



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:06 PM UTC

PDB ID : 7PKQ / pdb_00007pkq
EMDB ID : EMD-13477
Title : Small subunit of the Chlamydomonas reinhardtii mitoribosome
Authors : Waltz, F.; Soufari, H.; Hashem, Y.
Deposited on : 2021-08-26
Resolution : 4.20 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:

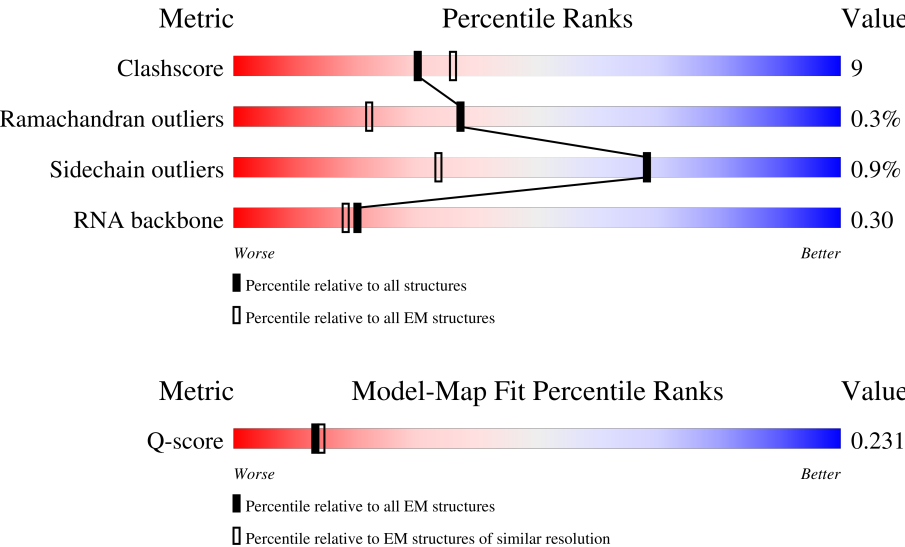
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	B	883	
2	C	999	
3	D	425	

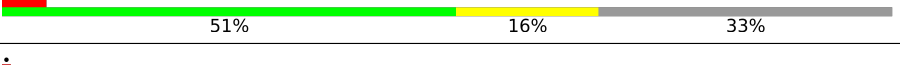
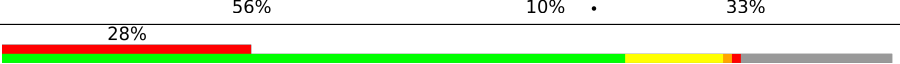
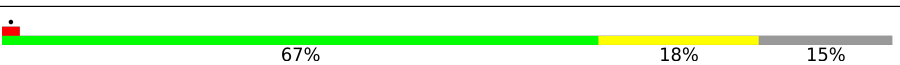
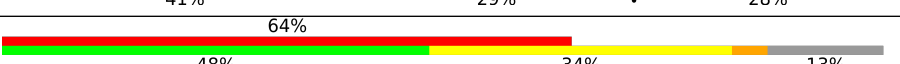
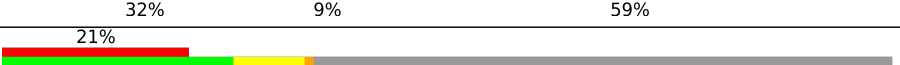
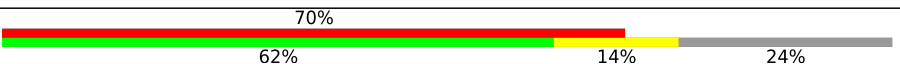
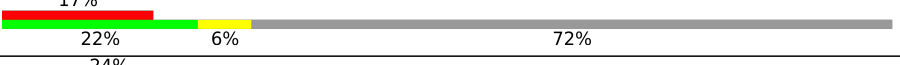
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Mol	Chain	Length	Quality of chain
4	K	186	
5	L	271	
5	M	271	
5	N	271	
6	O	516	
7	P	416	
8	U	33	
9	V	152	
10	W	54	
11	X	81	
12	Y	108	
13	Z	571	
14	d	415	
15	f	122	
16	p	88	
17	r	356	
18	w	193	
19	1	101	
20	4	415	
21	2	213	
22	3	393	
23	a	253	
24	b	530	
25	e	368	
26	o	319	

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Mol	Chain	Length	Quality of chain
27	z	133	
28	v	190	
29	q	220	
30	l	128	
31	h	412	
32	k	233	
33	j	612	
34	m	124	
35	n	112	
36	u	136	
37	s	116	
38	g	324	
39	i	446	
40	x	485	
41	c	490	
42	y	209	

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 70313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	53	Total	C	N	O	S	0	0
			386	235	81	69	1		

- Molecule 2 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	369	Total	C	N	O	S	0	0
			2766	1742	518	503	3		

- Molecule 3 is a protein called mS45-insert.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	425	Total	C	N	O	0	0
			2125	1275	425	425		

- Molecule 4 is a protein called mS31/46.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	186	Total	C	N	O	0	0
			930	558	186	186		

- Molecule 5 is a protein called mS105.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	175	Total	C	N	O	S	0	0
			1373	861	226	284	2		
5	M	174	Total	C	N	O	S	0	0
			1370	862	225	281	2		
5	N	195	Total	C	N	O	S	0	0
			1479	926	247	304	2		

- Molecule 6 is a protein called mS106.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	236	Total	C	N	O	S	0	0
			1710	1069	327	309	5		

- Molecule 7 is a protein called mS107.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	337	Total	C	N	O	S	0	0
			2601	1647	492	456	6		

- Molecule 8 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	33	Total	C	N	O	0	0
			165	99	33	33		

- Molecule 9 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	152	Total	C	N	O	0	0
			760	456	152	152		

- Molecule 10 is a protein called Unk3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	54	Total	C	N	O	0	0
			270	162	54	54		

- Molecule 11 is a protein called Unk4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	81	Total	C	N	O	0	0
			405	243	81	81		

- Molecule 12 is a protein called Unk5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	108	Total	C	N	O	0	0
			540	324	108	108		

- Molecule 13 is a protein called Unk6.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	571	Total	C	N	O	0	0
			2855	1713	571	571		

- Molecule 14 is a protein called uS4m.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	d	129	Total	C	N	O	S	0
			923	581	173	162	7	0

- Molecule 15 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	f	103	Total	C	N	O	S	0
			824	533	145	142	4	0

- Molecule 16 is a protein called bS16m.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	p	79	Total	C	N	O	S	0
			627	395	117	113	2	0

- Molecule 17 is a protein called bS18m.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	56	Total	C	N	O	S	0
			459	295	93	70	1	0

- Molecule 18 is a protein called mS26.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	w	155	Total	C	N	O	S	0
			1245	768	252	224	1	0

- Molecule 19 is a RNA chain called S1 rRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1	93	Total	C	N	O	P	0
			1986	886	352	655	93	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	52	A	-	insertion	GB 12503
1	53	C	-	insertion	GB 12503

- Molecule 20 is a RNA chain called S4 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	415	Total	C	N	O	P	0	0
			8811	3946	1532	2918	415		

- Molecule 21 is a RNA chain called S2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	213	Total	C	N	O	P	0	0
			4533	2024	798	1498	213		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	66	U	G	conflict	GB 12503
2	67	U	A	conflict	GB 12503
2	68	U	C	conflict	GB 12503
2	69	U	G	conflict	GB 12503
2	70	U	C	conflict	GB 12503
2	71	U	C	conflict	GB 12503
2	72	U	A	conflict	GB 12503
2	73	U	A	conflict	GB 12503
2	75	U	A	conflict	GB 12503

- Molecule 22 is a RNA chain called S3 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	393	Total	C	N	O	P	0	0
			8405	3759	1534	2719	393		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	U	deletion	GB 12503
3	?	-	G	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	A	deletion	GB 12503
3	?	-	A	deletion	GB 12503
3	?	-	U	deletion	GB 12503

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Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	G	deletion	GB 12503
3	?	-	C	deletion	GB 12503
3	251	G	A	conflict	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	U	deletion	GB 12503
3	?	-	C	deletion	GB 12503
3	?	-	A	deletion	GB 12503

- Molecule 23 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	212	Total	C	N	O	S	0	0
			1562	965	301	291	5		

- Molecule 24 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	241	Total	C	N	O	S	0	0
			1824	1153	341	322	8		

- Molecule 25 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	176	Total	C	N	O	S	0	0
			1403	882	275	238	8		

- Molecule 26 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	163	Total	C	N	O	S	0	0
			1284	802	249	228	5		

- Molecule 27 is a protein called mS34.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	z	85	Total	C	N	O	0	0
			667	427	118	122		

- Molecule 28 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	128	Total	C	N	O	S	0	0
			1003	632	189	180	2		

- Molecule 29 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	147	Total	C	N	O	S	0	0
			1128	709	217	201	1		

- Molecule 30 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	106	Total	C	N	O	S	0	0
			805	501	160	140	4		

- Molecule 31 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	351	Total	C	N	O	S	0	0
			2711	1709	504	484	14		

- Molecule 32 is a protein called uS11m.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	k	99	Total	C	N	O	0	0
			729	458	130	141		

- Molecule 33 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	164	Total	C	N	O	S	0	0
			1211	765	222	219	5		

- Molecule 34 is a protein called Mitochondrial ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	89	Total	C	N	O	S	0	0
			685	430	128	126	1		

- Molecule 35 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	97	Total	C	N	O	S	0	0
			779	479	163	133	4		

- Molecule 36 is a protein called Plastid-specific ribosomal protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	u	24	Total	C	N	O	S	0	0
			199	120	45	34			

- Molecule 37 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	87	Total	C	N	O	S	0	0
			678	438	120	117	3		

- Molecule 38 is a protein called uS7m,Ribosomal_S7 domain-containing protein,Ribosomal_S7 domain-containing protein,Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	132	Total	C	N	O	S	0	0
			909	561	179	165	4		

- Molecule 39 is a protein called 30S ribosomal protein S9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	154	Total	C	N	O	S	0	0
			1019	622	198	194	5		

- Molecule 40 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	368	Total	C	N	O	S	0	0
			2647	1661	490	490	6		

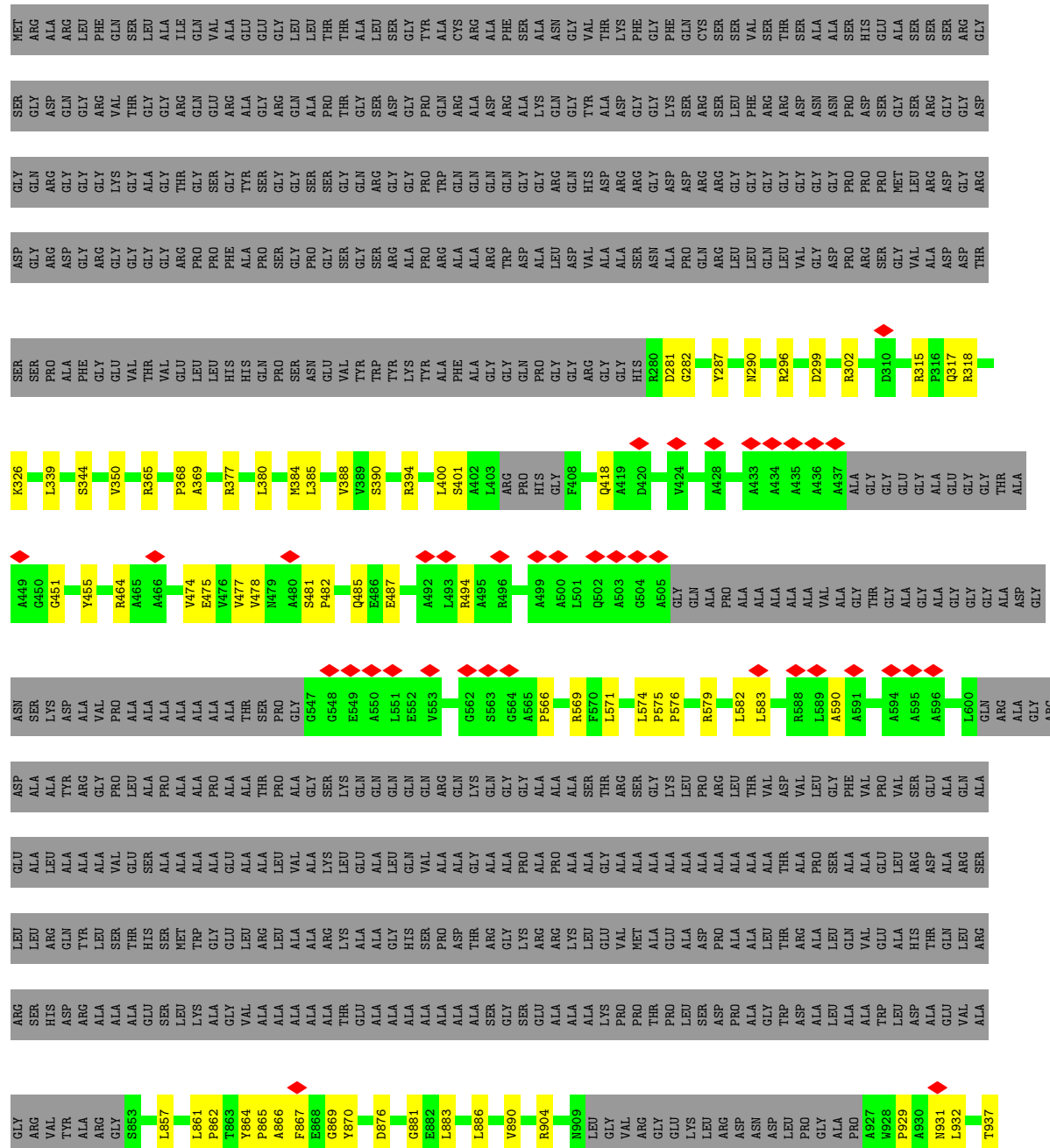
- Molecule 41 is a protein called Ribosomal_S3_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	c	135	Total	C	N	O	S	0	0
			1012	643	186	181	2		

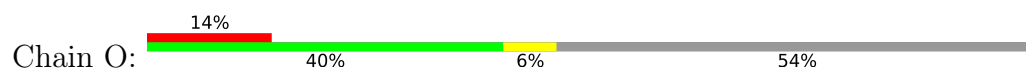
- Molecule 42 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	61	Total	C	N	O	S	0	0
			510	319	101	88	2		

- Molecule 2: mS45

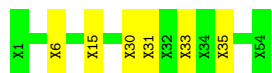


Chain M:

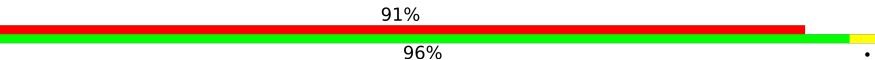


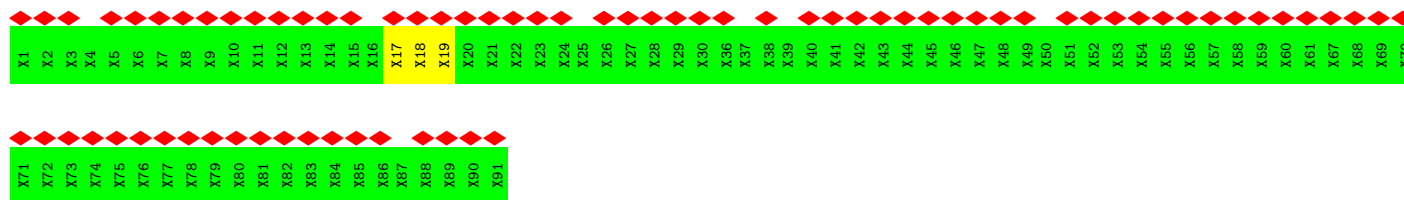
- Molecule 10: Unk3

Chain W:  89% 11%

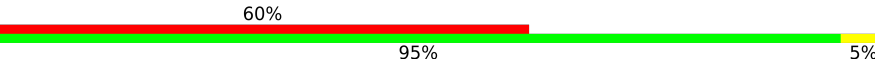


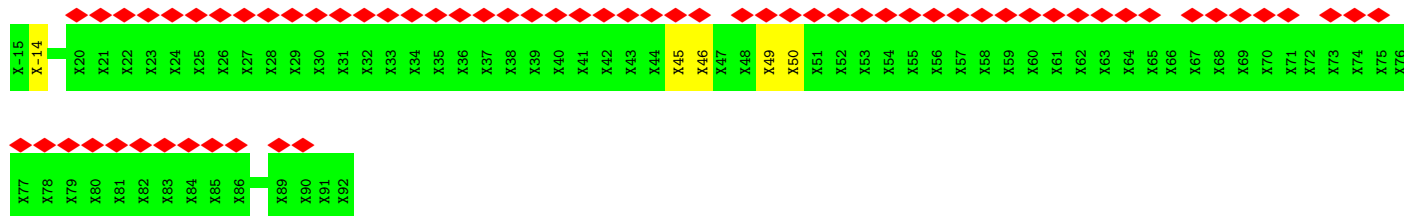
- Molecule 11: Unk4

Chain X:  91% 96% .

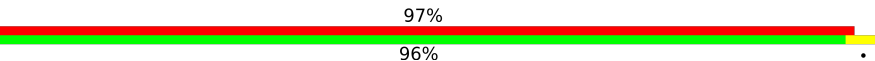


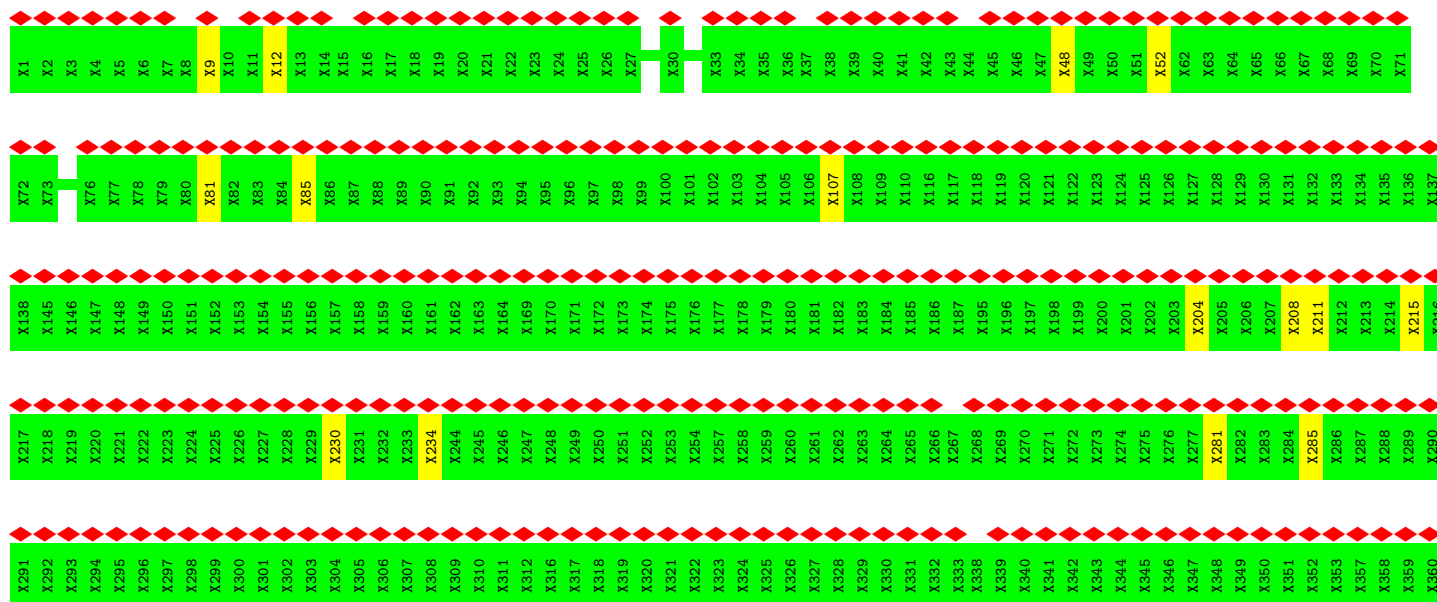
- Molecule 12: Unk5

Chain Y:  60% 95% 5%



- Molecule 13: Unk6

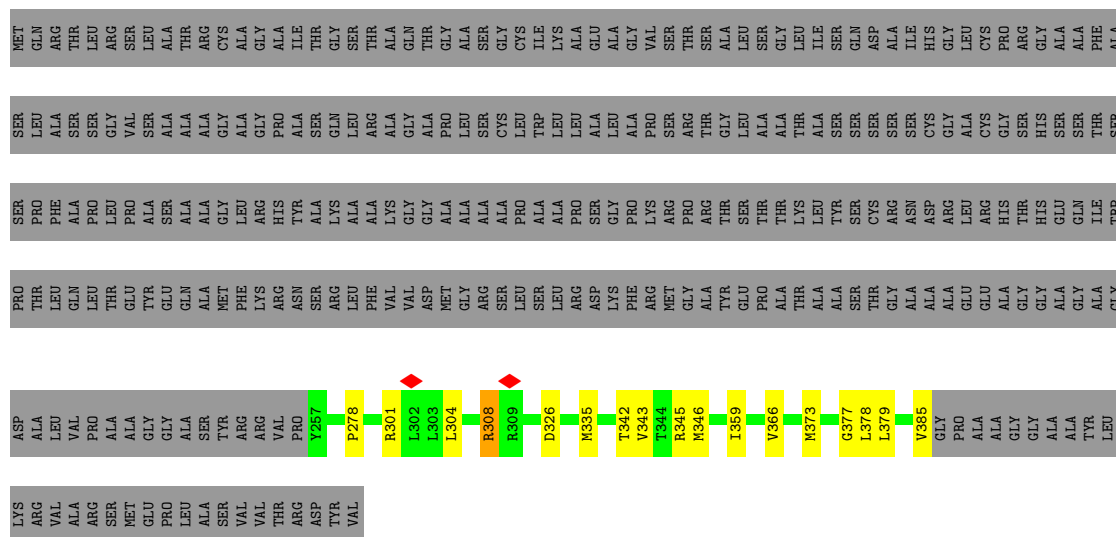
Chain Z:  97% 96% .





