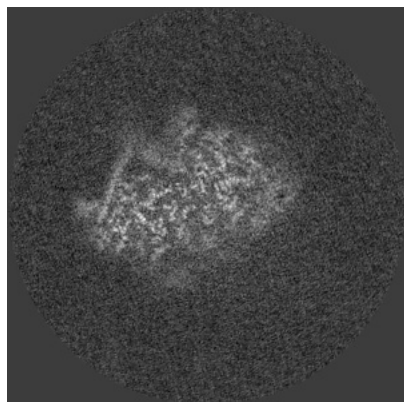


Y Index: 139

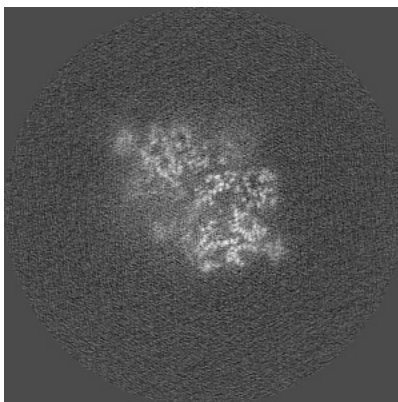


Z Index: 179

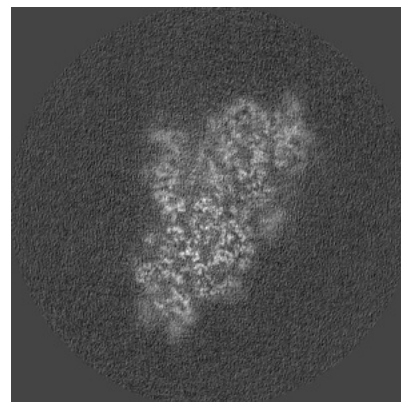
6.3.2 Raw map



X Index: 149



Y Index: 200

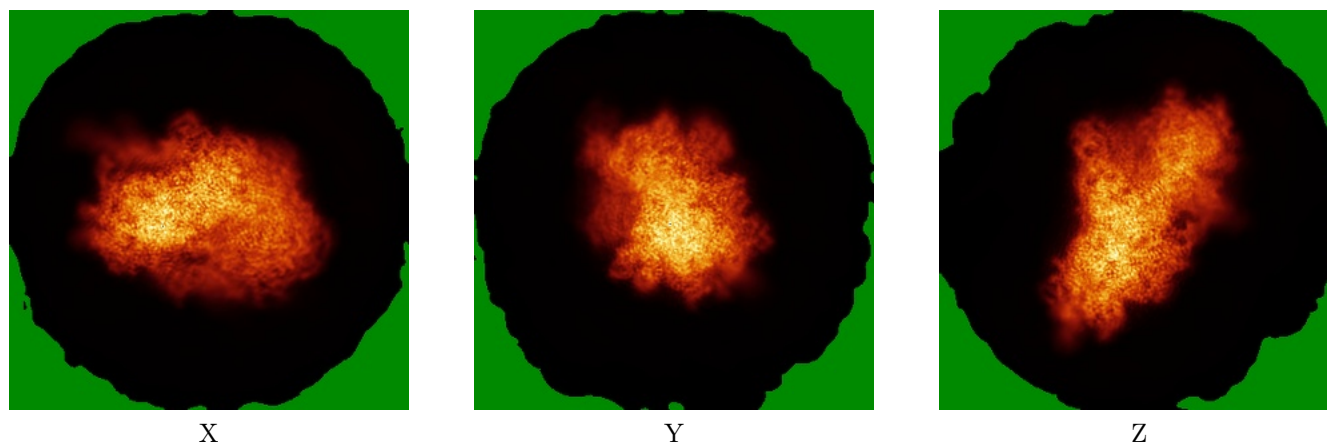


