



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:52 PM UTC

PDB ID : 7WTW / pdb_00007wtw
EMDB ID : EMD-32803
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-A3
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2022-02-05
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

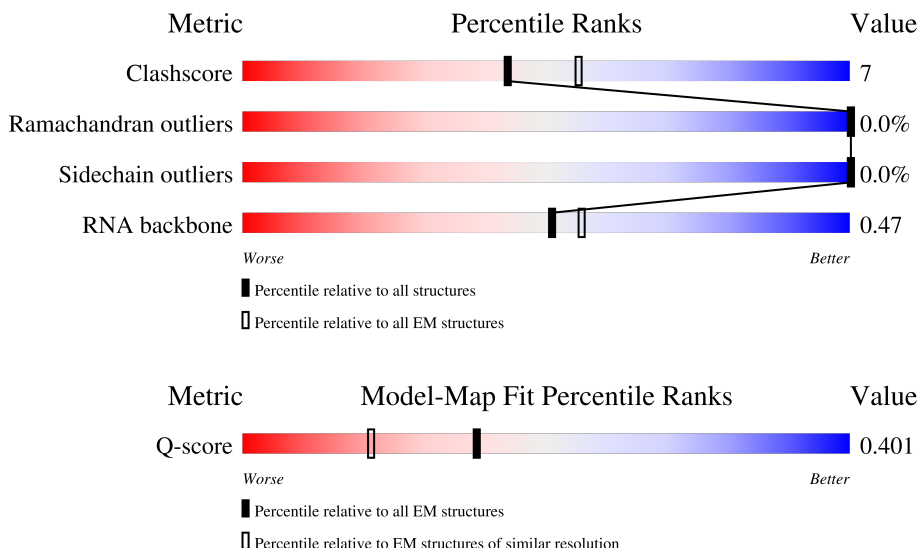
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	b	84	

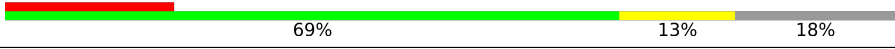
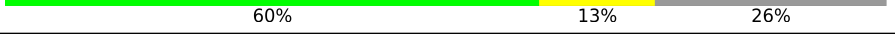
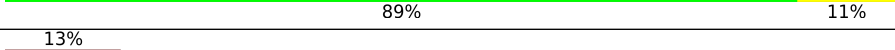
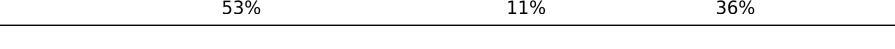
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Mol	Chain	Length	Quality of chain
4	B	264	
5	c	69	
6	E	263	
7	e	59	
8	F	204	
9	H	194	
10	G	249	
11	Z	125	
12	Y	133	
13	x	252	
14	X	143	
15	w	437	
16	t	475	
17	W	130	
18	u	804	
19	T	145	
20	S	152	
21	Q	146	
22	P	145	
23	O	151	
24	N	151	
25	L	158	
26	J	194	
27	I	208	
28	r	125	

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Mol	Chain	Length	Quality of chain
29	q	207	
30	K	1297	
31	M	132	
32	f	156	
33	z	230	
34	A	295	
35	C	293	
36	V	83	
37	y	412	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 87147 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	1586	Total	C	N	O	P	0	0
			33870	15116	6080	11088	1586		

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	81	Total	C	N	O	S	0	0
			673	420	137	114	2		

- Molecule 3 is a protein called 40S ribosomal protein S27.

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

- Molecule 4 is a protein called 40S ribosomal protein S3a.

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 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

- Molecule 6 is a protein called 40S ribosomal protein S4, 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 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	20	Total	C	N	O	S	0	0
			179	110	43	25	1		

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

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

- Molecule 10 is a protein called 40S ribosomal protein S6.

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

- Molecule 11 is a protein called 40S ribosomal protein S25.

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

- Molecule 12 is a protein called 40S ribosomal protein S24.

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

- Molecule 13 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	x	175	Total	C	N	O	S	0	0
			1372	881	249	238	4		

- Molecule 14 is a protein called 40S ribosomal protein S23.

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

- Molecule 15 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	332	Total	C	N	O	S	0	0
			2617	1676	478	454	9		

- Molecule 16 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	t	108	Total	C	N	O	S	0	0
			931	578	177	173	3		

- Molecule 17 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 18 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	642	Total	C	N	O	S	0	0
			5168	3315	928	901	24		

- Molecule 19 is a protein called 40S ribosomal protein S19.

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

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	127	Total	C	N	O	S	0	0
			1054	669	205	179	1		

- Molecule 21 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	125	Total	C	N	O	S	0	0
			998	637	185	173	3		

- Molecule 22 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	121	Total	C	N	O	S	0	0
			1006	643	186	170	7		

- Molecule 23 is a protein called 40S ribosomal protein S14.

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

- Molecule 24 is a protein called 40S ribosomal protein S13.

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

- Molecule 25 is a protein called 40S ribosomal protein S11.

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

- Molecule 26 is a protein called 40S ribosomal protein S9.

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

- Molecule 27 is a protein called 40S ribosomal protein S8.

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

- Molecule 28 is a protein called Multifunctional methyltransferase subunit TRM112-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	r	118	Total	C	N	O	S	0	0
			940	601	166	166	7		

- Molecule 29 is a protein called Probable 18S rRNA (guanine-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	202	Total	C	N	O	S	0	0
			1571	999	264	297	11		

- Molecule 30 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	993	Total	C	N	O	S	0	0
			7707	4938	1337	1387	45		

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Ribosome biogenesis protein SLX9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	52	Total	C	N	O	S	0	0
			416	255	80	79	2		

- Molecule 34 is a protein called 40S ribosomal protein SA.

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

- Molecule 35 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	216	Total	C	N	O	S	0	0
			1674	1085	287	292	10		

- Molecule 36 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 37 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	265	Total	C	N	O	S	0	0
			2091	1324	384	373	10		

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

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





• Molecule 4: 40S ribosomal protein S3a

Chain B: 64% 17% 19%



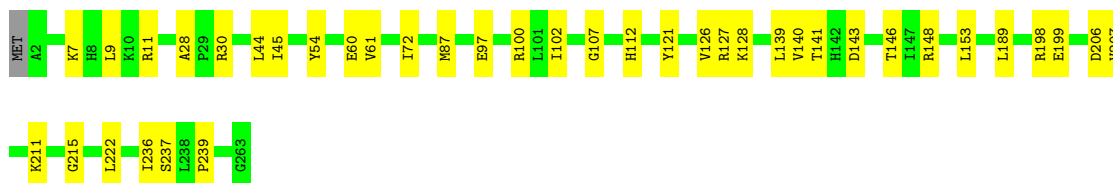
• Molecule 5: 40S ribosomal protein S28

Chain c: 70% 19% 12%



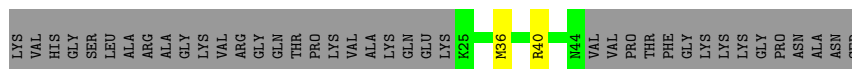
• Molecule 6: 40S ribosomal protein S4, X isoform

Chain E: 85% 15%



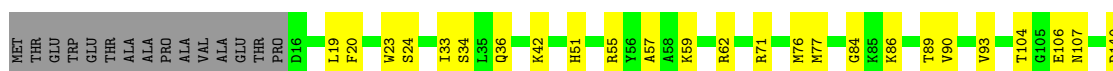
• Molecule 7: 40S ribosomal protein S30

Chain e: 31% 66%



• Molecule 8: 40S ribosomal protein S5

Chain F: 75% 18% 7%





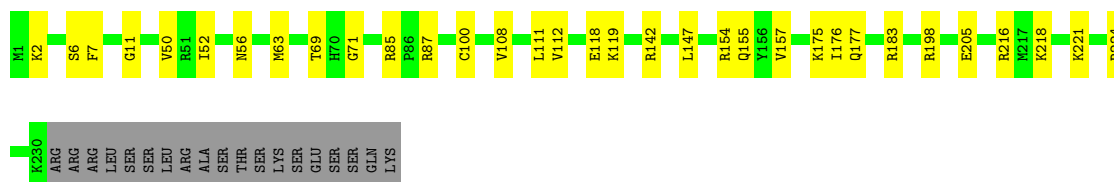
- Molecule 9: 40S ribosomal protein S7

Chain H: 78% 18%



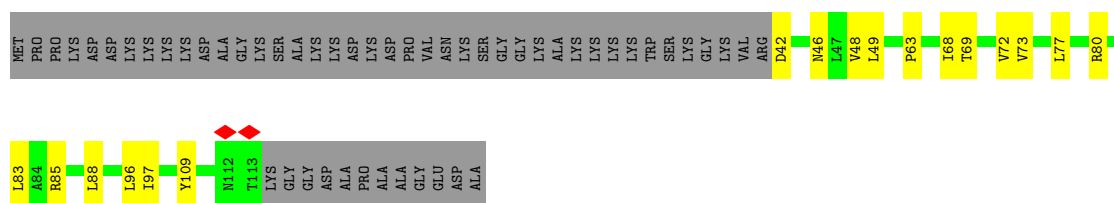
- Molecule 10: 40S ribosomal protein S6

Chain G: 79% 13% 8%



- Molecule 11: 40S ribosomal protein S25

Chain Z: 44% 14% 42%



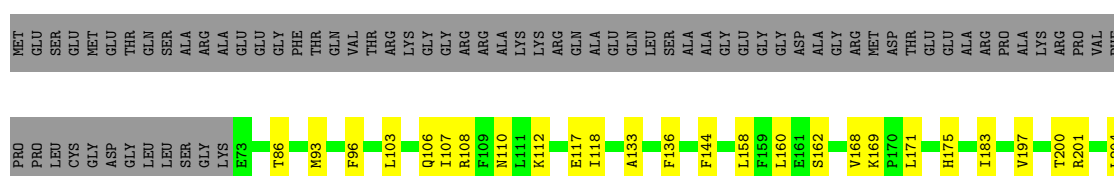
- Molecule 12: 40S ribosomal protein S24

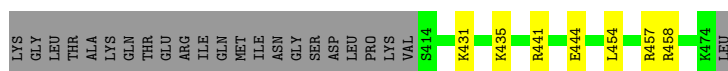
Chain Y: 80% 14% 7%



- Molecule 13: RNA-binding protein PNO1

Chain x: 55% 14% 31%





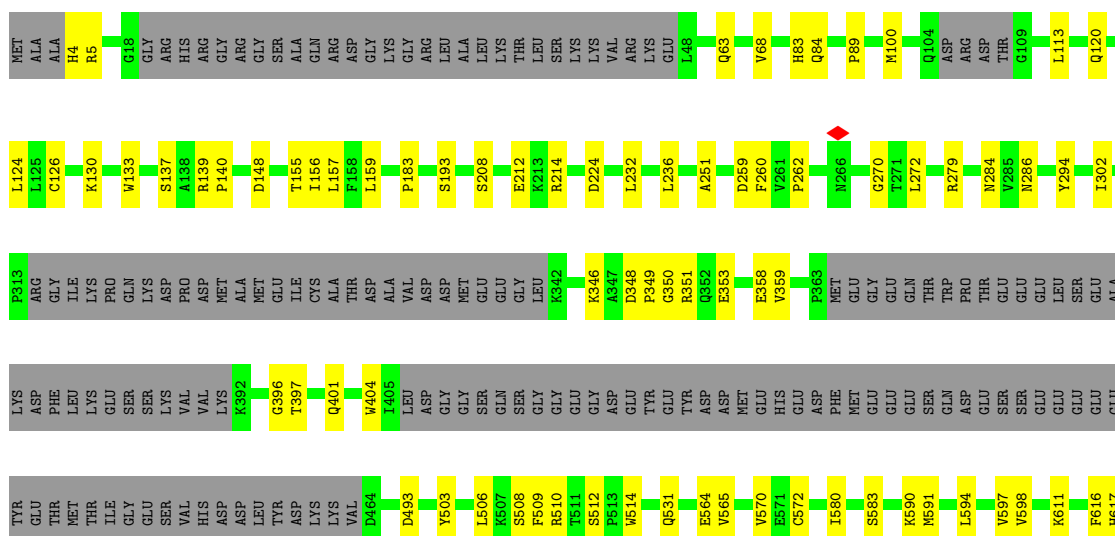
- Molecule 17: 40S ribosomal protein S15a

Chain W: 89% 10%



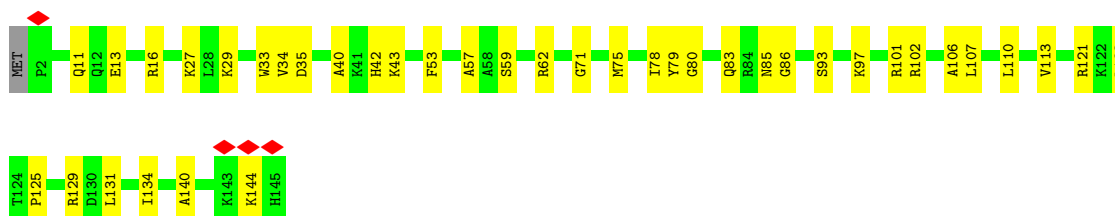
- Molecule 18: Pre-rRNA-processing protein TSR1 homolog

Chain u: 68% 12% 20%



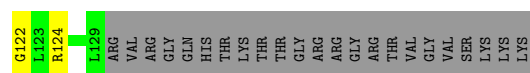
- Molecule 19: 40S ribosomal protein S19

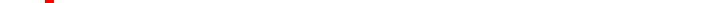
Chain T: 72% 27%

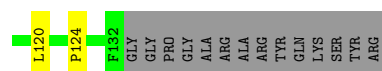


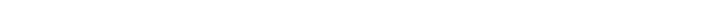
- Molecule 20: 40S ribosomal protein S18

Chain S: 63% 20% 16%

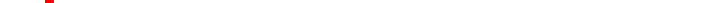


- Chain Q:  63% 23% 14%



- Chain P:  61% 23% 17%

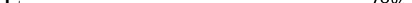


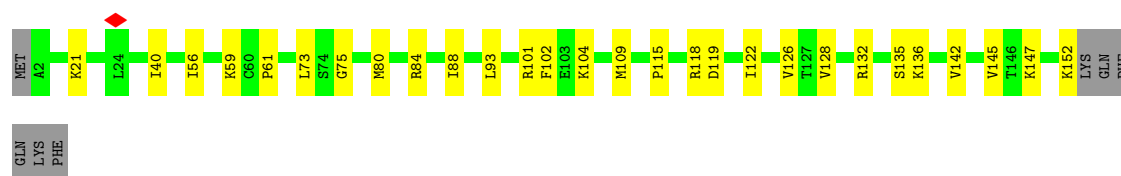
- Chain O:  70% 19% 11%



- Chain N: 91% 8%

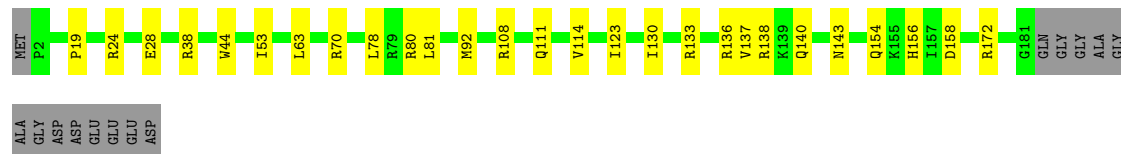


- Chain L:  78% 18%



- Molecule 26: 40S ribosomal protein S9

Chain J: 79% 14% 7%



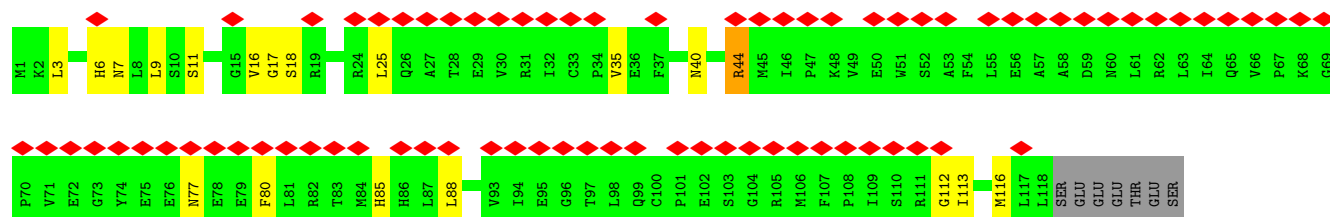
- Molecule 27: 40S ribosomal protein S8

Chain I: 77% 21%



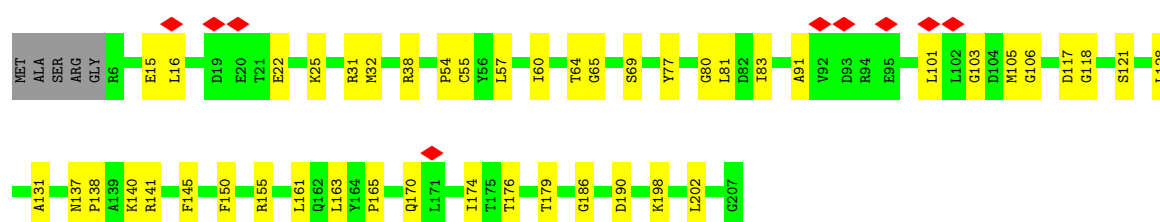
- Molecule 28: Multifunctional methyltransferase subunit TRM112-like protein