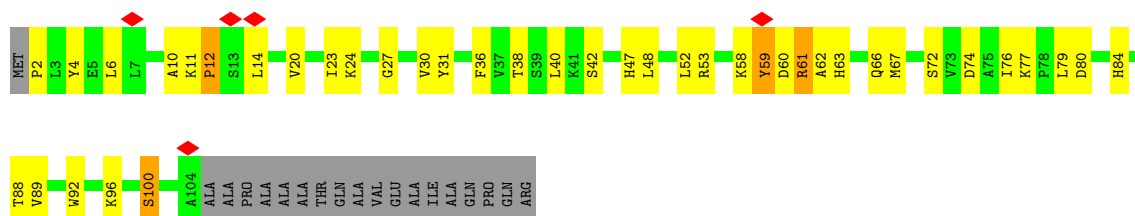
• Molecule 14: uS4m

Chain d: 27% . 69%



• Molecule 15: Mitochondrial ribosomal protein S6

Chain f: 51% 30% . 16%

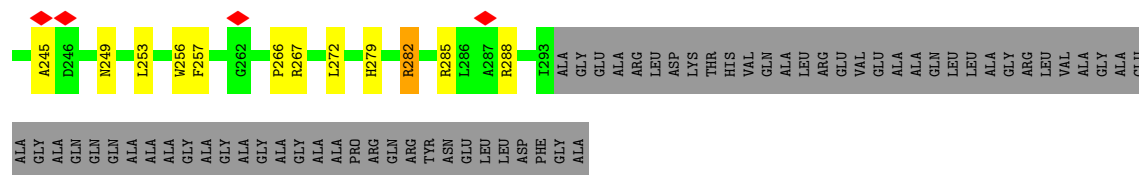


• Molecule 16: bS16m

Frequency	Percentage
Often	70%
Sometimes	18%
Rarely	10%

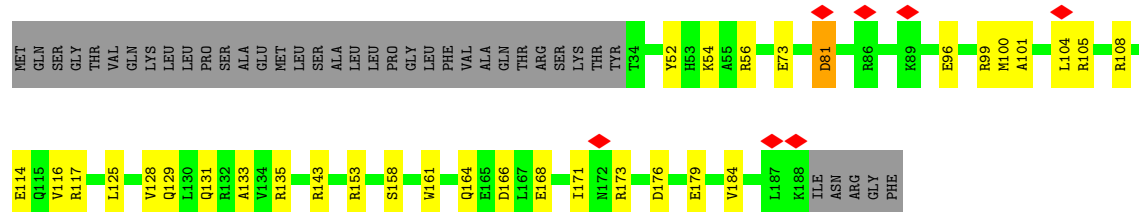


Response	Percentage
Yes	12%
No	84%



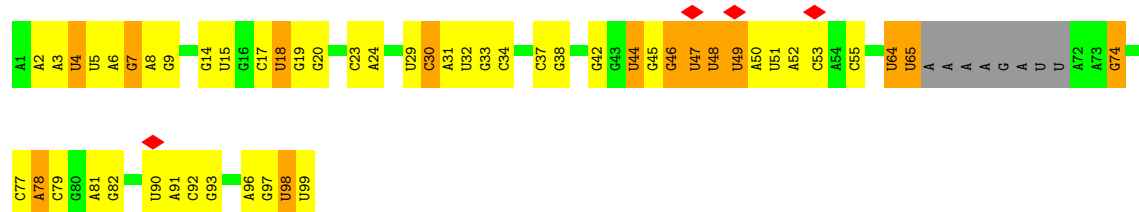
- Molecule 18: mS26

Frequency	Percentage
Daily	63%
Weekly	17%
Monthly	20%

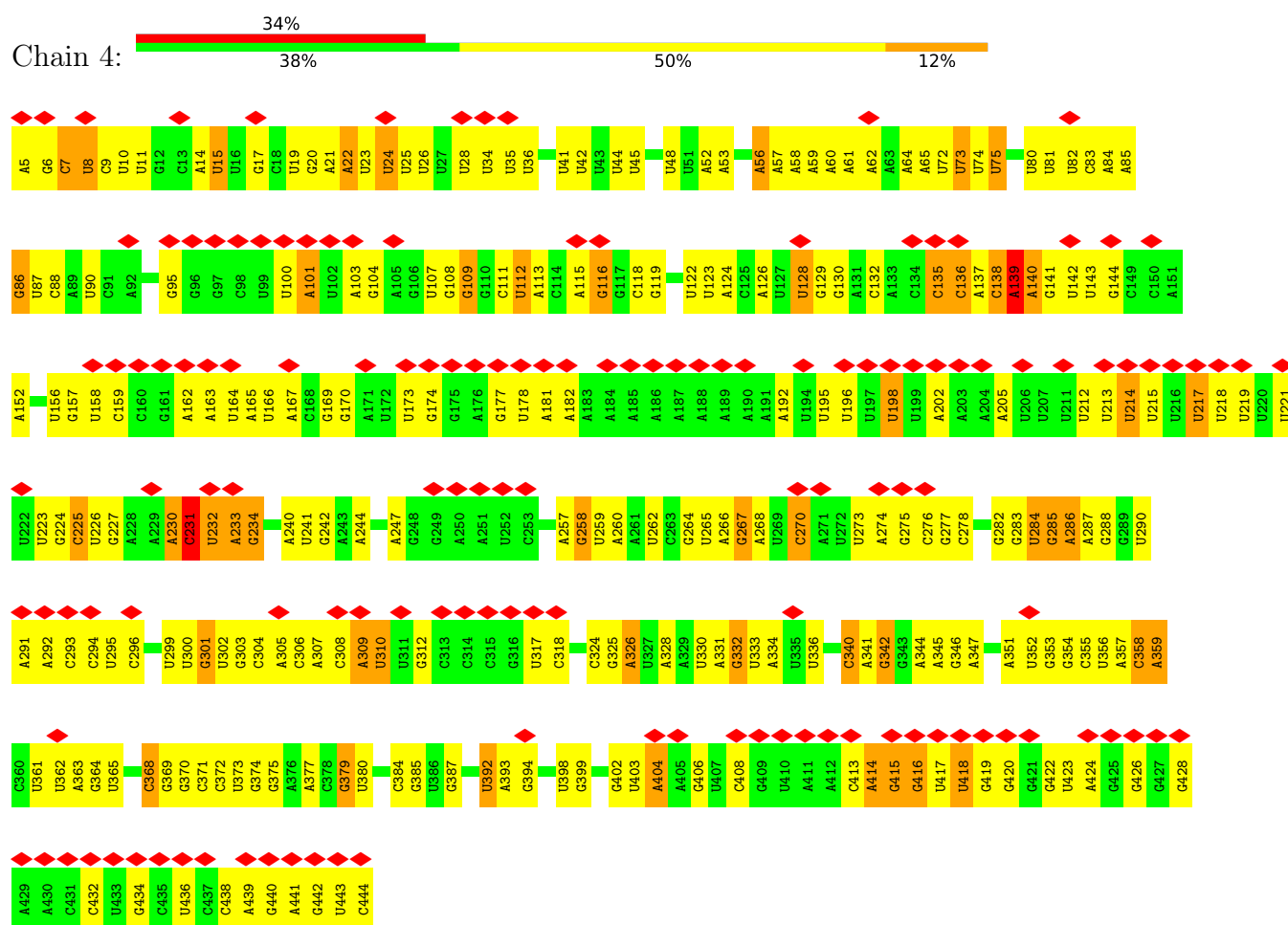


- Molecule 19: S1 rRNA

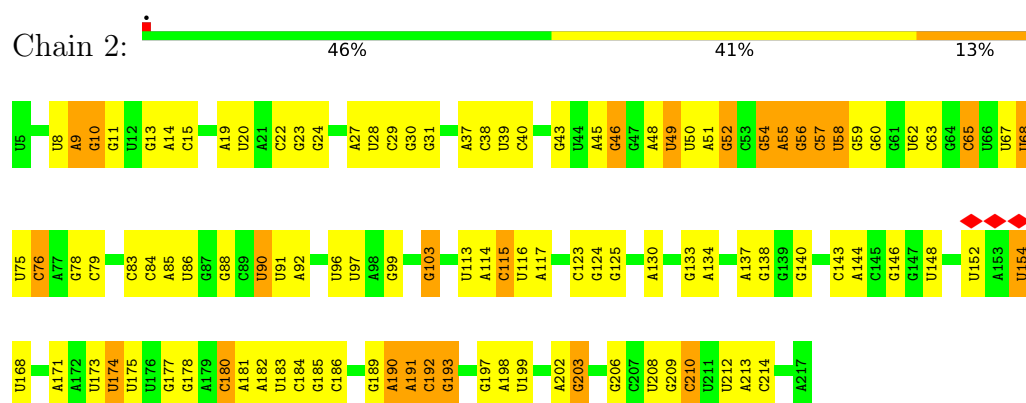
Frequency	Percentage
Daily	41%
Often	38%
Sometimes	14%
Never	8%



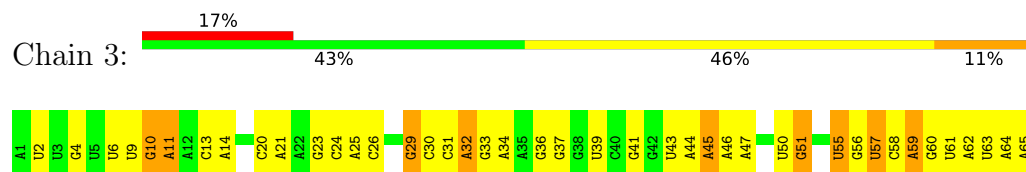
- Molecule 20: S4 rRNA

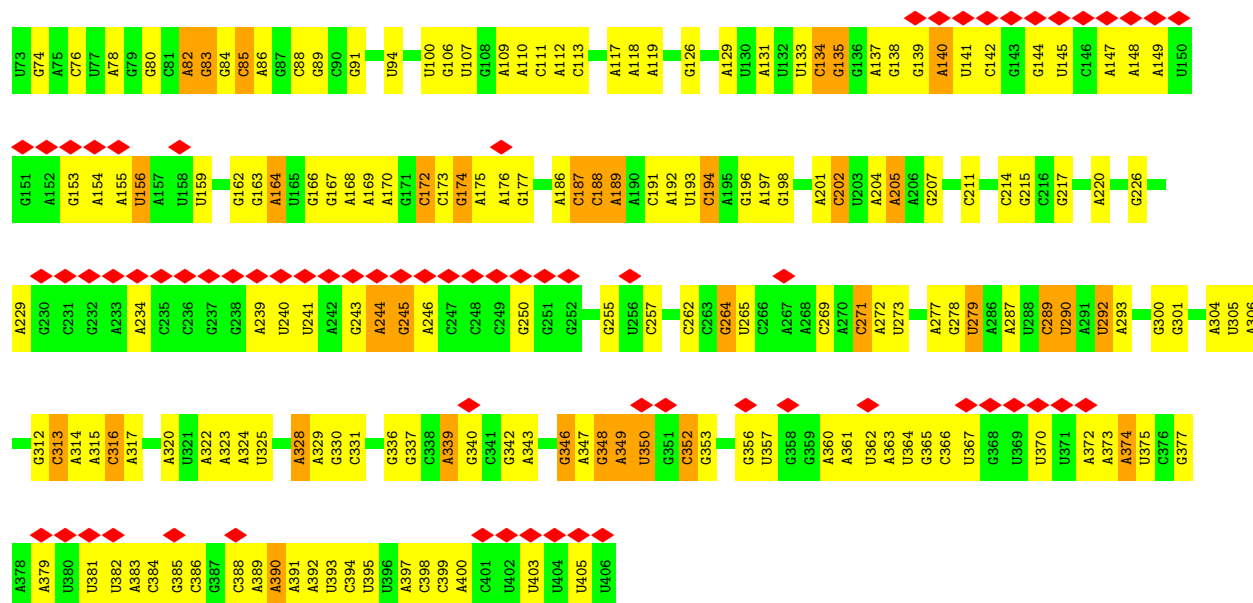


• Molecule 21: S2 rRNA

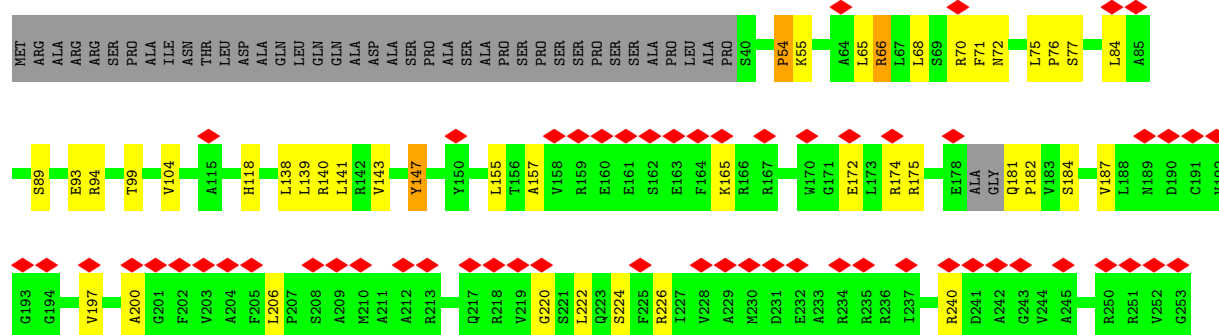


• Molecule 22: S3 rRNA

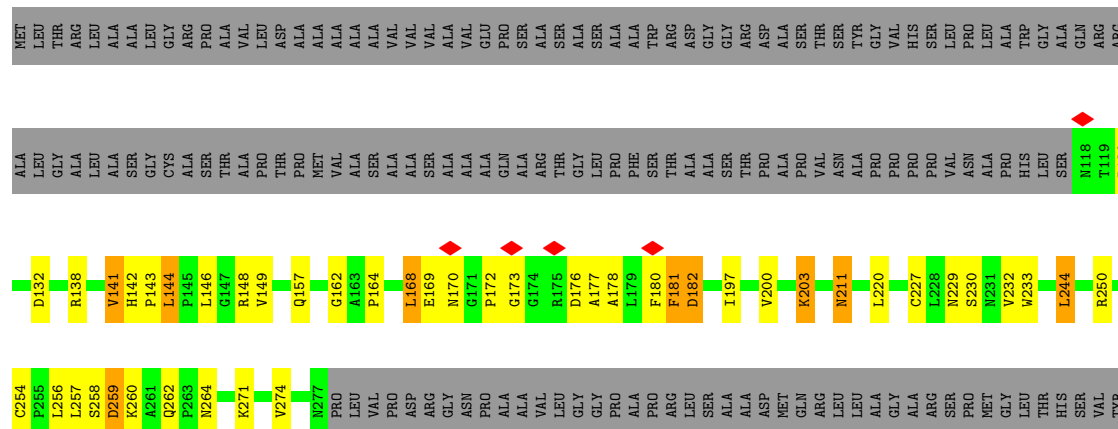
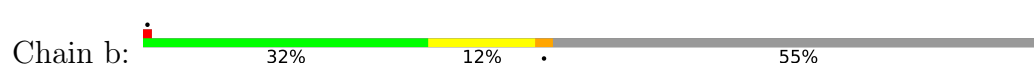


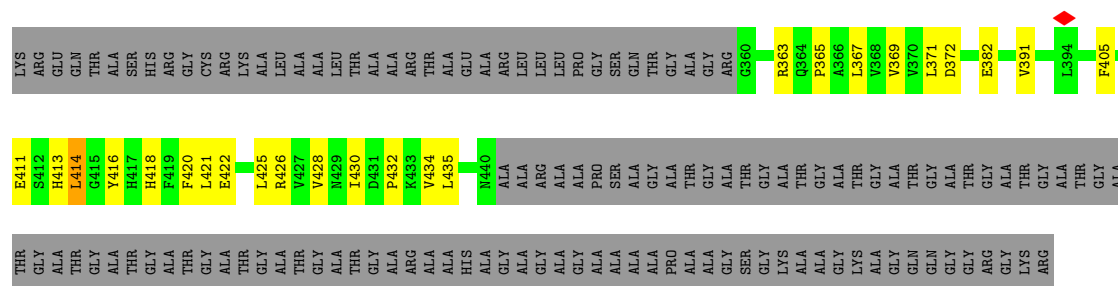


• Molecule 23: bS1m

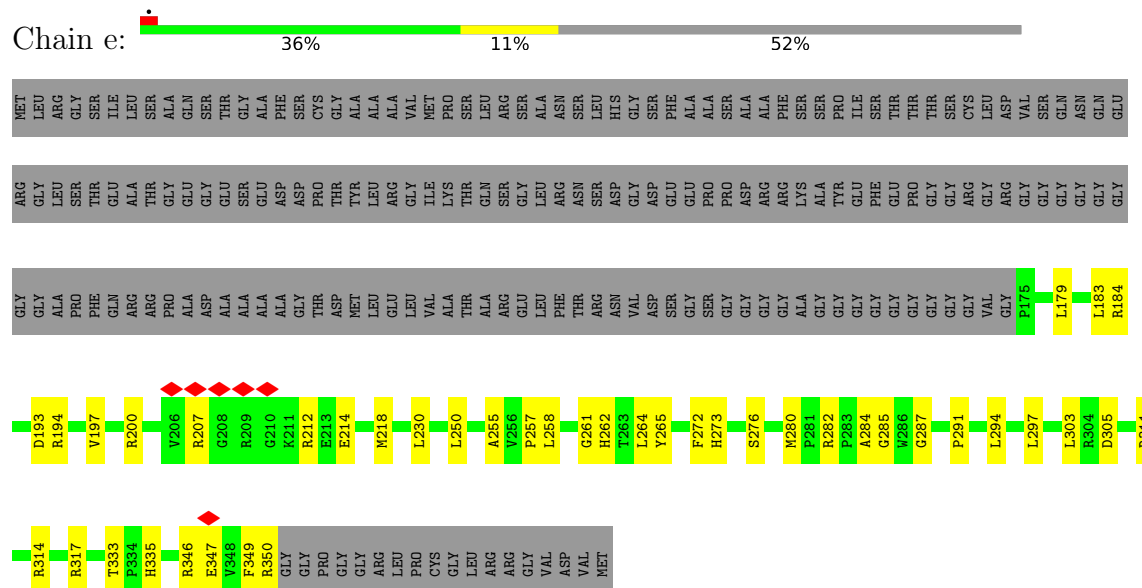


• Molecule 24: uS2m

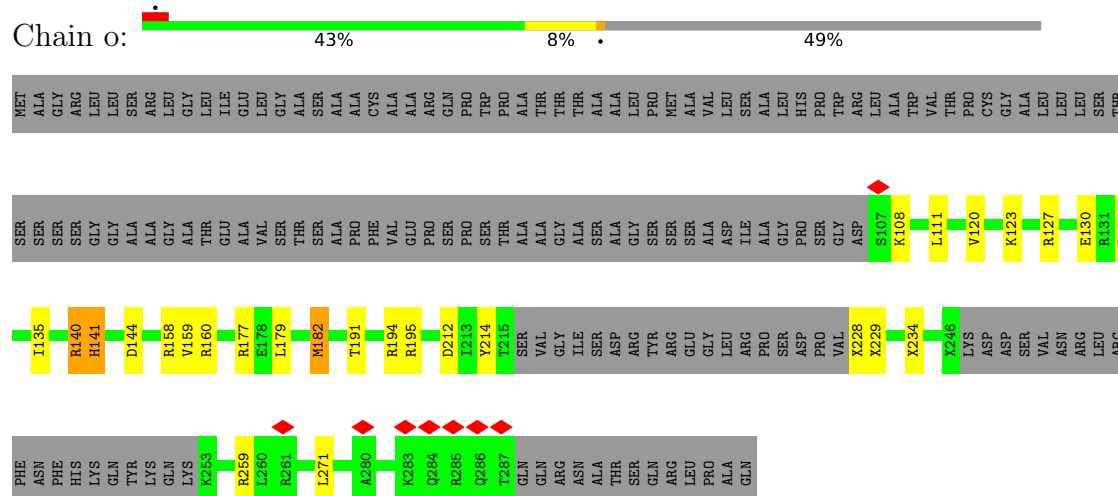




• Molecule 25: S5 DRBM domain-containing protein



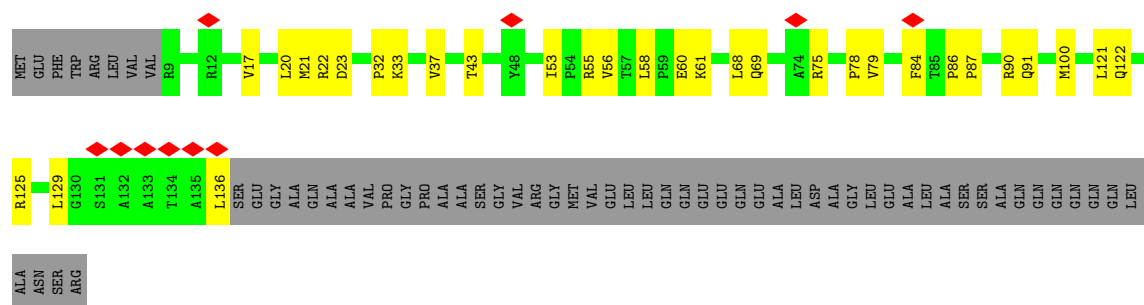
• Molecule 26: uS15m



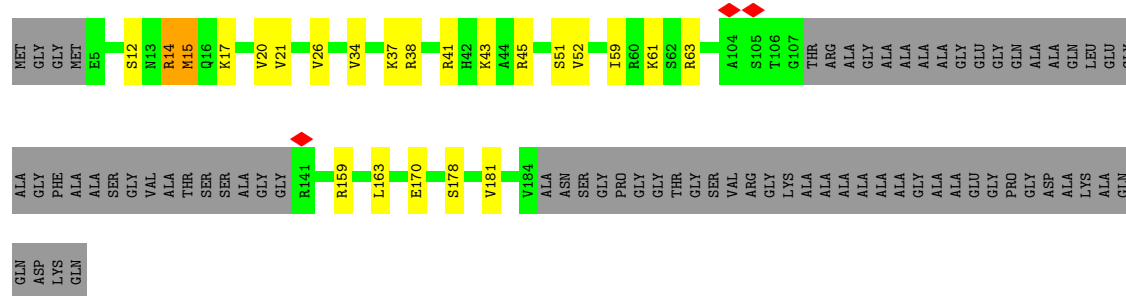
• Molecule 27: mS34



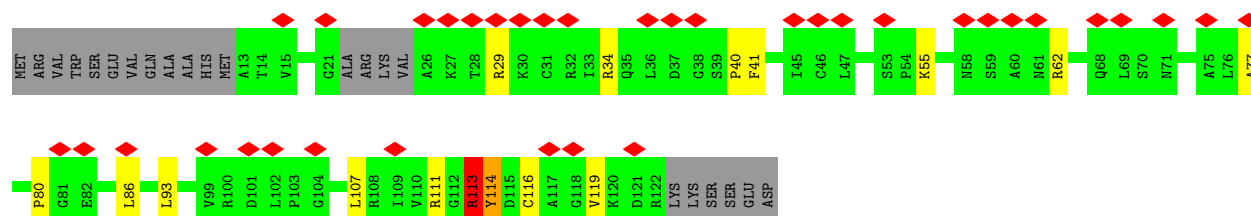
- Molecule 28: mS23



- Molecule 29: uS17m



- Molecule 30: uS12m

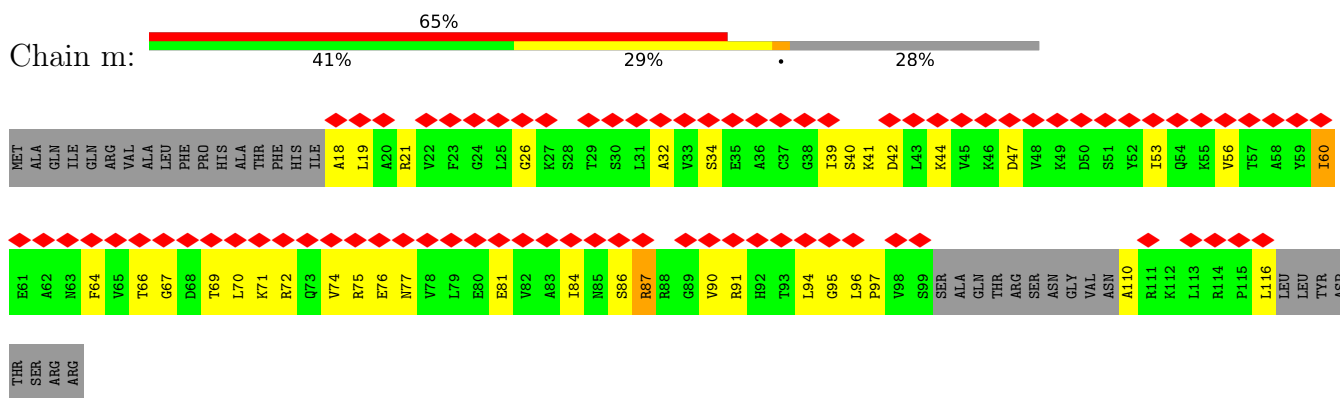


- Molecule 31: uS8m

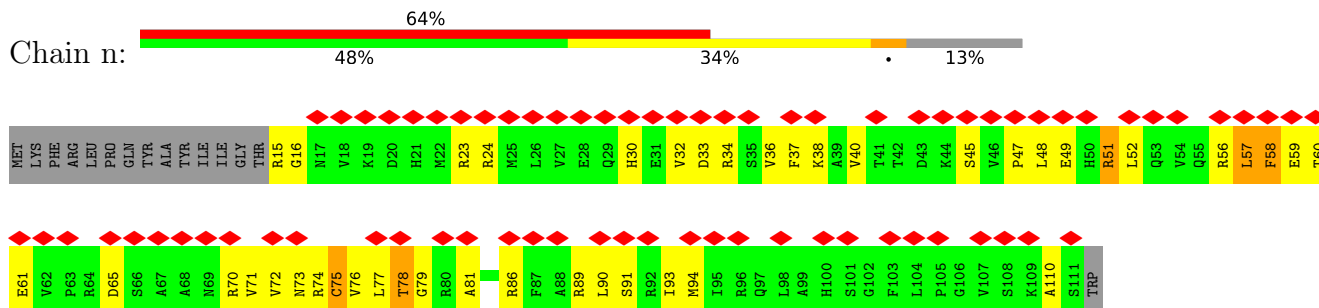




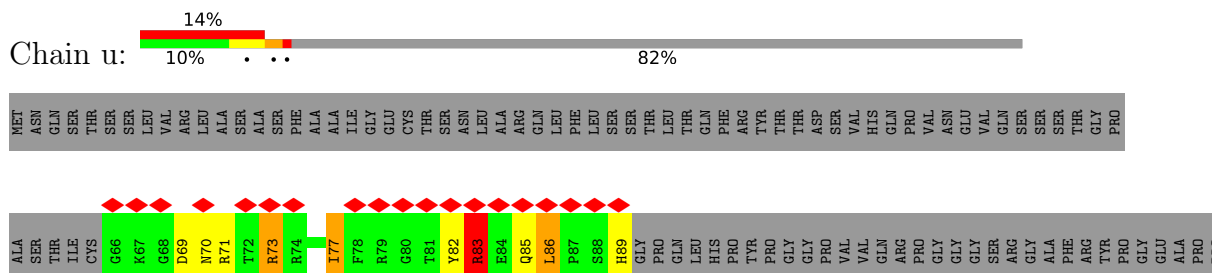
- Molecule 34: Mitochondrial ribosomal protein S13



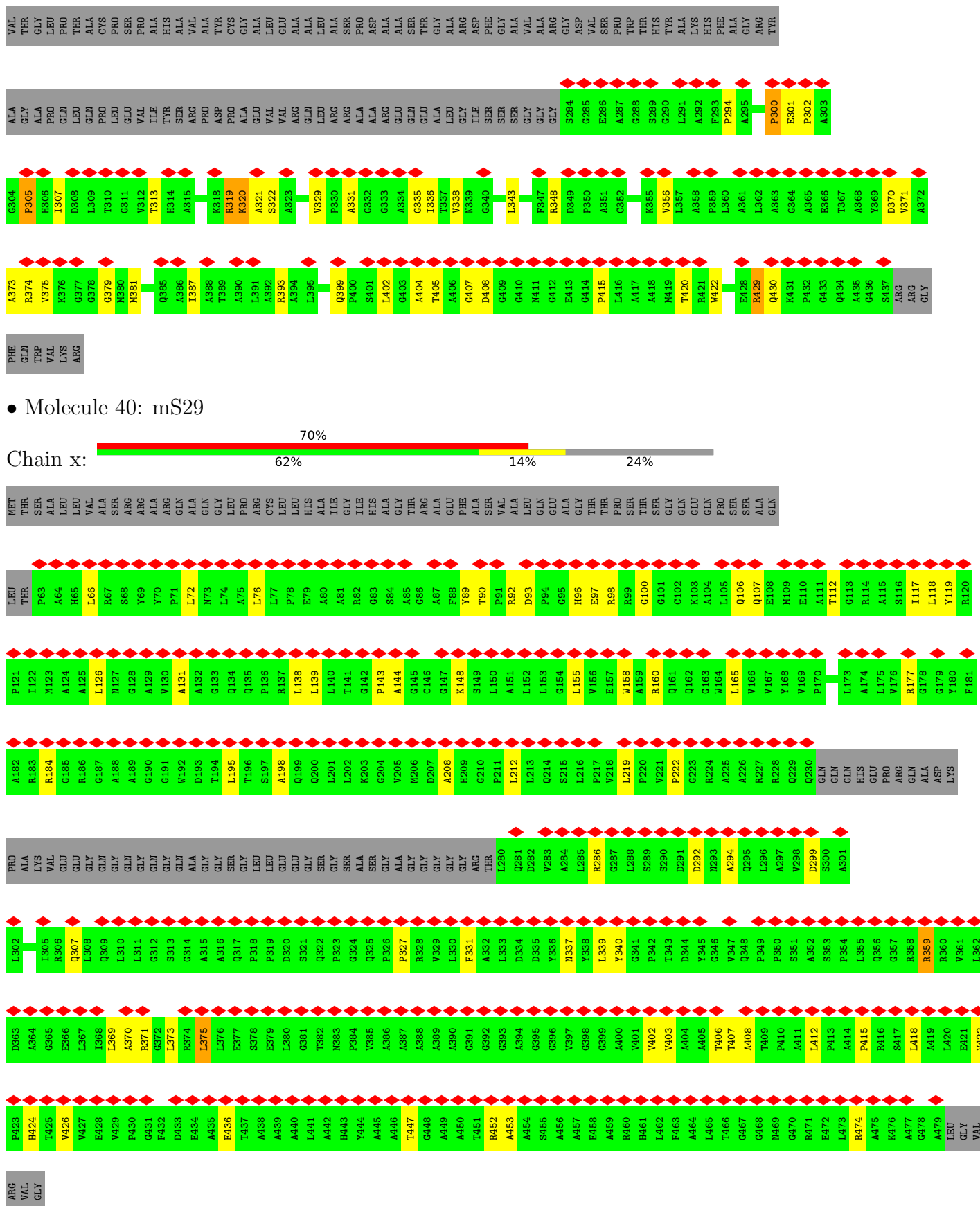
- Molecule 35: Mitochondrial ribosomal protein S14