Z Index: 175

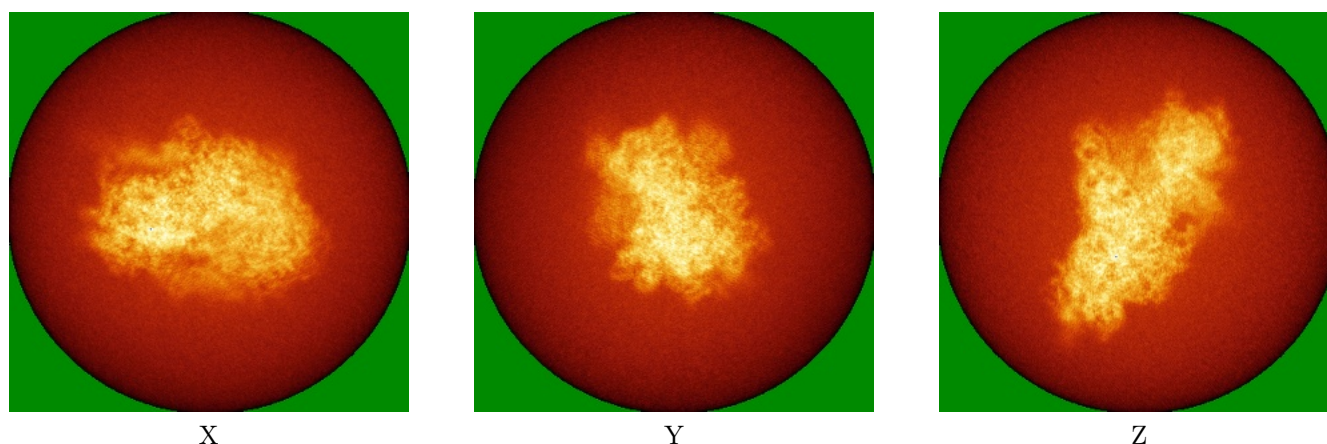
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

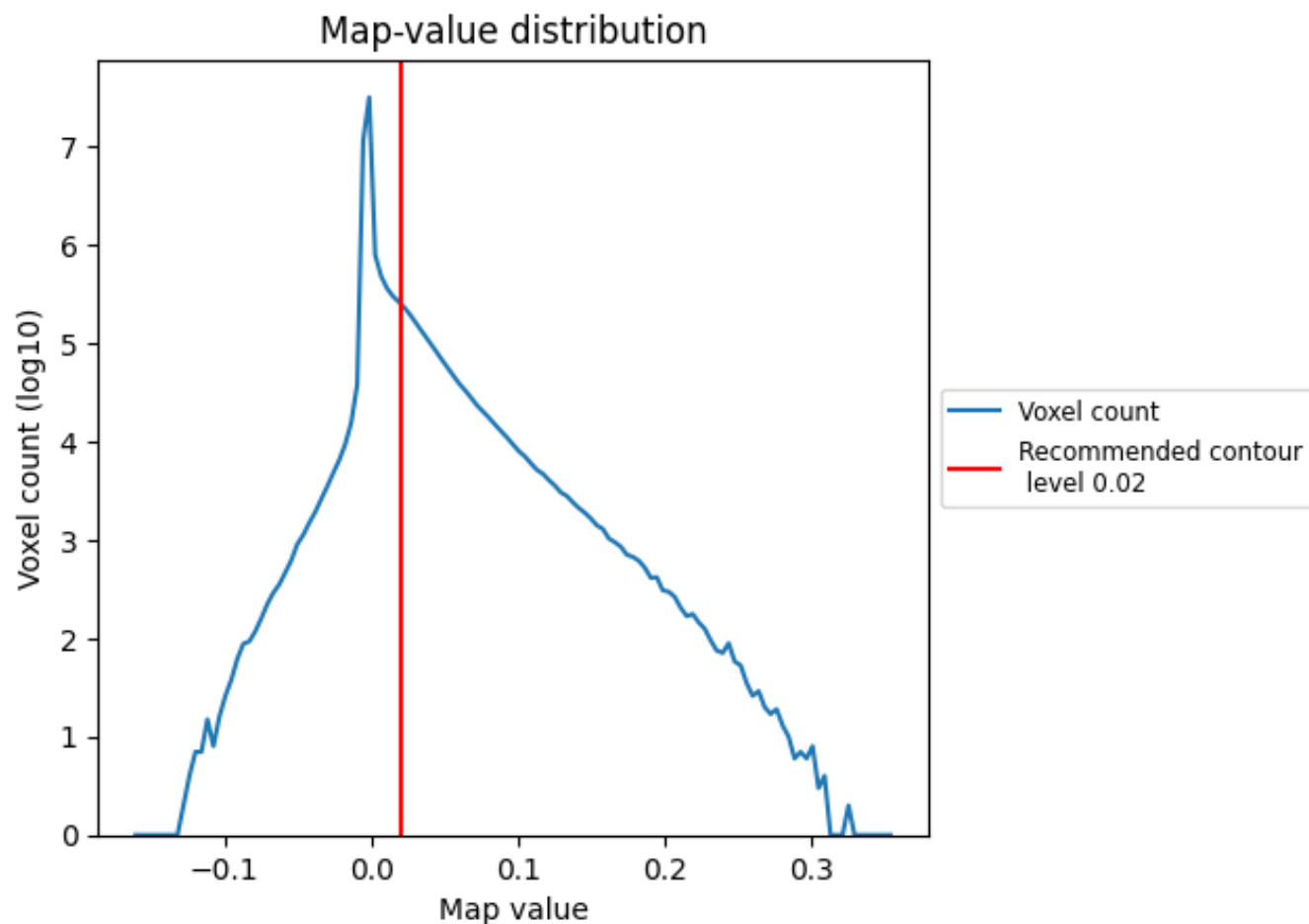
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