Chain r: 62% 79% 14% 6%

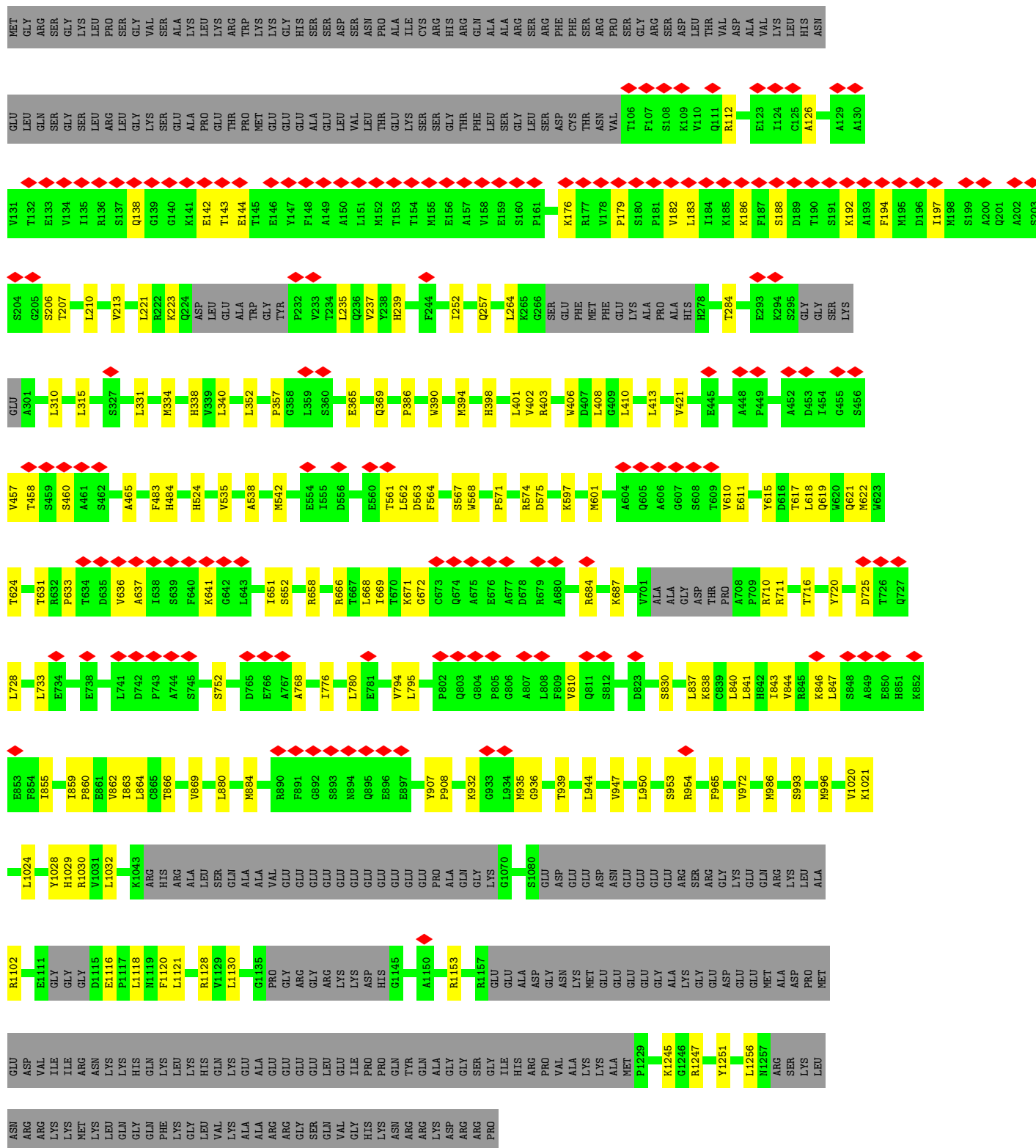


- Molecule 29: Probable 18S rRNA (guanine-N(7))-methyltransferase

Chain q: 75% 22%

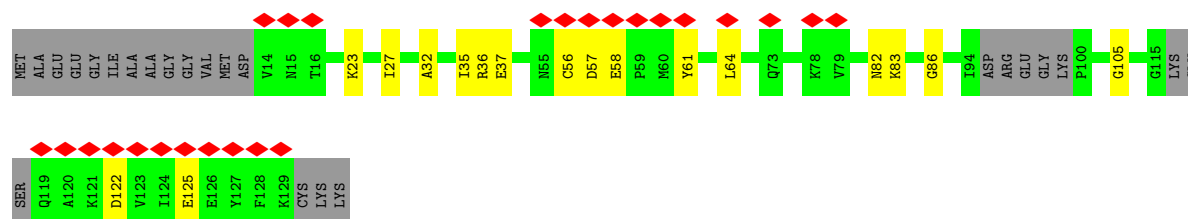


- Molecule 30: RRP12-like protein



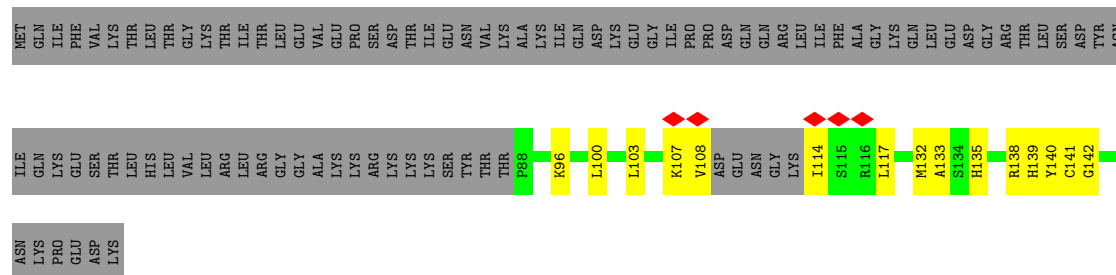
- Molecule 31: 40S ribosomal protein S12





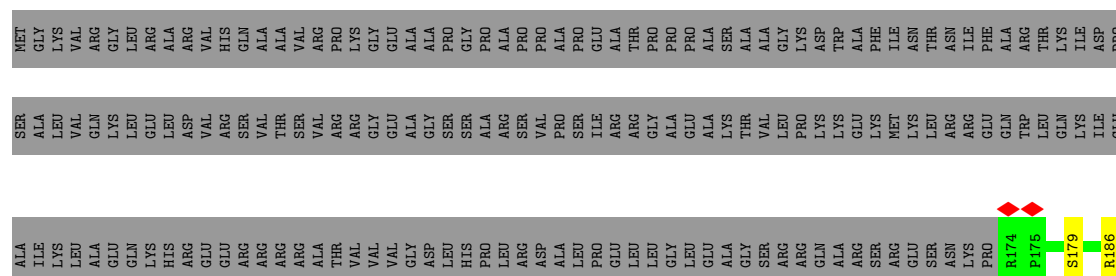
- Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain f: 27% 10% 63%



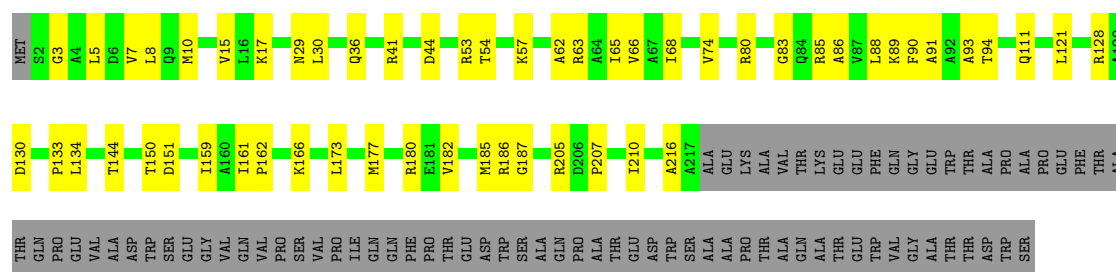
- Molecule 33: Ribosome biogenesis protein SLX9 homolog

Chain z: 9% 17% 5% 77%



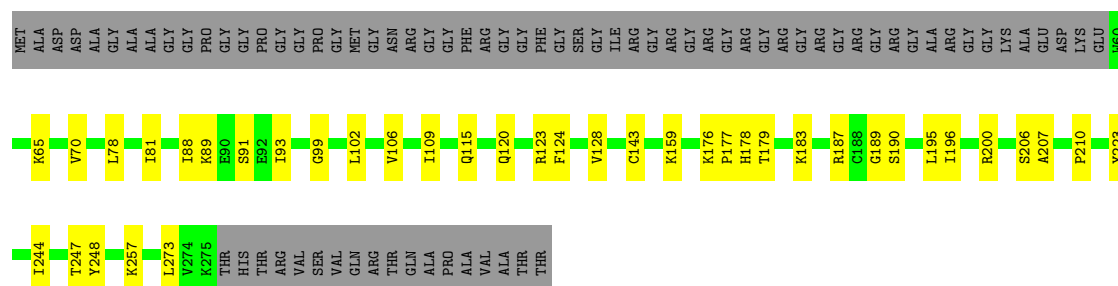
- Molecule 34: 40S ribosomal protein SA

Chain A: 55% 19% 27%



- Molecule 35: 40S ribosomal protein S2

Chain C:  60% 13% 26%



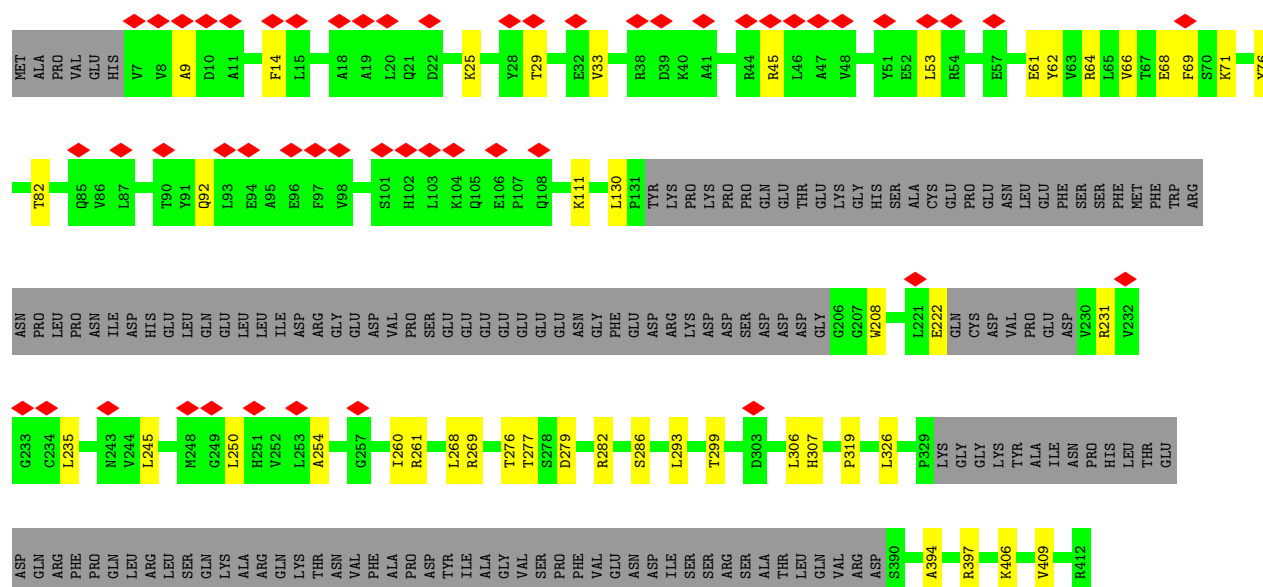
- Molecule 36: 40S ribosomal protein S21

Chain V:  89% 11%



- Molecule 37: RNA-binding protein NOB1

Chain y:  13% 53% 11% 36%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.479	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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, G7M

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	0.19	1/37837 (0.0%)	0.36	0/58946
2	R	0.17	0/680	0.44	0/905
3	b	0.17	0/653	0.44	0/876
4	B	0.21	0/1756	0.52	0/2350
5	c	0.20	0/473	0.50	0/633
6	E	0.22	0/2118	0.44	0/2849
7	e	0.18	0/180	0.37	0/232
8	F	0.15	0/1515	0.44	0/2037
9	H	0.20	0/1524	0.50	0/2042
10	G	0.18	0/1885	0.42	0/2510
11	Z	0.22	0/580	0.62	0/780
12	Y	0.19	0/1031	0.39	0/1370
13	x	0.26	0/1394	0.58	0/1880
14	X	0.23	0/1116	0.52	0/1490
15	w	0.16	0/2664	0.41	0/3597
16	t	0.19	0/942	0.53	0/1246
17	W	0.23	0/1050	0.50	0/1406
18	u	0.22	1/5296 (0.0%)	0.45	0/7154
19	T	0.18	0/1142	0.49	0/1530
20	S	0.21	0/1071	0.55	0/1437
21	Q	0.18	0/1012	0.45	0/1356
22	P	0.18	0/1025	0.48	0/1369
23	O	0.21	0/1022	0.58	0/1372
24	N	0.18	0/1226	0.40	0/1649
25	L	0.21	0/1250	0.40	0/1673
26	J	0.23	0/1524	0.50	2/2035 (0.1%)
27	I	0.23	0/1711	0.49	0/2282
28	r	0.17	0/961	0.47	0/1301
29	q	0.15	0/1606	0.39	0/2170
30	K	0.17	0/7851	0.44	0/10624
31	M	0.16	0/845	0.40	0/1134
32	f	0.15	0/474	0.49	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	z	0.21	0/420	0.54	1/564 (0.2%)
34	A	0.20	0/1742	0.46	0/2367
35	C	0.22	0/1710	0.49	0/2310
36	V	0.16	0/643	0.38	0/860
37	y	0.19	0/2130	0.51	3/2874 (0.1%)
All	All	0.20	2/92059 (0.0%)	0.42	6/131836 (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
18	u	0	1
27	I	0	1
28	r	0	1
33	z	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	u	564	GLU	CA-CB	5.94	1.61	1.52
1	2	1639	G7M	O3'-P	5.04	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	137	VAL	CA-C-N	5.57	132.18	121.54
26	J	137	VAL	C-N-CA	5.57	132.18	121.54
37	y	68	GLU	CA-C-N	-5.50	110.86	121.58
37	y	68	GLU	C-N-CA	-5.50	110.86	121.58
33	z	199	GLU	N-CA-CB	5.22	117.98	110.20
37	y	68	GLU	N-CA-CB	5.21	117.87	110.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	I	66	SER	Peptide
28	r	44	ARG	Peptide