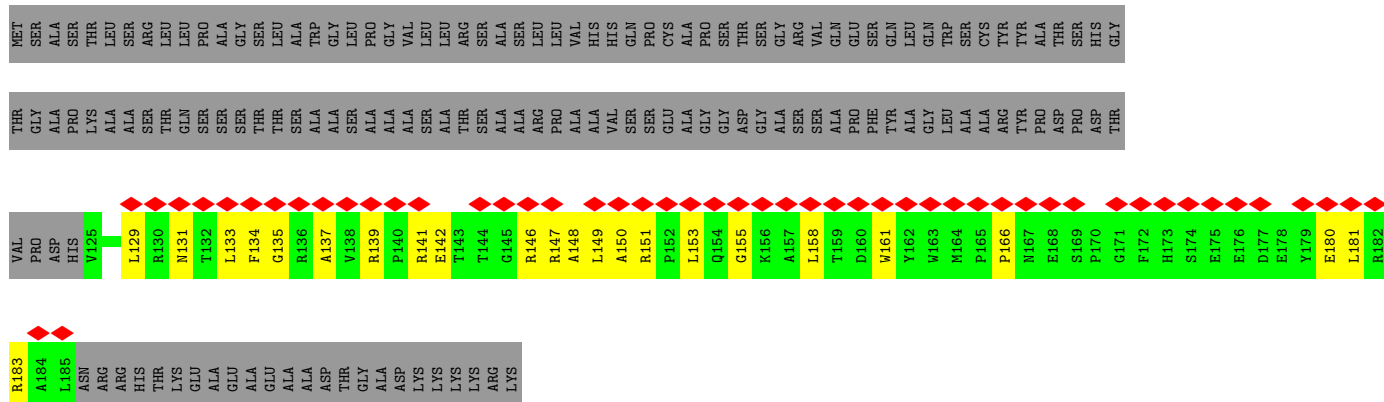
- Molecule 36: Plastid-specific ribosomal protein 4







Chain c:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	406.8, 406.8, 406.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.13, 1.13, 1.13	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.95	0/390	1.35	2/526 (0.4%)
2	C	0.36	0/2806	0.79	1/3811 (0.0%)
5	L	0.36	0/1399	0.71	0/1893
5	M	0.37	0/1397	0.75	0/1891
5	N	0.34	0/1416	0.71	0/1916
6	O	0.31	0/1737	0.76	0/2357
7	P	0.31	0/2647	0.67	0/3590
14	d	0.88	0/934	1.25	2/1262 (0.2%)
15	f	0.97	0/845	1.37	6/1144 (0.5%)
16	p	0.94	0/647	1.41	6/880 (0.7%)
17	r	0.42	0/469	1.08	4/633 (0.6%)
18	w	0.38	0/1263	0.92	2/1698 (0.1%)
19	1	0.43	0/2219	0.64	3/3455 (0.1%)
20	4	0.46	0/9843	0.69	5/15307 (0.0%)
21	2	0.41	0/5065	0.61	2/7891 (0.0%)
22	3	0.44	0/9410	0.64	2/14662 (0.0%)
23	a	0.36	0/1584	0.86	4/2146 (0.2%)
24	b	0.92	0/1865	1.46	22/2541 (0.9%)
25	e	0.48	0/1436	0.91	0/1941
26	o	0.44	0/1209	0.95	5/1628 (0.3%)
27	z	0.37	0/687	0.85	0/935
28	v	0.37	0/1020	0.90	0/1380
29	q	0.40	0/1145	0.78	1/1549 (0.1%)
30	l	0.33	0/814	0.87	2/1088 (0.2%)
31	h	0.44	0/2764	0.84	2/3749 (0.1%)
32	k	0.70	0/735	1.47	10/994 (1.0%)
33	j	0.55	0/1068	0.96	3/1442 (0.2%)
34	m	0.54	0/690	1.10	4/926 (0.4%)
35	n	0.90	0/790	1.63	15/1059 (1.4%)
36	u	0.81	0/202	1.55	3/266 (1.1%)
37	s	0.91	0/696	1.40	1/945 (0.1%)
38	g	0.50	0/700	1.03	0/938
39	i	0.62	0/1031	1.22	10/1398 (0.7%)
40	x	0.48	0/2700	0.82	3/3682 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	c	0.52	0/1032	0.92	0/1399
42	y	0.88	0/524	1.28	1/708 (0.1%)
All	All	0.51	0/65179	0.86	121/93630 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	6
6	O	0	1
13	Z	0	4
23	a	0	1
25	e	0	2
26	o	0	1
27	z	0	3
28	v	0	1
29	q	0	1
30	l	0	1
31	h	0	2
33	j	0	4
38	g	0	2
39	i	0	4
41	c	0	1
All	All	0	34

There are no bond length outliers.

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	p	34	ASN	N-CA-C	-11.53	91.98	109.86
32	k	209	LEU	N-CA-C	-11.44	93.64	110.23
32	k	194	GLY	N-CA-C	10.83	124.03	111.36
32	k	212	THR	N-CA-C	-9.87	100.52	111.28
23	a	147	TYR	CA-C-N	9.34	136.11	122.29
23	a	147	TYR	C-N-CA	9.34	136.11	122.29
34	m	87	ARG	CG-CD-NE	-8.93	92.35	112.00
32	k	151	ALA	N-CA-C	-8.93	101.55	111.28
32	k	144	LEU	N-CA-C	-8.41	98.04	110.23
31	h	213	LYS	CA-CB-CG	8.13	130.35	114.10
35	n	59	GLU	N-CA-C	-8.00	101.26	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	p	16	VAL	N-CA-C	-7.94	102.20	113.07
36	u	77	ILE	N-CA-C	-7.91	101.76	113.39
26	o	141	HIS	N-CA-CB	-7.90	103.16	111.29
24	b	138	ARG	N-CA-C	-7.65	104.08	113.41
39	i	429	ARG	CB-CG-CD	-7.61	93.79	111.30
39	i	305	PRO	N-CA-CB	7.59	111.22	103.25
30	l	113	ARG	CA-C-N	7.53	135.91	121.54
30	l	113	ARG	C-N-CA	7.53	135.91	121.54
14	d	308	ARG	N-CA-C	7.49	119.08	111.07
24	b	176	ASP	N-CA-C	7.32	119.16	111.03
15	f	58	LYS	CA-C-O	-7.30	113.34	121.00
24	b	203	LYS	N-CA-C	-7.26	104.00	112.92
24	b	173	GLY	N-CA-C	-7.21	105.83	115.21
40	x	222	PRO	N-CA-CB	7.21	110.82	103.25
39	i	429	ARG	CG-CD-NE	7.15	127.73	112.00
39	i	302	PRO	N-CA-CB	7.10	110.09	103.41
39	i	320	LYS	N-CA-C	-7.10	95.67	110.80
22	3	290	U	N1-C1'-C2'	7.01	122.52	112.00
1	B	829	PRO	N-CA-CB	6.93	110.53	103.25
15	f	12	PRO	N-CA-C	6.92	123.36	113.47
31	h	50	ARG	N-CA-C	-6.89	100.56	108.49
20	4	223	U	N1-C1'-C2'	6.87	122.30	112.00
39	i	381	MET	CB-CG-SD	-6.85	92.14	112.70
32	k	181	LEU	N-CA-C	-6.84	103.82	111.28
16	p	35	PHE	N-CA-C	6.81	118.14	108.74
32	k	135	ILE	N-CA-C	6.67	117.44	108.11
23	a	54	PRO	N-CA-CB	6.64	110.22	103.25
14	d	278	PRO	N-CA-CB	6.64	110.22	103.25
35	n	75	CYS	CA-C-N	-6.63	116.23	122.66
35	n	75	CYS	C-N-CA	-6.63	116.23	122.66
39	i	319	ARG	CA-C-N	6.58	134.11	121.54
39	i	319	ARG	C-N-CA	6.58	134.11	121.54
24	b	162	GLY	CA-C-N	-6.47	115.31	123.15
24	b	162	GLY	C-N-CA	-6.47	115.31	123.15
29	q	15	MET	CB-CG-SD	-6.47	93.30	112.70
24	b	120	PRO	N-CA-CB	6.46	110.67	103.44
24	b	203	LYS	CB-CA-C	6.44	121.44	110.56
36	u	83	ARG	N-CA-C	-6.31	98.89	108.67
39	i	300	PRO	N-CA-CB	6.30	109.86	103.25
35	n	51	ARG	N-CA-C	-6.29	104.42	111.28
35	n	78	THR	N-CA-CB	6.29	121.11	110.49
18	w	73	GLU	N-CA-CB	6.26	119.98	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	180	PHE	N-CA-C	6.23	118.08	110.41
35	n	30	HIS	N-CA-C	-6.23	96.27	107.98
26	o	135	ILE	CG1-CB-CG2	-6.18	92.17	110.70
24	b	414	LEU	N-CA-C	-6.17	104.66	111.82
1	B	849	ARG	N-CA-C	6.17	117.88	111.03
20	4	139	A	C2'-C3'-O3'	6.15	122.92	113.70
16	p	68	PRO	N-CA-C	6.14	118.19	110.70
34	m	76	GLU	N-CA-CB	6.02	120.22	110.40
24	b	211	ASN	CB-CA-C	6.00	119.38	110.14
24	b	144	LEU	N-CA-C	5.98	116.48	109.60
19	l	4	U	N1-C1'-C2'	5.98	120.96	112.00
15	f	12	PRO	CB-CA-C	-5.92	103.64	113.06
24	b	132	ASP	CA-CB-CG	5.90	118.50	112.60
24	b	168	LEU	N-CA-CB	-5.90	103.53	113.15
36	u	73	ARG	N-CA-C	-5.86	105.79	113.17
19	l	44	U	C2'-C3'-O3'	5.84	122.47	113.70
24	b	181	PHE	CA-CB-CG	5.84	119.64	113.80
24	b	271	LYS	N-CA-C	-5.76	105.08	111.36
24	b	181	PHE	CB-CA-C	-5.74	97.44	110.07
20	4	217	U	N1-C1'-C2'	5.73	120.60	112.00
26	o	132	GLN	CA-CB-CG	5.73	125.55	114.10
39	i	294	PRO	N-CA-CB	5.71	109.89	102.86
35	n	45	SER	N-CA-C	-5.66	106.04	113.17
32	k	142	GLN	N-CA-C	-5.63	105.51	112.38
33	j	201	ARG	CB-CG-CD	5.59	124.15	111.30
35	n	58	PHE	CB-CA-C	5.56	118.07	110.06
32	k	184	SER	N-CA-C	-5.55	105.23	111.28
21	2	183	U	N1-C1'-C2'	5.52	120.27	112.00
24	b	141	VAL	N-CA-C	-5.51	105.00	110.62
32	k	145	ILE	N-CA-C	5.49	116.00	107.99
33	j	188	PRO	CA-C-N	-5.47	115.00	121.90
33	j	188	PRO	C-N-CA	-5.47	115.00	121.90
35	n	47	PRO	N-CA-C	-5.46	102.55	110.80
35	n	49	GLU	CA-C-O	-5.46	115.52	121.14
24	b	172	PRO	N-CA-C	-5.44	105.13	112.48
34	m	60	ILE	CA-C-N	-5.43	111.09	121.94
34	m	60	ILE	C-N-CA	-5.43	111.09	121.94
35	n	77	LEU	N-CA-C	-5.38	101.20	109.76
23	a	66	ARG	NE-CZ-NH2	5.38	124.04	119.20
20	4	231	C	N1-C1'-C2'	5.36	120.04	112.00
24	b	182	ASP	N-CA-CB	5.33	119.86	110.37
15	f	100	SER	N-CA-C	-5.32	106.56	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	r	242	LEU	CA-C-N	5.28	131.63	121.54
17	r	242	LEU	C-N-CA	5.28	131.63	121.54
37	s	56	ASP	CB-CA-C	5.28	120.93	110.42
16	p	17	GLY	CA-C-O	-5.27	118.79	122.22
42	y	166	PRO	CA-C-O	-5.24	112.58	118.98
15	f	61	ARG	N-CA-C	-5.24	106.84	113.23
16	p	37	ARG	N-CA-C	-5.22	107.29	113.97
24	b	274	VAL	N-CA-C	-5.22	102.20	109.45
40	x	375	LEU	CB-CG-CD2	-5.22	95.05	110.70
18	w	81	ASP	N-CA-C	5.19	121.27	109.81
35	n	61	GLU	N-CA-C	-5.16	105.73	111.36
24	b	181	PHE	CA-C-O	-5.12	115.61	121.40
2	C	861	LEU	CA-CB-CG	5.12	134.21	116.30
20	4	342	G	N9-C1'-C2'	5.11	119.67	112.00
22	3	289	C	N1-C1'-C2'	5.11	119.66	112.00
35	n	37	PHE	CB-CA-C	5.11	119.53	110.85
21	2	154	U	N1-C1'-C2'	5.09	119.63	112.00
15	f	59	TYR	N-CA-CB	5.09	119.09	110.49
17	r	242	LEU	CA-CB-CG	5.08	134.07	116.30
17	r	282	ARG	CB-CG-CD	5.06	122.93	111.30
40	x	359	ARG	CA-CB-CG	-5.04	104.01	114.10
19	l	64	U	C2'-C3'-O3'	5.03	121.24	113.70
26	o	182	MET	CB-CG-SD	5.03	127.78	112.70
35	n	57	LEU	CA-C-O	-5.02	115.45	120.77
35	n	91	SER	CA-C-O	-5.02	115.59	121.46
26	o	132	GLN	N-CA-CB	5.00	118.81	110.41

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	401	SER	Peptide
2	C	866	ALA	Peptide
2	C	867	PHE	Peptide
2	C	929	PRO	Peptide
2	C	931	ASN	Peptide
2	C	932	LEU	Peptide
6	O	323	ASP	Peptide
13	Z	107	UNK	Peptide
13	Z	12	UNK	Peptide
13	Z	477	UNK	Peptide
13	Z	9	UNK	Peptide