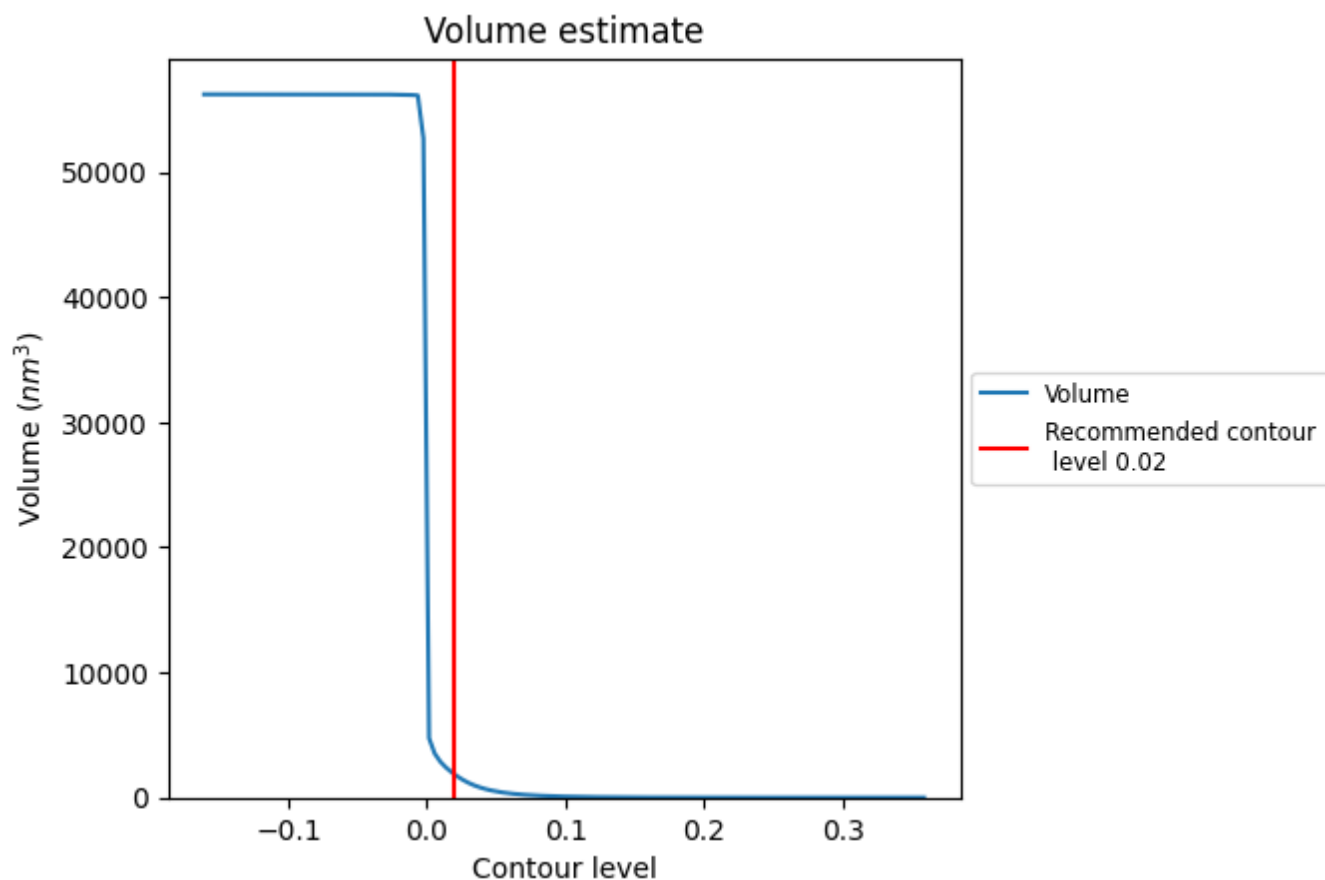
This section contains the results of statistical analysis of the map.