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Mol	Chain	Res	Type	Group
18	u	348	ASP	Peptide
33	z	222	MET	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	33870	0	17108	360	0
2	R	673	0	722	12	0
3	b	640	0	665	4	0
4	B	1729	0	1803	29	0
5	c	471	0	499	9	0
6	E	2076	0	2177	28	0
7	e	179	0	200	1	0
8	F	1494	0	1549	24	0
9	H	1501	0	1593	23	0
10	G	1862	0	2018	23	0
11	Z	574	0	627	14	0
12	Y	1014	0	1082	13	0
13	x	1372	0	1453	31	0
14	X	1098	0	1167	11	0
15	w	2617	0	2652	34	0
16	t	931	0	949	9	0
17	W	1033	0	1080	9	0
18	u	5168	0	5230	60	0
19	T	1122	0	1153	28	0
20	S	1054	0	1105	21	0
21	Q	998	0	1065	26	0
22	P	1006	0	1056	26	0
23	O	1009	0	1034	28	0
24	N	1202	0	1289	9	0
25	L	1229	0	1302	17	0
26	J	1499	0	1618	18	0
27	I	1682	0	1769	28	0
28	r	940	0	958	13	0
29	q	1571	0	1545	27	0
30	K	7707	0	7986	110	0
31	M	837	0	870	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	f	465	0	485	12	0
33	z	416	0	424	11	0
34	A	1705	0	1706	42	0
35	C	1674	0	1764	25	0
36	V	636	0	637	9	0
37	y	2091	0	2147	28	0
38	f	1	0	0	0	0
38	y	1	0	0	0	0
All	All	87147	0	72487	1004	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 (1004) 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)
17:W:101:PHE:O	17:W:128:PHE:HA	1.37	1.24
1:2:748:C:H42	1:2:794:A:N6	1.46	1.12
1:2:748:C:N4	1:2:794:A:H61	1.46	1.12
1:2:1609:C:N4	1:2:1630:A:H61	1.49	1.10
1:2:1609:C:H42	1:2:1630:A:N6	1.49	1.10
1:2:1710:C:H42	1:2:1823:A:N6	1.49	1.09
1:2:1710:C:N4	1:2:1823:A:H61	1.49	1.08
1:2:536:A:H61	1:2:548:C:N4	1.55	1.03
1:2:536:A:N6	1:2:548:C:H42	1.55	1.02
1:2:1215:C:H42	1:2:1220:A:N6	1.59	0.99
1:2:1398:G:H1	1:2:1448:A:H2	1.03	0.98
1:2:24:C:H42	1:2:650:A:N6	1.63	0.97
1:2:1232:U:H3	1:2:1527:C:H42	1.09	0.97
1:2:24:C:N4	1:2:650:A:H61	1.64	0.96
1:2:1335:G:H1	1:2:1492:U:H3	1.04	0.93
1:2:1215:C:N4	1:2:1220:A:H61	1.64	0.93
1:2:674:C:H42	1:2:1031:A:N6	1.66	0.93
1:2:674:C:N4	1:2:1031:A:H61	1.68	0.91
1:2:1232:U:H3	1:2:1527:C:N4	1.69	0.91
1:2:674:C:H42	1:2:1031:A:H61	0.95	0.90
1:2:1548:G:O6	1:2:1586:U:C4	2.26	0.88
1:2:8:U:O4	1:2:15:U:O4	1.92	0.88
1:2:1215:C:H42	1:2:1220:A:H61	0.90	0.87
1:2:1548:G:C6	1:2:1586:U:O4	2.28	0.87
1:2:536:A:H61	1:2:548:C:H42	0.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1236:G:H21	1:2:1522:A:H62	1.25	0.83
1:2:925:G:H1	1:2:1017:U:H3	1.24	0.82
1:2:1288:U:H3	1:2:1311:C:H42	1.24	0.81
32:f:133:ALA:HB3	32:f:140:TYR:O	1.81	0.81
1:2:1296:U:H3	1:2:1301:A:H62	1.28	0.80
1:2:1330:G:H1	1:2:1499:U:H3	0.83	0.80
8:F:157:GLY:O	8:F:161:ALA:HB2	1.82	0.80
30:K:538:ALA:O	30:K:542:MET:HB3	1.83	0.79
1:2:1534:C:C2	1:2:1598:G:N2	2.51	0.78
1:2:1277:C:O2	1:2:1322:G:N2	2.16	0.78
1:2:1282:A:H61	1:2:1316:C:N4	1.82	0.78
13:x:106:GLN:HE22	37:y:208:TRP:HB3	1.49	0.76
1:2:536:A:N1	1:2:548:C:N3	2.34	0.76
1:2:1472:C:H42	1:2:1476:A:H62	1.34	0.75
1:2:1282:A:N6	1:2:1316:C:H42	1.84	0.75
1:2:1398:G:N1	1:2:1448:A:H2	1.84	0.74
1:2:1710:C:N3	1:2:1823:A:N1	2.36	0.74
1:2:1609:C:N3	1:2:1630:A:N1	2.36	0.73
1:2:1748:G:H1	1:2:1786:U:H3	1.37	0.73
1:2:748:C:H42	1:2:794:A:H61	0.75	0.72
1:2:1288:U:H3	1:2:1311:C:N4	1.87	0.72
1:2:24:C:H42	1:2:650:A:H61	0.81	0.72
1:2:71:G:C6	1:2:79:A:C5	2.78	0.71
14:X:68:LYS:HD3	14:X:91:LEU:HD22	1.72	0.71
1:2:1302:G:O6	1:2:1307:U:O4	2.09	0.70
23:O:103:ASN:HB3	23:O:142:ARG:HG2	1.73	0.70
1:2:1616:U:O4	22:P:40:ARG:NH1	2.24	0.70
29:q:190:ASP:O	29:q:198:LYS:HA	1.91	0.70
5:c:46:VAL:HG22	8:F:140:ASP:HB3	1.73	0.70
1:2:749:U:O4	1:2:793:G:O6	2.10	0.70
1:2:1215:C:H41	1:2:1646:C:H41	1.40	0.70
1:2:1398:G:N1	1:2:1448:A:C2	2.52	0.69
1:2:748:C:N4	1:2:794:A:N6	2.21	0.68
9:H:76:GLN:HE22	9:H:94:PHE:HB2	1.57	0.68
23:O:98:ARG:NH1	23:O:99:ALA:O	2.26	0.68
6:E:198:ARG:HA	6:E:207:VAL:O	1.93	0.68
1:2:1282:A:H61	1:2:1316:C:H42	1.37	0.67
22:P:108:LYS:HB2	22:P:111:MET:HE1	1.76	0.67
30:K:687:LYS:HG3	30:K:728:LEU:HD13	1.75	0.67
4:B:165:ARG:HG2	4:B:169:MET:HE2	1.77	0.67
9:H:177:TYR:O	9:H:181:THR:HB	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:x:133:ALA:O	13:x:136:PHE:HB3	1.95	0.67
1:2:1548:G:C6	1:2:1586:U:C4	2.82	0.67
35:C:91:SER:HB2	35:C:159:LYS:HD2	1.76	0.67
1:2:24:C:N3	1:2:650:A:N1	2.43	0.66
1:2:1545:A:C5	1:2:1588:A:C6	2.84	0.66
30:K:188:SER:OG	30:K:192:LYS:NZ	2.27	0.66
21:Q:34:VAL:HG12	21:Q:70:VAL:HB	1.78	0.66
1:2:1606:G:H5'	19:T:86:GLY:HA2	1.77	0.65
21:Q:11:GLN:HB2	30:K:1120:PHE:HB2	1.79	0.65
30:K:197:ILE:HG21	30:K:213:VAL:HG21	1.78	0.65
1:2:104:A:H62	1:2:356:C:N4	1.95	0.65
13:x:168:VAL:HG23	23:O:149:ARG:HH11	1.61	0.65
18:u:251:ALA:HB3	18:u:583:SER:HB3	1.79	0.64
31:M:32:ALA:HB1	31:M:37:GLU:HB3	1.80	0.64
37:y:61:GLU:OE1	37:y:64:ARG:NH2	2.31	0.64
1:2:1871:C:N4	13:x:86:THR:OG1	2.31	0.64
35:C:109:ILE:HD11	35:C:124:PHE:HB3	1.80	0.64
1:2:71:G:N1	1:2:79:A:C5	2.66	0.64
1:2:64:A:H2	1:2:83:A:H62	1.43	0.64
1:2:507:G:OP1	12:Y:108:LYS:NZ	2.31	0.64
32:f:132:MET:HE2	32:f:139:HIS:HB3	1.77	0.64
1:2:957:A:H3'	1:2:958:G:H21	1.63	0.64
31:M:86:GLY:HA3	31:M:105:GLY:HA2	1.79	0.64
1:2:885:U:O2	1:2:902:G:C6	2.51	0.63
4:B:107:ARG:NH1	23:O:133:THR:O	2.31	0.63
9:H:93:VAL:HG21	9:H:133:LEU:HD12	1.80	0.63
22:P:87:PRO:HA	22:P:112:ILE:HD12	1.79	0.63
17:W:111:MET:HE3	17:W:116:ALA:HA	1.81	0.63
1:2:8:U:H3	1:2:1196:A:H62	1.47	0.63
1:2:1551:U:C4	1:2:1577:G:C6	2.86	0.63
8:F:33:ILE:O	8:F:36:GLN:NE2	2.30	0.63
10:G:69:THR:HG22	10:G:71:GLY:H	1.63	0.63
1:2:962:A:N1	1:2:1055:A:O2'	2.32	0.62
28:r:44:ARG:NH2	29:q:54:PRO:O	2.31	0.62
29:q:161:LEU:HB2	29:q:202:LEU:HB2	1.80	0.62
34:A:36:GLN:NE2	36:V:67:ASP:OD1	2.29	0.62
1:2:1398:G:O6	1:2:1448:A:N1	2.32	0.62
1:2:1682:C:OP2	15:w:34:ARG:NH2	2.33	0.62
30:K:950:LEU:HA	33:z:222:MET:HE1	1.82	0.62
1:2:1203:G:H2'	1:2:1204:A:H8	1.65	0.62
1:2:1849:G:OP2	16:t:441:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1534:C:O2	1:2:1598:G:N2	2.32	0.62
10:G:157:VAL:HG11	10:G:176:ILE:HD11	1.81	0.62
14:X:139:GLU:OE2	18:u:214:ARG:NH1	2.32	0.62
1:2:913:A:H2	9:H:99:ARG:H	1.48	0.61
1:2:1236:G:N2	1:2:1522:A:H62	1.98	0.61
1:2:1268:C:H4'	22:P:100:LYS:HG3	1.81	0.61
26:J:24:ARG:NH1	26:J:28:GLU:OE2	2.32	0.61
34:A:29:ASN:HB2	34:A:151:ASP:HB3	1.82	0.61
15:w:390:LYS:HA	15:w:393:LEU:HD12	1.83	0.61
35:C:176:LYS:HD3	35:C:177:PRO:HD2	1.82	0.61
1:2:674:C:N3	1:2:1031:A:N1	2.49	0.61
14:X:11:ARG:NH2	25:L:104:LYS:O	2.34	0.61
21:Q:45:ARG:O	21:Q:48:GLN:HB3	2.01	0.61
25:L:80:MET:HE2	25:L:122:ILE:HG13	1.82	0.60
1:2:798:G:HO2'	9:H:108:SER:HG	1.47	0.60
1:2:1282:A:N6	1:2:1316:C:N4	2.46	0.60
4:B:71:LEU:HD12	4:B:84:PHE:HE2	1.67	0.60
13:x:110:ASN:ND2	13:x:117:GLU:OE2	2.34	0.60
15:w:301:THR:HG23	15:w:304:GLU:H	1.66	0.60
1:2:1534:C:C2	1:2:1598:G:C2	2.90	0.60
37:y:25:LYS:HE2	37:y:231:ARG:HH22	1.66	0.60
1:2:1545:A:C6	1:2:1588:A:C6	2.90	0.60
1:2:1551:U:N3	1:2:1577:G:C6	2.70	0.60
19:T:11:GLN:OE1	19:T:62:ARG:NH2	2.35	0.60
23:O:44:VAL:HG13	23:O:53:ILE:HB	1.83	0.60
1:2:1565:C:OP2	19:T:102:ARG:NH2	2.34	0.60
18:u:302:ILE:HD13	18:u:346:LYS:HD2	1.84	0.60
24:N:30:SER:HB2	24:N:67:THR:HA	1.84	0.60
1:2:1203:G:H1'	35:C:115:GLN:HB3	1.84	0.59
29:q:186:GLY:HA2	30:K:1256:LEU:HG	1.82	0.59
10:G:85:ARG:O	10:G:87:ARG:NH1	2.35	0.59
1:2:104:A:N6	1:2:356:C:C4	2.70	0.59
1:2:480:G:H4'	18:u:68:VAL:HG11	1.84	0.59
1:2:1283:C:O2'	1:2:1313:A:N1	2.34	0.59
1:2:1629:C:H2'	1:2:1630:A:H8	1.67	0.59
28:r:3:LEU:HB2	28:r:88:LEU:HA	1.85	0.59
1:2:1091:C:HO2'	17:W:2:VAL:N	2.01	0.59
1:2:1290:G:C2	1:2:1310:U:O2	2.55	0.59
6:E:60:GLU:OE2	12:Y:20:ARG:NH1	2.36	0.59
27:I:3:ILE:O	27:I:30:GLY:N	2.36	0.59
1:2:1722:G:O6	1:2:1812:U:O2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:t:441:ARG:NH1	16:t:444:GLU:OE2	2.36	0.59
1:2:1778:C:H2'	1:2:1779:G:H8	1.68	0.58
22:P:28:MET:HE1	22:P:33:LEU:HD23	1.86	0.58
30:K:458:THR:HG23	30:K:460:SER:H	1.68	0.58
28:r:112:GLY:H	28:r:113:ILE:HD12	1.69	0.58
29:q:150:PHE:O	29:q:155:ARG:NH2	2.36	0.58
1:2:1455:A:N3	30:K:711:ARG:NH1	2.52	0.58
4:B:70:SER:OG	23:O:128:ARG:NH1	2.36	0.58
30:K:331:LEU:HA	30:K:334:MET:HG2	1.86	0.58
37:y:62:TYR:HD2	37:y:92:GLN:HG2	1.69	0.58
1:2:309:G:OP2	27:I:53:LYS:NZ	2.37	0.58
1:2:1232:U:O2	1:2:1527:C:N3	2.36	0.58
1:2:1545:A:C5	1:2:1588:A:N6	2.72	0.58
13:x:229:ILE:O	23:O:149:ARG:NH2	2.37	0.58
30:K:637:ALA:O	30:K:641:LYS:NZ	2.37	0.58
34:A:130:ASP:HB3	34:A:133:PRO:HG2	1.86	0.58
25:L:75:GLY:HA3	25:L:88:ILE:HD12	1.85	0.58
1:2:1024:A:OP2	24:N:124:ARG:NH2	2.37	0.58
1:2:1227:G:N2	1:2:1635:C:O2'	2.36	0.58
18:u:617:HIS:HB2	18:u:666:LEU:HB2	1.86	0.58
18:u:745:LEU:HD12	18:u:752:LYS:HG3	1.86	0.58
18:u:148:ASP:HB3	18:u:580:ILE:HD13	1.85	0.58
20:S:68:ILE:O	20:S:72:GLN:NE2	2.37	0.58
1:2:1821:U:H2'	1:2:1822:A:H8	1.68	0.57
17:W:101:PHE:O	17:W:128:PHE:CA	2.32	0.57
30:K:597:LYS:HG3	30:K:601:MET:HE1	1.86	0.57
1:2:1213:C:OP2	15:w:34:ARG:NH1	2.36	0.57
1:2:952:G:H21	23:O:52:THR:HG21	1.68	0.57
1:2:434:G:OP2	27:I:25:ARG:NH2	2.37	0.57
1:2:750:C:N4	1:2:751:G:O6	2.37	0.57
1:2:1546:G:N2	1:2:1670:C:O2	2.36	0.57
27:I:98:LYS:NZ	27:I:176:ALA:O	2.36	0.57
2:R:73:LEU:HB3	30:K:610:VAL:HG13	1.86	0.57
15:w:255:LEU:HD11	15:w:294:LEU:HD13	1.85	0.57
27:I:154:LYS:O	27:I:157:LYS:NZ	2.37	0.57
28:r:3:LEU:O	28:r:7:ASN:HB2	2.04	0.57
30:K:947:VAL:HA	30:K:950:LEU:HD12	1.87	0.57
12:Y:36:PRO:HG2	12:Y:39:GLU:HG2	1.87	0.57
1:2:1452:A:H61	1:2:1473:G:H21	1.51	0.57
8:F:59:LYS:HE3	8:F:62:ARG:HE	1.70	0.57
15:w:292:ILE:HD13	15:w:328:LYS:HZ3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1036:A:N3	1:2:1844:U:O2'	2.38	0.57
1:2:1551:U:C2	1:2:1577:G:N1	2.73	0.57
1:2:1811:C:O2'	18:u:63:GLN:OE1	2.23	0.57
10:G:218:LYS:HD2	10:G:221:LYS:HE3	1.87	0.57
15:w:230:MET:HE3	15:w:272:LEU:HD21	1.86	0.57
20:S:36:VAL:HG23	20:S:40:TYR:HB3	1.86	0.57
1:2:1473:G:N2	1:2:1476:A:OP2	2.38	0.57
18:u:157:LEU:HD11	18:u:232:LEU:HD21	1.85	0.57
19:T:35:ASP:HB2	20:S:46:ARG:HB3	1.87	0.57
19:T:59:SER:OG	19:T:79:TYR:OH	2.20	0.57
34:A:128:ARG:HH12	37:y:326:LEU:HD22	1.70	0.57
10:G:118:GLU:HG2	10:G:119:LYS:HG2	1.87	0.56
34:A:205:ARG:HH21	34:A:210:ILE:HG13	1.69	0.56
1:2:587:A:H5'	1:2:592:C:H41	1.69	0.56
12:Y:55:ILE:HG13	12:Y:75:ILE:HG12	1.87	0.56
21:Q:97:GLN:HB2	21:Q:105:LYS:HG3	1.85	0.56
32:f:107:LYS:O	32:f:114:ILE:N	2.38	0.56
1:2:1204:A:H61	18:u:5:ARG:H	1.53	0.56
1:2:1285:G:H5'	31:M:35:ILE:HD12	1.86	0.56
18:u:350:GLY:HA2	18:u:353:GLU:HB3	1.88	0.56
18:u:667:LEU:HB2	18:u:680:ALA:HB3	1.88	0.56
19:T:42:HIS:ND1	19:T:93:SER:OG	2.38	0.56
1:2:609:U:H2'	1:2:610:G:H8	1.71	0.56
18:u:284:ASN:ND2	18:u:286:ASN:OD1	2.39	0.56
1:2:948:C:H2'	1:2:949:G:H8	1.70	0.56
13:x:200:THR:HG22	13:x:213:GLY:HA3	1.86	0.56
22:P:61:ARG:NH2	22:P:88:GLU:O	2.39	0.56
1:2:1330:G:O6	1:2:1499:U:O4	2.22	0.56
20:S:14:ARG:NH2	20:S:17:ASN:OD1	2.36	0.56
30:K:1118:LEU:HD12	30:K:1128:ARG:HD2	1.86	0.56
18:u:113:LEU:HD11	18:u:120:GLN:HB2	1.88	0.56
21:Q:90:LYS:HA	21:Q:93:VAL:HG12	1.88	0.56
34:A:3:GLY:H	36:V:80:SER:HB3	1.71	0.56
18:u:89:PRO:HA	18:u:159:LEU:HB2	1.88	0.56
19:T:140:ALA:HA	19:T:144:LYS:HD3	1.87	0.56
1:2:70:G:H21	1:2:79:A:H62	1.54	0.56
34:A:216:ALA:HA	37:y:64:ARG:HG2	1.86	0.56
1:2:1293:A:N6	1:2:1302:G:C6	2.74	0.55
1:2:818:A:OP1	26:J:80:ARG:NH2	2.36	0.55
8:F:24:SER:O	8:F:107:ASN:ND2	2.39	0.55
19:T:40:ALA:HB3	19:T:43:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:89:SER:HB3	21:Q:112:LEU:HD11	1.89	0.55
1:2:1286:G:N2	1:2:1312:G:O2'	2.40	0.55
26:J:111:GLN:HE21	26:J:123:ILE:HG13	1.70	0.55
1:2:1542:C:OP2	19:T:79:TYR:OH	2.25	0.55
1:2:1726:G:C6	1:2:1809:A:N1	2.74	0.55
19:T:13:GLU:HA	19:T:16:ARG:HG2	1.86	0.55
1:2:885:U:O2	1:2:901:G:O6	2.24	0.55
1:2:1320:G:O2'	1:2:1322:G:N7	2.40	0.55
9:H:101:LEU:O	9:H:116:ARG:NH1	2.40	0.55
1:2:94:G:O2'	1:2:508:A:O2'	2.23	0.55
23:O:26:ASN:C	23:O:26:ASN:HD22	2.14	0.55
36:V:32:ILE:HG12	36:V:60:ARG:HD2	1.88	0.55
27:I:11:ARG:NH1	27:I:15:GLY:O	2.39	0.55
34:A:182:VAL:O	34:A:186:ARG:HB2	2.07	0.55
1:2:17:C:O2'	1:2:1194:A:N1	2.37	0.55
19:T:125:PRO:HB2	19:T:129:ARG:HH12	1.72	0.55
1:2:1284:A:H5'	1:2:1285:G:H8	1.71	0.55
25:L:119:ASP:O	25:L:147:LYS:NZ	2.40	0.55
30:K:1024:LEU:HD13	30:K:1028:TYR:HB3	1.89	0.55
6:E:45:ILE:HA	6:E:61:VAL:HG11	1.88	0.55
6:E:139:LEU:O	6:E:146:THR:HA	2.07	0.55
37:y:111:LYS:NZ	37:y:306:LEU:O	2.40	0.54
30:K:863:ILE:O	30:K:866:THR:OG1	2.25	0.54
1:2:1307:U:O2	32:f:138:ARG:NH2	2.31	0.54
11:Z:73:VAL:HG13	11:Z:77:LEU:HD12	1.90	0.54
18:u:493:ASP:N	18:u:493:ASP:OD1	2.41	0.54
23:O:135:ILE:HD12	23:O:136:PRO:HD2	1.90	0.54
34:A:57:LYS:HD2	34:A:159:ILE:HG23	1.88	0.54
1:2:380:G:OP1	27:I:56:ARG:NH2	2.40	0.54
1:2:928:G:H2'	1:2:929:G:C8	2.41	0.54
6:E:199:GLU:HB3	6:E:207:VAL:HB	1.90	0.54
11:Z:49:LEU:HB3	20:S:5:ILE:HG22	1.89	0.54
1:2:792:C:H2'	1:2:793:G:H8	1.72	0.54
1:2:1562:C:H5''	19:T:71:GLY:HA3	1.90	0.54
4:B:35:ALA:O	4:B:42:ARG:NH2	2.34	0.54
1:2:570:C:O2'	12:Y:34:THR:O	2.23	0.54
1:2:1064:C:H2'	1:2:1065:G:H8	1.72	0.54
1:2:1335:G:O6	1:2:1492:U:O4	2.26	0.54
13:x:183:ILE:HD11	13:x:229:ILE:HG23	1.90	0.54
30:K:844:VAL:HG21	30:K:884:MET:HE1	1.90	0.54
1:2:8:U:H3	1:2:1196:A:N6	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1124:C:H5''	4:B:150:ILE:HG12	1.90	0.54
11:Z:85:ARG:HA	11:Z:88:LEU:HG	1.90	0.54
29:q:105:MET:SD	29:q:105:MET:N	2.78	0.54
1:2:594:A:H61	1:2:643:A:H5''	1.72	0.53
1:2:944:A:H5''	23:O:134:PRO:HB3	1.90	0.53
1:2:1545:A:H4'	21:Q:74:GLY:HA2	1.89	0.53
1:2:1649:U:H2'	1:2:1650:A:H8	1.72	0.53
1:2:1761:U:N3	1:2:1771:G:N1	2.56	0.53
4:B:134:LEU:HB3	4:B:219:LYS:HB3	1.89	0.53
13:x:205:ALA:HB3	13:x:208:LYS:HB2	1.90	0.53
1:2:71:G:O6	1:2:79:A:N7	2.41	0.53
1:2:851:C:H5''	1:2:852:G:H5'	1.89	0.53
1:2:886:A:H1'	1:2:900:C:H42	1.73	0.53
1:2:1236:G:H21	1:2:1522:A:N6	2.03	0.53
14:X:101:LEU:HB3	14:X:124:LYS:HB2	1.89	0.53
30:K:386:PRO:O	30:K:390:TRP:HB2	2.08	0.53
35:C:187:ARG:NH2	35:C:189:GLY:O	2.41	0.53
11:Z:69:THR:HG22	11:Z:72:VAL:HG12	1.88	0.53
30:K:112:ARG:HE	30:K:126:ALA:HA	1.74	0.53
35:C:257:LYS:O	36:V:16:LYS:NZ	2.40	0.53
6:E:100:ARG:NH2	6:E:121:TYR:O	2.41	0.53
18:u:712:VAL:HG22	18:u:752:LYS:HG2	1.90	0.53
21:Q:44:PRO:HG2	21:Q:81:ILE:HD11	1.88	0.53
1:2:1005:G:OP2	4:B:162:ARG:NH1	2.41	0.53
27:I:103:LEU:HD13	27:I:170:LYS:HE2	1.91	0.53
30:K:684:ARG:HA	30:K:687:LYS:HE2	1.89	0.53
30:K:869:VAL:HG22	33:z:179:SER:HA	1.90	0.53
2:R:36:GLU:O	30:K:1153:ARG:NH2	2.42	0.53
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.89	0.53
11:Z:46:ASN:O	20:S:23:ARG:NH2	2.42	0.53
27:I:57:ALA:HB2	27:I:183:GLY:HA2	1.91	0.53
1:2:75:G:H1	10:G:155:GLN:HG3	1.73	0.53
1:2:1726:G:H2'	1:2:1727:G:H8	1.74	0.53
1:2:1757:G:C6	1:2:1776:G:C2	2.96	0.53
1:2:1757:G:O6	1:2:1775:U:C2	2.62	0.53
30:K:830:SER:OG	33:z:186:ARG:NH1	2.42	0.53
32:f:141:CYS:SG	32:f:142:GLY:N	2.81	0.53
35:C:99:GLY:HA2	35:C:102:LEU:HD13	1.91	0.53
37:y:71:LYS:HA	37:y:76:TYR:HB2	1.90	0.53
1:2:562:U:O4	26:J:172:ARG:NH2	2.42	0.53
1:2:1306:U:C4	1:2:1307:U:O4	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:128:LYS:HG2	6:E:140:VAL:HB	1.90	0.53
26:J:136:ARG:NH2	26:J:158:ASP:OD2	2.42	0.53
34:A:57:LYS:HG3	34:A:161:ILE:HD13	1.91	0.53
1:2:507:G:O6	12:Y:105:LYS:NZ	2.42	0.52
8:F:90:VAL:HA	8:F:93:VAL:HG22	1.91	0.52
30:K:535:VAL:HG11	30:K:568:TRP:HZ3	1.73	0.52
1:2:617:G:OP1	14:X:88:ASP:N	2.42	0.52
1:2:1289:U:O3'	15:w:278:LYS:NZ	2.43	0.52
12:Y:86:GLU:OE2	12:Y:90:ARG:NH1	2.37	0.52
1:2:1455:A:OP2	2:R:56:HIS:NE2	2.42	0.52
30:K:538:ALA:O	30:K:542:MET:CB	2.55	0.52
9:H:66:VAL:HG12	9:H:96:ALA:HB1	1.92	0.52
29:q:128:LEU:O	29:q:141:ARG:NH2	2.39	0.52
30:K:631:THR:HG23	30:K:671:LYS:HD2	1.92	0.52
31:M:58:GLU:HG3	32:f:100:LEU:HD11	1.91	0.52
1:2:884:C:N4	1:2:903:A:N6	2.58	0.52
15:w:330:ALA:HB2	15:w:360:LEU:HD23	1.91	0.52
23:O:61:LYS:HB3	23:O:76:LEU:HD23	1.91	0.52
2:R:63:ARG:O	30:K:574:ARG:NH2	2.41	0.52
18:u:676:HIS:CD2	18:u:786:PRO:HG3	2.45	0.52
34:A:30:LEU:HA	34:A:150:THR:HG22	1.91	0.52
21:Q:33:LYS:HB3	21:Q:69:ARG:HG2	1.92	0.52
30:K:401:LEU:HD11	30:K:408:LEU:HD23	1.91	0.52