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Mol	Chain	Res	Type	Group
23	a	71	PHE	Peptide
41	c	219	SER	Peptide
25	e	272	PHE	Peptide
25	e	349	PHE	Peptide
38	g	137	UNK	Peptide
38	g	139	UNK	Peptide
31	h	212	SER	Peptide
31	h	221	TYR	Peptide
39	i	319	ARG	Peptide
39	i	348	ARG	Peptide
39	i	379	GLY	Peptide
39	i	430	GLN	Peptide
33	j	147	TYR	Peptide
33	j	165	ALA	Peptide
33	j	190	ILE	Peptide
33	j	198	PHE	Peptide
30	l	113	ARG	Peptide
26	o	140	ARG	Peptide
29	q	14	ARG	Peptide
28	v	43	THR	Peptide
27	z	24	ASN	Peptide
27	z	44	TRP	Peptide
27	z	94	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	386	0	364	8	0
2	C	2766	0	2848	50	0
3	D	2125	0	461	7	0
4	K	930	0	193	4	0
5	L	1373	0	1304	41	0
5	M	1370	0	1302	24	0
5	N	1479	0	1339	28	0
6	O	1710	0	1751	19	0
7	P	2601	0	2693	44	0
8	U	165	0	38	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	760	0	169	7	0
10	W	270	0	67	6	0
11	X	405	0	93	2	0
12	Y	540	0	114	3	0
13	Z	2855	0	640	8	0
14	d	923	0	891	13	0
15	f	824	0	831	33	0
16	p	627	0	610	11	0
17	r	459	0	490	10	0
18	w	1245	0	1212	29	0
19	1	1986	0	1000	26	0
20	4	8811	0	4439	113	0
21	2	4533	0	2289	59	0
22	3	8405	0	4237	131	0
23	a	1562	0	1533	39	0
24	b	1824	0	1798	54	0
25	e	1403	0	1415	31	0
26	o	1284	0	1233	20	0
27	z	667	0	645	5	0
28	v	1003	0	1039	27	0
29	q	1128	0	1171	19	0
30	l	805	0	859	13	0
31	h	2711	0	2759	51	0
32	k	729	0	773	121	0
33	j	1211	0	1120	18	0
34	m	685	0	729	32	0
35	n	779	0	806	28	0
36	u	199	0	199	7	0
37	s	678	0	677	25	0
38	g	909	0	774	17	0
39	i	1019	0	976	18	0
40	x	2647	0	2649	45	0
41	c	1012	0	1013	20	0
42	y	510	0	499	19	0
All	All	70313	0	52042	1073	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1073) 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)
9:V:162:UNK:CB	20:4:48:U:C2'	2.19	1.20
32:k:189:ARG:HB3	32:k:217:VAL:HB	1.36	1.04
32:k:154:VAL:HG11	32:k:169:LYS:HB3	1.36	1.03
32:k:129:ASN:HD22	32:k:194:GLY:HA3	1.22	0.99
20:4:299:U:H3	22:3:343:A:H61	1.09	0.98
32:k:187:GLN:HG2	32:k:212:THR:HB	1.44	0.98
9:V:162:UNK:CB	20:4:48:U:O2'	2.12	0.97
32:k:150:SER:H	32:k:153:VAL:HB	1.27	0.97
9:V:162:UNK:CB	20:4:48:U:H2'	1.91	0.96
20:4:138:C:H42	20:4:152:A:N6	1.63	0.96
32:k:125:VAL:HB	32:k:188:VAL:HA	1.47	0.95
20:4:138:C:N4	20:4:152:A:H62	1.66	0.93
21:2:180:C:N4	21:2:198:A:H62	1.67	0.92
22:3:141:U:H5'	32:k:153:VAL:HA	1.52	0.92
21:2:180:C:H42	21:2:198:A:H62	0.94	0.91
32:k:139:THR:HB	32:k:145:ILE:HA	1.51	0.90
35:n:24:ARG:HD2	42:y:158:LEU:HD12	1.53	0.89
20:4:345:A:H62	20:4:379:G:H21	1.19	0.89
9:V:162:UNK:CB	20:4:48:U:C3'	2.50	0.89
41:c:179:GLY:O	41:c:183:ARG:HG3	1.74	0.88
15:f:11:LYS:HD2	15:f:12:PRO:HD2	1.54	0.87
32:k:187:GLN:HA	32:k:213:SER:H	1.39	0.87
21:2:180:C:H42	21:2:198:A:N6	1.74	0.85
20:4:259:U:H3	20:4:286:A:H62	1.20	0.84
20:4:101:A:H62	22:3:405:U:H3	1.24	0.84
19:1:19:G:H21	22:3:328:A:H62	1.23	0.83
22:3:137:A:H1'	32:k:144:LEU:HB3	1.58	0.83
32:k:189:ARG:HH11	32:k:217:VAL:HG21	1.43	0.82
32:k:191:LYS:HG3	32:k:218:THR:HA	1.62	0.82
24:b:211:ASN:HD21	24:b:220:LEU:HD21	1.44	0.81
20:4:345:A:H62	20:4:379:G:N2	1.77	0.81
22:3:126:G:H1	22:3:170:A:H2	1.27	0.80
9:V:162:UNK:CB	20:4:48:U:H3'	2.12	0.79
4:K:129:UNK:O	4:K:133:UNK:N	2.16	0.78
22:3:126:G:N1	22:3:170:A:C2	2.49	0.78
10:W:6:UNK:HA	14:d:345:ARG:HH22	1.48	0.77
32:k:136:LEU:HD11	32:k:200:ALA:HB1	1.66	0.77
20:4:345:A:N6	20:4:379:G:H21	1.82	0.77
6:O:482:GLY:O	6:O:486:ALA:HB3	1.84	0.77
32:k:185:SER:HA	32:k:210:THR:O	1.84	0.76
22:3:142:C:H5'	32:k:148:TYR:OH	1.87	0.74
15:f:100:SER:HA	18:w:153:ARG:HH12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:11:LYS:HD2	15:f:12:PRO:CD	2.20	0.72
32:k:129:ASN:ND2	32:k:194:GLY:HA3	2.01	0.72
32:k:187:GLN:HB3	32:k:213:SER:HB3	1.69	0.72
22:3:32:A:H62	22:3:41:G:N2	1.88	0.71
32:k:134:ILE:HG23	32:k:151:ALA:HB2	1.70	0.71
35:n:60:THR:HG21	37:s:13:VAL:HG11	1.71	0.71
32:k:121:LEU:HB2	32:k:183:TYR:HA	1.73	0.71
32:k:138:LEU:HD21	32:k:181:LEU:HG	1.73	0.71
38:g:230:ARG:HH22	38:g:253:LEU:HD12	1.55	0.70
20:4:259:U:H2'	20:4:260:A:H8	1.56	0.70
40:x:143:PRO:O	40:x:148:LYS:NZ	2.25	0.70
10:W:15:UNK:CB	14:d:346:MET:HE1	2.22	0.70
20:4:138:C:H42	20:4:152:A:H62	0.82	0.70
42:y:137:ALA:HB3	42:y:139:ARG:HH11	1.56	0.70
33:j:116:GLU:HB2	33:j:237:GLN:HB2	1.72	0.69
23:a:66:ARG:HH21	28:v:56:VAL:HG22	1.56	0.69
24:b:413:HIS:HB3	24:b:416:TYR:H	1.57	0.69
20:4:58:A:O2'	24:b:260:LYS:HD3	1.92	0.69
22:3:141:U:C5'	32:k:153:VAL:HA	2.22	0.69
32:k:134:ILE:HD13	32:k:197:LYS:HA	1.75	0.69
5:M:155:VAL:HB	5:M:166:PHE:HB2	1.75	0.69
19:1:19:G:N2	22:3:328:A:H62	1.91	0.68
32:k:156:TYR:HD2	32:k:160:ARG:HB2	1.57	0.68
15:f:27:GLY:O	15:f:31:TYR:HB2	1.92	0.68
22:3:34:A:H62	30:l:62:ARG:HH22	1.41	0.68
5:M:126:ASN:HB2	5:M:156:SER:HB2	1.74	0.68
18:w:161:TRP:HE1	26:o:111:LEU:HB3	1.59	0.68
32:k:151:ALA:HB1	32:k:166:ALA:HB1	1.75	0.68
32:k:125:VAL:HG23	32:k:186:VAL:CG1	2.24	0.67
32:k:150:SER:N	32:k:153:VAL:HB	2.06	0.67
2:C:377:ARG:NH1	3:D:345:UNK:O	2.28	0.67
27:z:45:GLU:HB3	27:z:64:TYR:HB2	1.75	0.67
34:m:84:ILE:HG23	37:s:79:MET:HE3	1.74	0.67
34:m:19:LEU:HA	34:m:21:ARG:HE	1.59	0.67
29:q:34:VAL:HG22	31:h:216:GLN:HB3	1.77	0.67
34:m:32:ALA:HA	40:x:359:ARG:HH12	1.59	0.67
5:N:163:VAL:HG23	5:N:185:LYS:HG2	1.76	0.66
37:s:5:THR:HA	37:s:9:PRO:HB3	1.76	0.66
32:k:125:VAL:HG23	32:k:186:VAL:HG12	1.77	0.66
32:k:186:VAL:C	32:k:212:THR:H	2.04	0.66
7:P:158:ARG:HH22	20:4:359:A:H4'	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:129:LEU:HD11	5:N:227:LEU:HD22	1.79	0.65
32:k:137:THR:HA	32:k:148:TYR:HA	1.78	0.65
32:k:139:THR:HG22	32:k:145:ILE:HG23	1.76	0.65
32:k:127:ILE:HG13	32:k:190:LEU:HA	1.79	0.65
32:k:135:ILE:HG23	32:k:148:TYR:HD2	1.61	0.65
22:3:142:C:P	32:k:152:GLY:HA3	2.37	0.65
22:3:137:A:C1'	32:k:144:LEU:HB3	2.27	0.65
32:k:135:ILE:HG12	32:k:150:SER:HB3	1.79	0.64
39:i:336:ILE:HA	39:i:371:VAL:HB	1.79	0.64
5:N:112:THR:HB	5:N:131:VAL:H	1.61	0.64
20:4:403:U:H5''	30:l:55:LYS:HD3	1.79	0.64
22:3:142:C:OP2	32:k:152:GLY:HA3	1.97	0.64
2:C:566:PRO:HA	2:C:569:ARG:HD2	1.78	0.64
32:k:124:ILE:O	32:k:139:THR:HG23	1.98	0.64
22:3:32:A:N6	22:3:41:G:H21	1.96	0.64
33:j:120:GLN:HB3	33:j:233:GLN:HB3	1.80	0.64
6:O:507:LEU:HD23	6:O:510:LYS:HD3	1.80	0.63
40:x:92:ARG:HD2	40:x:97:GLU:HA	1.79	0.63
21:2:9:A:H61	21:2:30:G:H1	1.45	0.63
24:b:227:CYS:O	24:b:264:ASN:ND2	2.31	0.63
34:m:90:VAL:O	34:m:94:LEU:HB2	1.98	0.63
31:h:300:TRP:HE1	31:h:305:LEU:HG	1.62	0.63
12:Y:-14:UNK:HA	23:a:89:SER:HB3	1.80	0.63
15:f:6:LEU:HD11	15:f:92:TRP:HB2	1.81	0.63
18:w:125:LEU:HA	18:w:128:VAL:HG12	1.80	0.63
35:n:56:ARG:HE	37:s:16:LEU:HD23	1.63	0.63
24:b:164:PRO:HD2	24:b:181:PHE:H	1.64	0.63
31:h:104:CYS:HB3	31:h:169:LEU:HB2	1.79	0.63
32:k:127:ILE:HG23	32:k:136:LEU:HD13	1.80	0.63
35:n:52:LEU:O	35:n:56:ARG:HB2	1.98	0.63
28:v:53:ILE:HD12	28:v:55:ARG:HH21	1.63	0.63
5:L:123:GLU:HG2	5:L:159:LYS:HD3	1.81	0.63
40:x:337:ASN:ND2	40:x:415:PRO:O	2.32	0.63
1:B:834:HIS:HB2	42:y:134:PHE:HE2	1.64	0.62
20:4:19:U:H2'	20:4:20:G:H8	1.65	0.62
20:4:392:U:H2'	20:4:393:A:H8	1.64	0.62
22:3:137:A:H1'	32:k:144:LEU:CB	2.29	0.62
15:f:23:ILE:HG21	15:f:40:LEU:HD21	1.81	0.62
24:b:144:LEU:HD22	24:b:178:ALA:HA	1.80	0.62
2:C:904:ARG:HH22	2:C:974:VAL:HG22	1.65	0.62
24:b:197:ILE:HD11	24:b:369:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:196:ASN:HA	32:k:199:TYR:HD1	1.63	0.62
41:c:211:LYS:O	41:c:211:LYS:HG2	2.00	0.62
31:h:172:ARG:HE	31:h:204:LEU:HD21	1.65	0.62
20:4:260:A:H61	20:4:285:G:H1'	1.64	0.61
23:a:68:LEU:HD21	24:b:141:VAL:HG12	1.82	0.61
16:p:33:LEU:HG	16:p:38:LEU:HD22	1.81	0.61
21:2:130:A:H61	21:2:140:G:H1	1.48	0.61
22:3:167:G:H2'	22:3:168:A:H8	1.66	0.61
32:k:126:HIS:HD2	32:k:217:VAL:HG11	1.66	0.61
34:m:96:LEU:HD12	34:m:97:PRO:HD2	1.82	0.61
40:x:148:LYS:HE3	40:x:407:THR:HA	1.83	0.61
5:N:155:VAL:HB	5:N:166:PHE:HB2	1.82	0.61
32:k:137:THR:HG22	32:k:139:THR:HG22	1.83	0.61
5:N:123:GLU:OE2	5:N:217:ARG:NH2	2.33	0.60
24:b:200:VAL:HB	28:v:37:VAL:HG21	1.83	0.60
23:a:187:VAL:HG23	23:a:220:GLY:H	1.66	0.60
22:3:193:U:OP1	26:o:127:ARG:NH2	2.33	0.60
32:k:136:LEU:HD11	32:k:200:ALA:CB	2.31	0.60
5:N:162:ARG:HD2	5:N:182:LEU:HD11	1.84	0.60
40:x:331:PHE:HB2	40:x:402:VAL:HG12	1.83	0.60
5:L:157:VAL:HB	5:L:164:LEU:HB3	1.83	0.60
16:p:33:LEU:HB3	16:p:34:ASN:O	2.01	0.60
22:3:138:G:H4'	32:k:146:LYS:HA	1.82	0.60
19:1:19:G:H21	22:3:328:A:N6	1.98	0.60
33:j:144:PRO:HG3	33:j:164:LEU:HD11	1.84	0.60
42:y:153:LEU:HG	42:y:155:GLY:H	1.67	0.60
22:3:131:A:N1	22:3:166:G:N2	2.50	0.60
32:k:156:TYR:HA	32:k:160:ARG:HE	1.66	0.59
34:m:18:ALA:N	34:m:40:SER:O	2.34	0.59
6:O:309:GLY:O	6:O:313:ALA:HB2	2.03	0.59
7:P:226:GLY:HA2	7:P:290:ASN:HD22	1.67	0.59
25:e:218:MET:HE3	25:e:230:LEU:HD22	1.85	0.59
31:h:71:MET:HE1	31:h:242:PRO:HD3	1.83	0.59
20:4:259:U:H3	20:4:286:A:N6	1.96	0.59
22:3:400:A:H1'	37:s:68:LYS:HA	1.85	0.59
40:x:89:TYR:OH	40:x:98:ARG:NH1	2.36	0.59
15:f:47:HIS:HA	15:f:61:ARG:HA	1.85	0.59
22:3:138:G:H5'	32:k:146:LYS:HE2	1.83	0.59
5:M:157:VAL:HB	5:M:164:LEU:HB2	1.85	0.59
7:P:386:ARG:NH2	7:P:409:TYR:OH	2.36	0.59
8:U:28:UNK:O	8:U:30:UNK:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:343:VAL:HA	14:d:346:MET:HG2	1.83	0.59
31:h:114:ASP:HA	31:h:117:LYS:HE2	1.85	0.59
31:h:162:PHE:H	31:h:165:ARG:HH12	1.50	0.59
5:N:148:ILE:O	5:N:228:ARG:NH1	2.36	0.58
22:3:32:A:N6	22:3:41:G:N2	2.50	0.58
31:h:72:LYS:NZ	31:h:76:MET:SD	2.76	0.58
7:P:38:GLY:O	7:P:68:ARG:NH2	2.36	0.58
20:4:332:G:H1	20:4:392:U:H3	1.51	0.58
21:2:60:G:OP1	29:q:45:ARG:NH2	2.36	0.58
21:2:43:G:N3	31:h:61:GLN:NE2	2.51	0.58
19:1:46:G:H3'	19:1:47:U:H4'	1.84	0.58
5:L:154:ASN:HA	5:L:167:GLU:HA	1.84	0.58
10:W:33:UNK:C	10:W:35:UNK:N	2.61	0.58
32:k:198:GLN:HG2	32:k:199:TYR:N	2.18	0.58
2:C:315:ARG:NH2	2:C:317:GLN:OE1	2.36	0.58
31:h:126:ASP:OD2	31:h:178:ARG:NH1	2.35	0.58
32:k:196:ASN:HA	32:k:199:TYR:CD1	2.39	0.58
42:y:139:ARG:HH12	42:y:146:ARG:HE	1.50	0.58
22:3:243:G:N7	22:3:244:A:N6	2.52	0.58
36:u:89:HIS:CE1	42:y:151:ARG:HH22	2.22	0.58
5:N:114:LEU:HD11	5:N:234:LYS:HE2	1.86	0.57
5:N:124:GLU:HB3	5:N:158:ALA:HB3	1.86	0.57
13:Z:204:UNK:O	13:Z:208:UNK:N	2.37	0.57
17:r:253:LEU:HA	17:r:257:PHE:HB2	1.86	0.57
20:4:104:G:H1	22:3:403:U:H3	1.51	0.57
39:i:402:LEU:HD12	39:i:415:PRO:HD2	1.85	0.57
24:b:256:LEU:HD11	24:b:365:PRO:HD3	1.86	0.57
31:h:174:ASP:HB2	31:h:199:PRO:HG2	1.85	0.57
32:k:129:ASN:HD22	32:k:194:GLY:CA	2.07	0.57
2:C:365:ARG:HE	2:C:369:ALA:HA	1.70	0.57
20:4:336:U:H3	20:4:387:G:H1	1.53	0.57
24:b:244:LEU:HD11	24:b:365:PRO:HG3	1.87	0.57
32:k:150:SER:H	32:k:153:VAL:CB	2.10	0.57
1:B:847:THR:HB	1:B:856:ASN:HB3	1.86	0.57
21:2:40:C:H1'	29:q:61:LYS:HZ1	1.70	0.57
37:s:49:ARG:HB2	37:s:85:GLY:HA2	1.85	0.57
14:d:343:VAL:HG21	14:d:359:ILE:HD11	1.85	0.57
21:2:59:G:H1'	29:q:15:MET:HE3	1.87	0.57
26:o:195:ARG:NH2	26:o:214:TYR:OH	2.38	0.57
17:r:249:ASN:HB2	18:w:184:VAL:HG23	1.86	0.57
31:h:79:TYR:OH	31:h:114:ASP:OD2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:244:LEU:HD11	31:h:291:LEU:HD12	1.86	0.57
2:C:961:GLY:HA2	16:p:58:HIS:HE2	1.70	0.56
34:m:47:ASP:OD1	40:x:90:THR:N	2.33	0.56
22:3:126:G:N1	22:3:170:A:H2	1.94	0.56
34:m:64:PHE:HE2	34:m:70:LEU:HB2	1.70	0.56
39:i:329:VAL:HB	39:i:370:ASP:HB3	1.86	0.56
18:w:96:GLU:HA	18:w:99:ARG:HG3	1.86	0.56
23:a:76:PRO:O	28:v:61:LYS:NZ	2.38	0.56
35:n:57:LEU:HG	35:n:58:PHE:H	1.69	0.56
38:g:187:ASN:OD1	38:g:262:ARG:NH2	2.38	0.56
39:i:404:ALA:H	39:i:420:THR:HG21	1.70	0.56
23:a:187:VAL:HG12	23:a:197:VAL:HG22	1.87	0.56
22:3:144:G:O6	32:k:161:LYS:NZ	2.38	0.56
26:o:229:UNK:O	29:q:14:ARG:NH2	2.39	0.56
24:b:418:HIS:O	24:b:422:GLU:HB2	2.05	0.56
7:P:216:ARG:HD3	7:P:320:LEU:HD23	1.87	0.56
7:P:395:GLY:H	7:P:399:GLU:HG2	1.70	0.56
19:l:15:U:OP1	25:e:200:ARG:NH2	2.39	0.56
22:3:305:U:H2'	22:3:306:A:H8	1.71	0.56
25:e:183:LEU:HD21	25:e:250:LEU:HG	1.88	0.56
20:4:58:A:H1'	24:b:258:SER:OG	2.06	0.56
22:3:360:A:H2'	22:3:361:A:C8	2.41	0.56
23:a:174:ARG:NH2	28:v:69:GLN:O	2.39	0.55
38:g:207:PRO:O	38:g:208:ARG:NH1	2.37	0.55
32:k:156:TYR:CG	32:k:166:ALA:HB2	2.41	0.55
24:b:425:LEU:HA	24:b:428:VAL:HG12	1.88	0.55
2:C:380:LEU:O	2:C:384:MET:HB3	2.06	0.55
4:K:28:UNK:HA	41:c:148:HIS:NE2	2.20	0.55
40:x:100:GLY:O	40:x:106:GLN:NE2	2.39	0.55
32:k:191:LYS:HG3	32:k:219:PRO:HD3	1.88	0.55
40:x:131:ALA:HB2	40:x:158:TRP:HH2	1.71	0.55
22:3:312:G:N2	22:3:315:A:OP2	2.40	0.55
41:c:224:ASP:O	41:c:255:ARG:NH1	2.35	0.55
13:Z:281:UNK:O	13:Z:285:UNK:N	2.40	0.55
31:h:60:ASN:OD1	31:h:64:GLN:NE2	2.40	0.55
32:k:129:ASN:OD1	32:k:134:ILE:HB	2.06	0.55
5:L:130:HIS:NE2	5:N:191:GLU:OE1	2.36	0.55
7:P:40:ARG:HH12	21:2:63:C:H5'	1.70	0.55
17:r:267:ARG:NH1	17:r:272:LEU:O	2.39	0.55
23:a:65:LEU:HD21	24:b:182:ASP:HA	1.88	0.55
31:h:120:ARG:NH2	31:h:121:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:65:ASP:HA	35:n:70:ARG:HD2	1.89	0.55
22:3:239:A:N6	22:3:245:G:OP2	2.40	0.55
7:P:220:LEU:HD21	7:P:320:LEU:HG	1.89	0.55
21:2:56:G:O6	21:2:85:A:N6	2.40	0.55
35:n:74:ARG:HG2	35:n:81:ALA:HA	1.89	0.55
2:C:281:ASP:OD1	2:C:281:ASP:N	2.40	0.54
18:w:143:ARG:NH2	22:3:112:A:O2'	2.41	0.54
20:4:259:U:C2	20:4:286:A:N6	2.68	0.54
23:a:172:GLU:HA	23:a:175:ARG:HB2	1.88	0.54
28:v:86:PRO:HG2	28:v:91:GLN:HE21	1.72	0.54
32:k:125:VAL:HA	32:k:137:THR:O	2.06	0.54
2:C:865:PRO:HG2	25:e:265:TYR:HA	1.88	0.54
20:4:129:G:H2'	20:4:130:G:H8	1.71	0.54
25:e:287:GLY:N	25:e:305:ASP:OD1	2.38	0.54
32:k:134:ILE:CD1	32:k:197:LYS:HA	2.37	0.54
35:n:73:ASN:HD21	35:n:86:ARG:HD2	1.72	0.54
38:g:265:ARG:O	38:g:269:HIS:ND1	2.34	0.54
7:P:33:LEU:HD22	7:P:57:PHE:HE1	1.73	0.54
7:P:326:GLY:HA3	7:P:370:THR:HG22	1.90	0.54
1:B:834:HIS:HB2	42:y:134:PHE:CE2	2.43	0.54
2:C:869:GLY:O	31:h:280:ARG:NH2	2.41	0.54
7:P:30:PRO:HA	7:P:33:LEU:HD12	1.88	0.54
16:p:56:LEU:HB3	16:p:62:LEU:HD12	1.90	0.54
19:1:65:U:O2	19:1:74:G:N2	2.41	0.54
7:P:59:THR:HA	7:P:62:MET:HE2	1.90	0.54
17:r:285:ARG:NH2	22:3:187:C:O3'	2.38	0.54
20:4:169:G:H21	20:4:244:A:H62	1.54	0.54
20:4:347:A:O2'	20:4:377:A:N6	2.40	0.54
22:3:126:G:O6	22:3:170:A:N1	2.41	0.54
23:a:147:TYR:HE2	24:b:148:ARG:HG3	1.73	0.54
26:o:160:ARG:HG2	26:o:271:LEU:HD21	1.89	0.54
26:o:228:UNK:O	29:q:41:ARG:NH2	2.41	0.54
30:l:41:PHE:HB3	30:l:93:LEU:HD11	1.90	0.54
13:Z:498:UNK:O	13:Z:502:UNK:N	2.41	0.54
20:4:232:U:H3'	20:4:233:A:H2'	1.90	0.54
20:4:267:G:H2'	20:4:268:A:C8	2.43	0.54
24:b:169:GLU:OE2	24:b:177:ALA:N	2.40	0.54
31:h:120:ARG:HG3	31:h:127:GLY:HA2	1.90	0.54
39:i:374:ARG:HE	39:i:375:VAL:H	1.54	0.54
16:p:79:ASP:N	16:p:79:ASP:OD1	2.41	0.54
19:1:7:G:H4'	25:e:291:PRO:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:156:TYR:O	32:k:161:LYS:HD3	2.07	0.54
18:w:101:ALA:O	18:w:105:ARG:HB3	2.06	0.54
22:3:100:U:H5'	31:h:81:ASN:ND2	2.23	0.54
5:L:162:ARG:HH21	5:L:182:LEU:HG	1.73	0.53
20:4:258:G:N2	20:4:286:A:OP2	2.41	0.53
22:3:58:C:H4'	22:3:60:G:H4'	1.89	0.53
23:a:141:LEU:HA	23:a:157:ALA:HB2	1.90	0.53
40:x:452:ARG:NH1	40:x:453:ALA:O	2.41	0.53
42:y:142:GLU:H	42:y:147:ARG:NH1	2.06	0.53
1:B:847:THR:HB	1:B:856:ASN:HD22	1.74	0.53
20:4:21:A:H2'	20:4:22:A:C4	2.44	0.53
21:2:40:C:H1'	29:q:61:LYS:NZ	2.23	0.53
21:2:58:U:O2'	29:q:43:LYS:NZ	2.40	0.53
23:a:165:LYS:HG3	23:a:200:ALA:HB1	1.90	0.53
40:x:184:ARG:HH22	40:x:299:ASP:HB2	1.74	0.53
20:4:300:U:H2'	20:4:301:G:C8	2.43	0.53
6:O:460:GLY:HA2	6:O:492:LEU:HD11	1.90	0.53
24:b:430:ILE:HG23	24:b:435:LEU:HD11	1.91	0.53
32:k:121:LEU:N	32:k:183:TYR:HA	2.23	0.53
32:k:135:ILE:CG2	32:k:148:TYR:HD2	2.21	0.53
22:3:36:G:H2'	22:3:37:G:H8	1.72	0.53
2:C:365:ARG:NH2	2:C:368:PRO:O	2.40	0.53
5:L:192:SER:O	5:M:112:THR:OG1	2.26	0.53
22:3:106:G:N2	22:3:205:A:N1	2.56	0.53
22:3:316:C:H2'	22:3:317:A:H8	1.73	0.53
24:b:203:LYS:HZ2	28:v:33:LYS:HG2	1.74	0.53
31:h:71:MET:HE1	31:h:241:HIS:HA	1.90	0.53
40:x:160:ARG:HH22	40:x:208:ALA:HB1	1.74	0.53
5:L:124:GLU:HB3	5:L:158:ALA:HB3	1.91	0.53
7:P:71:HIS:NE2	7:P:75:GLN:OE1	2.42	0.53
22:3:118:A:H1'	22:3:186:A:H5'	1.90	0.53
22:3:346:G:H2'	22:3:347:A:C8	2.44	0.53
40:x:138:LEU:HB2	40:x:403:VAL:HG22	1.91	0.53
20:4:336:U:O2	20:4:387:G:N2	2.41	0.53
21:2:43:G:H1'	31:h:61:GLN:HE22	1.73	0.53
31:h:330:ARG:NH1	31:h:333:GLU:OE2	2.42	0.53
41:c:162:PRO:HG3	41:c:237:GLY:HA2	1.90	0.53
14:d:304:LEU:HD11	14:d:335:MET:HE1	1.91	0.53
14:d:366:VAL:HG22	14:d:385:VAL:HG23	1.91	0.53
32:k:123:GLY:HA3	32:k:186:VAL:HG13	1.91	0.53
32:k:127:ILE:CG2	32:k:136:LEU:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:132:ASN:O	32:k:161:LYS:NZ	2.42	0.53
6:O:285:ARG:HH12	6:O:289:LEU:HG	1.74	0.52
7:P:368:VAL:HA	7:P:371:LEU:HD12	1.92	0.52
40:x:72:LEU:HD21	40:x:117:ILE:HG12	1.91	0.52
2:C:482:PRO:HA	2:C:485:GLN:HG2	1.91	0.52
7:P:46:MET:HE2	7:P:65:LEU:HD11	1.90	0.52
17:r:245:ALA:O	17:r:279:HIS:NE2	2.42	0.52
34:m:90:VAL:O	34:m:94:LEU:CB	2.57	0.52
37:s:76:GLN:HE22	37:s:78:ALA:HB3	1.73	0.52
7:P:197:ASP:OD1	7:P:289:ARG:NH1	2.43	0.52
18:w:100:MET:O	18:w:104:LEU:HB2	2.09	0.52
32:k:139:THR:HB	32:k:145:ILE:CA	2.33	0.52
32:k:151:ALA:HB3	32:k:161:LYS:HG3	1.92	0.52
18:w:100:MET:HG3	18:w:104:LEU:HD12	1.90	0.52
24:b:244:LEU:HB2	24:b:382:GLU:HB3	1.90	0.52
36:u:77:ILE:HG22	36:u:82:TYR:HB3	1.92	0.52
2:C:876:ASP:OD2	31:h:313:ARG:NH2	2.43	0.52
5:L:126:ASN:HB2	5:L:156:SER:HB2	1.90	0.52
20:4:57:A:H4'	24:b:250:ARG:O	2.09	0.52
29:q:12:SER:HB3	29:q:20:VAL:HB	1.91	0.52
40:x:107:GLN:OE1	40:x:474:ARG:NH1	2.42	0.52
40:x:219:LEU:O	40:x:307:GLN:NE2	2.42	0.52
41:c:233:LYS:NZ	41:c:260:ALA:O	2.39	0.52
5:L:163:VAL:HG23	5:L:185:LYS:HA	1.90	0.52
15:f:36:PHE:CD1	18:w:164:GLN:HG2	2.44	0.52
18:w:116:VAL:HG12	31:h:157:TYR:HD2	1.75	0.52
22:3:214:C:O3'	26:o:259:ARG:NH1	2.42	0.52
33:j:123:GLU:HB3	33:j:126:TYR:HD2	1.75	0.52
39:i:373:ALA:HB1	39:i:387:ILE:HD11	1.91	0.52
2:C:478:VAL:O	2:C:485:GLN:NE2	2.33	0.52
20:4:259:U:H2'	20:4:260:A:C8	2.39	0.52
30:l:80:PRO:HG2	30:l:111:ARG:HD3	1.92	0.52
15:f:4:TYR:CE2	15:f:76:ILE:HD11	2.45	0.52
20:4:19:U:H2'	20:4:20:G:C8	2.44	0.52
35:n:75:CYS:SG	35:n:76:VAL:N	2.83	0.52
39:i:343:LEU:HD11	39:i:356:VAL:HG11	1.92	0.52
2:C:481:SER:O	2:C:485:GLN:NE2	2.38	0.52
24:b:259:ASP:OD1	24:b:259:ASP:N	2.41	0.52
19:1:98:U:H3	21:2:38:C:H42	1.58	0.51
35:n:23:ARG:HH21	35:n:70:ARG:HD3	1.75	0.51
2:C:940:VAL:HA	16:p:29:MET:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:108:ILE:HD12	7:P:152:LEU:HD22	1.92	0.51
28:v:17:VAL:O	28:v:21:MET:HB2	2.10	0.51
30:l:111:ARG:HH22	30:l:119:VAL:H	1.57	0.51
34:m:34:SER:HB2	34:m:39:ILE:HB	1.92	0.51
5:M:209:GLN:HB3	5:N:74:LEU:HD13	1.91	0.51
15:f:80:ASP:O	15:f:84:HIS:HB2	2.10	0.51
22:3:138:G:C4'	32:k:146:LYS:HA	2.40	0.51
22:3:277:A:N1	31:h:95:ARG:NH2	2.58	0.51
22:3:366:C:OP1	22:3:386:C:N4	2.37	0.51
26:o:194:ARG:NH2	26:o:212:ASP:OD2	2.44	0.51
27:z:97:LEU:HD21	27:z:102:LEU:HD13	1.92	0.51
32:k:126:HIS:H	32:k:137:THR:HB	1.74	0.51
36:u:70:ASN:OD1	36:u:71:ARG:N	2.44	0.51
40:x:76:LEU:HD22	40:x:160:ARG:HB3	1.92	0.51
20:4:118:C:H2'	20:4:119:G:H8	1.75	0.51
31:h:290:GLU:OE2	31:h:292:ARG:NH1	2.43	0.51
32:k:153:VAL:HG13	32:k:177:ARG:HH22	1.75	0.51
7:P:227:PRO:O	7:P:287:GLN:NE2	2.44	0.51
13:Z:230:UNK:O	13:Z:234:UNK:N	2.43	0.51
15:f:38:THR:HA	18:w:161:TRP:CE3	2.45	0.51
21:2:103:G:H22	21:2:115:C:H5'	1.74	0.51
25:e:197:VAL:HG12	25:e:317:ARG:HB3	1.92	0.51
32:k:154:VAL:HG21	32:k:166:ALA:O	2.10	0.51
40:x:339:LEU:HG	40:x:370:ALA:HB1	1.92	0.51
20:4:109:G:H5'	37:s:49:ARG:HH22	1.75	0.51
22:3:100:U:H5''	31:h:81:ASN:HD22	1.74	0.51
22:3:262:C:H1'	22:3:313:C:H41	1.76	0.51
32:k:123:GLY:C	32:k:186:VAL:HG13	2.36	0.51
26:o:127:ARG:HA	26:o:130:GLU:HG3	1.92	0.51
6:O:381:ALA:HA	6:O:384:LEU:HD12	1.93	0.51
20:4:158:U:O2'	40:x:177:ARG:NH1	2.43	0.51
22:3:29:G:H22	22:3:45:A:H5'	1.75	0.51
25:e:257:PRO:HG3	28:v:22:ARG:HD2	1.92	0.51
34:m:69:THR:HG23	34:m:72:ARG:HH22	1.76	0.51
9:V:49:UNK:O	9:V:53:UNK:N	2.44	0.51
32:k:125:VAL:N	32:k:187:GLN:O	2.44	0.51
32:k:156:TYR:CD2	32:k:166:ALA:HB2	2.46	0.51
7:P:96:ARG:HA	7:P:100:LEU:HD12	1.91	0.51
15:f:74:ASP:O	15:f:77:LYS:NZ	2.44	0.51
19:1:82:G:H1'	21:2:162:G:H5'	1.93	0.51
20:4:135:C:H2'	20:4:136:C:H4'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:178:SER:HB3	29:q:181:VAL:HG23	1.93	0.51
31:h:191:GLN:HB2	31:h:307:ARG:HH21	1.76	0.51
42:y:141:ARG:H	42:y:147:ARG:HH22	1.58	0.51
5:L:74:LEU:O	5:L:78:LEU:HB2	2.11	0.50
5:M:226:TYR:O	5:M:230:LEU:HB2	2.11	0.50
7:P:59:THR:HG21	7:P:108:ILE:HD13	1.92	0.50
28:v:121:LEU:HB3	28:v:125:ARG:HH21	1.75	0.50
37:s:66:ASN:OD1	37:s:69:SER:N	2.43	0.50
38:g:213:ASP:O	38:g:216:THR:OG1	2.26	0.50
41:c:225:LEU:HA	41:c:255:ARG:HD2	1.92	0.50
31:h:239:CYS:HB2	31:h:247:ILE:HG13	1.92	0.50
5:L:84:TYR:HA	5:L:87:LYS:HE3	1.94	0.50
18:w:129:GLN:O	18:w:133:ALA:HB3	2.10	0.50
21:2:192:C:H5''	21:2:193:G:H5''	1.93	0.50
24:b:233:TRP:HH2	24:b:363:ARG:HB3	1.76	0.50
32:k:192:GLY:H	32:k:218:THR:HG23	1.76	0.50
34:m:32:ALA:N	40:x:359:ARG:HH22	2.10	0.50
1:B:867:LEU:HA	42:y:133:LEU:HD11	1.94	0.50
2:C:881:GLY:HA2	25:e:346:ARG:HH11	1.77	0.50
5:L:73:SER:OG	5:L:74:LEU:N	2.45	0.50
19:1:19:G:H2'	19:1:20:G:H8	1.75	0.50
22:3:194:C:OP1	26:o:158:ARG:NH1	2.44	0.50
40:x:337:ASN:HA	40:x:340:TYR:HD2	1.77	0.50
2:C:939:PRO:HB3	2:C:960:ALA:HA	1.93	0.50
5:M:118:ARG:NH1	5:M:217:ARG:O	2.44	0.50
7:P:157:THR:OG1	7:P:198:ARG:NH1	2.44	0.50
18:w:52:TYR:OH	18:w:56:ARG:NH2	2.44	0.50
20:4:116:G:H1	22:3:367:U:H3	1.59	0.50
20:4:174:G:O3'	34:m:77:ASN:ND2	2.44	0.50
22:3:66:A:H2'	22:3:67:G:C8	2.47	0.50
5:L:212:LYS:O	5:L:216:ASP:CB	2.60	0.50
5:M:225:GLU:OE1	5:M:228:ARG:NH2	2.44	0.50
22:3:138:G:H5'	32:k:146:LYS:CE	2.42	0.50
24:b:372:ASP:HA	24:b:411:GLU:HG2	1.94	0.50
32:k:181:LEU:HB3	32:k:183:TYR:CD1	2.47	0.50
3:D:261:UNK:HA	3:D:265:UNK:HA	1.94	0.50
15:f:96:LYS:HE2	22:3:191:C:OP1	2.11	0.50
5:L:91:ARG:NH2	5:L:95:ILE:O	2.45	0.50
5:M:106:THR:O	5:M:115:THR:OG1	2.29	0.50
20:4:230:A:O2'	20:4:234:G:N7	2.41	0.50
20:4:310:U:O2	20:4:415:G:N2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:184:SER:HA	23:a:224:SER:HA	1.93	0.50
24:b:230:SER:O	24:b:262:GLN:NE2	2.45	0.50
26:o:159:VAL:HG23	26:o:179:LEU:HD11	1.93	0.50
37:s:89:PRO:HG2	37:s:91:LYS:HD3	1.94	0.50
39:i:331:ALA:HB3	39:i:370:ASP:HB2	1.94	0.50
2:C:942:VAL:HA	16:p:32:GLY:H	1.77	0.50
15:f:48:LEU:HD12	15:f:60:ASP:HA	1.94	0.50
18:w:131:GLN:O	18:w:135:ARG:HB2	2.12	0.50
23:a:84:LEU:HG	28:v:78:PRO:HB2	1.93	0.50
40:x:198:ALA:HB2	40:x:369:LEU:HD22	1.92	0.50
40:x:118:LEU:HD21	40:x:436:GLU:HB2	1.94	0.49
2:C:282:GLY:O	2:C:318:ARG:NH1	2.45	0.49
5:L:130:HIS:HB3	5:L:133:SER:HB2	1.94	0.49
22:3:66:A:H2'	22:3:67:G:H8	1.76	0.49
34:m:34:SER:O	34:m:39:ILE:N	2.42	0.49
42:y:129:LEU:O	42:y:133:LEU:HB2	2.11	0.49
11:X:18:UNK:HA	42:y:181:LEU:HD21	1.93	0.49
21:2:57:C:O2'	21:2:88:G:N2	2.45	0.49
22:3:57:U:O2'	22:3:61:U:OP1	2.30	0.49
2:C:494:ARG:HH22	2:C:574:LEU:HA	1.76	0.49
5:L:149:SER:HA	5:L:228:ARG:HH21	1.78	0.49
5:L:166:PHE:HE1	5:L:180:VAL:HG23	1.77	0.49
7:P:109:THR:HG21	7:P:170:ARG:HG3	1.94	0.49
14:d:301:ARG:HD3	14:d:308:ARG:HG3	1.95	0.49
19:1:48:U:H4'	19:1:49:U:H5''	1.93	0.49
22:3:192:A:OP1	26:o:123:LYS:NZ	2.46	0.49
25:e:179:LEU:HD23	25:e:184:ARG:HH21	1.77	0.49
37:s:13:VAL:HG22	37:s:17:GLN:HE21	1.77	0.49
5:L:213:TYR:O	5:L:217:ARG:NH1	2.40	0.49
23:a:76:PRO:HA	24:b:168:LEU:CD1	2.43	0.49
32:k:167:ALA:HB1	32:k:200:ALA:HB2	1.95	0.49
33:j:177:TRP:NE1	33:j:179:ARG:HE	2.10	0.49
42:y:131:ASN:O	42:y:135:GLY:N	2.46	0.49
5:N:107:GLU:OE1	5:N:234:LYS:NZ	2.43	0.49
37:s:29:TRP:CD1	37:s:38:GLN:H	2.30	0.49
5:M:191:GLU:O	5:N:130:HIS:NE2	2.40	0.49
20:4:10:U:H3	20:4:95:G:H1	1.59	0.49
20:4:282:G:H2'	20:4:283:G:H8	1.77	0.49
20:4:303:G:O6	22:3:339:A:N6	2.45	0.49
33:j:197:GLN:HB3	35:n:110:ALA:HB3	1.94	0.49
38:g:194:VAL:HA	38:g:207:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:205:A:H4'	40:x:371:ARG:HH21	1.77	0.49
23:a:206:LEU:HD13	23:a:240:ARG:HA	1.95	0.49
32:k:191:LYS:HA	32:k:218:THR:OG1	2.12	0.49
31:h:219:LEU:HD11	31:h:258:PRO:HB2	1.95	0.49
20:4:287:A:O2'	38:g:221:LYS:NZ	2.46	0.48
23:a:182:PRO:HB2	23:a:224:SER:HB3	1.94	0.48
31:h:120:ARG:NH1	31:h:152:GLU:OE2	2.46	0.48
13:Z:508:UNK:O	13:Z:512:UNK:N	2.46	0.48
18:w:54:LYS:NZ	21:2:23:G:OP1	2.45	0.48
20:4:7:C:O2'	20:4:103:A:OP1	2.31	0.48
20:4:178:U:O2'	20:4:181:A:O4'	2.30	0.48
22:3:362:U:H2'	22:3:363:A:H8	1.77	0.48
31:h:115:MET:HB2	31:h:246:LEU:HD13	1.94	0.48
31:h:128:PHE:HB3	31:h:169:LEU:HD23	1.96	0.48
32:k:132:ASN:C	32:k:161:LYS:HZ2	2.20	0.48
32:k:211:ILE:H	32:k:211:ILE:HD13	1.77	0.48
18:w:108:ARG:NH1	29:q:170:GLU:OE1	2.46	0.48
2:C:864:TYR:O	25:e:350:ARG:NH2	2.46	0.48
5:M:160:GLY:O	5:M:185:LYS:NZ	2.44	0.48
6:O:278:LEU:O	6:O:282:ARG:CB	2.61	0.48
17:r:288:ARG:NH1	22:3:172:C:N3	2.62	0.48
3:D:456:UNK:O	3:D:460:UNK:N	2.47	0.48
5:N:116:LEU:HB2	5:N:127:VAL:HB	1.94	0.48
15:f:11:LYS:CD	15:f:12:PRO:HD2	2.37	0.48
16:p:20:ASP:H	16:p:30:HIS:CD2	2.31	0.48
22:3:293:A:OP2	31:h:213:LYS:NZ	2.46	0.48
23:a:84:LEU:HD22	23:a:138:LEU:HB3	1.95	0.48
24:b:391:VAL:HG22	24:b:405:PHE:HB2	1.95	0.48
32:k:132:ASN:O	32:k:161:LYS:HB3	2.12	0.48
7:P:289:ARG:NH2	7:P:290:ASN:OD1	2.46	0.48
15:f:100:SER:HA	18:w:153:ARG:NH1	2.26	0.48
22:3:140:A:H2	22:3:153:G:H21	1.62	0.48
1:B:847:THR:HG22	1:B:860:LEU:HD13	1.96	0.48
2:C:350:VAL:HG12	3:D:298:UNK:O	2.14	0.48
12:Y:46:UNK:O	12:Y:50:UNK:CB	2.61	0.48
20:4:57:A:H2'	20:4:58:A:H8	1.79	0.48
20:4:325:G:H3'	20:4:326:A:H8	1.79	0.48
23:a:72:ASN:OD1	28:v:90:ARG:NH2	2.47	0.48
25:e:333:THR:HG22	25:e:335:HIS:H	1.79	0.48
5:L:91:ARG:HH12	5:L:96:SER:HA	1.79	0.48
11:X:17:UNK:O	11:X:19:UNK:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:58:A:H5''	24:b:254:CYS:SG	2.54	0.48
24:b:256:LEU:CD1	24:b:365:PRO:HD3	2.43	0.48
30:l:86:LEU:HD21	30:l:116:CYS:HB2	1.96	0.48
5:L:78:LEU:HD22	5:L:247:GLU:HB2	1.95	0.48
20:4:152:A:H5''	36:u:73:ARG:HH22	1.79	0.48
28:v:68:LEU:HD22	28:v:75:ARG:HG3	1.96	0.48
32:k:122:GLU:HB2	32:k:141:LYS:HG2	1.94	0.48
34:m:91:ARG:HD2	34:m:96:LEU:HB3	1.95	0.48
19:1:5:U:C4	25:e:280:MET:HE1	2.49	0.48
20:4:415:G:N3	20:4:416:G:N2	2.62	0.48
21:2:143:C:H2'	21:2:144:A:H8	1.79	0.48
33:j:181:ARG:NH1	33:j:197:GLN:OE1	2.47	0.48
35:n:34:ARG:HG3	35:n:38:LYS:NZ	2.29	0.48
41:c:187:ALA:O	41:c:191:ALA:HB2	2.13	0.48
21:2:84:C:H2'	21:2:85:A:C8	2.49	0.47
22:3:364:U:H2'	22:3:365:G:H8	1.79	0.47
28:v:58:LEU:HG	28:v:60:GLU:H	1.79	0.47
31:h:162:PHE:H	31:h:165:ARG:NH1	2.12	0.47
39:i:408:ASP:OD1	39:i:408:ASP:N	2.46	0.47