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.

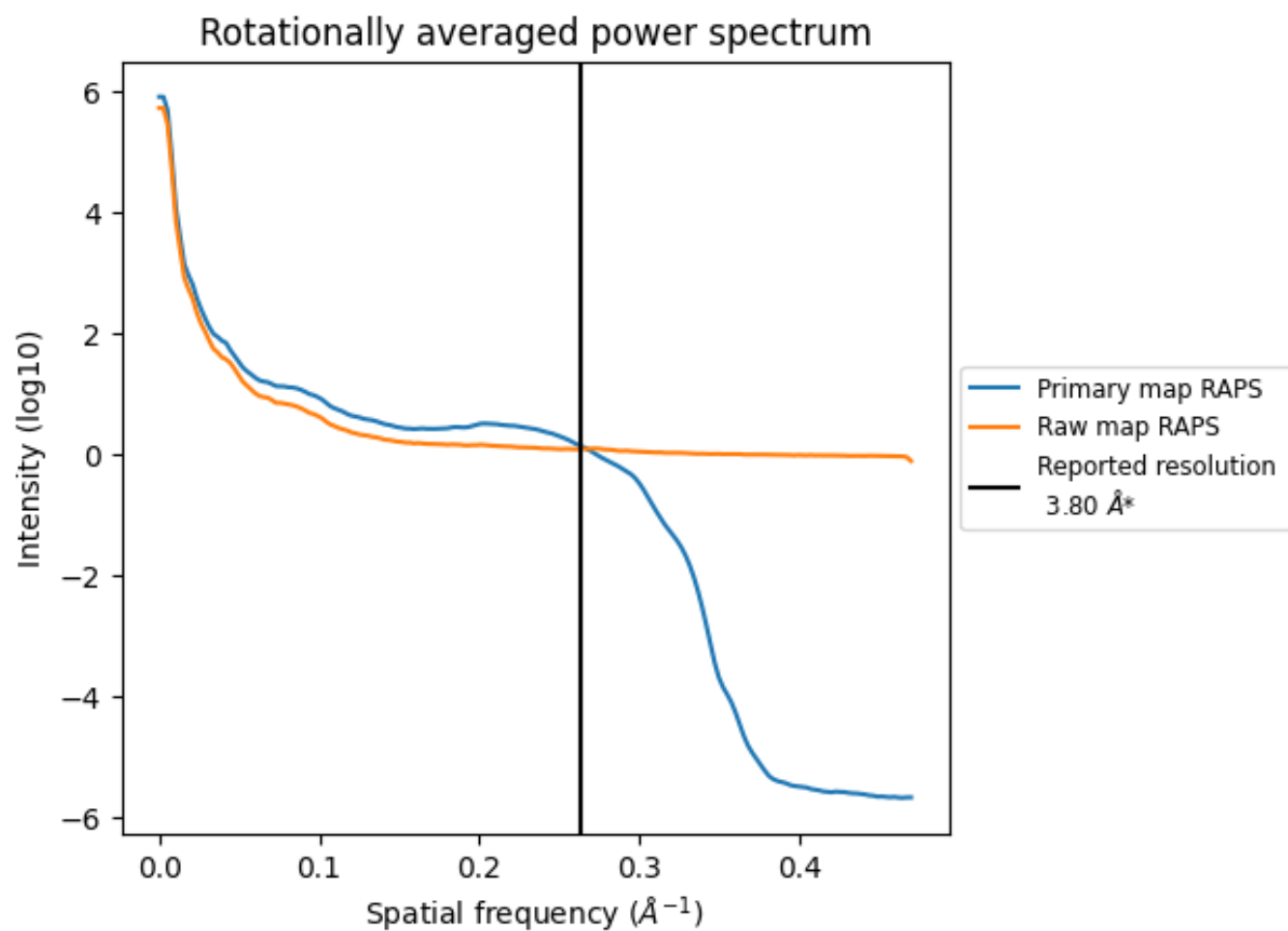
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1850 nm³; this corresponds to an approximate mass of 1671 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 ⓘ