11:Z:96:LEU:HD12	11:Z:97:ILE:HG12	1.92	0.52
27:I:148:LYS:HD3	27:I:152:ARG:HH21	1.74	0.52
30:K:365:GLU:OE1	30:K:369:GLN:NE2	2.42	0.52
37:y:282:ARG:HH22	37:y:286:SER:HA	1.74	0.52
1:2:84:A:N3	1:2:150:A:O2'	2.41	0.52
1:2:1310:U:OP2	31:M:36:ARG:NH2	2.43	0.52
1:2:1452:A:H61	1:2:1473:G:N2	2.07	0.52
1:2:1725:U:H2'	1:2:1726:G:H8	1.75	0.52
1:2:1761:U:O2	1:2:1771:G:N2	2.43	0.52
4:B:33:VAL:HA	4:B:96:CYS:HB3	1.91	0.52
1:2:30:C:O2'	1:2:596:U:OP1	2.28	0.52
1:2:218:U:O2	27:I:184:ARG:NH1	2.38	0.52
1:2:980:A:H2'	1:2:981:A:C8	2.45	0.52
1:2:1025:U:OP1	1:2:1090:C:O2'	2.29	0.52
20:S:26:ILE:HD11	20:S:52:LEU:HA	1.92	0.52
3:b:3:LEU:HD23	17:W:22:LYS:HD3	1.91	0.51
19:T:83:GLN:HE21	19:T:85:ASN:HB3	1.75	0.51
25:L:126:VAL:HG12	25:L:145:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:390:TRP:CD2	30:K:394:MET:HE1	2.45	0.51
34:A:17:LYS:HG3	34:A:173:LEU:HD11	1.91	0.51
1:2:433:A:H5''	27:I:22:HIS:HB3	1.93	0.51
7:e:36:MET:HE3	7:e:40:ARG:HH12	1.75	0.51
29:q:121:SER:HB3	29:q:161:LEU:HA	1.92	0.51
1:2:1452:A:N6	1:2:1473:G:H21	2.07	0.51
1:2:1854:U:H2'	1:2:1855:G:H8	1.76	0.51
6:E:148:ARG:NH2	10:G:205:GLU:OE1	2.38	0.51
1:2:1677:U:OP1	8:F:71:ARG:NH2	2.44	0.51
9:H:15:LYS:NZ	9:H:16:PRO:O	2.43	0.51
27:I:162:LEU:HD11	27:I:191:GLU:HG2	1.92	0.51
30:K:860:PRO:HG2	33:z:194:ARG:HG2	1.92	0.51
1:2:128:U:H5'	1:2:129:C:H5	1.75	0.51
13:x:201:ARG:HG2	15:w:19:LEU:HD13	1.93	0.51
18:u:126:CYS:O	18:u:130:LYS:N	2.44	0.51
30:K:908:PRO:HB3	33:z:200:LEU:HD23	1.91	0.51
35:C:244:ILE:O	35:C:247:THR:OG1	2.21	0.51
1:2:884:C:H42	1:2:903:A:N6	2.07	0.51
6:E:54:TYR:OH	6:E:97:GLU:OE1	2.25	0.51
1:2:681:U:O2'	1:2:1160:U:OP1	2.28	0.51
1:2:1819:A:O2'	16:t:458:ARG:NH1	2.44	0.51
4:B:142:PHE:O	4:B:208:HIS:N	2.41	0.51
18:u:262:PRO:HA	18:u:270:GLY:HA3	1.93	0.51
35:C:70:VAL:HG11	35:C:93:ILE:HG12	1.92	0.51
1:2:928:G:H1	1:2:1013:U:H3	1.59	0.51
1:2:1348:G:O6	1:2:1381:G:O6	2.29	0.51
23:O:34:PHE:HB3	23:O:41:PHE:HB2	1.91	0.51
24:N:37:ILE:HD11	24:N:63:VAL:HG21	1.92	0.51
30:K:936:GLY:O	30:K:939:THR:OG1	2.28	0.51
30:K:1024:LEU:HD12	30:K:1032:LEU:HD11	1.91	0.51
34:A:36:GLN:O	34:A:53:ARG:NH1	2.43	0.51
6:E:126:VAL:HG12	6:E:141:THR:HG22	1.93	0.51
26:J:53:ILE:HD13	26:J:81:LEU:HD21	1.93	0.51
1:2:868:G:O2'	9:H:113:LYS:O	2.29	0.51
5:c:13:ARG:NH1	5:c:14:VAL:O	2.44	0.51
22:P:60:LEU:HA	22:P:76:VAL:HG21	1.91	0.51
30:K:206:SER:OG	30:K:207:THR:N	2.44	0.51
1:2:1312:G:O6	31:M:36:ARG:NH1	2.39	0.50
1:2:1534:C:O2	1:2:1598:G:C2	2.64	0.50
10:G:52:ILE:HA	10:G:111:LEU:HD23	1.93	0.50
15:w:355:ARG:NH2	16:t:247:SER:OG	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:11:LEU:HD12	17:W:74:VAL:HB	1.93	0.50
30:K:944:LEU:HA	30:K:947:VAL:HG12	1.93	0.50
1:2:671:A:O2'	1:2:1089:G:OP2	2.27	0.50
1:2:1757:G:O6	1:2:1775:U:O2	2.27	0.50
4:B:137:LEU:HD13	4:B:215:VAL:HG22	1.93	0.50
37:y:14:PHE:O	37:y:45:ARG:NH2	2.44	0.50
1:2:54:A:OP1	12:Y:111:LYS:NZ	2.37	0.50
1:2:1290:G:N1	1:2:1310:U:C2	2.79	0.50
18:u:597:VAL:HG23	18:u:685:MET:HB2	1.94	0.50
30:K:838:LYS:O	30:K:841:LEU:HB3	2.10	0.50
27:I:65:PHE:O	27:I:73:THR:HA	2.11	0.50
29:q:15:GLU:HG3	29:q:83:ILE:HG12	1.94	0.50
37:y:254:ALA:HB2	37:y:260:ILE:HD11	1.93	0.50
16:t:454:LEU:HD23	16:t:457:ARG:HH21	1.76	0.50
18:u:272:LEU:HD22	18:u:565:VAL:HG11	1.93	0.50
29:q:55:CYS:HB3	29:q:117:ASP:HB3	1.94	0.50
1:2:1780:G:H2'	1:2:1781:A:C8	2.46	0.50
2:R:21:TYR:OH	2:R:62:GLN:OE1	2.29	0.50
4:B:124:HIS:HA	4:B:137:LEU:O	2.12	0.50
1:2:928:G:N2	3:b:68:GLY:O	2.38	0.50
26:J:138:ARG:HB3	26:J:156:HIS:HB3	1.94	0.50
30:K:953:SER:OG	30:K:954:ARG:N	2.45	0.50
1:2:581:U:OP1	26:J:133:ARG:NH2	2.42	0.50
1:2:1726:G:O6	1:2:1809:A:C6	2.64	0.50
21:Q:11:GLN:HG2	30:K:1121:LEU:HG	1.94	0.50
34:A:187:GLY:HA2	36:V:45:ARG:HH12	1.76	0.50
37:y:277:THR:HG22	37:y:279:ASP:H	1.77	0.50
1:2:1451:G:OP1	2:R:32:LYS:NZ	2.42	0.49
20:S:114:LEU:HB3	20:S:122:GLY:HA3	1.93	0.49
1:2:1652:G:N1	1:2:1673:U:C2	2.80	0.49
8:F:19:LEU:HB3	8:F:23:TRP:HB2	1.92	0.49
15:w:354:TYR:OH	16:t:256:LEU:O	2.30	0.49
20:S:35:GLY:HA3	20:S:99:LEU:HA	1.93	0.49
22:P:29:SER:OG	22:P:30:TYR:N	2.44	0.49
9:H:144:ILE:HB	17:W:52:ILE:HB	1.94	0.49
10:G:142:ARG:HG2	10:G:147:LEU:HB2	1.94	0.49
13:x:169:LYS:HB3	23:O:149:ARG:CZ	2.42	0.49
1:2:640:A:H2'	1:2:641:A:C8	2.47	0.49
5:c:17:VAL:HA	5:c:30:VAL:HG23	1.93	0.49
21:Q:53:GLU:OE1	21:Q:85:ARG:NH2	2.37	0.49
26:J:19:PRO:O	26:J:24:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:564:PHE:HB2	30:K:567:SER:HB3	1.93	0.49
1:2:1619:A:OP2	22:P:44:ARG:NH1	2.45	0.49
34:A:85:ARG:HH21	34:A:89:LYS:HD2	1.77	0.49
37:y:268:LEU:HB3	37:y:293:LEU:HB3	1.94	0.49
1:2:1297:U:N3	1:2:1300:U:OP2	2.45	0.49
4:B:182:LYS:NZ	4:B:231:LEU:HD13	2.28	0.49
6:E:54:TYR:O	12:Y:15:ASN:ND2	2.45	0.49
1:2:156:G:OP1	10:G:2:LYS:NZ	2.40	0.49
18:u:503:TYR:HB3	18:u:769:LEU:HB3	1.94	0.49
24:N:5:HIS:HD2	24:N:121:ARG:HE	1.60	0.49
30:K:264:LEU:HD11	30:K:284:THR:HG21	1.95	0.49
1:2:220:U:H2'	1:2:221:A:H8	1.77	0.49
1:2:678:U:H3	1:2:1027:A:H62	1.61	0.49
1:2:884:C:N4	1:2:903:A:H61	2.11	0.49
1:2:983:A:OP1	1:2:1073:U:O2'	2.31	0.49
13:x:112:LYS:NZ	37:y:130:LEU:O	2.31	0.49
13:x:205:ALA:N	13:x:208:LYS:O	2.45	0.49
20:S:86:ARG:HH21	20:S:106:LYS:HD2	1.77	0.49
30:K:810:VAL:HG11	30:K:846:LYS:HE3	1.94	0.49
35:C:206:SER:HB3	35:C:210:PRO:HB2	1.94	0.49
37:y:29:THR:HG22	37:y:53:LEU:HD11	1.95	0.49
1:2:1226:G:N1	1:2:1639:G7M:OP2	2.39	0.49
30:K:357:PRO:O	30:K:403:ARG:NH2	2.45	0.49
6:E:9:LEU:HB2	6:E:30:ARG:HD2	1.94	0.49
15:w:185:TYR:HA	15:w:188:VAL:HG12	1.95	0.49
4:B:78:GLU:HG3	4:B:79:VAL:H	1.78	0.48
18:u:84:GLN:HB2	18:u:279:ARG:HH22	1.78	0.48
23:O:95:ILE:HG21	23:O:116:LEU:HD21	1.95	0.48
30:K:669:ILE:HD11	30:K:720:TYR:HD1	1.78	0.48
30:K:986:MET:HE1	30:K:1020:VAL:HA	1.95	0.48
34:A:5:LEU:HG	34:A:7:VAL:HG12	1.94	0.48
1:2:309:G:OP2	27:I:55:TYR:OH	2.28	0.48
5:c:66:ARG:NH2	15:w:27:ASN:OD1	2.45	0.48
30:K:666:ARG:NH1	30:K:716:THR:OG1	2.44	0.48
31:M:64:LEU:HD23	32:f:103:LEU:HD12	1.94	0.48
34:A:90:PHE:O	34:A:93:ALA:HB3	2.13	0.48
34:A:94:THR:OG1	34:A:186:ARG:NH2	2.42	0.48
1:2:398:A:OP1	1:2:399:C:O2'	2.28	0.48
1:2:909:G:H2'	1:2:910:G:H8	1.78	0.48
2:R:77:GLU:HB2	30:K:610:VAL:HG21	1.95	0.48
16:t:366:LEU:HD11	18:u:531:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:83:HIS:NE2	18:u:155:THR:OG1	2.35	0.48
30:K:315:LEU:HB3	30:K:352:LEU:HD13	1.94	0.48
30:K:947:VAL:HG21	30:K:965:PHE:HB3	1.96	0.48
33:z:201:LEU:O	33:z:207:ARG:NH1	2.42	0.48
1:2:106:C:H2'	1:2:107:A:H8	1.79	0.48
1:2:1265:A:O2'	18:u:705:LYS:NZ	2.34	0.48
6:E:44:LEU:HD13	6:E:72:ILE:HD11	1.95	0.48
13:x:206:ASP:OD1	13:x:207:VAL:N	2.47	0.48
18:u:644:LEU:HG	18:u:650:LEU:HD12	1.95	0.48
30:K:524:HIS:HB2	30:K:1130:LEU:HD22	1.95	0.48
34:A:187:GLY:HA2	36:V:45:ARG:HH22	1.78	0.48
1:2:71:G:C6	1:2:79:A:C6	3.00	0.48
1:2:530:U:H2'	1:2:531:A:H8	1.77	0.48
13:x:169:LYS:HB3	23:O:149:ARG:NH1	2.28	0.48
28:r:44:ARG:NH2	29:q:77:TYR:OH	2.45	0.48
31:M:83:LYS:HA	31:M:105:GLY:HA3	1.93	0.48
1:2:78:C:H1'	10:G:175:LYS:HB2	1.95	0.48
6:E:211:LYS:HZ3	6:E:215:GLY:HA2	1.77	0.48
34:A:41:ARG:HH21	37:y:319:PRO:HB2	1.78	0.48
1:2:618:C:H41	14:X:67:ARG:HH21	1.60	0.48
1:2:1725:U:H2'	1:2:1726:G:C8	2.48	0.48
1:2:1758:G:H2'	1:2:1759:G:C8	2.49	0.48
19:T:80:GLY:CA	19:T:93:SER:O	2.62	0.48
1:2:1239:U:H4'	22:P:124:LYS:HD2	1.94	0.48
1:2:1736:G:H2'	1:2:1737:G:C8	2.49	0.48
30:K:561:THR:OG1	30:K:563:ASP:OD1	2.31	0.48
1:2:1282:A:N1	1:2:1316:C:N3	2.62	0.48
1:2:1776:G:H2'	1:2:1777:G:C8	2.49	0.48
4:B:139:CYS:HB2	4:B:172:MET:HE1	1.94	0.48
13:x:106:GLN:NE2	37:y:208:TRP:HB3	2.24	0.48
30:K:235:LEU:O	30:K:239:HIS:ND1	2.46	0.48
1:2:1013:U:OP1	1:2:1129:G:O2'	2.31	0.47
1:2:1652:G:C2	1:2:1673:U:O2	2.67	0.47
21:Q:82:TYR:HD1	21:Q:85:ARG:HD3	1.79	0.47
27:I:101:ILE:HD12	27:I:190:LEU:HD11	1.95	0.47
1:2:954:U:O2	23:O:55:ARG:NH2	2.46	0.47
1:2:1330:G:N2	1:2:1499:U:O2	2.33	0.47
8:F:77:MET:HE2	8:F:86:LYS:HB3	1.95	0.47
15:w:338:ASN:HA	15:w:341:PHE:HD2	1.79	0.47
19:T:131:LEU:HA	19:T:134:ILE:HG22	1.97	0.47
30:K:410:LEU:HD13	30:K:413:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:483:PHE:O	30:K:484:HIS:ND1	2.47	0.47
1:2:942:G:OP1	4:B:216:LYS:NZ	2.44	0.47
1:2:1010:G:H2'	1:2:1011:A:C8	2.49	0.47
4:B:145:LYS:HE3	4:B:149:GLN:HG2	1.96	0.47
21:Q:42:ILE:HG22	21:Q:44:PRO:HD2	1.95	0.47
21:Q:68:ILE:HD12	21:Q:88:ILE:HG12	1.95	0.47
30:K:142:GLU:HA	30:K:143:THR:HA	1.55	0.47
1:2:1292:C:N3	32:f:138:ARG:NH2	2.51	0.47
5:c:36:ASP:N	5:c:36:ASP:OD1	2.46	0.47
9:H:51:ILE:HD11	9:H:176:VAL:HG22	1.97	0.47
18:u:155:THR:HG21	18:u:236:LEU:HD22	1.95	0.47
27:I:61:ASP:OD1	27:I:61:ASP:N	2.48	0.47
30:K:402:VAL:HA	30:K:406:TRP:HA	1.96	0.47
30:K:571:PRO:HB3	30:K:574:ARG:HH21	1.80	0.47
30:K:935:MET:SD	30:K:939:THR:OG1	2.67	0.47
1:2:106:C:H2'	1:2:107:A:C8	2.50	0.47
1:2:1776:G:H2'	1:2:1777:G:H8	1.79	0.47
18:u:124:LEU:HB3	18:u:133:TRP:HB2	1.95	0.47
1:2:677:G:N1	1:2:1027:A:OP2	2.45	0.47
1:2:902:G:H2'	1:2:903:A:H8	1.79	0.47
1:2:1821:U:H2'	1:2:1822:A:C8	2.49	0.47
18:u:358:GLU:HG2	18:u:359:VAL:HG23	1.96	0.47
18:u:594:LEU:HG	18:u:656:ALA:HB3	1.97	0.47
19:T:29:LYS:HE3	19:T:106:ALA:HB2	1.96	0.47
1:2:122:G:H21	6:E:146:THR:HG21	1.80	0.47
1:2:1268:C:O2	22:P:97:TYR:OH	2.28	0.47
1:2:1562:C:H2'	1:2:1563:G:H8	1.79	0.47
14:X:67:ARG:HB2	14:X:115:ILE:HG21	1.97	0.47
18:u:401:GLN:HE22	22:P:121:ILE:H	1.63	0.47
30:K:733:LEU:HD23	30:K:768:ALA:HB1	1.97	0.47
30:K:780:LEU:HD11	30:K:795:LEU:HD11	1.96	0.47
1:2:71:G:N1	1:2:79:A:C4	2.83	0.47
1:2:1545:A:C4	1:2:1588:A:N6	2.83	0.47
13:x:103:LEU:HD22	13:x:133:ALA:HB2	1.96	0.47
19:T:33:TRP:HZ2	19:T:102:ARG:HG3	1.79	0.47
19:T:71:GLY:HA2	19:T:121:ARG:HH21	1.78	0.47
29:q:163:LEU:HG	29:q:165:PRO:HD3	1.96	0.47
32:f:108:VAL:HB	32:f:114:ILE:HG12	1.97	0.47
1:2:943:U:H2'	1:2:944:A:C8	2.50	0.47
1:2:1726:G:C6	1:2:1809:A:C6	3.03	0.47
13:x:171:LEU:HD22	13:x:175:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:A:54:THR:HB	34:A:162:PRO:HG2	1.97	0.47
20:S:120:HIS:H	22:P:118:GLU:HB2	1.79	0.47
23:O:75:MET:HG3	23:O:118:ALA:HB2	1.96	0.47
25:L:128:VAL:HG12	25:L:142:VAL:HA	1.96	0.47
37:y:66:VAL:HA	37:y:69:PHE:CE2	2.50	0.47
1:2:795:A:H2'	1:2:796:G:H8	1.80	0.46
15:w:313:THR:HA	15:w:348:LYS:HD3	1.97	0.46
18:u:508:SER:H	18:u:512:SER:HB2	1.80	0.46
30:K:257:GLN:HG2	30:K:310:LEU:HD21	1.96	0.46
30:K:394:MET:O	30:K:398:HIS:ND1	2.38	0.46
30:K:633:PRO:HB2	30:K:636:VAL:HB	1.97	0.46
35:C:78:LEU:HD12	35:C:81:ILE:HD13	1.97	0.46
1:2:659:G:O2'	1:2:662:G:O2'	2.29	0.46
8:F:77:MET:SD	8:F:84:GLY:N	2.89	0.46
12:Y:110:ARG:O	12:Y:114:MET:HG2	2.15	0.46
20:S:124:ARG:NH1	22:P:123:TYR:OH	2.48	0.46
29:q:65:GLY:O	29:q:69:SER:N	2.44	0.46
30:K:176:LYS:O	30:K:223:LYS:NZ	2.47	0.46
30:K:1021:LYS:O	30:K:1029:HIS:NE2	2.47	0.46
1:2:677:G:OP1	24:N:124:ARG:NH1	2.48	0.46
1:2:1620:A:H5''	1:2:1621:U:H3	1.80	0.46
8:F:42:LYS:HD2	8:F:42:LYS:HA	1.66	0.46
25:L:115:PRO:O	25:L:118:ARG:NH1	2.47	0.46
6:E:127:ARG:N	6:E:140:VAL:O	2.44	0.46
14:X:10:ALA:HB2	25:L:101:ARG:HB3	1.96	0.46
15:w:259:ARG:HH12	15:w:299:THR:HG23	1.80	0.46
25:L:73:LEU:HD12	25:L:109:MET:HE1	1.97	0.46
29:q:80:GLY:O	29:q:101:LEU:N	2.47	0.46
29:q:176:THR:HA	29:q:179:THR:HG22	1.97	0.46
37:y:394:ALA:HA	37:y:397:ARG:HH21	1.80	0.46
1:2:1393:G:O6	1:2:1477:U:O2	2.33	0.46
9:H:145:ARG:HB2	9:H:155:LYS:HZ1	1.81	0.46
30:K:621:GLN:O	30:K:624:THR:OG1	2.24	0.46
30:K:932:LYS:HB3	30:K:972:VAL:HG13	1.96	0.46
34:A:10:MET:HE3	34:A:15:VAL:HG12	1.98	0.46
1:2:71:G:C6	1:2:79:A:N7	2.84	0.46
1:2:1486:A:OP1	30:K:1030:ARG:NH1	2.48	0.46
1:2:1736:G:H2'	1:2:1737:G:H8	1.81	0.46
8:F:51:HIS:ND1	21:Q:82:TYR:OH	2.48	0.46
13:x:204:LEU:HA	13:x:209:VAL:HA	1.98	0.46
28:r:17:GLY:HA2	28:r:18:SER:HA	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:668:LEU:O	30:K:672:GLY:N	2.48	0.46
35:C:88:ILE:HG23	35:C:93:ILE:HD12	1.96	0.46
1:2:93:U:H1'	6:E:7:LYS:HD2	1.97	0.46
10:G:221:LYS:HA	10:G:224:ARG:HE	1.81	0.46
20:S:20:ILE:HD11	20:S:33:ILE:HB	1.97	0.46
26:J:63:LEU:HD12	26:J:70:ARG:HB2	1.97	0.46
28:r:6:HIS:CE1	28:r:25:LEU:HD11	2.50	0.46
37:y:9:ALA:HA	37:y:235:LEU:HB2	1.97	0.46
1:2:165:G:OP2	1:2:165:G:N2	2.38	0.46
2:R:62:GLN:HE22	30:K:617:THR:HG23	1.80	0.46
11:Z:49:LEU:HA	11:Z:83:LEU:HD21	1.98	0.46
25:L:93:LEU:HG	25:L:102:PHE:HB3	1.97	0.46
29:q:131:ALA:HB2	29:q:138:PRO:HG3	1.98	0.46
34:A:44:ASP:OD1	34:A:44:ASP:N	2.48	0.46
35:C:176:LYS:O	35:C:200:ARG:NH2	2.49	0.46
1:2:1189:A:H4'	14:X:34:THR:HG21	1.98	0.46
17:W:27:ILE:HG13	17:W:61:ILE:HB	1.98	0.46
37:y:245:LEU:HD13	37:y:250:LEU:HD22	1.97	0.46
1:2:974:C:O2	23:O:55:ARG:NH1	2.49	0.46
1:2:1639:G7M:H5'	29:q:32:MET:HE1	1.97	0.46
1:2:1709:G:C2	1:2:1824:A:C2	3.04	0.46
4:B:123:ALA:HB2	4:B:165:ARG:HG3	1.97	0.46
6:E:87:MET:HE1	6:E:236:ILE:HD13	1.97	0.46
11:Z:48:VAL:HG21	20:S:23:ARG:HA	1.97	0.46
21:Q:86:GLN:NE2	21:Q:120:LEU:O	2.49	0.46
1:2:31:U:O2'	1:2:643:A:N1	2.48	0.45
1:2:1275:G:N2	1:2:1324:G:O2'	2.46	0.45
9:H:69:LEU:O	9:H:73:GLN:HG2	2.15	0.45
13:x:197:VAL:HG11	13:x:241:ILE:HG13	1.98	0.45
35:C:196:ILE:HB	35:C:223:TYR:HB2	1.98	0.45
37:y:406:LYS:HE3	37:y:409:VAL:HG11	1.97	0.45
1:2:223:C:H2'	1:2:224:A:C8	2.51	0.45
1:2:1183:A:H2'	1:2:1184:G:H8	1.81	0.45
3:b:34:ASP:O	3:b:79:PHE:HA	2.16	0.45
9:H:73:GLN:HB3	9:H:135:PHE:CE1	2.52	0.45
30:K:652:SER:O	30:K:658:ARG:NH2	2.42	0.45
34:A:134:LEU:HD11	34:A:144:THR:HG21	1.97	0.45
1:2:1472:C:N4	1:2:1476:A:H62	2.07	0.45
13:x:214:SER:OG	13:x:217:ASN:OD1	2.34	0.45
22:P:82:ASP:OD1	22:P:82:ASP:N	2.46	0.45
26:J:108:ARG:NH2	26:J:154:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:A:62:ALA:HA	34:A:65:ILE:HG22	1.97	0.45
1:2:220:U:H2'	1:2:221:A:C8	2.50	0.45
2:R:66:VAL:HG11	30:K:618:LEU:HG	1.98	0.45
4:B:144:LYS:HE3	4:B:206:PRO:HB2	1.99	0.45
16:t:431:LYS:O	16:t:435:LYS:HG2	2.16	0.45
26:J:28:GLU:OE1	26:J:44:TRP:NE1	2.50	0.45
27:I:22:HIS:ND1	27:I:23:LYS:O	2.48	0.45
30:K:221:LEU:HD11	30:K:237:VAL:HG12	1.99	0.45
30:K:421:VAL:HG13	30:K:483:PHE:HZ	1.80	0.45
34:A:182:VAL:O	34:A:186:ARG:CB	2.64	0.45
34:A:207:PRO:HA	34:A:210:ILE:HG22	1.98	0.45
37:y:282:ARG:NH1	37:y:286:SER:OG	2.49	0.45
1:2:77:A:C8	10:G:154:ARG:HD3	2.51	0.45
1:2:1515:G:H2'	1:2:1516:G:H8	1.82	0.45
6:E:107:GLY:HA2	6:E:189:LEU:HG	1.98	0.45
13:x:171:LEU:HD11	23:O:149:ARG:HH22	1.81	0.45
1:2:115:U:H2'	1:2:116:U:C6	2.51	0.45
1:2:383:G:H4'	25:L:132:ARG:HD2	1.99	0.45
1:2:1205:C:O2	18:u:4:HIS:ND1	2.36	0.45
1:2:1220:A:N3	1:2:1677:U:O2'	2.45	0.45
22:P:95:GLY:HA2	22:P:104:GLN:HA	1.98	0.45
1:2:4:C:H4'	35:C:207:ALA:HB2	1.99	0.45
1:2:374:G:OP1	25:L:59:LYS:NZ	2.42	0.45
1:2:943:U:H2'	1:2:944:A:H8	1.81	0.45
1:2:1778:C:H2'	1:2:1779:G:C8	2.48	0.45
12:Y:64:PHE:O	26:J:140:GLN:NE2	2.49	0.45
14:X:41:PHE:O	14:X:76:LYS:NZ	2.43	0.45
21:Q:42:ILE:O	21:Q:45:ARG:NH1	2.50	0.45
1:2:420:G:O2'	1:2:660:C:N3	2.49	0.45
1:2:1004:U:H2'	1:2:1005:G:H8	1.81	0.45
1:2:1333:U:O2	1:2:1495:G:O6	2.35	0.45
1:2:1646:C:O2	1:2:1678:A:N6	2.49	0.45
1:2:1743:G:H21	1:2:1791:A:H62	1.65	0.45
1:2:1748:G:H2'	1:2:1749:G:H8	1.81	0.45
21:Q:24:HIS:HE2	21:Q:26:LYS:HD3	1.82	0.45
25:L:40:ILE:HD13	25:L:61:PRO:HB2	1.98	0.45
29:q:137:ASN:HB3	29:q:140:LYS:HB3	1.98	0.45
1:2:1329:U:H2'	1:2:1330:G:C8	2.52	0.45
5:c:20:ARG:HA	5:c:28:THR:HA	1.99	0.45
6:E:102:ILE:HD12	6:E:239:PRO:HD3	1.99	0.45
18:u:616:PHE:HZ	18:u:627:PRO:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:33:LYS:O	21:Q:69:ARG:HA	2.17	0.45
22:P:59:ARG:HH12	22:P:77:LYS:H	1.64	0.45
1:2:1228:A:H2'	1:2:1229:G:C8	2.52	0.45
1:2:1565:C:H41	19:T:101:ARG:HH12	1.65	0.45
26:J:114:VAL:HG21	26:J:130:ILE:HD11	1.99	0.45
30:K:574:ARG:NH1	30:K:575:ASP:OD1	2.50	0.45
30:K:1247:ARG:NH2	30:K:1251:TYR:OH	2.50	0.45
31:M:122:ASP:HA	31:M:125:GLU:HG2	1.97	0.45
37:y:269:ARG:HG3	37:y:276:THR:HG22	1.99	0.45
1:2:678:U:O4	1:2:1027:A:N7	2.51	0.44
2:R:67:ARG:HH12	30:K:568:TRP:HD1	1.64	0.44
11:Z:42:ASP:OD1	11:Z:42:ASP:N	2.47	0.44