5:M:138:GLU:OE1	5:N:42:UNK:N	2.47	0.47
5:N:75:SER:HA	5:N:78:LEU:HD12	1.95	0.47
22:3:65:A:H1'	30:l:40:PRO:HB3	1.96	0.47
35:n:93:ILE:HG13	35:n:94:MET:SD	2.54	0.47
41:c:202:VAL:HG13	41:c:252:VAL:HG22	1.95	0.47
13:Z:211:UNK:O	13:Z:215:UNK:N	2.47	0.47
22:3:111:C:H2'	22:3:112:A:H8	1.79	0.47
22:3:348:G:N3	22:3:352:C:N4	2.59	0.47
22:3:372:A:C6	37:s:68:LYS:HB3	2.49	0.47
26:o:191:THR:HG22	26:o:214:TYR:HA	1.97	0.47
32:k:151:ALA:HB3	32:k:161:LYS:CG	2.44	0.47
19:1:19:G:H5'	22:3:85:C:H42	1.80	0.47
19:1:30:C:N4	21:2:174:U:O4'	2.47	0.47
21:2:190:A:H3'	21:2:191:A:H8	1.80	0.47
22:3:24:C:H2'	22:3:25:A:H8	1.78	0.47
22:3:372:A:H2'	22:3:373:A:C8	2.49	0.47
32:k:140:ASP:CG	32:k:146:LYS:HE3	2.39	0.47
35:n:33:ASP:HA	35:n:36:VAL:HG12	1.96	0.47
37:s:75:VAL:HG23	37:s:79:MET:HG2	1.96	0.47
22:3:202:C:O2'	26:o:144:ASP:OD1	2.29	0.47
24:b:211:ASN:HD22	24:b:371:LEU:HB2	1.80	0.47
29:q:21:VAL:HG11	29:q:59:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:117:ILE:HG12	33:j:236:MET:HG3	1.96	0.47
33:j:197:GLN:CB	35:n:110:ALA:HB3	2.44	0.47
5:L:127:VAL:HG22	5:L:155:VAL:HG22	1.96	0.47
5:N:159:LYS:HD2	5:N:162:ARG:HH22	1.79	0.47
18:w:176:ASP:OD1	18:w:176:ASP:N	2.47	0.47
38:g:177:VAL:HA	38:g:180:VAL:HG12	1.97	0.47
40:x:72:LEU:HD11	40:x:117:ILE:HG23	1.96	0.47
2:C:339:LEU:HD22	2:C:344:SER:HA	1.96	0.47
2:C:583:LEU:HD22	2:C:590:ALA:HB2	1.97	0.47
7:P:59:THR:HB	7:P:107:ASP:HB3	1.96	0.47
20:4:107:U:H2'	20:4:108:G:C8	2.49	0.47
20:4:414:A:HO2'	20:4:442:G:HO2'	1.61	0.47
21:2:184:C:H2'	21:2:185:G:C8	2.49	0.47
22:3:162:G:H2'	22:3:163:G:H8	1.80	0.47
32:k:138:LEU:N	32:k:147:THR:O	2.47	0.47
34:m:42:ASP:O	40:x:98:ARG:NH2	2.48	0.47
34:m:71:LYS:HA	34:m:74:VAL:HG12	1.97	0.47
35:n:15:ARG:N	35:n:79:GLY:HA3	2.30	0.47
35:n:33:ASP:OD1	35:n:34:ARG:N	2.48	0.47
40:x:93:ASP:HB2	40:x:96:HIS:CG	2.49	0.47
40:x:337:ASN:HB3	40:x:418:LEU:HD21	1.97	0.47
2:C:290:ASN:OD1	2:C:326:LYS:NZ	2.33	0.47
5:N:220:THR:HG23	5:N:223:LEU:H	1.79	0.47
6:O:372:ALA:HA	6:O:375:LEU:HG	1.96	0.47
20:4:5:A:H2'	20:4:6:G:C8	2.50	0.47
21:2:60:G:N1	21:2:84:C:O2	2.48	0.47
22:3:395:U:H4'	35:n:72:VAL:HG21	1.97	0.47
32:k:154:VAL:CG1	32:k:169:LYS:HB3	2.26	0.47
14:d:377:GLY:HA3	14:d:378:LEU:HA	1.69	0.47
25:e:276:SER:HB2	25:e:311:ARG:HB2	1.97	0.47
20:4:107:U:H1'	37:s:47:TYR:CE2	2.49	0.47
20:4:265:U:H5''	36:u:83:ARG:HE	1.80	0.47
21:2:45:A:H2'	21:2:46:G:C8	2.50	0.47
22:3:214:C:H2'	22:3:215:G:C8	2.50	0.47
23:a:55:LYS:HE2	28:v:56:VAL:HA	1.96	0.47
39:i:307:ILE:HA	39:i:313:THR:HA	1.97	0.47
2:C:296:ARG:NH1	3:D:929:UNK:O	2.47	0.46
5:L:151:VAL:O	5:L:170:SER:N	2.38	0.46
18:w:129:GLN:O	18:w:133:ALA:CB	2.63	0.46
18:w:158:SER:HA	18:w:161:TRP:HB3	1.97	0.46
20:4:59:A:H2'	20:4:60:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:e:258:LEU:HD12	25:e:261:GLY:HA2	1.96	0.46
32:k:125:VAL:HG11	32:k:188:VAL:HG22	1.96	0.46
37:s:26:HIS:HB2	37:s:30:TRP:H	1.80	0.46
40:x:66:LEU:HA	40:x:119:TYR:HD2	1.79	0.46
2:C:571:LEU:HA	2:C:574:LEU:HD12	1.97	0.46
5:L:212:LYS:O	5:L:216:ASP:HB2	2.16	0.46
7:P:168:PRO:HB3	7:P:210:PHE:CD1	2.50	0.46
10:W:6:UNK:HA	14:d:345:ARG:NH2	2.24	0.46
20:4:8:U:H4'	20:4:9:C:H5''	1.97	0.46
20:4:328:A:C6	20:4:394:G:C6	3.03	0.46
21:2:52:G:N1	21:2:90:U:O2	2.48	0.46
21:2:184:C:H2'	21:2:185:G:H8	1.80	0.46
40:x:370:ALA:HA	40:x:373:LEU:HB2	1.97	0.46
41:c:220:TRP:HZ3	41:c:222:TRP:HB2	1.80	0.46
20:4:270:C:OP2	35:n:73:ASN:HB3	2.16	0.46
23:a:139:LEU:HD23	23:a:141:LEU:HD11	1.97	0.46
34:m:44:LYS:HD3	34:m:44:LYS:HA	1.73	0.46
39:i:338:VAL:HG12	39:i:373:ALA:HB3	1.97	0.46
20:4:57:A:H2'	20:4:58:A:C8	2.50	0.46
21:2:130:A:N6	21:2:140:G:H1	2.13	0.46
33:j:117:ILE:HD13	33:j:134:LEU:HD23	1.96	0.46
7:P:209:ASN:OD1	21:2:10:G:N2	2.47	0.46
15:f:24:LYS:HE3	18:w:168:GLU:CG	2.45	0.46
19:1:23:C:H2'	19:1:24:A:C8	2.50	0.46
22:3:24:C:H2'	22:3:25:A:C8	2.51	0.46
24:b:168:LEU:HA	28:v:61:LYS:HZ1	1.81	0.46
15:f:74:ASP:OD1	15:f:74:ASP:N	2.49	0.46
16:p:38:LEU:HD21	16:p:56:LEU:HD11	1.97	0.46
17:r:282:ARG:NH1	22:3:189:A:OP1	2.45	0.46
21:2:54:G:H5''	21:2:55:A:H5'	1.97	0.46
22:3:82:A:H4'	22:3:271:C:H2'	1.97	0.46
40:x:337:ASN:H	40:x:406:THR:HG1	1.64	0.46
5:M:129:LEU:HD23	5:M:227:LEU:HD23	1.97	0.46
15:f:88:THR:HG23	15:f:89:VAL:HG13	1.97	0.46
20:4:340:C:H2'	20:4:341:A:H8	1.79	0.46
23:a:99:THR:HG22	23:a:155:LEU:HD13	1.97	0.46
4:K:132:UNK:O	4:K:136:UNK:N	2.48	0.46
5:L:104:LYS:N	5:L:117:THR:O	2.44	0.46
5:M:92:PRO:HG2	5:M:95:ILE:HG12	1.98	0.46
7:P:168:PRO:HD2	21:2:30:G:H5'	1.98	0.46
19:1:5:U:O4	25:e:280:MET:HE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:163:G:H2'	22:3:164:A:H8	1.81	0.46
24:b:253:HIS:CG	24:b:254:CYS:H	2.33	0.46
28:v:20:LEU:HD11	28:v:32:PRO:HG2	1.96	0.46
31:h:101:VAL:HG12	31:h:103:PHE:H	1.80	0.46
32:k:178:ALA:HB3	32:k:209:LEU:HG	1.97	0.46
39:i:320:LYS:HD3	39:i:322:SER:H	1.79	0.46
23:a:65:LEU:HD13	24:b:164:PRO:HG3	1.98	0.46
38:g:190:PRO:N	38:g:265:ARG:HH12	2.14	0.46
41:c:185:PHE:HB3	41:c:220:TRP:HZ2	1.81	0.46
5:L:81:GLU:HA	5:L:84:TYR:HB3	1.98	0.46
20:4:75:U:OP1	33:j:181:ARG:NH2	2.47	0.46
21:2:28:U:H2'	21:2:29:C:C6	2.51	0.46
22:3:399:C:H2'	22:3:400:A:H8	1.81	0.46
23:a:181:GLN:O	23:a:226:ARG:NH1	2.49	0.46
31:h:82:PHE:O	31:h:86:SER:HB3	2.16	0.46
31:h:82:PHE:HA	31:h:111:LEU:HD22	1.98	0.46
38:g:261:ALA:O	38:g:265:ARG:HB3	2.16	0.46
19:1:78:A:H61	21:2:133:G:H1'	1.81	0.45
40:x:139:LEU:HB3	40:x:426:VAL:HG12	1.98	0.45
6:O:375:LEU:HD11	6:O:416:VAL:HG23	1.98	0.45
19:1:23:C:H2'	19:1:24:A:H8	1.81	0.45
20:4:240:A:H5''	34:m:26:GLY:H	1.81	0.45
21:2:23:G:H2'	21:2:24:G:H8	1.81	0.45
22:3:364:U:H2'	22:3:365:G:C8	2.51	0.45
35:n:48:LEU:O	35:n:51:ARG:NH1	2.49	0.45
5:L:100:PRO:O	5:L:103:PHE:N	2.49	0.45
7:P:67:ARG:HD2	21:2:69:U:P	2.56	0.45
22:3:145:U:O4	32:k:132:ASN:HA	2.16	0.45
22:3:301:G:H1	22:3:325:U:H3	1.64	0.45
32:k:125:VAL:HG23	32:k:186:VAL:HG11	1.97	0.45
33:j:211:THR:OG1	33:j:212:ASN:N	2.50	0.45
35:n:15:ARG:HB3	35:n:16:GLY:H	1.56	0.45
6:O:427:ALA:HB2	6:O:459:LEU:HD23	1.97	0.45
24:b:257:LEU:HD13	24:b:363:ARG:HG3	1.99	0.45
35:n:32:VAL:CG1	42:y:153:LEU:HD11	2.45	0.45
5:N:130:HIS:HE1	5:N:132:ASN:HB2	1.81	0.45
6:O:309:GLY:O	6:O:313:ALA:CB	2.63	0.45
15:f:10:ALA:HB3	15:f:63:HIS:HB3	1.97	0.45
17:r:266:PRO:HB3	22:3:173:C:H5'	1.98	0.45
20:4:156:U:H2'	20:4:157:G:H8	1.82	0.45
22:3:399:C:H2'	22:3:400:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:211:ASN:HD21	24:b:220:LEU:CD2	2.21	0.45
2:C:287:TYR:HA	2:C:290:ASN:HD22	1.82	0.45
2:C:862:PRO:HG2	25:e:284:ALA:HB3	1.98	0.45
5:L:232:TYR:O	5:L:236:GLN:OE1	2.35	0.45
31:h:105:LEU:HD12	31:h:166:LEU:HD13	1.97	0.45
32:k:134:ILE:O	32:k:150:SER:HA	2.17	0.45
40:x:126:LEU:HG	40:x:155:LEU:HD13	1.98	0.45
40:x:165:LEU:HD13	40:x:212:LEU:HD23	1.98	0.45
2:C:299:ASP:OD1	2:C:302:ARG:N	2.40	0.45
2:C:475:GLU:HA	2:C:478:VAL:HG22	1.97	0.45
6:O:278:LEU:O	6:O:282:ARG:HB2	2.16	0.45
22:3:173:C:H3'	22:3:174:G:H2'	1.98	0.45
23:a:104:VAL:HG23	24:b:414:LEU:HD21	1.98	0.45
34:m:19:LEU:HA	34:m:19:LEU:HD23	1.87	0.45
40:x:331:PHE:HD2	40:x:375:LEU:HD21	1.82	0.45
2:C:979:ARG:HH22	16:p:18:TRP:HE1	1.63	0.45
5:N:159:LYS:HB3	5:N:162:ARG:HH12	1.80	0.45
6:O:289:LEU:HD23	6:O:289:LEU:HA	1.89	0.45
26:o:108:LYS:HA	26:o:111:LEU:HD12	1.98	0.45
26:o:179:LEU:HA	26:o:182:MET:HE2	1.98	0.45
32:k:127:ILE:O	32:k:191:LYS:N	2.49	0.45
32:k:134:ILE:HD13	32:k:197:LYS:CA	2.45	0.45
1:B:838:ARG:HE	1:B:841:ARG:HH11	1.65	0.45
5:M:166:PHE:HE1	5:M:180:VAL:HG13	1.82	0.45
22:3:82:A:H3'	22:3:83:G:H8	1.80	0.45
24:b:244:LEU:HD13	24:b:244:LEU:HA	1.81	0.45
32:k:122:GLU:CB	32:k:141:LYS:HG2	2.46	0.45
37:s:44:ILE:O	37:s:63:GLY:N	2.48	0.45
15:f:11:LYS:HG2	15:f:14:LEU:HD11	1.98	0.45
20:4:173:U:H2'	20:4:174:G:C8	2.52	0.45
35:n:38:LYS:HD2	35:n:58:PHE:HB3	1.97	0.45
2:C:400:LEU:HD11	2:C:487:GLU:HG2	1.98	0.44
5:M:112:THR:OG1	5:M:130:HIS:NE2	2.50	0.44
5:N:114:LEU:HB2	5:N:129:LEU:HB2	1.99	0.44
19:1:8:A:H2'	19:1:9:G:H8	1.82	0.44
20:4:60:A:H2'	20:4:61:A:C8	2.52	0.44
21:2:181:A:H2'	21:2:182:A:H8	1.82	0.44
25:e:212:ARG:NH1	25:e:214:GLU:OE2	2.44	0.44
32:k:186:VAL:O	32:k:211:ILE:HA	2.16	0.44
34:m:41:LYS:HA	34:m:41:LYS:HD2	1.74	0.44
38:g:159:UNK:O	38:g:163:UNK:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:151:VAL:N	5:L:170:SER:O	2.47	0.44
7:P:302:ALA:O	7:P:347:LYS:NZ	2.42	0.44
20:4:398:U:H2'	20:4:399:G:H8	1.81	0.44
32:k:187:GLN:HA	32:k:213:SER:O	2.17	0.44
33:j:175:LEU:HD12	33:j:176:PRO:HD2	1.98	0.44
5:N:158:ALA:HB1	5:N:185:LYS:HE2	1.98	0.44
6:O:418:VAL:HG12	6:O:422:ARG:HH12	1.82	0.44
20:4:139:A:H2'	20:4:140:A:C8	2.52	0.44
20:4:306:C:O2	20:4:309:A:O2'	2.34	0.44
22:3:366:C:H2'	22:3:367:U:H6	1.83	0.44
28:v:100:MET:HE3	28:v:100:MET:HB3	1.75	0.44
31:h:250:ALA:HB2	31:h:276:ARG:HG2	2.00	0.44
34:m:21:ARG:HH22	34:m:44:LYS:HD3	1.83	0.44
2:C:418:GLN:HG2	2:C:464:ARG:HG2	1.99	0.44
5:N:116:LEU:HD11	5:N:226:TYR:HE2	1.83	0.44
13:Z:48:UNK:O	13:Z:52:UNK:N	2.51	0.44
21:2:143:C:H2'	21:2:144:A:C8	2.53	0.44
22:3:347:A:H2'	22:3:349:A:H8	1.81	0.44
34:m:87:ARG:HA	34:m:90:VAL:HG22	1.99	0.44
34:m:91:ARG:HA	34:m:91:ARG:HD3	1.79	0.44
2:C:957:TYR:HE1	2:C:959:ALA:HB2	1.82	0.44
7:P:35:TRP:CZ3	21:2:65:C:H5''	2.52	0.44
19:1:5:U:O4	31:h:231:ARG:NH2	2.50	0.44
22:3:36:G:H2'	22:3:37:G:C8	2.52	0.44
32:k:125:VAL:HG22	32:k:137:THR:O	2.17	0.44
32:k:190:LEU:HD12	32:k:216:ASP:HB2	1.99	0.44
34:m:75:ARG:HH22	34:m:116:LEU:HA	1.83	0.44
5:L:102:PRO:HD2	5:L:118:ARG:HD2	2.00	0.44
22:3:126:G:C6	22:3:170:A:N1	2.86	0.44
22:3:133:U:O2	22:3:163:G:N2	2.48	0.44
23:a:93:GLU:HB3	23:a:94:ARG:HD2	2.00	0.44
31:h:286:GLU:HG2	31:h:294:VAL:HG22	1.99	0.44
35:n:94:MET:SD	35:n:94:MET:N	2.90	0.44
15:f:2:PRO:HB2	15:f:4:TYR:CE1	2.53	0.44
15:f:30:VAL:HG12	15:f:79:LEU:HD21	2.00	0.44
20:4:22:A:H2'	20:4:24:U:H3	1.82	0.44
22:3:365:G:N3	22:3:384:C:O2'	2.47	0.44
25:e:346:ARG:HD2	25:e:347:GLU:H	1.83	0.44
32:k:129:ASN:CB	32:k:197:LYS:HB2	2.48	0.44
32:k:185:SER:HB3	32:k:212:THR:HA	1.99	0.44
34:m:56:VAL:O	34:m:60:ILE:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:PRO:HA	2:C:576:PRO:HD3	1.86	0.44
8:U:9:UNK:C	8:U:11:UNK:N	2.81	0.44
8:U:28:UNK:C	8:U:30:UNK:N	2.81	0.44
15:f:72:SER:OG	26:o:120:VAL:HA	2.18	0.44
21:2:19:A:N1	27:z:72:GLN:NE2	2.66	0.44
21:2:76:C:O3'	29:q:63:ARG:NH1	2.51	0.44
24:b:432:PRO:HA	24:b:435:LEU:HD13	1.99	0.44
37:s:26:HIS:CD2	37:s:31:ASN:HB2	2.53	0.44
5:M:152:ALA:HA	5:M:169:GLU:HA	2.00	0.44
19:1:18:U:O3'	22:3:85:C:N4	2.51	0.44
20:4:15:U:P	41:c:207:ARG:HH22	2.41	0.44
20:4:17:G:H1	20:4:87:U:H3	1.64	0.44
20:4:259:U:O4	20:4:286:A:N7	2.50	0.44
20:4:358:C:H42	20:4:368:C:H41	1.65	0.44
22:3:71:C:OP1	25:e:314:ARG:NH2	2.51	0.44
23:a:68:LEU:CD2	24:b:141:VAL:HG12	2.48	0.44
24:b:430:ILE:HD11	24:b:434:VAL:HG11	2.00	0.44
27:z:47:VAL:N	27:z:62:TRP:O	2.47	0.44
42:y:180:GLU:OE1	42:y:183:ARG:NH1	2.50	0.44
7:P:204:LEU:HD21	7:P:293:VAL:HG22	1.98	0.43
18:w:114:GLU:HG3	18:w:117:ARG:NH1	2.33	0.43
24:b:422:GLU:OE2	24:b:426:ARG:NE	2.51	0.43
32:k:151:ALA:O	32:k:154:VAL:HG23	2.17	0.43
38:g:190:PRO:HD3	38:g:265:ARG:HH22	1.82	0.43
41:c:207:ARG:HD3	41:c:245:MET:HE2	2.00	0.43
10:W:15:UNK:HA	14:d:385:VAL:HG12	2.00	0.43
20:4:262:U:H3	20:4:283:G:H1	1.65	0.43
22:3:361:A:H2'	22:3:362:U:C6	2.53	0.43
23:a:77:SER:CB	24:b:170:ASN:HD21	2.32	0.43
2:C:975:TYR:HE2	3:D:937:UNK:CB	2.31	0.43
5:L:75:SER:OG	5:L:247:GLU:OE1	2.36	0.43
20:4:111:C:H5''	20:4:112:U:H5''	1.99	0.43
22:3:13:C:H2'	22:3:14:A:C8	2.53	0.43
22:3:197:A:H2'	22:3:198:G:H8	1.83	0.43
23:a:72:ASN:HB3	28:v:84:PHE:HA	2.01	0.43
23:a:172:GLU:OE1	23:a:226:ARG:NH2	2.51	0.43
30:l:77:ALA:HA	30:l:107:LEU:HB2	1.99	0.43
31:h:58:MET:O	31:h:64:GLN:NE2	2.51	0.43
32:k:151:ALA:HB1	32:k:166:ALA:CB	2.46	0.43
32:k:171:ALA:HB1	32:k:204:LEU:HG	2.00	0.43
39:i:399:GLN:OE1	39:i:402:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:c:235:ASP:OD1	41:c:236:TYR:N	2.51	0.43
2:C:474:VAL:HA	2:C:477:VAL:HG12	1.99	0.43
7:P:151:ASP:HA	7:P:154:VAL:HG22	2.01	0.43
22:3:328:A:H2'	22:3:329:A:C8	2.53	0.43
22:3:362:U:OP1	34:m:110:ALA:N	2.52	0.43
23:a:184:SER:HB2	23:a:222:LEU:HD11	1.99	0.43
32:k:190:LEU:HG	32:k:215:ALA:O	2.18	0.43
12:Y:45:UNK:O	12:Y:49:UNK:N	2.51	0.43
15:f:10:ALA:N	15:f:63:HIS:O	2.52	0.43
19:1:92:C:H2'	19:1:93:G:H8	1.84	0.43
20:4:152:A:N1	20:4:283:G:H1'	2.33	0.43
31:h:237:PHE:HB2	31:h:249:ASP:HB3	2.00	0.43
41:c:202:VAL:HG22	41:c:252:VAL:HG13	1.98	0.43
5:M:103:PHE:HB3	5:M:116:LEU:HD22	2.01	0.43
20:4:101:A:N6	22:3:405:U:H3	2.05	0.43
20:4:260:A:N6	20:4:285:G:H1'	2.31	0.43
20:4:273:U:H3'	22:3:390:A:H61	1.82	0.43
20:4:398:U:H2'	20:4:399:G:C8	2.54	0.43
21:2:177:G:H2'	21:2:178:G:H8	1.83	0.43
22:3:169:A:H2'	22:3:170:A:C8	2.54	0.43
39:i:429:ARG:HA	39:i:429:ARG:HD2	1.75	0.43
40:x:66:LEU:HA	40:x:66:LEU:HD23	1.88	0.43
6:O:437:LEU:HB3	6:O:442:LEU:HB2	2.00	0.43
7:P:370:THR:HA	7:P:373:VAL:HG12	2.00	0.43
15:f:53:ARG:HD2	15:f:53:ARG:HA	1.88	0.43
22:3:140:A:N6	22:3:156:U:O2	2.47	0.43
23:a:143:VAL:HA	23:a:155:LEU:HA	2.00	0.43
40:x:292:ASP:OD1	40:x:292:ASP:N	2.51	0.43
3:D:260:UNK:O	3:D:265:UNK:N	2.52	0.43
22:3:325:U:OP2	30:l:34:ARG:NH1	2.52	0.43
32:k:136:LEU:HB2	32:k:149:THR:OG1	2.18	0.43
41:c:178:TRP:NE1	41:c:182:GLU:OE1	2.51	0.43
2:C:385:LEU:HA	2:C:388:VAL:HG22	2.01	0.43
5:L:95:ILE:HA	5:L:226:TYR:CE1	2.54	0.43
6:O:325:LEU:HD11	6:O:329:PRO:HD3	2.00	0.43
6:O:499:ASP:OD1	6:O:500:GLN:N	2.51	0.43
21:2:49:U:O4	22:3:320:A:H1'	2.18	0.43
22:3:137:A:O2'	32:k:144:LEU:HB2	2.17	0.43
25:e:179:LEU:HD12	25:e:179:LEU:HA	1.89	0.43
25:e:255:ALA:HB3	28:v:23:ASP:HA	2.00	0.43
25:e:262:HIS:CD2	25:e:284:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:117:ILE:HB	33:j:207:LEU:HB2	2.01	0.43
36:u:69:ASP:OD1	36:u:70:ASN:N	2.52	0.43
5:L:99:PRO:HA	5:L:100:PRO:HD3	1.84	0.43
23:a:75:LEU:HD21	28:v:79:VAL:HG21	2.00	0.43
23:a:76:PRO:HA	24:b:168:LEU:HD11	2.01	0.43
31:h:239:CYS:HA	31:h:261:VAL:HA	2.00	0.43
39:i:393:ARG:HH22	39:i:422:TRP:HE3	1.66	0.43
1:B:829:PRO:HA	42:y:150:ALA:HB1	2.01	0.42
19:1:8:A:H5''	25:e:317:ARG:HH22	1.84	0.42
21:2:96:U:H2'	21:2:97:U:H6	1.83	0.42
24:b:143:PRO:HD2	24:b:413:HIS:CE1	2.54	0.42
24:b:146:LEU:HD23	24:b:146:LEU:HA	1.88	0.42
28:v:20:LEU:HD23	28:v:20:LEU:HA	1.91	0.42
38:g:185:VAL:C	38:g:189:LYS:HZ2	2.27	0.42
15:f:42:SER:O	18:w:179:GLU:HB2	2.19	0.42
15:f:52:LEU:HG	15:f:53:ARG:H	1.84	0.42
20:4:198:U:N3	20:4:202:A:C6	2.87	0.42
22:3:336:G:H5'	25:e:207:ARG:HD2	2.00	0.42
24:b:157:GLN:HA	31:h:103:PHE:HE1	1.84	0.42
33:j:129:MET:HE3	33:j:129:MET:HB3	1.86	0.42
39:i:320:LYS:HD3	39:i:321:ALA:N	2.34	0.42
18:w:166:ASP:OD1	18:w:166:ASP:N	2.49	0.42
22:3:370:U:H3	22:3:374:A:H2	1.66	0.42
25:e:282:ARG:HA	25:e:282:ARG:HD3	1.75	0.42
32:k:156:TYR:CE1	32:k:166:ALA:HA	2.54	0.42
40:x:195:LEU:HD13	40:x:294:ALA:HA	2.01	0.42
5:N:79:ARG:NH2	5:N:247:GLU:OE1	2.53	0.42
7:P:92:VAL:HG13	7:P:148:LEU:HD22	2.01	0.42
7:P:158:ARG:NH1	20:4:359:A:O3'	2.51	0.42
20:4:198:U:O2'	40:x:286:ARG:NH2	2.51	0.42
21:2:43:G:OP1	29:q:38:ARG:NH1	2.52	0.42
22:3:196:G:H2'	22:3:197:A:H8	1.84	0.42
31:h:172:ARG:HD3	31:h:204:LEU:HD11	2.00	0.42
32:k:157:LYS:H	32:k:160:ARG:HG3	1.85	0.42
5:L:129:LEU:HD13	5:L:231:ILE:HB	2.00	0.42
5:L:214:LEU:HD23	5:L:214:LEU:HA	1.91	0.42
14:d:342:THR:HG21	14:d:379:LEU:HD13	2.01	0.42
20:4:57:A:H5''	24:b:250:ARG:HA	2.02	0.42
20:4:122:U:H2'	20:4:123:U:C6	2.54	0.42
20:4:214:U:H2'	20:4:215:U:C6	2.54	0.42
22:3:279:U:P	31:h:133:ARG:HH22	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:l:113:ARG:NH2	30:l:114:TYR:OH	2.52	0.42
32:k:142:GLN:HB2	32:k:144:LEU:HG	2.01	0.42
2:C:937:THR:OG1	2:C:938:ARG:N	2.52	0.42
5:L:203:ASP:HB3	5:L:206:LEU:HG	2.02	0.42
19:1:30:C:H41	21:2:174:U:H5'	1.85	0.42
20:4:11:U:O2'	20:4:14:A:OP2	2.36	0.42
22:3:55:U:H2'	22:3:56:G:H8	1.84	0.42
32:k:156:TYR:CG	32:k:166:ALA:CB	3.02	0.42
40:x:422:VAL:O	40:x:424:HIS:ND1	2.47	0.42
5:L:104:LYS:O	5:L:117:THR:N	2.49	0.42
5:M:242:TRP:HE3	5:M:243:LEU:HD22	1.85	0.42
15:f:40:LEU:HD12	15:f:67:MET:HA	2.02	0.42
20:4:5:A:H2'	20:4:6:G:H8	1.84	0.42
24:b:420:PHE:HD2	24:b:421:LEU:HD12	1.85	0.42
31:h:176:PHE:HZ	31:h:192:PRO:HG2	1.85	0.42
34:m:91:ARG:O	34:m:95:GLY:N	2.35	0.42
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.80	0.42
5:L:238:GLU:OE1	5:L:241:ASN:ND2	2.46	0.42
20:4:173:U:H2'	20:4:174:G:H8	1.85	0.42
20:4:284:U:H3'	20:4:285:G:C8	2.54	0.42
20:4:356:U:O2	20:4:370:G:C2	2.73	0.42
39:i:335:GLY:O	39:i:371:VAL:N	2.45	0.42
2:C:886:LEU:O	2:C:890:VAL:HB	2.20	0.42
17:r:238:VAL:HA	17:r:256:TRP:HZ3	1.85	0.42
21:2:30:G:H2'	21:2:31:G:H8	1.85	0.42
21:2:123:C:H2'	21:2:124:G:C8	2.54	0.42
22:3:163:G:H2'	22:3:164:A:C8	2.54	0.42
24:b:200:VAL:HG11	24:b:367:LEU:HD22	2.01	0.42
24:b:229:ASN:HB3	24:b:428:VAL:HG22	2.02	0.42
26:o:140:ARG:HG3	26:o:141:HIS:HB2	2.01	0.42
28:v:86:PRO:HA	28:v:87:PRO:HD3	1.91	0.42
32:k:211:ILE:HB	32:k:213:SER:O	2.20	0.42
22:3:137:A:H2	32:k:145:ILE:HB	1.85	0.42
32:k:121:LEU:HB2	32:k:183:TYR:CA	2.46	0.42
32:k:142:GLN:HB2	32:k:144:LEU:CD2	2.49	0.42
35:n:89:ARG:HA	42:y:161:TRP:CH2	2.55	0.42
36:u:85:GLN:NE2	36:u:86:LEU:O	2.52	0.42
40:x:144:ALA:HB2	40:x:408:ALA:HB3	2.01	0.42
5:L:171:ASP:OD1	5:L:174:SER:N	2.53	0.41
5:M:79:ARG:HH22	5:M:82:VAL:HG11	1.85	0.41
15:f:12:PRO:HG3	15:f:62:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:11:A:N6	22:3:59:A:O4'	2.53	0.41
27:z:34:ASP:OD1	27:z:34:ASP:N	2.49	0.41
32:k:204:LEU:HA	32:k:207:ALA:HB3	2.01	0.41
34:m:81:GLU:OE2	34:m:86:SER:OG	2.36	0.41
35:n:65:ASP:OD1	35:n:65:ASP:N	2.53	0.41
5:N:156:SER:HB2	5:N:163:VAL:HG11	2.01	0.41
7:P:58:ASP:OD1	7:P:58:ASP:N	2.46	0.41
13:Z:81:UNK:O	13:Z:85:UNK:N	2.52	0.41
20:4:128:U:OP1	38:g:231:ARG:NH2	2.53	0.41
20:4:129:G:H2'	20:4:130:G:C8	2.53	0.41
29:q:159:ARG:O	29:q:163:LEU:HD12	2.20	0.41
32:k:211:ILE:HG13	32:k:214:LEU:HB2	2.01	0.41
5:L:108:ALA:HB3	5:L:111:ASP:HB2	2.02	0.41
7:P:378:GLN:HA	7:P:379:PRO:HD3	1.93	0.41
20:4:59:A:H2'	20:4:60:A:C8	2.55	0.41
20:4:404:A:OP1	30:l:55:LYS:NZ	2.53	0.41
22:3:91:G:O3'	26:o:177:ARG:NH2	2.54	0.41
32:k:156:TYR:CD2	32:k:160:ARG:HB2	2.46	0.41
32:k:188:VAL:N	32:k:213:SER:O	2.44	0.41
33:j:185:ILE:HG12	33:j:195:MET:HE1	2.02	0.41
5:M:79:ARG:HH12	5:M:82:VAL:HG21	1.84	0.41
19:1:97:G:H1	21:2:39:U:H3	1.68	0.41
21:2:174:U:H1'	21:2:203:G:H22	1.85	0.41
21:2:198:A:H3'	21:2:199:U:H6	1.84	0.41
22:3:63:U:H2'	22:3:64:A:H8	1.85	0.41
28:v:129:LEU:HD23	28:v:129:LEU:HA	1.93	0.41
7:P:67:ARG:HD2	21:2:69:U:OP1	2.19	0.41
22:3:362:U:H2'	22:3:363:A:C8	2.54	0.41
23:a:165:LYS:HZ2	28:v:136:LEU:HB2	1.84	0.41
32:k:192:GLY:H	32:k:218:THR:CG2	2.33	0.41
34:m:18:ALA:O	34:m:21:ARG:NE	2.54	0.41
5:L:206:LEU:HD11	5:M:81:GLU:HG3	2.02	0.41
5:M:162:ARG:HE	5:M:182:LEU:HD21	1.85	0.41
14:d:373:MET:HE1	21:2:210:C:H5''	2.01	0.41
22:3:134:C:N4	22:3:135:G:O6	2.54	0.41
22:3:217:G:H2'	22:3:264:G:N2	2.36	0.41
23:a:55:LYS:HE2	28:v:56:VAL:HG23	2.02	0.41
37:s:10:TYR:CD2	37:s:54:LEU:HD21	2.56	0.41
38:g:210:LEU:HD11	38:g:214:GLN:HB2	2.02	0.41
39:i:405:THR:HG23	39:i:407:GLY:H	1.84	0.41
40:x:165:LEU:HB2	40:x:327:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:979:ARG:NH2	16:p:18:TRP:HE1	2.19	0.41
5:N:127:VAL:HG13	5:N:155:VAL:HG22	2.03	0.41
7:P:43:LEU:HA	7:P:46:MET:HG3	2.02	0.41
7:P:392:TRP:O	7:P:402:ARG:NH2	2.41	0.41
15:f:38:THR:HA	18:w:161:TRP:HE3	1.84	0.41
20:4:56:A:H2'	20:4:57:A:H8	1.86	0.41
20:4:225:C:H2'	20:4:226:U:C6	2.55	0.41
22:3:71:C:H4'	22:3:72:U:H3'	2.03	0.41
22:3:142:C:OP1	32:k:152:GLY:HA3	2.20	0.41
25:e:294:LEU:HA	25:e:297:LEU:HB2	2.01	0.41
32:k:123:GLY:CA	32:k:186:VAL:HG13	2.50	0.41
22:3:348:G:O2'	22:3:350:U:OP2	2.31	0.41
22:3:348:G:H1'	22:3:352:C:H42	1.86	0.41
24:b:148:ARG:HB3	24:b:149:VAL:H	1.70	0.41
41:c:220:TRP:CZ3	41:c:222:TRP:HB2	2.56	0.41
2:C:390:SER:O	2:C:394:ARG:HG2	2.20	0.41
2:C:870:TYR:CE2	25:e:347:GLU:HB2	2.56	0.41
5:M:106:THR:OG1	5:M:115:THR:OG1	2.35	0.41
5:N:75:SER:OG	5:N:247:GLU:OE1	2.39	0.41
6:O:282:ARG:HA	6:O:285:ARG:HB2	2.02	0.41
7:P:220:LEU:HD22	7:P:324:ALA:HB2	2.03	0.41
14:d:326:ASP:HA	25:e:285:GLY:HA3	2.03	0.41
15:f:20:VAL:HG13	18:w:171:ILE:HG21	2.02	0.41
17:r:285:ARG:NH1	22:3:188:C:O5'	2.41	0.41
20:4:72:U:H2'	20:4:73:U:C5	2.56	0.41
20:4:107:U:H1'	37:s:47:TYR:HE2	1.86	0.41
20:4:419:G:H2'	20:4:420:G:C8	2.56	0.41
21:2:60:G:H4'	29:q:17:LYS:HE2	2.02	0.41
22:3:50:U:H2'	22:3:51:G:C8	2.55	0.41
24:b:220:LEU:HD13	24:b:220:LEU:HA	1.91	0.41
25:e:193:ASP:OD1	25:e:194:ARG:N	2.50	0.41
25:e:264:LEU:HG	25:e:303:LEU:HD11	2.02	0.41
26:o:234:UNK:HA	29:q:52:VAL:HG23	2.02	0.41
32:k:127:ILE:HG13	32:k:190:LEU:HD23	2.02	0.41
35:n:36:VAL:O	35:n:40:VAL:HG23	2.21	0.41
35:n:40:VAL:HG22	42:y:148:ALA:HB3	2.02	0.41
37:s:74:GLU:OE2	37:s:75:VAL:N	2.54	0.41
41:c:129:GLU:HG3	41:c:130:VAL:HG23	2.03	0.41
41:c:211:LYS:O	41:c:211:LYS:CG	2.66	0.41
42:y:142:GLU:H	42:y:147:ARG:HH12	1.68	0.41
2:C:571:LEU:O	2:C:579:ARG:NE	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:w:81:ASP:OD1	18:w:81:ASP:N	2.48	0.41
23:a:65:LEU:HD22	24:b:164:PRO:HG2	2.03	0.41
31:h:173:THR:H	31:h:178:ARG:HH12	1.69	0.41
33:j:186:ARG:N	33:j:194:GLY:O	2.34	0.41
40:x:412:LEU:HD23	40:x:412:LEU:HA	1.89	0.41
9:V:194:UNK:O	31:h:330:ARG:NH2	2.52	0.40
15:f:6:LEU:O	15:f:66:GLN:HA	2.21	0.40
20:4:418:U:O2'	20:4:419:G:O4'	2.38	0.40
21:2:68:U:O2'	21:2:69:U:O5'	2.39	0.40
21:2:113:U:P	30:l:29:ARG:HH21	2.44	0.40
23:a:118:HIS:HD2	23:a:140:ARG:HH21	1.68	0.40
24:b:232:VAL:C	24:b:233:TRP:HD1	2.29	0.40
29:q:26:VAL:HG22	29:q:37:LYS:HG2	2.03	0.40
30:l:113:ARG:HA	30:l:113:ARG:HD2	1.62	0.40
38:g:273:LEU:HD13	38:g:276:ARG:HH12	1.86	0.40
19:1:82:G:N3	21:2:161:A:O2'	2.54	0.40
20:4:86:G:H2'	20:4:87:U:C6	2.55	0.40
22:3:137:A:C2	32:k:145:ILE:HB	2.56	0.40
22:3:372:A:N1	37:s:68:LYS:HB3	2.34	0.40
23:a:70:ARG:HD3	23:a:70:ARG:HA	1.78	0.40
2:C:582:LEU:HD23	2:C:582:LEU:HA	1.92	0.40
7:P:35:TRP:HZ3	21:2:65:C:H5''	1.86	0.40
7:P:38:GLY:HA2	7:P:68:ARG:HE	1.86	0.40
10:W:30:UNK:O	10:W:31:UNK:CB	2.69	0.40
18:w:173:ARG:HE	18:w:173:ARG:HB2	1.69	0.40
22:3:10:G:H1'	22:3:11:A:H2'	2.04	0.40
22:3:292:U:H2'	22:3:293:A:C8	2.57	0.40
29:q:51:SER:O	29:q:51:SER:OG	2.35	0.40
34:m:84:ILE:HG22	34:m:86:SER:HB3	2.03	0.40
2:C:857:LEU:HA	2:C:857:LEU:HD23	1.89	0.40
7:P:215:LEU:HD22	7:P:297:LEU:HG	2.02	0.40
20:4:231:C:H42	37:s:85:GLY:HA3	1.85	0.40
22:3:62:A:H2'	22:3:63:U:C6	2.57	0.40
33:j:249:ASP:OD1	33:j:250:VAL:N	2.55	0.40
34:m:53:ILE:HA	34:m:56:VAL:HG22	2.03	0.40
37:s:49:ARG:HB2	37:s:85:GLY:CA	2.50	0.40
37:s:68:LYS:HE3	37:s:68:LYS:HB2	1.85	0.40
38:g:221:LYS:HE3	38:g:225:GLN:HE22	1.86	0.40
41:c:178:TRP:CG	41:c:218:LYS:HE3	2.57	0.40
2:C:451:GLY:O	2:C:455:TYR:N	2.51	0.40
4:K:24:UNK:O	4:K:28:UNK:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:78:LEU:HD11	5:L:246:VAL:HG13	2.03	0.40
5:N:130:HIS:CE1	5:N:132:ASN:HB2	2.56	0.40
6:O:359:LEU:HD11	6:O:390:VAL:HG13	2.02	0.40
28:v:122:GLN:HA	28:v:125:ARG:HE	1.87	0.40
31:h:109:SER:H	31:h:112:ALA:HB3	1.86	0.40
40:x:112:THR:HB	40:x:447:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	51/883 (6%)	44 (86%)	6 (12%)	1 (2%)	6	32
2	C	355/999 (36%)	341 (96%)	14 (4%)	0	100	100
5	L	171/271 (63%)	164 (96%)	7 (4%)	0	100	100
5	M	170/271 (63%)	166 (98%)	4 (2%)	0	100	100
5	N	173/271 (64%)	172 (99%)	1 (1%)	0	100	100
6	O	232/516 (45%)	224 (97%)	8 (3%)	0	100	100
7	P	329/416 (79%)	325 (99%)	4 (1%)	0	100	100
14	d	127/415 (31%)	117 (92%)	10 (8%)	0	100	100
15	f	101/122 (83%)	96 (95%)	4 (4%)	1 (1%)	12	47
16	p	77/88 (88%)	68 (88%)	9 (12%)	0	100	100
17	r	54/356 (15%)	50 (93%)	4 (7%)	0	100	100
18	w	153/193 (79%)	139 (91%)	14 (9%)	0	100	100
23	a	208/253 (82%)	192 (92%)	15 (7%)	1 (0%)	24	62
24	b	237/530 (45%)	216 (91%)	20 (8%)	1 (0%)	30	66
25	e	174/368 (47%)	156 (90%)	17 (10%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	o	140/319 (44%)	134 (96%)	6 (4%)	0	100	100
27	z	81/133 (61%)	73 (90%)	8 (10%)	0	100	100
28	v	126/190 (66%)	117 (93%)	9 (7%)	0	100	100
29	q	143/220 (65%)	136 (95%)	7 (5%)	0	100	100
30	l	102/128 (80%)	91 (89%)	10 (10%)	1 (1%)	12	47
31	h	345/412 (84%)	320 (93%)	25 (7%)	0	100	100
32	k	97/233 (42%)	97 (100%)	0	0	100	100
33	j	128/612 (21%)	113 (88%)	15 (12%)	0	100	100
34	m	85/124 (68%)	80 (94%)	3 (4%)	2 (2%)	4	28
35	n	95/112 (85%)	90 (95%)	4 (4%)	1 (1%)	11	45
36	u	22/136 (16%)	21 (96%)	1 (4%)	0	100	100
37	s	83/116 (72%)	75 (90%)	7 (8%)	1 (1%)	10	42
38	g	83/324 (26%)	79 (95%)	4 (5%)	0	100	100
39	i	152/446 (34%)	135 (89%)	14 (9%)	3 (2%)	6	32
40	x	364/485 (75%)	338 (93%)	26 (7%)	0	100	100
41	c	133/490 (27%)	123 (92%)	10 (8%)	0	100	100
42	y	59/209 (28%)	56 (95%)	3 (5%)	0	100	100
All	All	4850/10641 (46%)	4548 (94%)	289 (6%)	13 (0%)	37	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	829	PRO
15	f	59	TYR
23	a	54	PRO
30	l	114	TYR
39	i	300	PRO
34	m	67	GLY
35	n	78	THR
37	s	56	ASP
25	e	273	HIS
34	m	66	THR
39	i	305	PRO
24	b	142	HIS
39	i	301	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	
1	B	31/567 (6%)	30 (97%)	1 (3%)	34	56
2	C	267/664 (40%)	267 (100%)	0	100	100
5	L	151/207 (73%)	151 (100%)	0	100	100
5	M	150/207 (72%)	150 (100%)	0	100	100
5	N	152/207 (73%)	152 (100%)	0	100	100
6	O	155/354 (44%)	155 (100%)	0	100	100
7	P	258/296 (87%)	258 (100%)	0	100	100
14	d	83/304 (27%)	83 (100%)	0	100	100
15	f	88/101 (87%)	88 (100%)	0	100	100
16	p	65/74 (88%)	65 (100%)	0	100	100
17	r	48/248 (19%)	48 (100%)	0	100	100
18	w	116/162 (72%)	116 (100%)	0	100	100
23	a	152/197 (77%)	152 (100%)	0	100	100
24	b	185/356 (52%)	183 (99%)	2 (1%)	65	73
25	e	145/273 (53%)	145 (100%)	0	100	100
26	o	124/243 (51%)	124 (100%)	0	100	100
27	z	66/99 (67%)	66 (100%)	0	100	100
28	v	102/148 (69%)	102 (100%)	0	100	100
29	q	113/145 (78%)	113 (100%)	0	100	100
30	l	86/105 (82%)	86 (100%)	0	100	100
31	h	280/315 (89%)	280 (100%)	0	100	100
32	k	77/161 (48%)	51 (66%)	26 (34%)	0	2
33	j	110/399 (28%)	110 (100%)	0	100	100
34	m	75/105 (71%)	75 (100%)	0	100	100
35	n	85/98 (87%)	83 (98%)	2 (2%)	43	63
36	u	20/110 (18%)	18 (90%)	2 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	s	71/95 (75%)	71 (100%)	0	100	100
38	g	71/209 (34%)	71 (100%)	0	100	100
39	i	84/311 (27%)	84 (100%)	0	100	100
40	x	251/336 (75%)	251 (100%)	0	100	100
41	c	92/342 (27%)	92 (100%)	0	100	100
42	y	52/159 (33%)	51 (98%)	1 (2%)	50	66
All	All	3805/7597 (50%)	3771 (99%)	34 (1%)	68	75