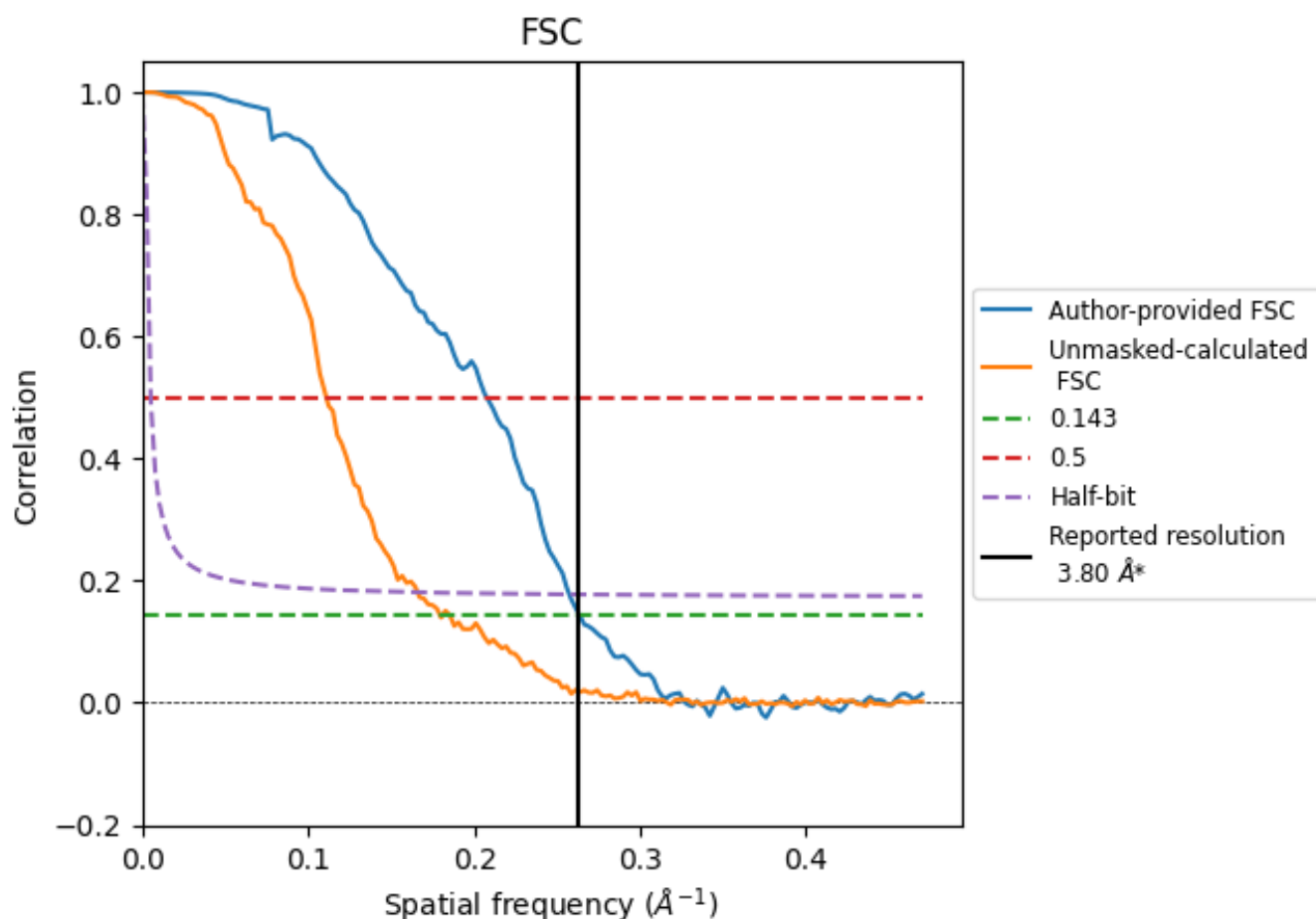


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

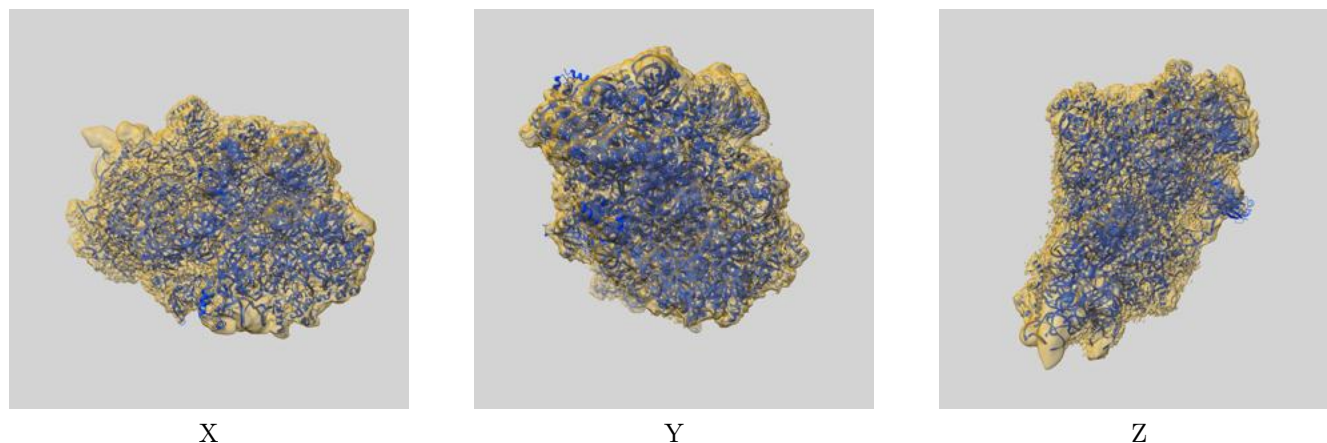
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.82	3.89
Unmasked-calculated*	5.57	9.01	6.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.57 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