18:u:139:ARG:HH11	18:u:140:PRO:HD2	1.81	0.44
26:J:24:ARG:O	26:J:28:GLU:HG3	2.17	0.44
29:q:60:ILE:HD13	29:q:81:LEU:HD23	1.98	0.44
30:K:855:ILE:O	30:K:859:ILE:HG12	2.17	0.44
1:2:382:C:H2'	1:2:383:G:H8	1.82	0.44
1:2:1310:U:H5''	31:M:36:ARG:HH21	1.82	0.44
15:w:315:CYS:SG	15:w:316:SER:N	2.90	0.44
30:K:615:TYR:HA	30:K:618:LEU:HD12	1.98	0.44
34:A:68:ILE:HD11	34:A:121:LEU:HG	1.99	0.44
35:C:123:ARG:HB3	35:C:143:CYS:SG	2.56	0.44
1:2:996:A:H2'	1:2:997:A:C8	2.52	0.44
1:2:1228:A:H2'	1:2:1229:G:H8	1.82	0.44
1:2:1497:G:OP1	15:w:376:VAL:N	2.50	0.44
1:2:1816:G:H2'	1:2:1817:G:H8	1.82	0.44
5:c:55:VAL:HB	8:F:34:SER:HA	2.00	0.44
8:F:104:THR:HG23	8:F:106:GLU:HG3	1.99	0.44
10:G:63:MET:HE3	10:G:100:CYS:HA	1.98	0.44
18:u:776:LYS:HB3	18:u:776:LYS:HE2	1.86	0.44
35:C:187:ARG:HE	35:C:187:ARG:HB3	1.60	0.44
1:2:28:U:H2'	1:2:29:G:C8	2.53	0.44
5:c:46:VAL:HG21	5:c:56:LEU:HD11	2.00	0.44
18:u:401:GLN:HA	18:u:404:TRP:HB2	1.99	0.44
22:P:28:MET:HE2	22:P:36:LEU:HD12	1.99	0.44
27:I:141:ARG:HB3	27:I:145:ILE:HB	1.99	0.44
34:A:66:VAL:HG21	34:A:185:MET:HG3	1.99	0.44
35:C:248:TYR:HE2	36:V:26:ALA:H	1.65	0.44
9:H:128:ALA:HA	9:H:131:GLU:HG2	1.99	0.44
13:x:162:SER:HB2	23:O:107:THR:HG21	1.99	0.44
18:u:396:GLY:HA2	22:P:104:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1817:G:H2'	1:2:1818:A:C8	2.52	0.44
15:w:365:LEU:HD11	15:w:400:ALA:HB1	1.99	0.44
22:P:50:ARG:H	22:P:53:GLN:NE2	2.16	0.44
1:2:28:U:H2'	1:2:29:G:H8	1.81	0.44
1:2:1398:G:C6	1:2:1448:A:N1	2.86	0.44
1:2:1856:C:H2'	1:2:1857:G:C8	2.53	0.44
8:F:143:PRO:HA	8:F:146:ARG:HB2	1.99	0.44
13:x:93:MET:HA	13:x:96:PHE:CE2	2.53	0.44
15:w:268:LEU:HB2	15:w:307:ILE:HD13	1.98	0.44
19:T:113:VAL:HA	19:T:123:LEU:HA	1.98	0.44
21:Q:19:ALA:HB2	21:Q:75:GLY:HA3	1.99	0.44
28:r:35:VAL:HB	28:r:85:HIS:HE1	1.83	0.44
34:A:80:ARG:HH12	34:A:166:LYS:HA	1.82	0.44
1:2:171:A:H5''	10:G:177:GLN:HG2	1.99	0.44
1:2:1296:U:O4	1:2:1301:A:N7	2.51	0.44
9:H:46:THR:HG23	9:H:65:PRO:HD3	2.00	0.44
18:u:260:PHE:HB2	18:u:570:VAL:HG21	1.99	0.44
1:2:317:C:OP2	10:G:183:ARG:NH1	2.43	0.44
1:2:823:U:H5	26:J:143:ASN:HB2	1.83	0.44
1:2:1295:A:H2'	1:2:1296:U:H6	1.83	0.44
1:2:1651:A:H2'	1:2:1652:G:H8	1.82	0.44
1:2:1679:A:N6	8:F:57:ALA:O	2.51	0.44
6:E:206:ASP:HB2	6:E:222:LEU:HB2	2.00	0.44
8:F:168:THR:HG22	8:F:170:ALA:H	1.83	0.44
9:H:17:ASP:OD1	9:H:18:GLU:N	2.44	0.44
15:w:395:THR:O	15:w:398:LYS:N	2.50	0.44
20:S:44:VAL:HG13	20:S:70:ILE:HG21	2.00	0.44
34:A:177:MET:HE3	34:A:180:ARG:NH2	2.33	0.44
18:u:598:VAL:HB	18:u:680:ALA:HB1	1.99	0.43
20:S:109:GLU:HA	20:S:112:GLU:HG2	2.00	0.43
21:Q:32:ILE:HG23	21:Q:68:ILE:HD11	2.00	0.43
25:L:56:ILE:O	25:L:84:ARG:NH2	2.40	0.43
34:A:83:GLY:O	34:A:86:ALA:HB3	2.18	0.43
1:2:1598:G:OP1	11:Z:80:ARG:NH1	2.48	0.43
21:Q:49:TYR:O	21:Q:53:GLU:N	2.51	0.43
22:P:72:LYS:HD2	22:P:73:PRO:HD2	2.00	0.43
27:I:37:LYS:HE2	27:I:95:THR:HG22	1.99	0.43
28:r:116:MET:HB2	29:q:103:GLY:HA3	1.99	0.43
30:K:138:GLN:HB2	30:K:144:GLU:HB2	2.00	0.43
1:2:126:G:OP2	10:G:198:ARG:NH1	2.51	0.43
1:2:1548:G:C5	1:2:1586:U:O4	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1854:U:H5''	23:O:147:ARG:HH21	1.84	0.43
6:E:143:ASP:OD1	6:E:143:ASP:N	2.49	0.43
12:Y:21:LYS:O	12:Y:74:MET:HA	2.18	0.43
19:T:57:ALA:HB1	19:T:107:LEU:HD21	2.00	0.43
4:B:25:PHE:HZ	23:O:53:ILE:HA	1.83	0.43
4:B:65:ARG:HB2	4:B:88:THR:HB	2.00	0.43
30:K:619:GLN:HA	30:K:622:MET:HG3	1.99	0.43
1:2:528:A:H2'	1:2:529:A:H8	1.83	0.43
1:2:929:G:H2'	1:2:930:C:O4'	2.18	0.43
6:E:198:ARG:CA	6:E:207:VAL:O	2.63	0.43
9:H:47:ALA:HB3	9:H:63:PHE:HB2	1.98	0.43
15:w:362:PHE:HA	15:w:365:LEU:HB2	2.01	0.43
27:I:201:LYS:HA	27:I:201:LYS:HD3	1.87	0.43
32:f:135:HIS:HB2	32:f:138:ARG:HG2	2.00	0.43
1:2:1290:G:C2	1:2:1310:U:C2	3.07	0.43
18:u:193:SER:OG	18:u:224:ASP:OD2	2.33	0.43
30:K:210:LEU:HA	30:K:213:VAL:HG12	2.01	0.43
30:K:710:ARG:NH1	30:K:752:SER:OG	2.52	0.43
9:H:159:ASP:OD2	24:N:19:ARG:NH1	2.51	0.43
22:P:61:ARG:NH2	22:P:88:GLU:OE1	2.52	0.43
23:O:39:ASP:OD1	23:O:39:ASP:N	2.48	0.43
27:I:150:ASP:HA	27:I:153:LYS:HG2	2.01	0.43
30:K:182:VAL:O	30:K:186:LYS:HG3	2.18	0.43
30:K:562:LEU:HD11	30:K:611:GLU:HG3	1.99	0.43
34:A:5:LEU:HD21	34:A:8:LEU:HD12	2.01	0.43
35:C:115:GLN:HA	35:C:120:GLN:HA	2.00	0.43
1:2:795:A:H2'	1:2:796:G:C8	2.52	0.43
1:2:1593:C:H2'	1:2:1594:A:H8	1.83	0.43
6:E:126:VAL:HA	6:E:141:THR:HA	2.01	0.43
27:I:34:ALA:HB2	27:I:56:ARG:HD2	2.01	0.43
28:r:77:ASN:HB2	28:r:80:PHE:HD2	1.84	0.43
30:K:776:ILE:HG13	30:K:794:VAL:HG11	2.00	0.43
1:2:528:A:H2'	1:2:529:A:C8	2.53	0.43
1:2:884:C:N3	1:2:903:A:C6	2.87	0.43
1:2:1279:C:H2'	1:2:1280:G:C8	2.54	0.43
1:2:1285:G:O6	31:M:82:ASN:ND2	2.52	0.43
1:2:1726:G:H2'	1:2:1727:G:C8	2.53	0.43
1:2:886:A:C6	1:2:888:U:C4	3.06	0.43
1:2:1004:U:H2'	1:2:1005:G:C8	2.54	0.43
1:2:1616:U:OP2	22:P:43:ARG:NH1	2.51	0.43
18:u:508:SER:O	18:u:510:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:745:LEU:H	18:u:751:MET:HA	1.84	0.43
21:Q:33:LYS:HZ2	21:Q:69:ARG:HE	1.67	0.43
25:L:135:SER:OG	25:L:136:LYS:N	2.51	0.43
30:K:864:LEU:HD23	30:K:864:LEU:HA	1.88	0.43
1:2:952:G:H2'	1:2:953:C:C6	2.54	0.42
1:2:1195:A:H2'	1:2:1196:A:C8	2.54	0.42
1:2:1619:A:O2'	22:P:82:ASP:OD2	2.32	0.42
4:B:109:LYS:O	4:B:113:MET:HB2	2.18	0.42
10:G:7:PHE:O	10:G:11:GLY:N	2.51	0.42
10:G:56:ASN:HB2	10:G:108:VAL:HG12	2.00	0.42
18:u:208:SER:O	18:u:212:GLU:HB2	2.19	0.42
18:u:358:GLU:HA	18:u:590:LYS:HA	2.00	0.42
18:u:594:LEU:HD22	18:u:687:VAL:HG22	2.01	0.42
19:T:34:VAL:HG13	19:T:53:PHE:HE2	1.84	0.42
24:N:87:ASP:OD1	24:N:87:ASP:N	2.52	0.42
30:K:862:VAL:HG22	30:K:880:LEU:HD23	2.01	0.42
1:2:51:U:H2'	1:2:52:G:C8	2.54	0.42
4:B:62:LEU:HA	4:B:65:ARG:HG2	2.01	0.42
6:E:112:HIS:NE2	6:E:237:SER:OG	2.44	0.42
8:F:55:ARG:HH22	21:Q:124:PRO:HG2	1.84	0.42
15:w:365:LEU:HA	15:w:368:ARG:NH1	2.35	0.42
20:S:74:PRO:HB2	20:S:79:ILE:HD13	2.01	0.42
30:K:179:PRO:HG2	30:K:183:LEU:HG	2.01	0.42
1:2:1290:G:H5''	15:w:235:ARG:HH11	1.83	0.42
1:2:1468:C:H2'	1:2:1469:A:H8	1.84	0.42
18:u:598:VAL:HG11	18:u:667:LEU:HD13	2.00	0.42
28:r:40:ASN:O	28:r:44:ARG:HG2	2.20	0.42
37:y:222:GLU:O	37:y:261:ARG:NH2	2.43	0.42
1:2:1314:U:H5'	15:w:316:SER:HB3	2.02	0.42
1:2:1323:U:H3'	1:2:1324:G:H8	1.85	0.42
4:B:185:VAL:O	4:B:189:ILE:HG12	2.18	0.42
15:w:188:VAL:HA	15:w:191:VAL:HB	2.00	0.42
19:T:97:LYS:HB3	19:T:101:ARG:HH21	1.83	0.42
21:Q:41:MET:HE3	21:Q:41:MET:HB3	1.91	0.42
22:P:100:LYS:HG2	22:P:101:THR:HG23	2.01	0.42
30:K:844:VAL:HA	30:K:847:LEU:HB2	2.00	0.42
34:A:111:GLN:NE2	35:C:89:LYS:O	2.52	0.42
1:2:909:G:H2'	1:2:910:G:C8	2.55	0.42
1:2:1051:G:H2'	1:2:1052:A:C8	2.55	0.42
1:2:1144:A:H2'	1:2:1145:A:C8	2.54	0.42
1:2:1565:C:H41	19:T:101:ARG:NH1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:100:MET:HE2	18:u:137:SER:HB3	2.01	0.42
19:T:75:MET:HA	19:T:78:ILE:HD12	2.02	0.42
19:T:125:PRO:HB2	19:T:129:ARG:NH1	2.35	0.42
27:I:74:ARG:HD2	27:I:108:PRO:HB2	2.01	0.42
30:K:338:HIS:CE1	30:K:340:LEU:HB2	2.54	0.42
34:A:65:ILE:HD11	34:A:74:VAL:HG11	2.00	0.42
5:c:31:ARG:NH1	5:c:41:SER:OG	2.53	0.42
13:x:158:LEU:HD23	13:x:158:LEU:HA	1.93	0.42
18:u:294:TYR:OH	18:u:572:CYS:SG	2.62	0.42
18:u:349:PRO:HG2	18:u:351:ARG:HD2	2.01	0.42
29:q:170:GLN:O	29:q:174:ILE:HG13	2.19	0.42
30:K:1245:LYS:HA	30:K:1245:LYS:HD2	1.78	0.42
35:C:106:VAL:HG23	35:C:128:VAL:HG12	2.00	0.42
35:C:178:HIS:ND1	35:C:179:THR:HG23	2.34	0.42
1:2:434:G:OP1	27:I:23:LYS:HG2	2.20	0.42
1:2:1037:G:H4'	1:2:1845:A:H4'	2.00	0.42
8:F:76:MET:HB2	8:F:89:THR:HG23	2.01	0.42
9:H:69:LEU:HD13	9:H:96:ALA:HB2	2.01	0.42
20:S:22:GLY:HA2	20:S:56:ALA:HB3	2.01	0.42
34:A:7:VAL:HG13	34:A:8:LEU:HG	2.02	0.42
1:2:903:A:H2'	1:2:904:A:C8	2.55	0.42
1:2:1492:U:H2'	1:2:1493:C:C6	2.55	0.42
6:E:153:LEU:HD13	10:G:216:ARG:HD2	2.02	0.42
11:Z:68:ILE:HB	11:Z:109:TYR:HB2	2.02	0.42
29:q:31:ARG:NH1	29:q:38:ARG:HH22	2.17	0.42
32:f:96:LYS:HA	32:f:96:LYS:HD2	1.90	0.42
1:2:107:A:H2'	1:2:108:G:C8	2.55	0.42
1:2:1214:A:OP2	15:w:36:LYS:NZ	2.44	0.42
1:2:1593:C:H2'	1:2:1594:A:C8	2.55	0.42
11:Z:49:LEU:HD11	20:S:3:LEU:HD23	2.02	0.42
30:K:651:ILE:HA	30:K:658:ARG:HG2	2.01	0.42
30:K:993:SER:HB2	30:K:996:MET:HB3	2.02	0.42
1:2:531:A:H2'	1:2:532:C:C6	2.55	0.42
1:2:1203:G:H2'	1:2:1204:A:C8	2.51	0.42
1:2:1329:U:H2'	1:2:1330:G:H8	1.85	0.42
2:R:62:GLN:O	30:K:621:GLN:NE2	2.53	0.42
23:O:117:ARG:O	23:O:121:ARG:HG2	2.20	0.42
29:q:106:GLY:HA2	29:q:145:PHE:HB2	2.02	0.42
30:K:840:LEU:HA	30:K:843:ILE:HG12	2.02	0.42
30:K:880:LEU:HD12	30:K:880:LEU:HA	1.87	0.42
2:R:34:VAL:O	2:R:38:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:x:107:ILE:HG22	13:x:118:ILE:HG23	2.02	0.41
13:x:229:ILE:HD12	23:O:149:ARG:NH1	2.35	0.41
1:2:1565:C:H2'	1:2:1566:G:C8	2.55	0.41
18:u:733:THR:HG22	18:u:765:VAL:HG12	2.02	0.41
37:y:33:VAL:HG12	37:y:82:THR:HB	2.02	0.41
15:w:179:PRO:HB2	15:w:180:ARG:H	1.66	0.41
30:K:223:LYS:HA	30:K:223:LYS:HD3	1.81	0.41
1:2:1025:U:C4	1:2:1026:C:N4	2.88	0.41
15:w:365:LEU:HD13	15:w:368:ARG:NH1	2.35	0.41
27:I:67:TRP:CZ2	27:I:109:TYR:HB3	2.55	0.41
37:y:299:THR:HB	37:y:307:HIS:CE1	2.54	0.41
1:2:604:A:N3	1:2:639:C:O2'	2.49	0.41
1:2:613:G:N2	1:2:626:G:OP1	2.48	0.41
1:2:948:C:H2'	1:2:949:G:C8	2.54	0.41
1:2:1051:G:H2'	1:2:1052:A:H8	1.85	0.41
1:2:1551:U:H1'	1:2:1558:C:C2	2.55	0.41
4:B:219:LYS:HB2	4:B:219:LYS:HE3	1.85	0.41
13:x:241:ILE:HD12	13:x:241:ILE:HA	1.98	0.41
18:u:259:ASP:OD1	18:u:260:PHE:N	2.48	0.41
19:T:27:LYS:HG3	19:T:110:LEU:HD22	2.02	0.41
21:Q:16:LYS:HD2	21:Q:16:LYS:HA	1.76	0.41
25:L:21:LYS:NZ	27:I:117:TYR:OH	2.54	0.41
30:K:1102:ARG:HD2	30:K:1102:ARG:HA	1.87	0.41
1:2:118:C:H1'	1:2:445:A:C5	2.56	0.41
1:2:931:C:H2'	1:2:932:G:C8	2.56	0.41
1:2:1195:A:H2'	1:2:1196:A:H8	1.85	0.41
8:F:140:ASP:OD1	8:F:141:VAL:N	2.52	0.41
9:H:9:VAL:HG23	9:H:24:SER:HB2	2.03	0.41
10:G:50:VAL:HA	10:G:112:VAL:O	2.21	0.41
13:x:108:ARG:HD3	37:y:208:TRP:CD2	2.55	0.41
13:x:144:PHE:CE2	13:x:160:LEU:HD11	2.56	0.41
15:w:361:VAL:HG11	15:w:397:GLN:HG2	2.03	0.41
19:T:80:GLY:HA3	19:T:93:SER:O	2.21	0.41
30:K:907:TYR:HB3	33:z:214:ILE:HG13	2.02	0.41
30:K:947:VAL:HG11	30:K:965:PHE:HD1	1.85	0.41
1:2:70:G:N2	1:2:79:A:H62	2.17	0.41
1:2:290:U:H2'	1:2:291:G:H3'	2.02	0.41
1:2:1598:G:OP1	20:S:55:ARG:NH2	2.54	0.41
4:B:28:LYS:NZ	23:O:51:GLU:OE2	2.44	0.41
9:H:177:TYR:O	9:H:181:THR:CB	2.67	0.41
18:u:156:ILE:HG13	18:u:183:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C:65:LYS:HE2	35:C:273:LEU:HD23	2.02	0.41
1:2:1491:G:H2'	1:2:1492:U:C6	2.54	0.41
1:2:1686:G:H2'	1:2:1687:C:C6	2.56	0.41
11:Z:63:PRO:HG3	11:Z:96:LEU:HD13	2.03	0.41
30:K:837:LEU:HB3	30:K:880:LEU:HD22	2.02	0.41
1:2:523:A:OP2	26:J:38:ARG:NH1	2.53	0.41
1:2:617:G:N7	14:X:67:ARG:NH1	2.57	0.41
1:2:1238:U:H1'	22:P:126:VAL:HG23	2.02	0.41
6:E:199:GLU:N	6:E:207:VAL:O	2.49	0.41
8:F:20:PHE:HB2	8:F:23:TRP:CD1	2.56	0.41
8:F:155:CYS:SG	8:F:159:ARG:NH1	2.93	0.41
9:H:168:HIS:CD2	9:H:168:HIS:H	2.38	0.41
15:w:354:TYR:HB3	16:t:251:ARG:HD2	2.01	0.41
18:u:591:MET:HB3	18:u:591:MET:HE3	1.81	0.41
20:S:86:ARG:HE	20:S:106:LYS:HD2	1.86	0.41
24:N:70:LYS:HG3	24:N:73:ARG:HG3	2.01	0.41
30:K:457:VAL:HG23	30:K:465:ALA:HB1	2.03	0.41
30:K:725:ASP:N	30:K:725:ASP:OD1	2.53	0.41
30:K:860:PRO:HG3	33:z:197:PHE:CD2	2.56	0.41
30:K:1116:GLU:O	30:K:1128:ARG:NH1	2.53	0.41
31:M:56:CYS:SG	31:M:61:TYR:OH	2.70	0.41
33:z:197:PHE:O	33:z:201:LEU:HB2	2.21	0.41
34:A:57:LYS:HE2	36:V:70:LEU:HD21	2.03	0.41
1:2:1468:C:H2'	1:2:1469:A:C8	2.56	0.41
18:u:397:THR:HG23	18:u:401:GLN:HB2	2.02	0.41
18:u:745:LEU:HD12	18:u:752:LYS:HE2	2.02	0.41
27:I:165:GLN:O	27:I:169:GLY:N	2.51	0.41
29:q:57:LEU:HA	29:q:118:GLY:O	2.21	0.41
34:A:130:ASP:O	34:A:134:LEU:HD23	2.21	0.41
35:C:183:LYS:HA	35:C:195:LEU:O	2.21	0.41
1:2:186:C:H2'	1:2:187:G:H8	1.86	0.40
1:2:1099:G:O2'	1:2:1100:A:H8	2.04	0.40
1:2:1681:U:O4	15:w:36:LYS:NZ	2.40	0.40
4:B:60:ASP:HA	4:B:63:LYS:HG2	2.02	0.40
15:w:368:ARG:NH2	15:w:404:LEU:HD13	2.36	0.40
18:u:611:LYS:HZ2	18:u:611:LYS:HG2	1.68	0.40
25:L:152:LYS:HE2	25:L:152:LYS:HB2	1.67	0.40
30:K:210:LEU:HB3	30:K:252:ILE:HD12	2.01	0.40
30:K:864:LEU:HD11	33:z:189:LEU:HG	2.03	0.40
31:M:23:LYS:O	31:M:27:ILE:HG12	2.21	0.40
33:z:211:LEU:HD23	33:z:211:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1596:U:OP2	11:Z:85:ARG:NH1	2.54	0.40
1:2:1810:U:H2'	1:2:1811:C:C6	2.56	0.40
4:B:182:LYS:HE3	4:B:182:LYS:HA	2.03	0.40
8:F:165:ASN:OD1	8:F:165:ASN:N	2.53	0.40
17:W:30:CYS:SG	17:W:31:SER:N	2.94	0.40
23:O:26:ASN:C	23:O:26:ASN:ND2	2.79	0.40
28:r:11:SER:HB2	28:r:16:VAL:HG21	2.03	0.40
29:q:22:GLU:HA	29:q:25:LYS:HG2	2.01	0.40
34:A:88:LEU:O	34:A:91:ALA:HB3	2.22	0.40
34:A:128:ARG:HD2	34:A:128:ARG:HA	1.85	0.40
1:2:1392:U:H2'	1:2:1393:G:C8	2.55	0.40
1:2:1845:A:H2'	1:2:1846:G:C8	2.57	0.40
3:b:82:LYS:HD3	24:N:25:TRP:CE2	2.55	0.40
8:F:198:ARG:HH22	29:q:16:LEU:HD13	1.87	0.40
10:G:2:LYS:HB2	10:G:108:VAL:HG23	2.03	0.40
18:u:506:LEU:HD11	18:u:514:TRP:HE3	1.86	0.40
30:K:194:PHE:HD1	30:K:197:ILE:HD12	1.84	0.40
34:A:177:MET:HE2	34:A:177:MET:HB3	1.97	0.40
1:2:1485:U:H2'	1:2:1486:A:H8	1.86	0.40
1:2:1611:G:H2'	1:2:1612:G:C8	2.56	0.40
4:B:193:ILE:O	4:B:197:ILE:HG12	2.21	0.40
12:Y:44:LEU:HD23	12:Y:44:LEU:HA	1.90	0.40
29:q:64:THR:HA	29:q:91:ALA:HB2	2.03	0.40
32:f:107:LYS:HE3	32:f:117:LEU:HD12	2.04	0.40
1:2:104:A:N6	1:2:356:C:C5	2.89	0.40
1:2:535:G:H2'	1:2:536:A:H8	1.86	0.40
1:2:1138:C:O2'	36:V:61:ARG:NH1	2.52	0.40
1:2:1143:A:H5'	35:C:190:SER:HB3	2.04	0.40
1:2:1282:A:N1	1:2:1316:C:C4	2.90	0.40
1:2:1285:G:H22	31:M:57:ASP:H	1.68	0.40
1:2:1797:U:H2'	1:2:1798:C:C6	2.57	0.40
10:G:6:SER:HB3	10:G:112:VAL:HG12	2.04	0.40
13:x:160:LEU:HD12	13:x:160:LEU:HA	1.86	0.40
26:J:78:LEU:HD22	26:J:92:MET:HA	2.02	0.40
28:r:6:HIS:HA	28:r:9:LEU:HD12	2.04	0.40
34:A:63:ARG:HG3	34:A:185:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	79/135 (58%)	75 (95%)	4 (5%)	0	100	100
3	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
4	B	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
5	c	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
6	E	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
7	e	18/59 (30%)	18 (100%)	0	0	100	100
8	F	187/204 (92%)	175 (94%)	12 (6%)	0	100	100
9	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
10	G	228/249 (92%)	224 (98%)	4 (2%)	0	100	100
11	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
12	Y	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
13	x	173/252 (69%)	165 (95%)	8 (5%)	0	100	100
14	X	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
15	w	322/437 (74%)	312 (97%)	10 (3%)	0	100	100
16	t	102/475 (22%)	92 (90%)	9 (9%)	1 (1%)	12	45
17	W	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
18	u	630/804 (78%)	606 (96%)	23 (4%)	1 (0%)	43	73
19	T	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
20	S	125/152 (82%)	121 (97%)	4 (3%)	0	100	100
21	Q	123/146 (84%)	118 (96%)	5 (4%)	0	100	100
22	P	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
23	O	133/151 (88%)	119 (90%)	13 (10%)	1 (1%)	16	50
24	N	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
25	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
26	J	178/194 (92%)	166 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
28	r	116/125 (93%)	109 (94%)	7 (6%)	0	100	100
29	q	200/207 (97%)	196 (98%)	4 (2%)	0	100	100
30	K	973/1297 (75%)	930 (96%)	43 (4%)	0	100	100
31	M	102/132 (77%)	101 (99%)	1 (1%)	0	100	100
32	f	53/156 (34%)	48 (91%)	5 (9%)	0	100	100
33	z	50/230 (22%)	47 (94%)	3 (6%)	0	100	100
34	A	214/295 (72%)	205 (96%)	9 (4%)	0	100	100
35	C	214/293 (73%)	205 (96%)	9 (4%)	0	100	100
36	V	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
37	y	257/412 (62%)	249 (97%)	8 (3%)	0	100	100
All	All	6568/8700 (76%)	6294 (96%)	271 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	u	509	PHE
23	O	22	ALA
16	t	261	GLU