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	841	ARG
24	b	244	LEU
24	b	259	ASP
32	k	121	LEU
32	k	124	ILE
32	k	127	ILE
32	k	134	ILE
32	k	136	LEU
32	k	138	LEU
32	k	139	THR
32	k	141	LYS
32	k	142	GLN
32	k	144	LEU
32	k	145	ILE
32	k	147	THR
32	k	150	SER
32	k	153	VAL
32	k	154	VAL
32	k	157	LYS
32	k	161	LYS
32	k	169	LYS
32	k	181	LEU
32	k	188	VAL
32	k	189	ARG
32	k	197	LYS
32	k	198	GLN
32	k	203	SER
32	k	211	ILE
32	k	217	VAL

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Mol	Chain	Res	Type
35	n	71	VAL
35	n	90	LEU
36	u	83	ARG
36	u	86	LEU
42	y	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	863	HIS
2	C	331	GLN
2	C	393	GLN
2	C	396	GLN
5	L	132	ASN
5	L	176	ASN
5	L	236	GLN
5	M	173	ASN
5	M	236	GLN
5	M	240	GLN
5	N	236	GLN
5	N	240	GLN
6	O	398	GLN
7	P	193	GLN
7	P	397	GLN
23	a	189	ASN
24	b	142	HIS
24	b	157	GLN
24	b	211	ASN
24	b	264	ASN
24	b	364	GLN
24	b	413	HIS
25	e	267	HIS
25	e	273	HIS
26	o	211	GLN
26	o	263	GLN
27	z	92	GLN
27	z	103	GLN
28	v	15	ASN
30	l	87	GLN
30	l	89	HIS
31	h	47	GLN
31	h	132	GLN