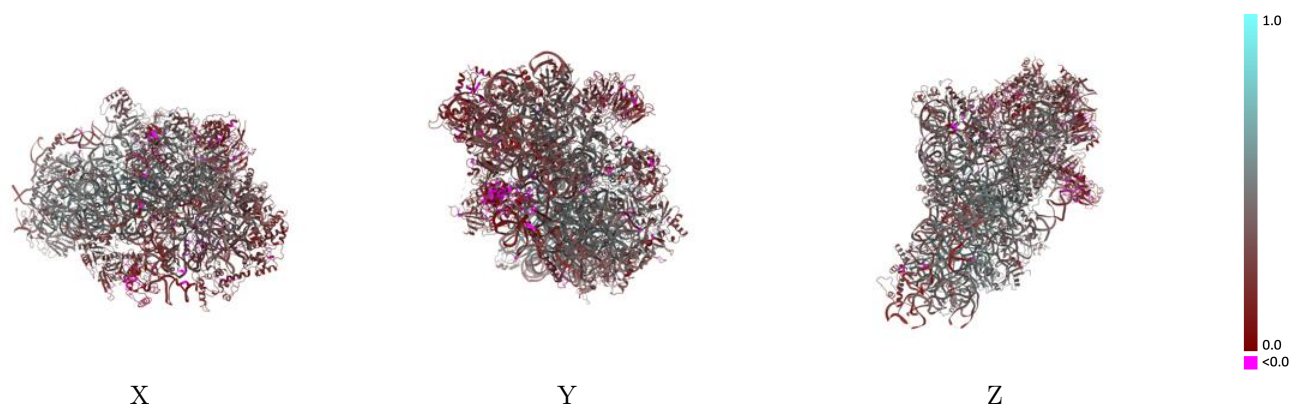
This section contains information regarding the fit between EMDB map EMD-39957 and PDB model 8ZDC. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



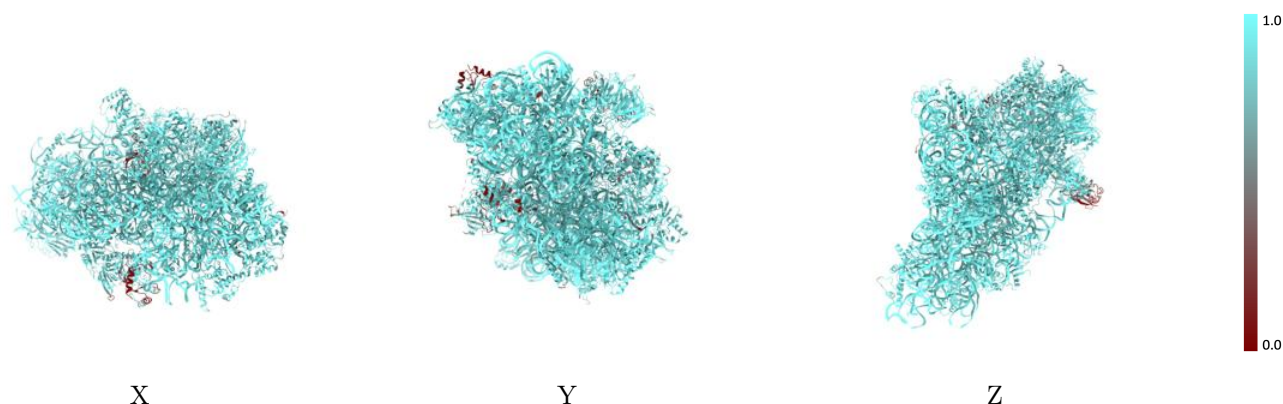
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