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	72/122 (59%)	72 (100%)	0	100	100
3	b	74/76 (97%)	74 (100%)	0	100	100
4	B	194/231 (84%)	194 (100%)	0	100	100
5	c	52/62 (84%)	52 (100%)	0	100	100
6	E	224/225 (100%)	224 (100%)	0	100	100
7	e	18/48 (38%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	159/170 (94%)	159 (100%)	0	100	100
9	H	167/174 (96%)	167 (100%)	0	100	100
10	G	200/218 (92%)	200 (100%)	0	100	100
11	Z	64/103 (62%)	64 (100%)	0	100	100
12	Y	108/115 (94%)	108 (100%)	0	100	100
13	x	148/208 (71%)	148 (100%)	0	100	100
14	X	113/115 (98%)	113 (100%)	0	100	100
15	w	263/370 (71%)	263 (100%)	0	100	100
16	t	103/434 (24%)	103 (100%)	0	100	100
17	W	112/113 (99%)	112 (100%)	0	100	100
18	u	561/705 (80%)	561 (100%)	0	100	100
19	T	114/115 (99%)	114 (100%)	0	100	100
20	S	111/132 (84%)	111 (100%)	0	100	100
21	Q	106/121 (88%)	106 (100%)	0	100	100
22	P	111/130 (85%)	111 (100%)	0	100	100
23	O	105/119 (88%)	104 (99%)	1 (1%)	68	80
24	N	130/131 (99%)	130 (100%)	0	100	100
25	L	135/142 (95%)	135 (100%)	0	100	100
26	J	160/168 (95%)	160 (100%)	0	100	100
27	I	178/180 (99%)	178 (100%)	0	100	100
28	r	105/112 (94%)	105 (100%)	0	100	100
29	q	168/171 (98%)	168 (100%)	0	100	100
30	K	846/1094 (77%)	846 (100%)	0	100	100
31	M	91/108 (84%)	91 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	z	44/185 (24%)	44 (100%)	0	100	100
34	A	180/243 (74%)	180 (100%)	0	100	100
35	C	182/225 (81%)	182 (100%)	0	100	100
36	V	67/67 (100%)	67 (100%)	0	100	100
37	y	233/367 (64%)	233 (100%)	0	100	100
All	All	5749/7439 (77%)	5748 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	O	26	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	62	GLN
4	B	43	ASN
4	B	53	GLN
6	E	98	ASN
6	E	157	ASN
8	F	29	GLN
8	F	82	ASN
9	H	76	GLN
14	X	46	HIS
16	t	269	GLN
16	t	365	GLN
17	W	15	ASN
18	u	59	GLN
18	u	180	GLN
18	u	190	GLN
18	u	401	GLN
18	u	604	ASN
19	T	83	GLN
20	S	105	ASN
22	P	46	ASN
22	P	114	HIS
23	O	26	ASN
23	O	38	ASN
24	N	62	GLN
25	L	19	ASN
26	J	111	GLN
26	J	156	HIS
27	I	52	ASN
27	I	64	ASN
27	I	155	ASN
28	r	40	ASN
30	K	369	GLN
30	K	428	HIS
30	K	576	HIS
30	K	621	GLN
30	K	688	ASN