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Mol	Chain	Res	Type
32	k	126	HIS
32	k	129	ASN
36	u	89	HIS
37	s	17	GLN
37	s	31	ASN
38	g	206	GLN
38	g	225	GLN
40	x	293	ASN
41	c	146	GLN
41	c	242	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	1	91/101 (90%)	39 (42%)	2 (2%)
20	4	407/415 (98%)	178 (43%)	8 (1%)
21	2	212/213 (99%)	77 (36%)	0
22	3	390/393 (99%)	135 (34%)	2 (0%)
All	All	1100/1122 (98%)	429 (39%)	12 (1%)

All (429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	1	2	A
19	1	3	A
19	1	4	U
19	1	6	A
19	1	7	G
19	1	14	G
19	1	17	C
19	1	18	U
19	1	29	U
19	1	30	C
19	1	31	A
19	1	32	U
19	1	33	G
19	1	34	C
19	1	37	C
19	1	38	G
19	1	42	G
19	1	44	U

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Mol	Chain	Res	Type
19	1	45	G
19	1	46	G
19	1	47	U
19	1	48	U
19	1	49	U
19	1	50	A
19	1	51	U
19	1	52	A
19	1	53	C
19	1	55	C
19	1	65	U
19	1	74	G
19	1	77	C
19	1	78	A
19	1	79	C
19	1	81	A
19	1	90	U
19	1	91	A
19	1	96	A
19	1	98	U
19	1	99	U
20	4	7	C
20	4	8	U
20	4	15	U
20	4	22	A
20	4	23	U
20	4	24	U
20	4	25	U
20	4	26	U
20	4	28	U
20	4	35	U
20	4	36	U
20	4	41	U
20	4	42	U
20	4	44	U
20	4	45	U
20	4	52	A
20	4	53	A
20	4	56	A
20	4	62	A
20	4	64	A
20	4	65	A

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Mol	Chain	Res	Type
20	4	73	U
20	4	74	U
20	4	75	U
20	4	80	U
20	4	81	U
20	4	82	U
20	4	83	C
20	4	84	A
20	4	85	A
20	4	86	G
20	4	88	C
20	4	90	U
20	4	100	U
20	4	101	A
20	4	109	G
20	4	112	U
20	4	113	A
20	4	115	A
20	4	116	G
20	4	124	A
20	4	126	A
20	4	128	U
20	4	132	C
20	4	135	C
20	4	136	C
20	4	137	A
20	4	138	C
20	4	139	A
20	4	140	A
20	4	141	G
20	4	142	U
20	4	143	U
20	4	144	G
20	4	159	C
20	4	162	A
20	4	163	A
20	4	164	U
20	4	165	A
20	4	166	U
20	4	167	A
20	4	170	G
20	4	177	G

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Mol	Chain	Res	Type
20	4	182	A
20	4	192	A
20	4	195	U
20	4	196	U
20	4	198	U
20	4	212	U
20	4	213	U
20	4	214	U
20	4	217	U
20	4	218	U
20	4	219	U
20	4	221	U
20	4	224	G
20	4	225	C
20	4	227	G
20	4	230	A
20	4	231	C
20	4	232	U
20	4	233	A
20	4	234	G
20	4	241	U
20	4	242	G
20	4	247	A
20	4	257	A
20	4	258	G
20	4	264	G
20	4	266	A
20	4	267	G
20	4	270	C
20	4	274	A
20	4	275	G
20	4	276	C
20	4	277	G
20	4	278	C
20	4	284	U
20	4	285	G
20	4	286	A
20	4	288	G
20	4	290	U
20	4	291	A
20	4	292	A
20	4	293	C

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Mol	Chain	Res	Type
20	4	294	C
20	4	296	C
20	4	301	G
20	4	302	U
20	4	304	C
20	4	305	A
20	4	307	A
20	4	308	C
20	4	309	A
20	4	310	U
20	4	312	G
20	4	317	U
20	4	318	C
20	4	324	C
20	4	326	A
20	4	330	U
20	4	331	A
20	4	332	G
20	4	333	U
20	4	334	A
20	4	340	C
20	4	342	G
20	4	344	A
20	4	346	G
20	4	351	A
20	4	352	U
20	4	353	G
20	4	354	G
20	4	355	C
20	4	357	A
20	4	358	C
20	4	359	A
20	4	361	U
20	4	362	U
20	4	363	A
20	4	364	G
20	4	365	U
20	4	368	C
20	4	369	G
20	4	371	C
20	4	372	C
20	4	373	U

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Mol	Chain	Res	Type
20	4	374	G
20	4	375	G
20	4	379	G
20	4	380	U
20	4	384	C
20	4	385	G
20	4	392	U
20	4	402	G
20	4	404	A
20	4	406	G
20	4	408	C
20	4	413	C
20	4	414	A
20	4	415	G
20	4	416	G
20	4	417	U
20	4	418	U
20	4	422	G
20	4	423	U
20	4	424	A
20	4	426	G
20	4	428	G
20	4	432	C
20	4	434	G
20	4	436	U
20	4	438	C
20	4	439	A
20	4	440	G
20	4	441	A
20	4	443	U
20	4	444	C
21	2	8	U
21	2	9	A
21	2	10	G
21	2	11	G
21	2	13	G
21	2	14	A
21	2	15	C
21	2	20	U
21	2	22	C
21	2	27	A
21	2	37	A

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Mol	Chain	Res	Type
21	2	46	G
21	2	48	A
21	2	49	U
21	2	50	U
21	2	51	A
21	2	52	G
21	2	54	G
21	2	55	A
21	2	56	G
21	2	57	C
21	2	58	U
21	2	62	U
21	2	65	C
21	2	67	U
21	2	68	U
21	2	70	U
21	2	72	U
21	2	75	U
21	2	76	C
21	2	78	G
21	2	79	C
21	2	83	C
21	2	86	U
21	2	90	U
21	2	91	U
21	2	92	A
21	2	99	G
21	2	103	G
21	2	114	A
21	2	115	C
21	2	116	U
21	2	117	A
21	2	125	G
21	2	134	A
21	2	137	A
21	2	138	G
21	2	146	G
21	2	148	U
21	2	152	U
21	2	154	U
21	2	155	G
21	2	160	C

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Mol	Chain	Res	Type
21	2	161	A
21	2	162	G
21	2	168	U
21	2	171	A
21	2	173	U
21	2	174	U
21	2	175	U
21	2	180	C
21	2	186	C
21	2	189	G
21	2	190	A
21	2	191	A
21	2	192	C
21	2	193	G
21	2	197	G
21	2	202	A
21	2	203	G
21	2	206	G
21	2	208	U
21	2	209	G
21	2	210	C
21	2	212	U
21	2	213	A
21	2	214	C
22	3	2	U
22	3	4	G
22	3	6	U
22	3	9	U
22	3	10	G
22	3	11	A
22	3	20	C
22	3	21	A
22	3	23	G
22	3	26	C
22	3	29	G
22	3	30	C
22	3	31	C
22	3	32	A
22	3	33	G
22	3	39	U
22	3	43	U
22	3	44	A

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Mol	Chain	Res	Type
22	3	45	A
22	3	47	A
22	3	51	G
22	3	55	U
22	3	57	U
22	3	59	A
22	3	66	A
22	3	74	G
22	3	76	C
22	3	78	A
22	3	80	G
22	3	82	A
22	3	83	G
22	3	84	G
22	3	85	C
22	3	86	A
22	3	88	C
22	3	89	G
22	3	94	U
22	3	107	U
22	3	109	A
22	3	110	A
22	3	113	C
22	3	117	A
22	3	119	A
22	3	129	A
22	3	134	C
22	3	135	G
22	3	139	G
22	3	140	A
22	3	147	A
22	3	148	A
22	3	149	A
22	3	154	A
22	3	155	A
22	3	156	U
22	3	159	U
22	3	164	A
22	3	172	C
22	3	174	G
22	3	175	A
22	3	176	A

Continued on next page...

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Mol	Chain	Res	Type
22	3	177	G
22	3	187	C
22	3	188	C
22	3	189	A
22	3	194	C
22	3	201	A
22	3	202	C
22	3	204	A
22	3	205	A
22	3	207	G
22	3	211	C
22	3	220	A
22	3	226	G
22	3	229	A
22	3	234	A
22	3	240	U
22	3	241	U
22	3	244	A
22	3	245	G
22	3	246	A
22	3	250	G
22	3	255	G
22	3	257	C
22	3	264	G
22	3	265	U
22	3	269	C
22	3	271	C
22	3	272	A
22	3	273	U
22	3	278	G
22	3	279	U
22	3	287	A
22	3	289	C
22	3	290	U
22	3	292	U
22	3	300	G
22	3	304	A
22	3	313	C
22	3	314	A
22	3	316	C
22	3	322	A
22	3	323	A

Continued on next page...

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Mol	Chain	Res	Type
22	3	324	A
22	3	328	A
22	3	330	G
22	3	331	C
22	3	337	G
22	3	339	A
22	3	340	G
22	3	342	G
22	3	346	G
22	3	348	G
22	3	349	A
22	3	350	U
22	3	352	C
22	3	353	G
22	3	356	G
22	3	357	U
22	3	374	A
22	3	375	U
22	3	377	G
22	3	379	A
22	3	381	U
22	3	382	U
22	3	383	A
22	3	385	G
22	3	388	C
22	3	389	A
22	3	390	A
22	3	391	A
22	3	392	A
22	3	393	U
22	3	394	C
22	3	397	A
22	3	398	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	1	44	U
19	1	64	U
20	4	34	U
20	4	139	A
20	4	165	A

Continued on next page...

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Mol	Chain	Res	Type
20	4	166	U
20	4	230	A
20	4	274	A
20	4	290	U
20	4	295	U
22	3	46	A
22	3	339	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	Z	18
20	4	8
3	D	7
9	V	5
11	X	2
22	3	2
8	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	608:UNK	C	652:UNK	N	59.09
1	V	85:UNK	C	87:UNK	N	51.40
1	V	194:UNK	C	206:UNK	N	47.06
1	Z	432:UNK	C	437:UNK	N	41.45
1	D	287:UNK	C	294:UNK	N	40.99
1	D	847:UNK	C	917:UNK	N	33.62
1	Z	312:UNK	C	316:UNK	N	31.86
1	Z	563:UNK	C	572:UNK	N	29.94
1	Z	52:UNK	C	62:UNK	N	29.83
1	V	149:UNK	C	151:UNK	N	27.09
1	X	61:UNK	C	67:UNK	N	26.04
1	Z	208:UNK	C	211:UNK	N	25.14
1	V	114:UNK	C	122:UNK	N	22.23
1	D	503:UNK	C	825:UNK	N	21.02
1	Z	234:UNK	C	244:UNK	N	20.95
1	Z	353:UNK	C	357:UNK	N	19.30
1	4	144:G	O3'	149:C	P	18.74
1	D	477:UNK	C	486:UNK	N	18.19
1	Z	277:UNK	C	281:UNK	N	17.65
1	X	30:UNK	C	36:UNK	N	17.30
1	Z	333:UNK	C	338:UNK	N	16.38
1	4	48:U	O3'	51:U	P	15.62
1	Z	138:UNK	C	145:UNK	N	14.83
1	Z	110:UNK	C	116:UNK	N	14.60
1	Z	254:UNK	C	257:UNK	N	14.41
1	D	212:UNK	C	217:UNK	N	13.12
1	3	100:U	O3'	106:G	P	12.55
1	D	160:UNK	C	166:UNK	N	12.12
1	4	199:U	O3'	202:A	P	11.13
1	D	369:UNK	C	376:UNK	N	11.07
1	Z	502:UNK	C	507:UNK	N	11.01
1	V	133:UNK	C	137:UNK	N	9.48
1	4	207:U	O3'	211:U	P	9.36
1	Z	187:UNK	C	195:UNK	N	8.89
1	Z	380:UNK	C	384:UNK	N	8.44
1	Z	164:UNK	C	169:UNK	N	7.72
1	3	279:U	O3'	286:A	P	7.37
1	4	28:U	O3'	34:U	P	7.28
1	Z	480:UNK	C	486:UNK	N	6.01
1	U	22:UNK	C	28:UNK	N	5.69
1	4	178:U	O3'	181:A	P	5.51
1	4	65:A	O3'	72:U	P	5.35
1	4	192:A	O3'	194:U	P	4.93

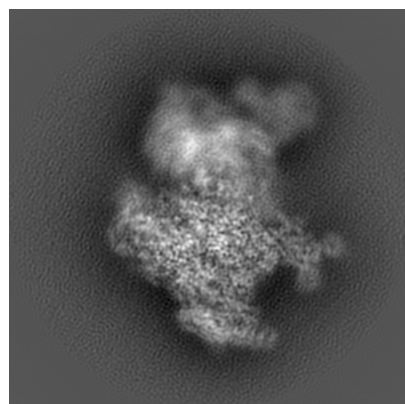
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13477. These allow visual inspection of the internal detail of the map and identification of artifacts.

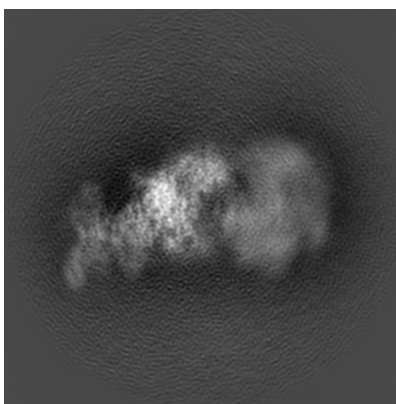
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

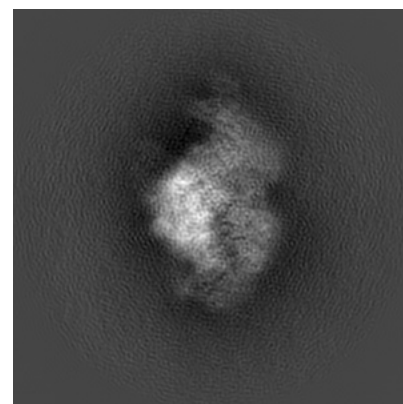
6.1.1 Primary map



X

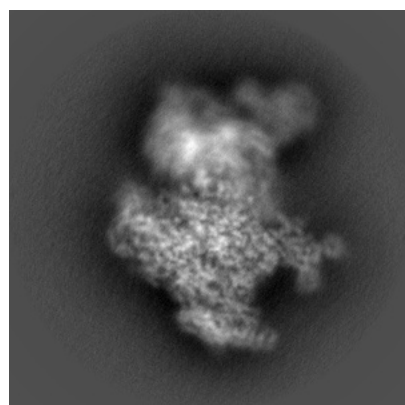


Y

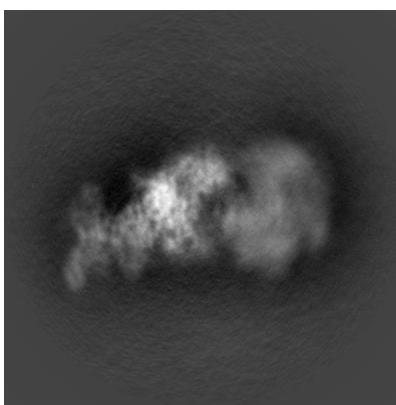


Z

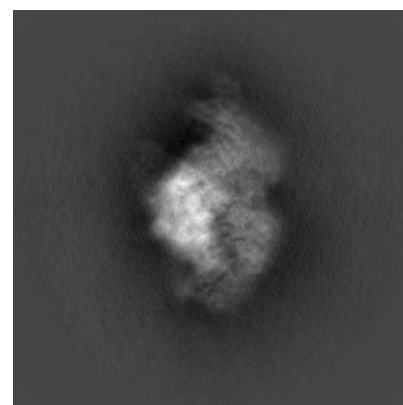
6.1.2 Raw map



X



Y

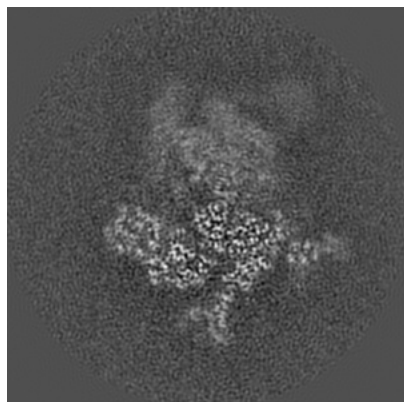


Z

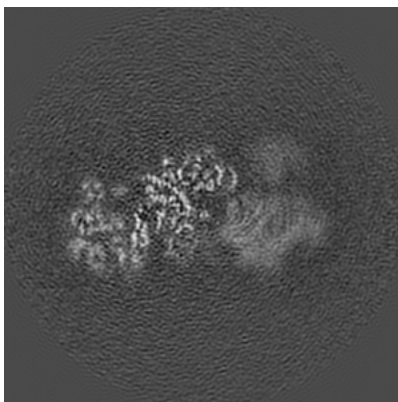
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

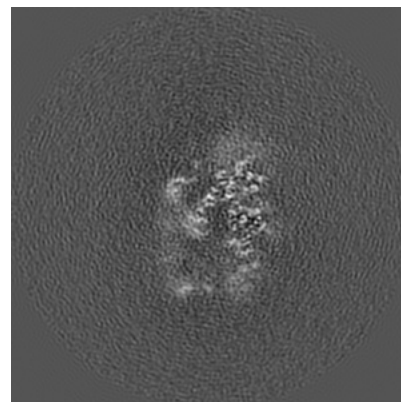
6.2.1 Primary map



X Index: 180

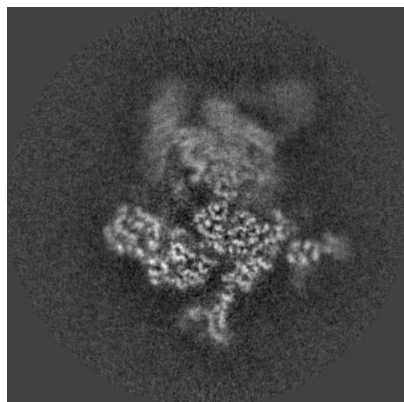


Y Index: 180

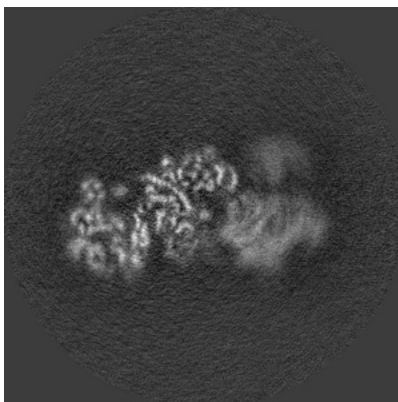


Z Index: 180

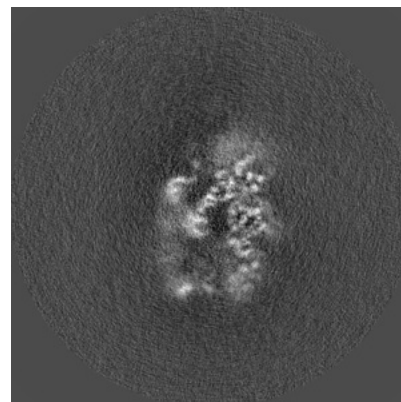
6.2.2 Raw map



X Index: 180



Y Index: 180

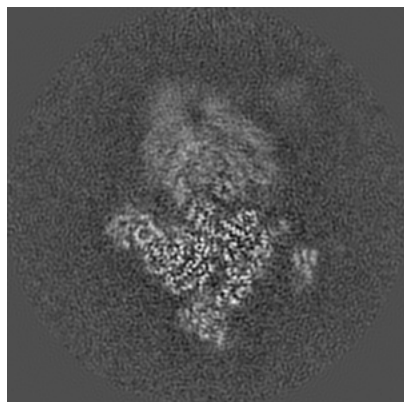


Z Index: 180

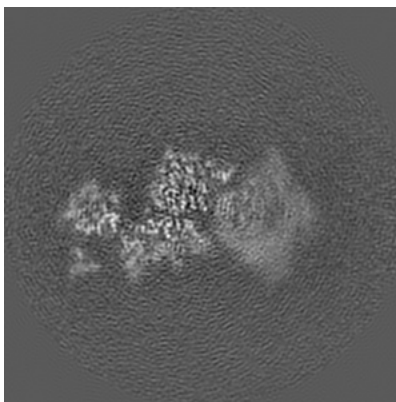
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

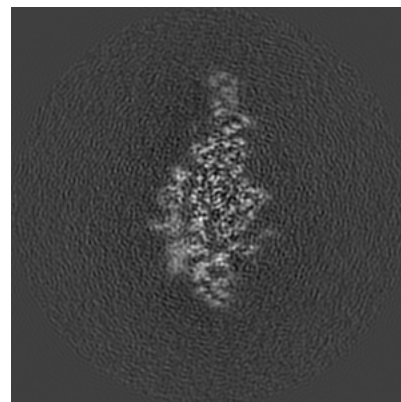
6.3.1 Primary map



X Index: 173

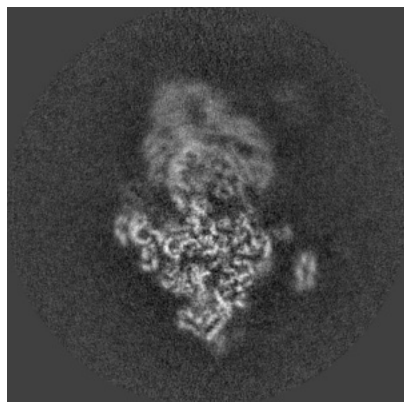


Y Index: 190

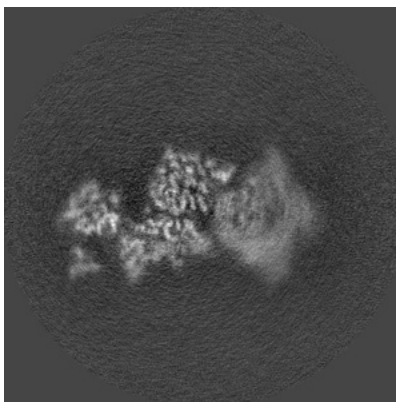


Z Index: 149

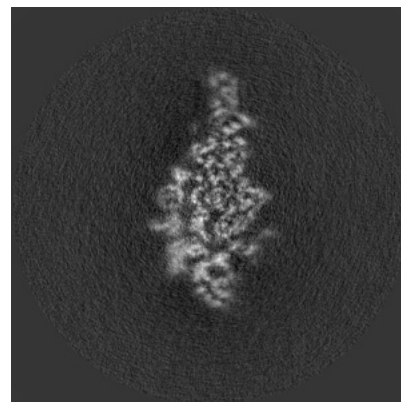
6.3.2 Raw map



X Index: 168



Y Index: 190

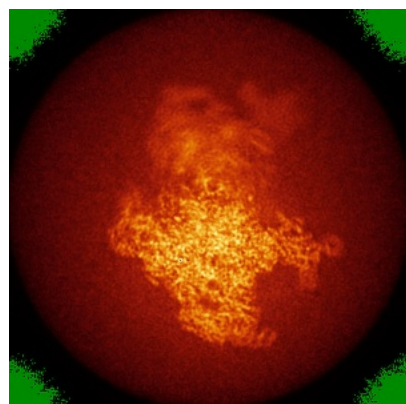


Z Index: 149

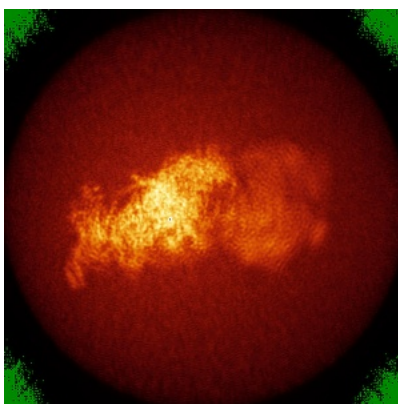
The images above show the largest variance slices of the map in three orthogonal directions.