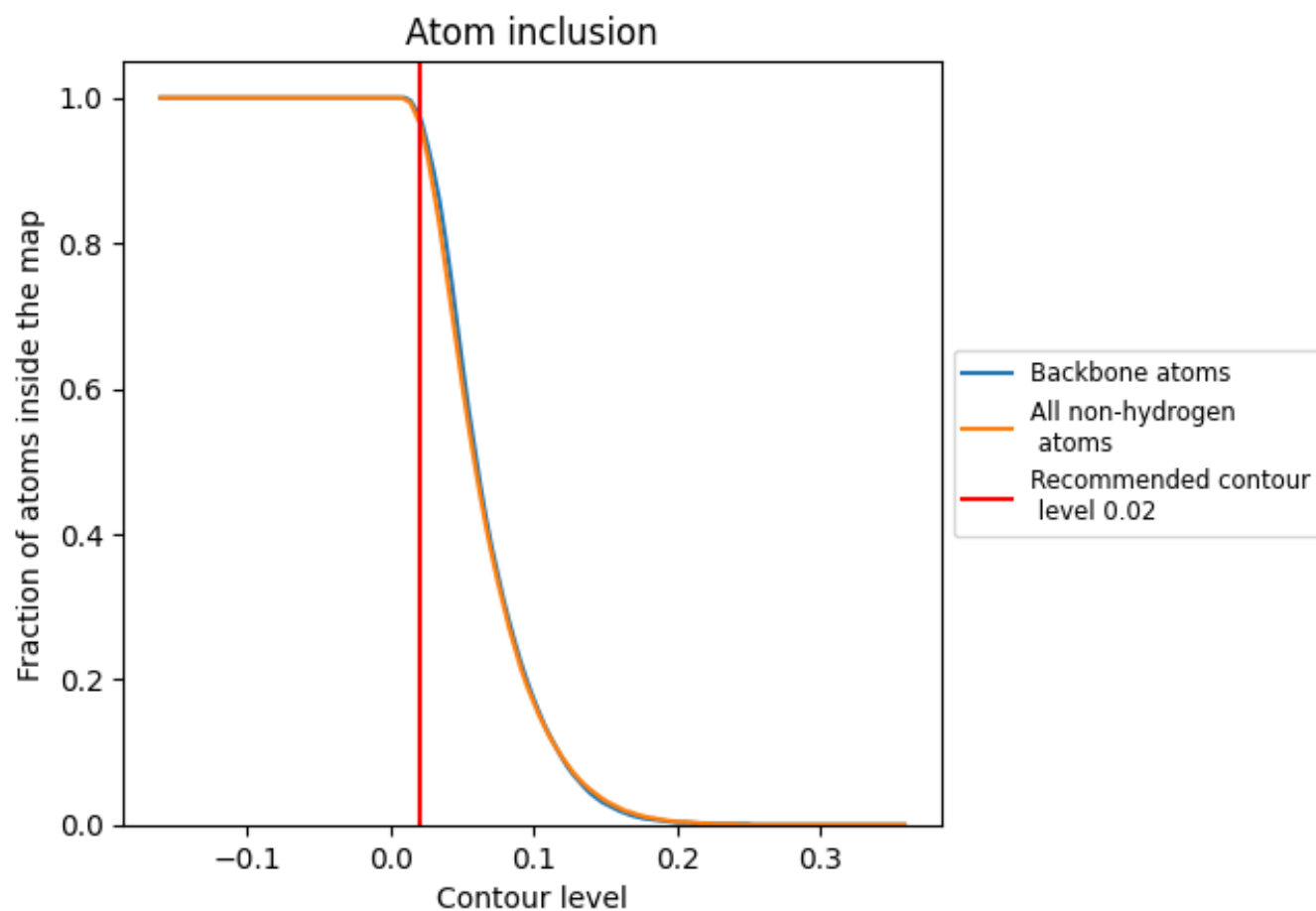
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.3680
2	 0.9940	 0.4010
A	 0.9810	 0.4410
B	 0.9640	 0.3850
C	 0.9840	 0.4620
D	 0.9700	 0.3680
E	 0.9900	 0.4870
F	 0.9840	 0.2950
G	 0.9770	 0.3940
H	 0.9670	 0.3460
I	 0.9700	 0.4130
J	 0.9930	 0.4390
K	 0.9680	 0.2700
L	 0.9930	 0.4940
M	 0.4810	 0.1070
N	 0.9940	 0.4480
O	 0.9800	 0.3600
P	 0.9600	 0.2360
Q	 0.9850	 0.3710
R	 0.9710	 0.3790
S	 0.9280	 0.2120
T	 0.9580	 0.2840
U	 0.9820	 0.3660
V	 0.9920	 0.4660
W	 0.9890	 0.5200
X	 0.9920	 0.4480
Y	 0.9870	 0.4550
Z	 0.9050	 0.1820
b	 0.9860	 0.4110
c	 0.9740	 0.2930
d	 0.9910	 0.3850
g	 0.9660	 0.2600
i	 0.4430	 0.1510
j	 0.7810	 0.1500
p	 0.8710	 0.1950



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Chain	Atom inclusion	Q-score
t	 0.8760	 0.2170
u	 0.9460	 0.2730
x	 0.9960	 0.4210
y	 0.8530	 0.2630