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Mol	Chain	Res	Type
30	K	730	ASN
30	K	977	HIS
31	M	28	HIS
35	C	113	GLN
35	C	115	GLN
35	C	267	GLN
37	y	129	HIS
37	y	402	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1568/1873 (83%)	354 (22%)	23 (1%)

All (354) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	8	U
1	2	14	C
1	2	17	C
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	62	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	103	A
1	2	113	G

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Mol	Chain	Res	Type
1	2	114	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	129	C
1	2	130	G
1	2	143	U
1	2	144	U
1	2	155	G
1	2	160	U
1	2	163	U
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	217	A
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	309	G
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	321	C
1	2	331	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	385	G
1	2	386	C
1	2	399	C
1	2	400	C

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Mol	Chain	Res	Type
1	2	407	G
1	2	409	C
1	2	413	G
1	2	418	A
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	493	A
1	2	496	C
1	2	525	A
1	2	540	U
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	568	C
1	2	573	U
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U

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Mol	Chain	Res	Type
1	2	595	U
1	2	598	G
1	2	600	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G
1	2	627	U
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	659	G
1	2	660	C
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	678	U
1	2	684	G
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	799	U
1	2	800	U
1	2	801	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	844	U
1	2	847	A

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Mol	Chain	Res	Type
1	2	869	A
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	881	G
1	2	885	U
1	2	886	A
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	896	U
1	2	898	U
1	2	908	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	933	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	981	A
1	2	990	A
1	2	991	G
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1026	C
1	2	1040	G
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1080	A
1	2	1083	A
1	2	1085	C

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Mol	Chain	Res	Type
1	2	1087	A
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1114	U
1	2	1115	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1121	G
1	2	1138	C
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1200	A
1	2	1202	U
1	2	1203	G
1	2	1206	G
1	2	1211	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1235	G
1	2	1238	U
1	2	1242	U
1	2	1265	A
1	2	1268	C
1	2	1269	G
1	2	1270	G
1	2	1271	C
1	2	1273	C
1	2	1284	A
1	2	1285	G

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Mol	Chain	Res	Type
1	2	1286	G
1	2	1293	A
1	2	1296	U
1	2	1298	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1304	U
1	2	1305	C
1	2	1307	U
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1323	U
1	2	1325	G
1	2	1326	U
1	2	1335	G
1	2	1337	C
1	2	1369	A
1	2	1371	U
1	2	1372	U
1	2	1376	A
1	2	1383	A
1	2	1387	G
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1445	U
1	2	1446	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1476	A
1	2	1477	U
1	2	1478	U

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Mol	Chain	Res	Type
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1501	C
1	2	1512	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1528	G
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1544	C
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1569	A
1	2	1570	G
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1617	G
1	2	1618	C
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1629	C
1	2	1639	G7M
1	2	1640	A
1	2	1646	C

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Mol	Chain	Res	Type
1	2	1647	A
1	2	1648	G
1	2	1654	G
1	2	1661	A
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1666	C
1	2	1669	G
1	2	1675	A
1	2	1680	G
1	2	1694	U
1	2	1705	C
1	2	1712	A
1	2	1721	U
1	2	1722	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1758	G
1	2	1761	U
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1801	A
1	2	1808	U
1	2	1826	G
1	2	1836	G
1	2	1839	U
1	2	1848	U
1	2	1849	G
1	2	1861	G
1	2	1864	U
1	2	1872	G
1	2	1873	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G

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Mol	Chain	Res	Type
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	417	C
1	2	465	A
1	2	604	A
1	2	749	U
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1264	C
1	2	1295	A
1	2	1304	U
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1601	A
1	2	1693	G
1	2	1726	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	G7M	2	1639	1	23,26,27	2.85	9 (39%)	34,39,42	1.83	10 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	2	1639	1	-	3/7/25/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	C4-N3	6.77	1.49	1.34
1	2	1639	G7M	C2-N2	6.69	1.49	1.34
1	2	1639	G7M	C2-N3	5.72	1.47	1.33
1	2	1639	G7M	C5-C6	4.17	1.54	1.43
1	2	1639	G7M	C5-N7	-3.74	1.34	1.39
1	2	1639	G7M	C2-N1	3.04	1.45	1.37
1	2	1639	G7M	C6-N1	3.01	1.44	1.38
1	2	1639	G7M	C8-N7	2.40	1.37	1.33
1	2	1639	G7M	O6-C6	-2.40	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	G7M	C2-N3-C4	4.89	120.73	112.30
1	2	1639	G7M	C5-C4-N3	-4.09	120.41	128.15
1	2	1639	G7M	C5-C6-N1	4.07	120.25	111.84
1	2	1639	G7M	O6-C6-C5	-2.99	121.34	128.01
1	2	1639	G7M	C2-N1-C6	-2.97	119.73	125.11
1	2	1639	G7M	N9-C4-N3	2.91	131.77	125.95
1	2	1639	G7M	CN7-N7-C5	2.85	130.35	126.80
1	2	1639	G7M	CN7-N7-C8	-2.26	121.36	124.79
1	2	1639	G7M	N1-C2-N3	-2.06	119.56	123.32
1	2	1639	G7M	N9-C8-N7	-2.01	107.59	112.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1639	G7M	O4'-C4'-C5'-O5'
1	2	1639	G7M	C3'-C4'-C5'-O5'
1	2	1639	G7M	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1639	G7M	2	0

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.

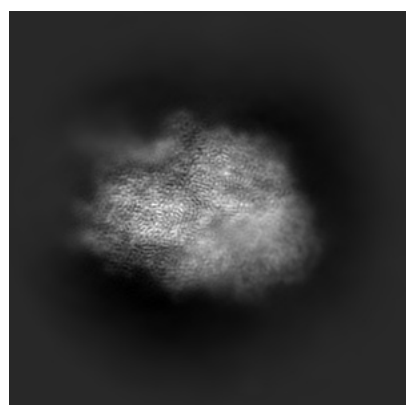
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32803. These allow visual inspection of the internal detail of the map and identification of artifacts.

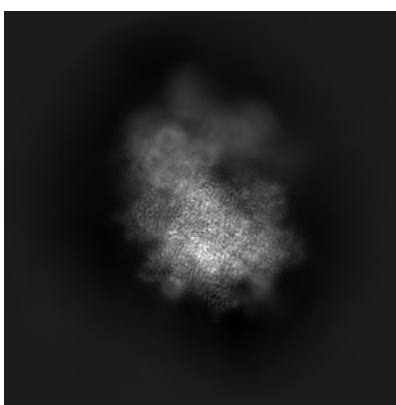
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

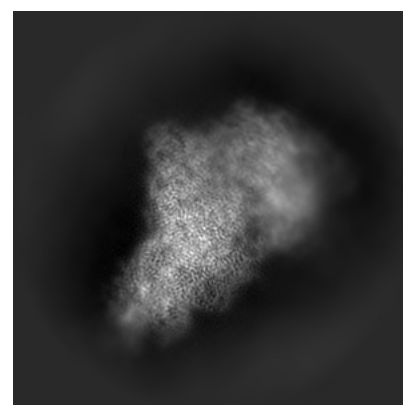
6.1.1 Primary map



X



Y

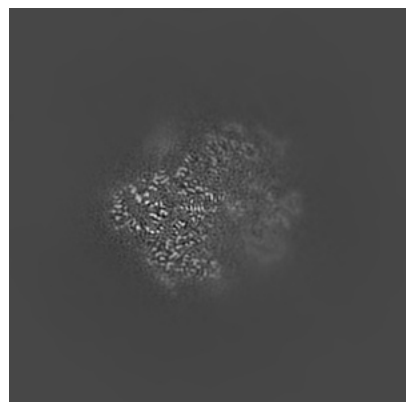


Z

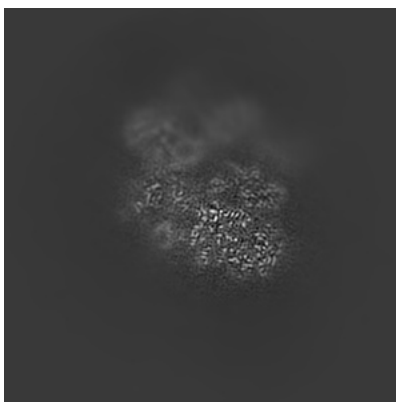
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

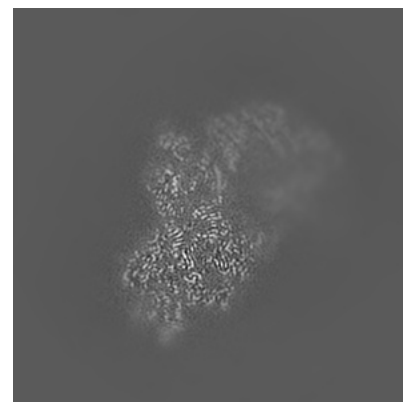
6.2.1 Primary map



X Index: 180



Y Index: 180

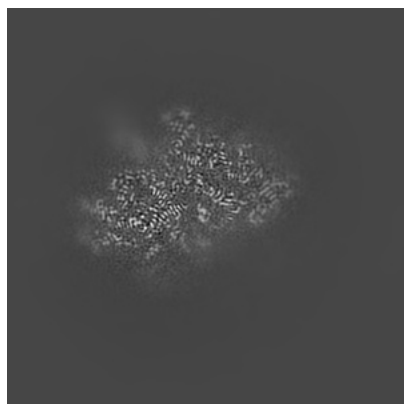


Z Index: 180

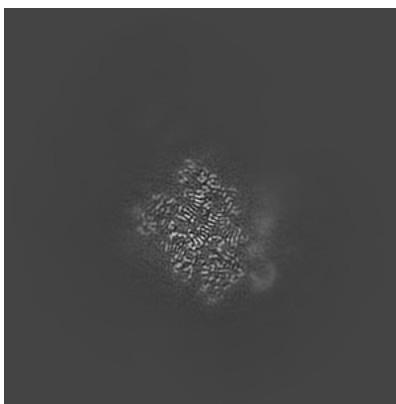
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

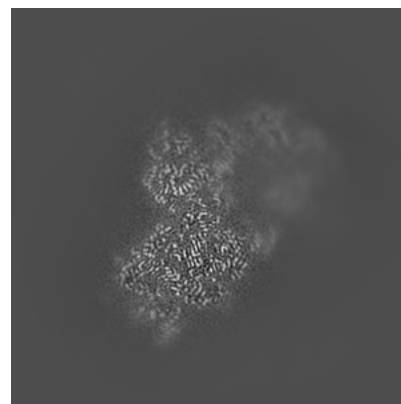
6.3.1 Primary map



X Index: 148



Y Index: 133

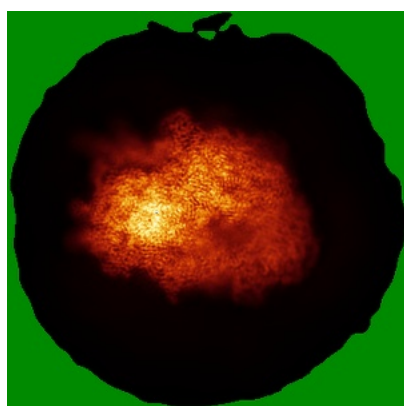


Z Index: 184

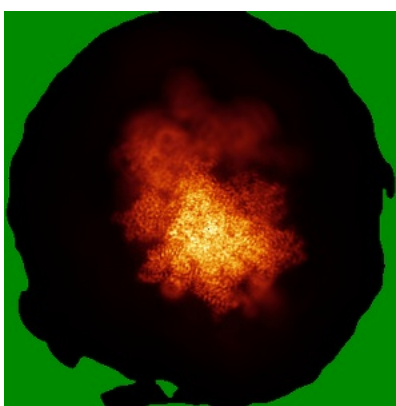
The images above show the largest variance slices of the map in three orthogonal directions.

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

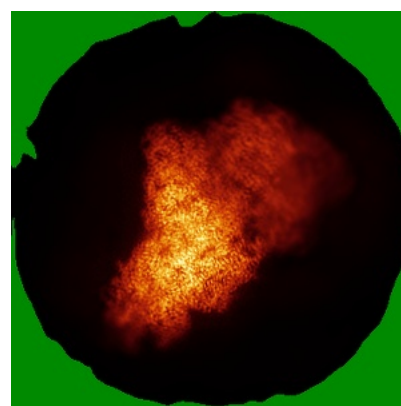
6.4.1 Primary map



X



Y

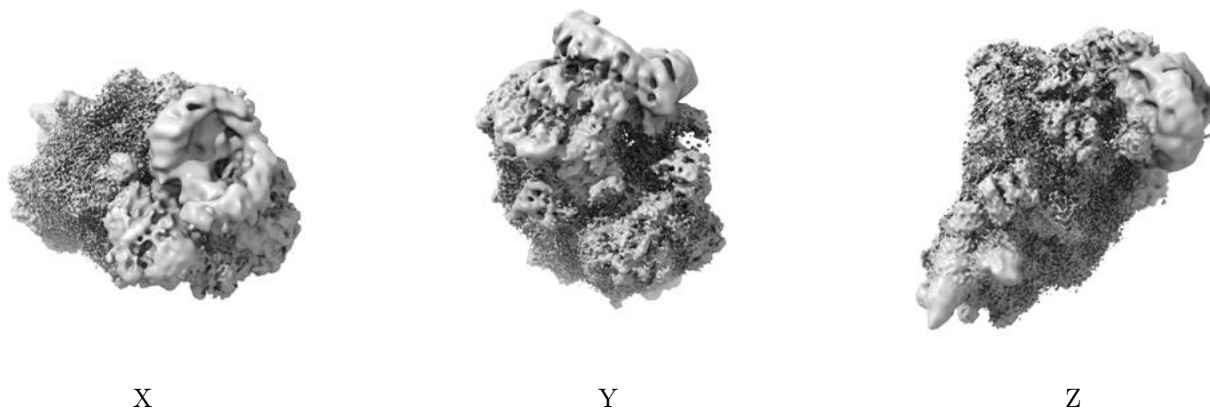


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

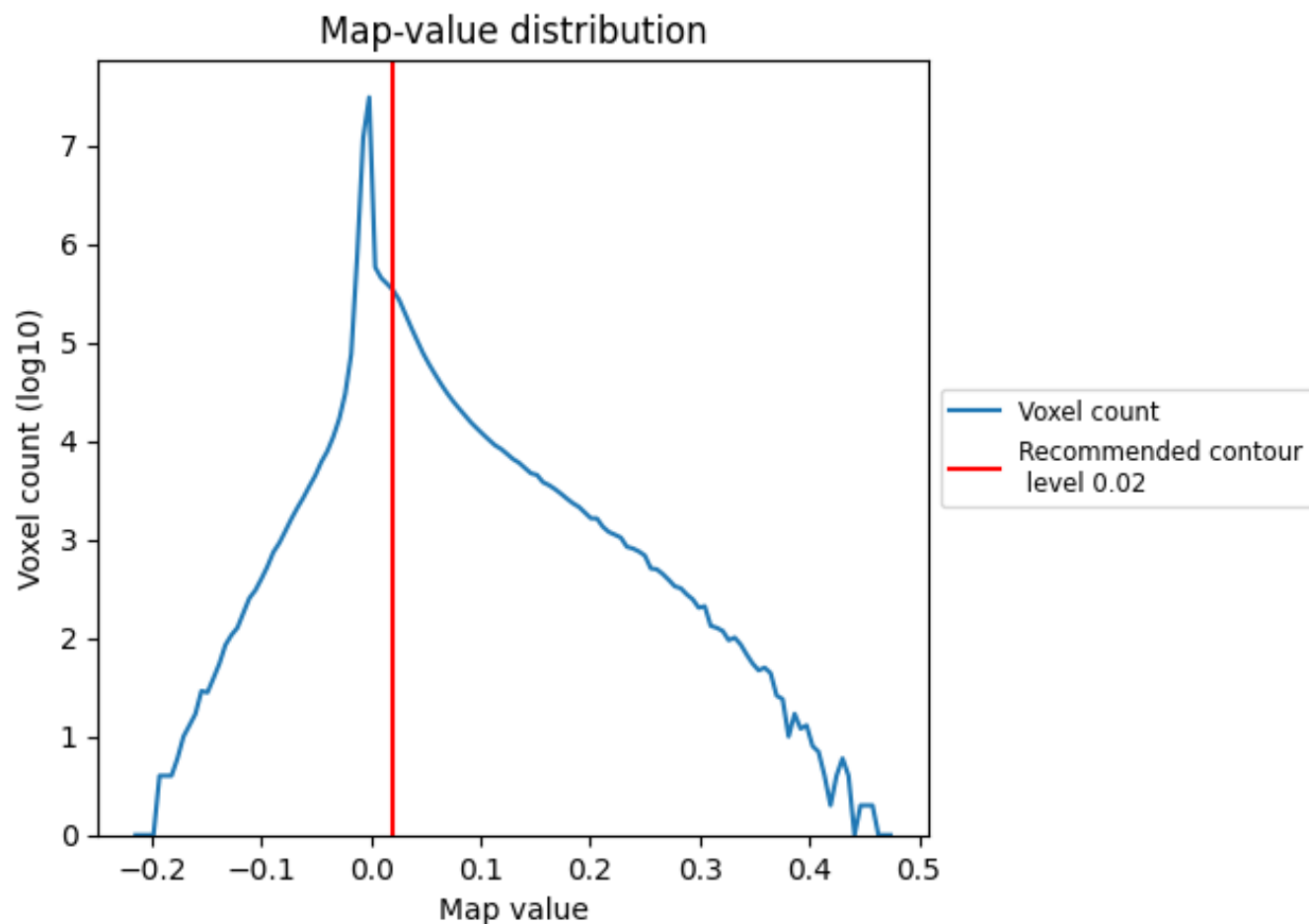
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

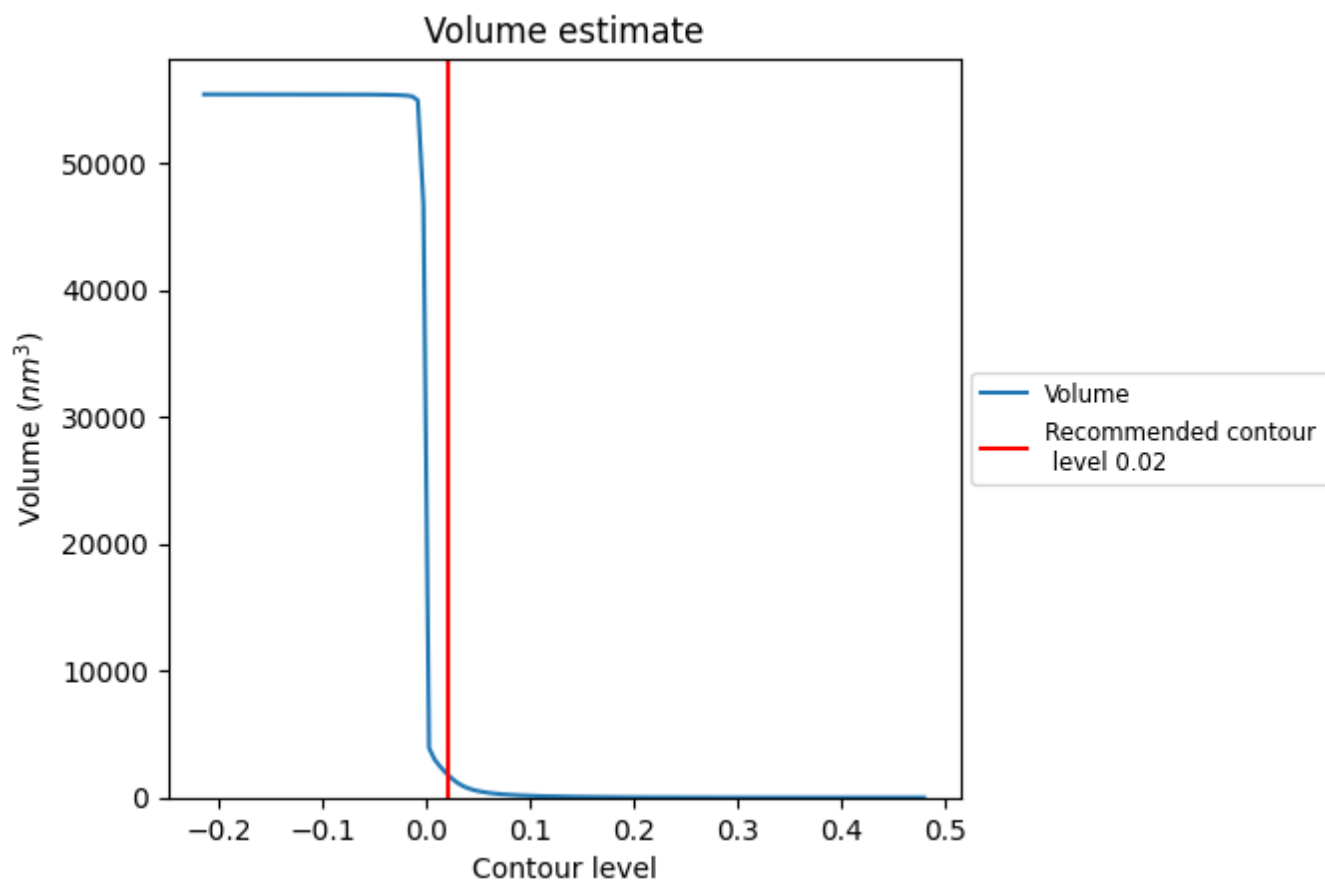
This section contains the results of statistical analysis of the map.

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.

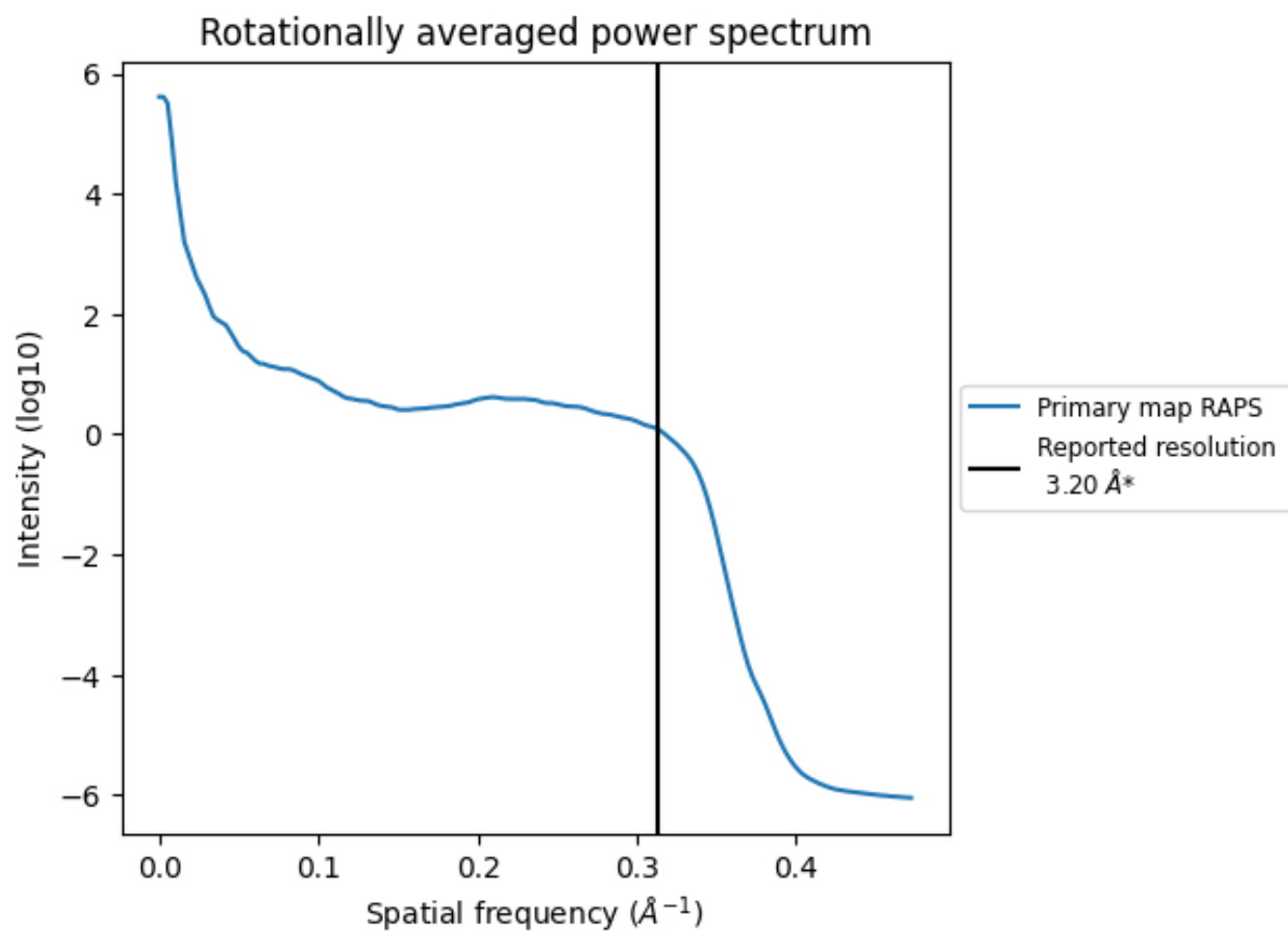
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1837 nm³; this corresponds to an approximate mass of 1660 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 ⓘ

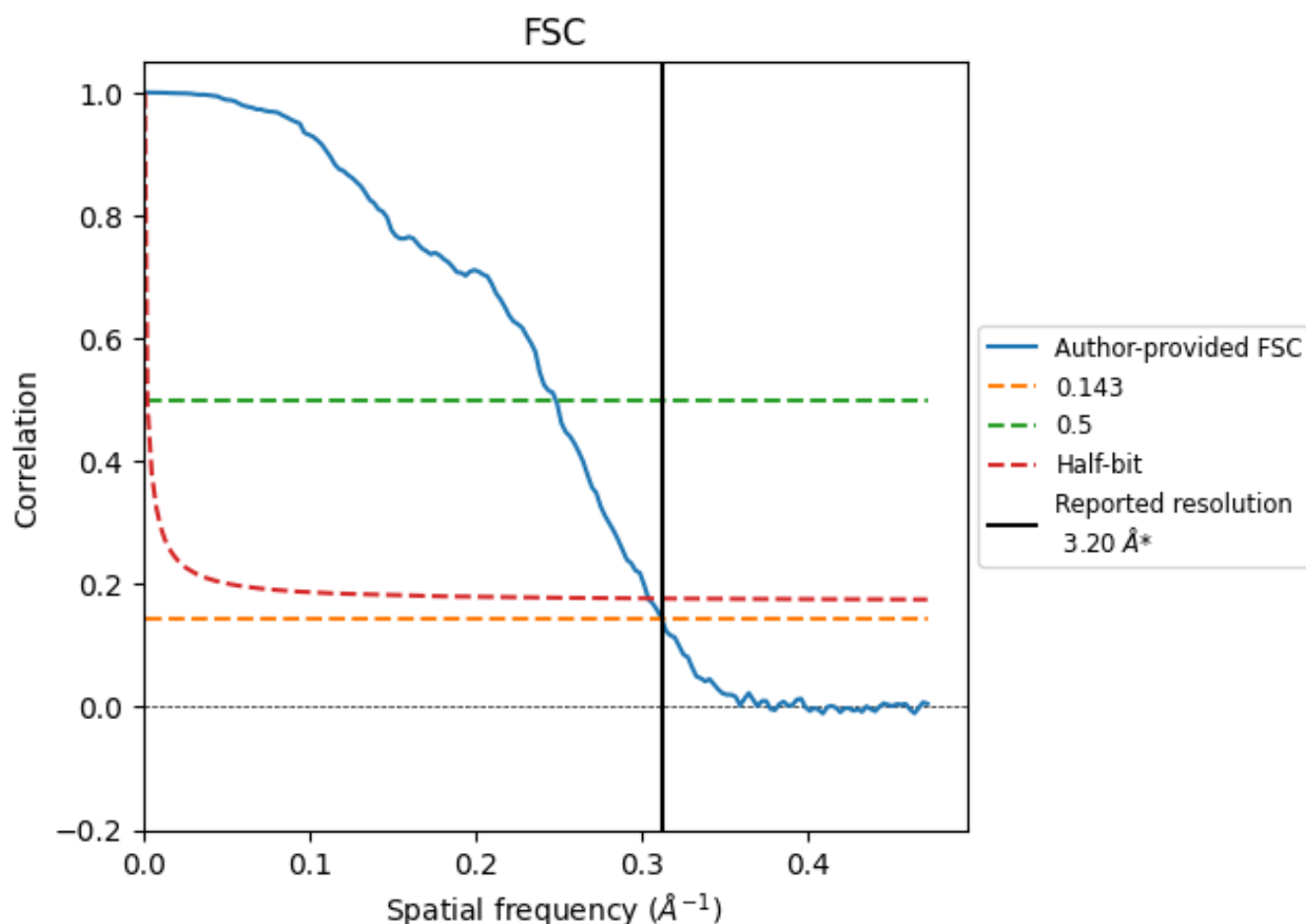


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

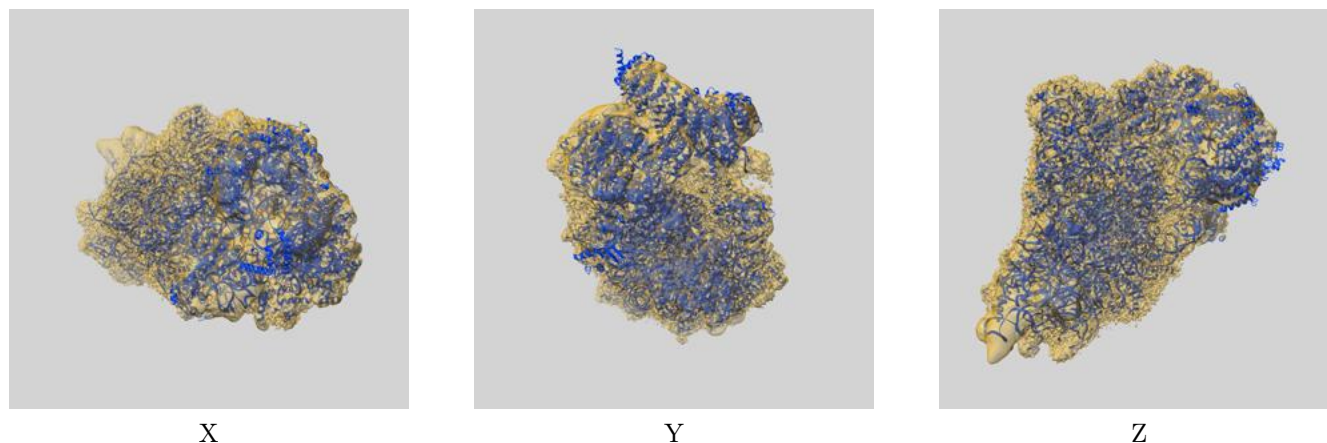
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	4.03	3.29
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

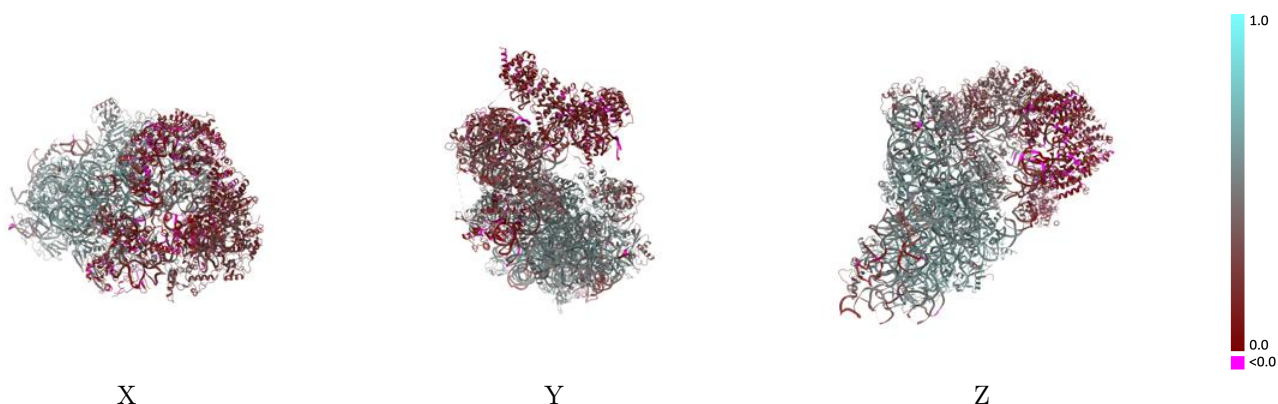
This section contains information regarding the fit between EMDB map EMD-32803 and PDB model 7WTW. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



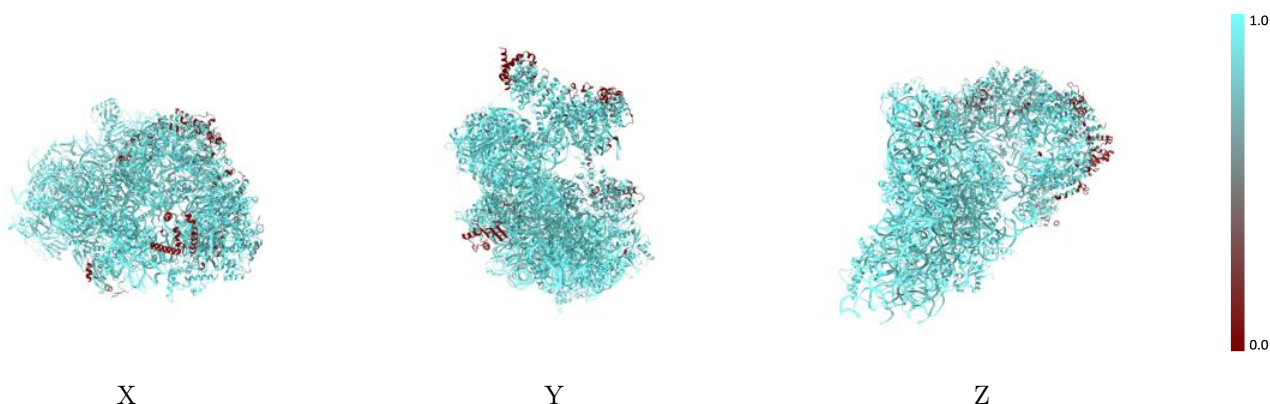
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



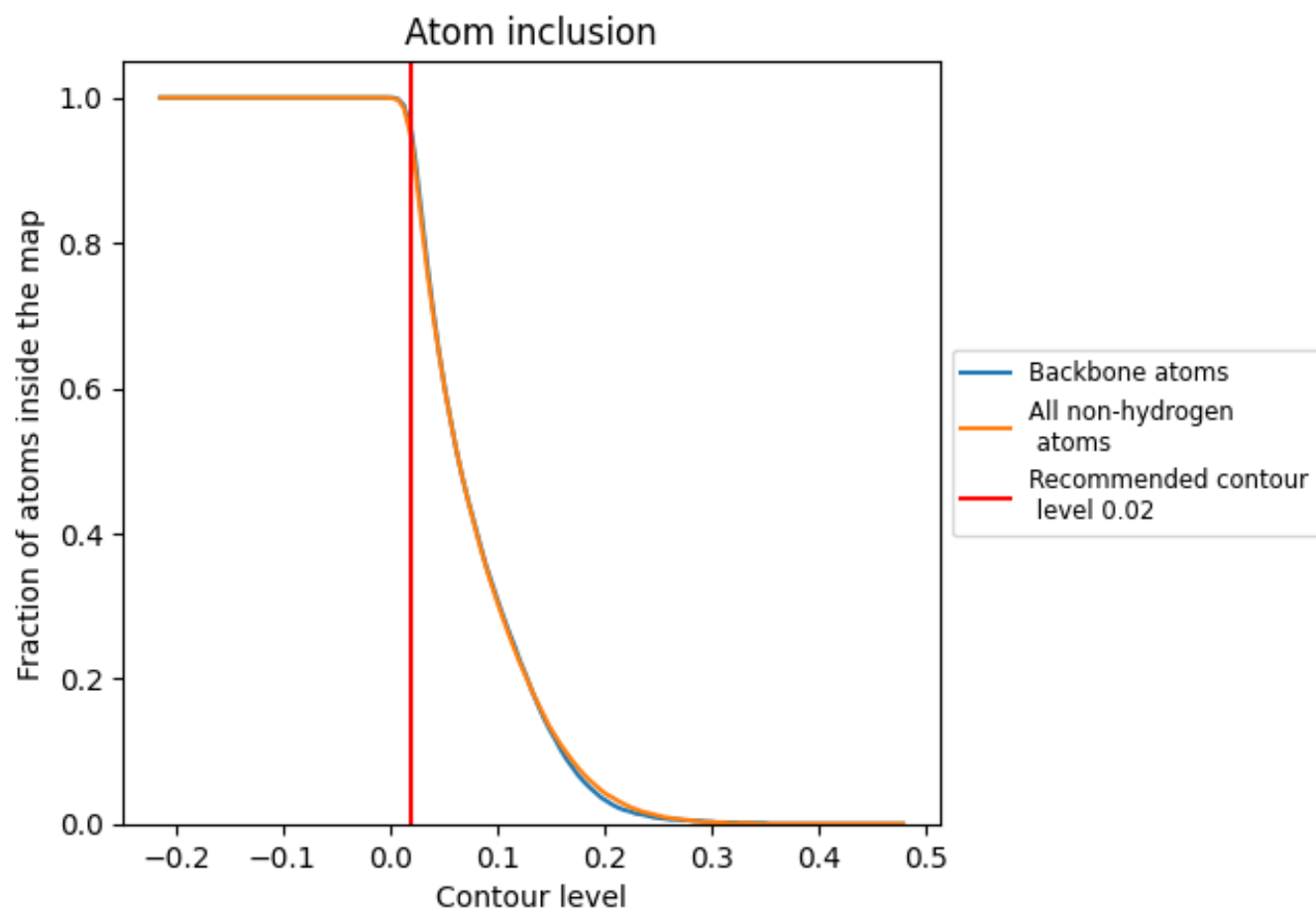
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 94% 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	 0.9440	 0.4010
2	 0.9940	 0.4510
A	 0.9600	 0.4620
B	 0.9550	 0.4550
C	 0.9840	 0.5100
E	 0.9960	 0.5850
F	 0.9620	 0.2950
G	 0.9830	 0.5020
H	 0.9700	 0.4570
I	 0.9780	 0.5120
J	 0.9910	 0.5740
K	 0.8010	 0.1280
L	 0.9820	 0.5500
M	 0.6760	 0.1160
N	 0.9940	 0.5510
O	 0.9780	 0.4750
P	 0.9740	 0.3230
Q	 0.9370	 0.2540
R	 0.9350	 0.1270
S	 0.9260	 0.2580
T	 0.9240	 0.2660
V	 0.9860	 0.5130
W	 0.9980	 0.5840
X	 0.9870	 0.5690
Y	 0.9970	 0.5740
Z	 0.8340	 0.2240
b	 0.9920	 0.5460
c	 0.9400	 0.3180
e	 1.0000	 0.5830
f	 0.8540	 0.0900
q	 0.8710	 0.1730
r	 0.2800	 0.1070
t	 0.9610	 0.3690
u	 0.9890	 0.4990
w	 0.8990	 0.1920



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Chain	Atom inclusion	Q-score
x	 0.9940	 0.4960
y	 0.7170	 0.3450
z	 0.5690	 0.0640