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

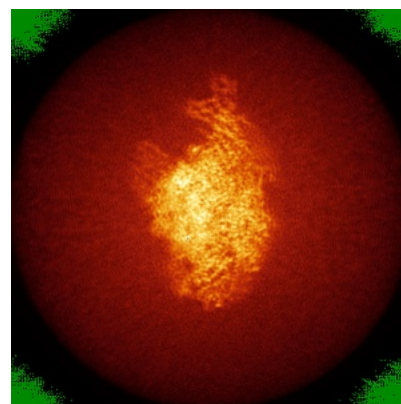
6.4.1 Primary map



X

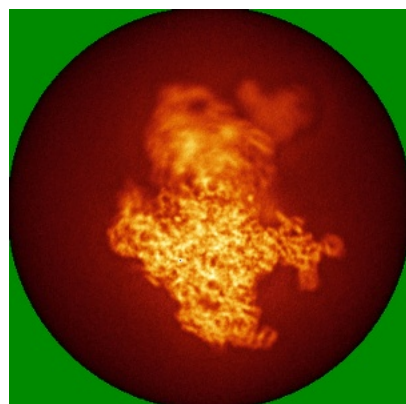


Y

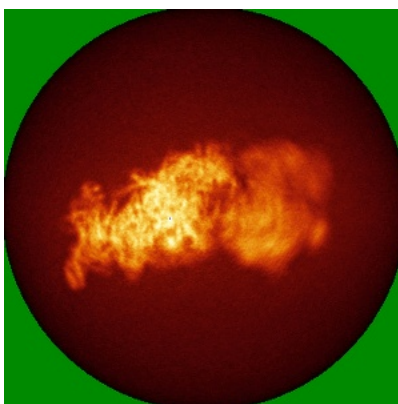


Z

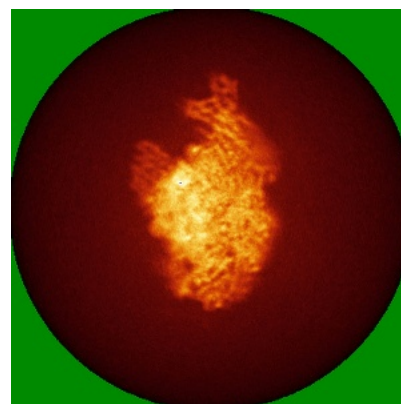
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

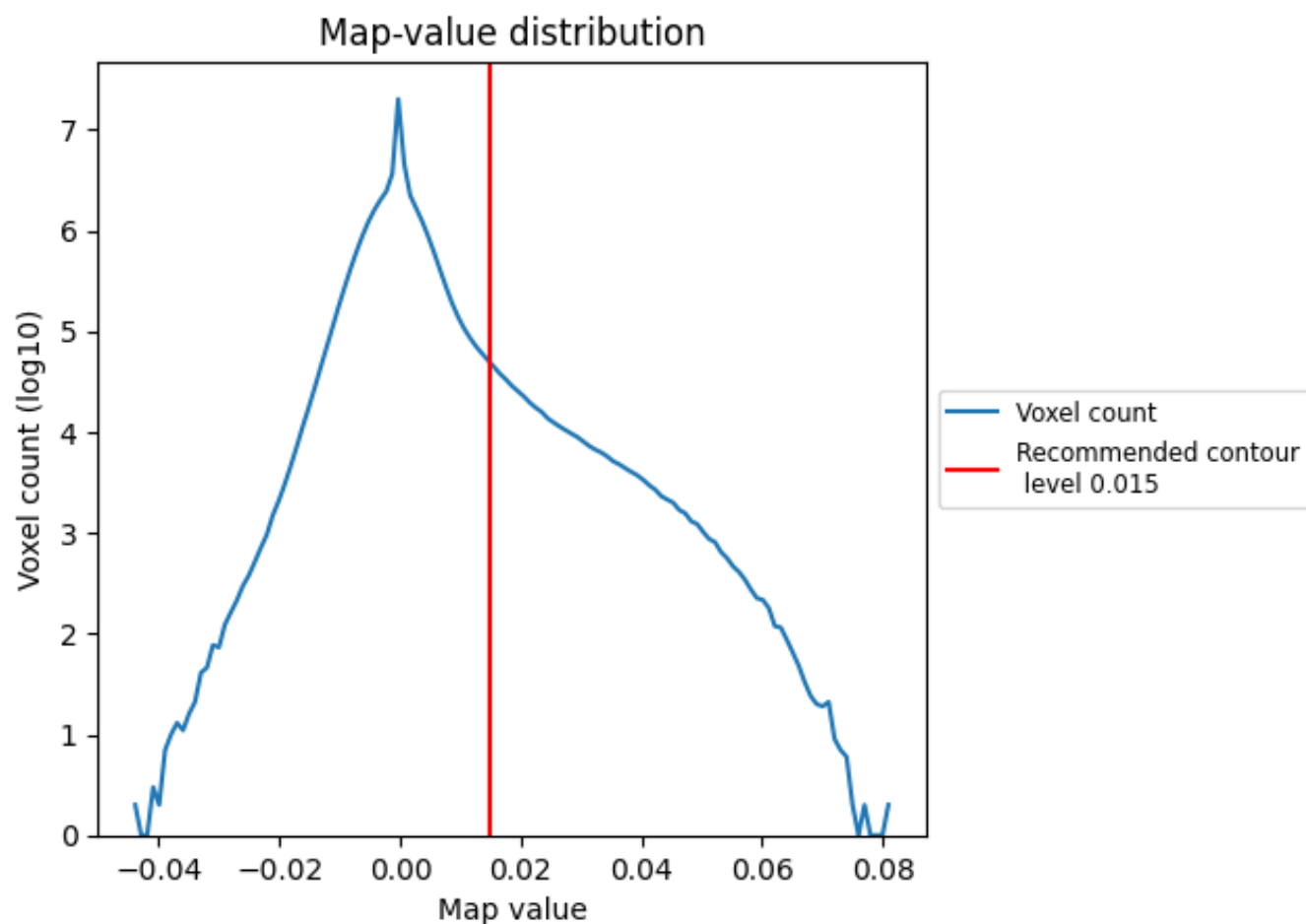
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

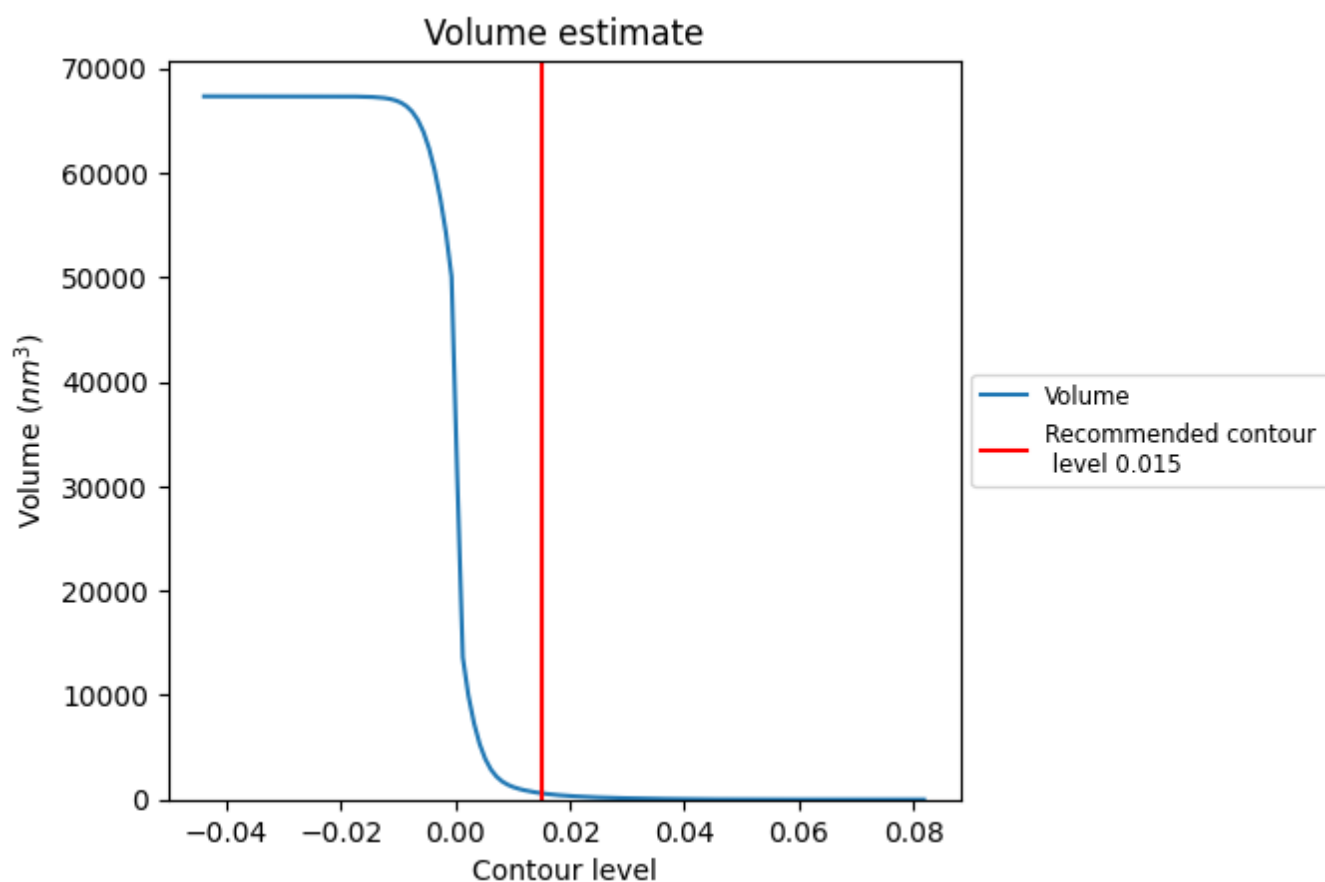
This section contains the results of statistical analysis of the map.

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.

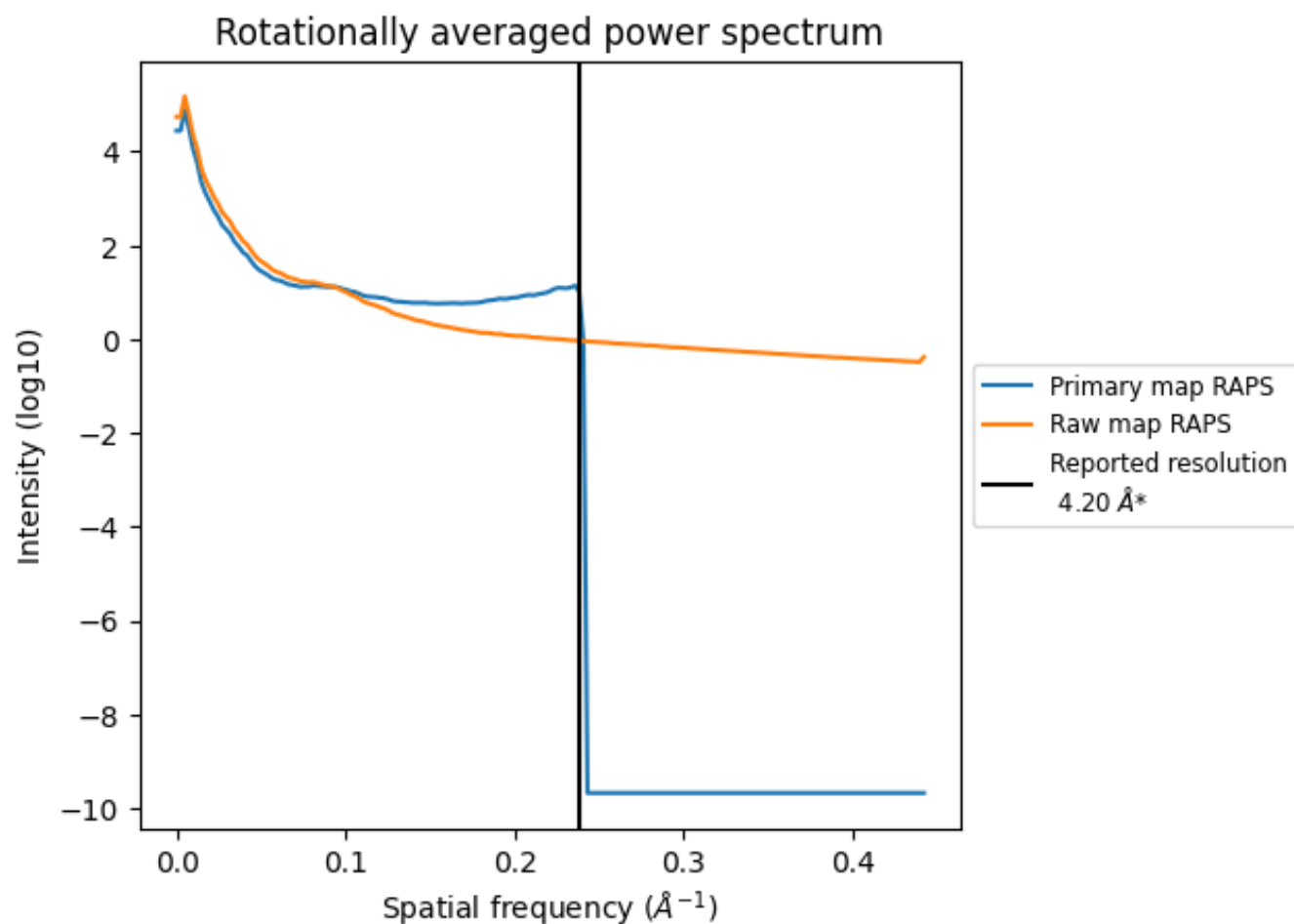
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 611 nm³; this corresponds to an approximate mass of 552 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 ⓘ

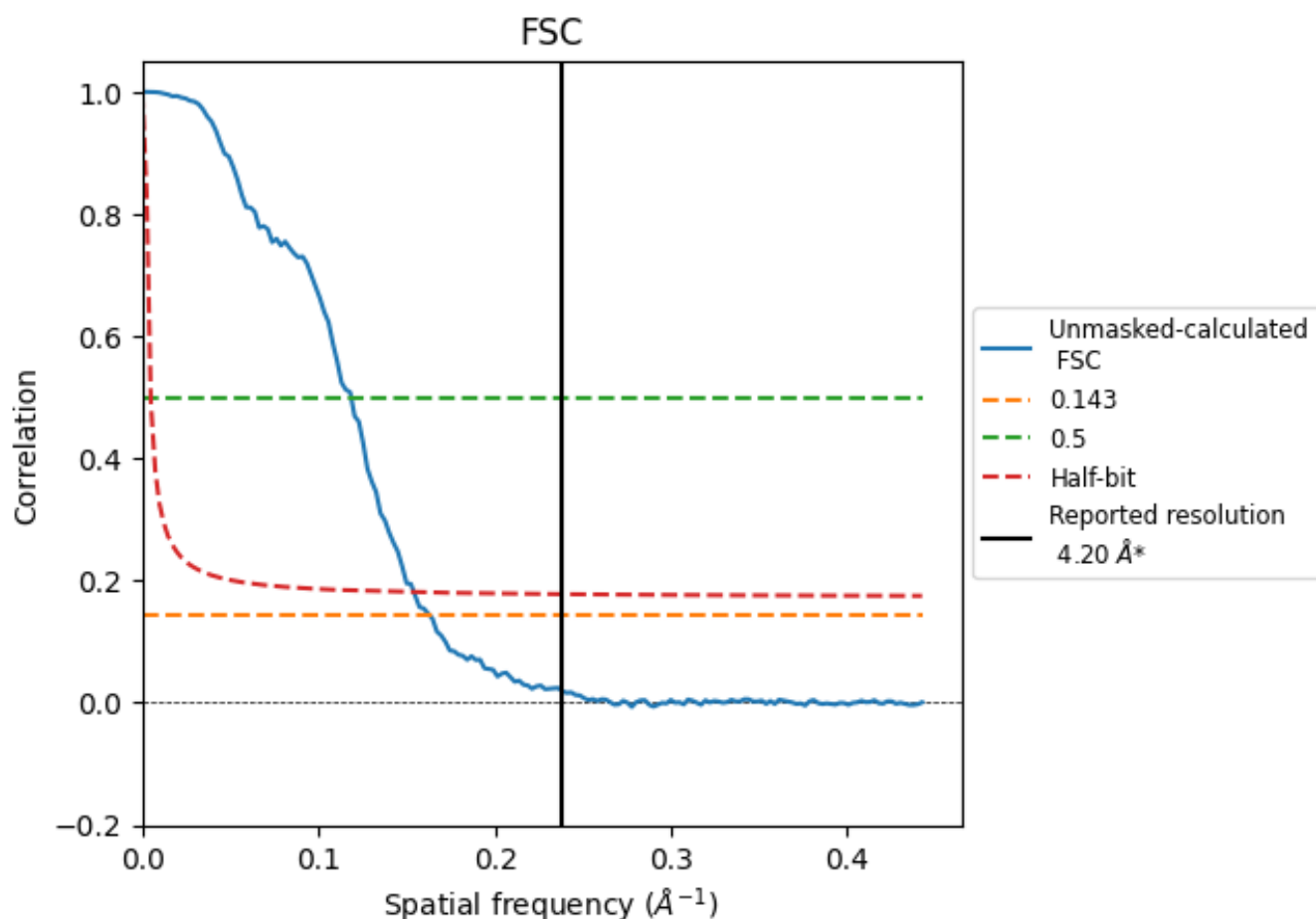


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.13	8.44	6.49

*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 6.13 differs from the reported value 4.2 by more than 10 %

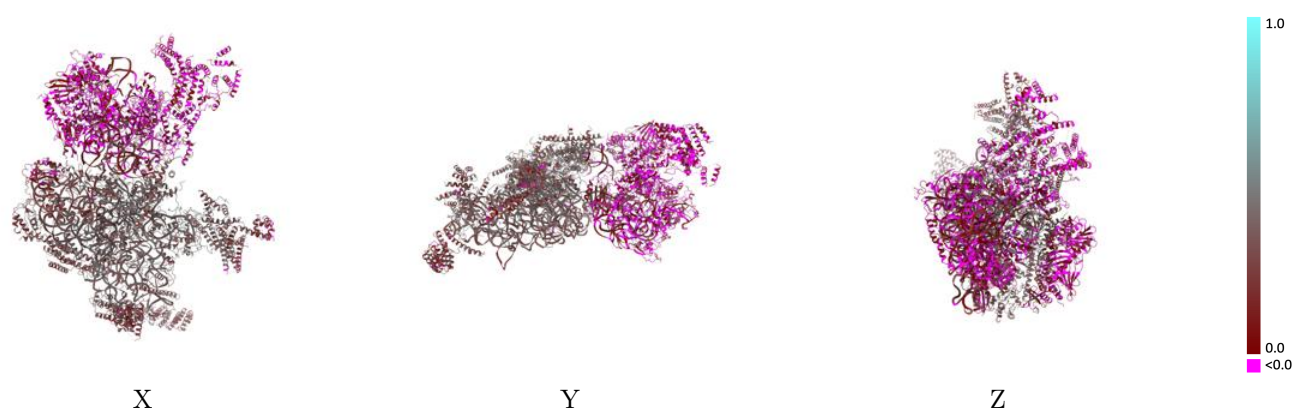
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13477 and PDB model 7PKQ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

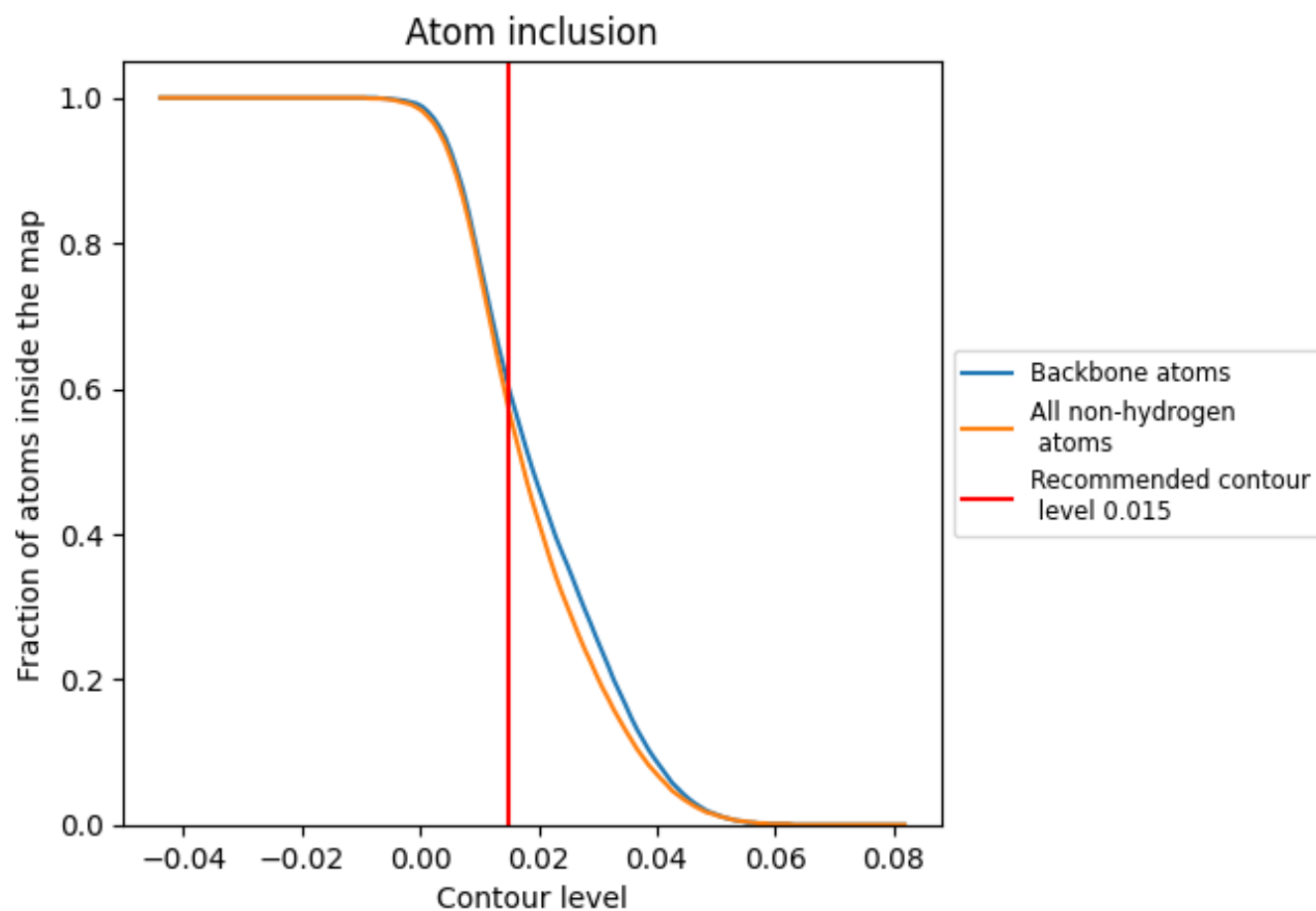


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.2310
1	 0.8810	 0.3540
2	 0.9110	 0.3690
3	 0.7290	 0.2880
4	 0.5200	 0.1300
B	 0.1950	 0.0660
C	 0.7330	 0.3360
D	 0.9320	 0.3970
K	 0.1620	 0.0320
L	 0.0760	 0.0090
M	 0.1230	 0.0230
N	 0.0640	 0.0210
O	 0.5260	 0.2440
P	 0.7770	 0.3220
U	 0.9270	 0.4520
V	 0.9410	 0.4120
W	 0.9110	 0.4700
X	 0.1730	 0.0620
Y	 0.3960	 0.1550
Z	 0.0570	 0.0200
a	 0.5790	 0.2910
b	 0.7600	 0.3630
c	 0.3550	 0.1170
d	 0.8110	 0.3920
e	 0.7760	 0.4110
f	 0.7620	 0.3340
g	 0.2090	 0.0470
h	 0.8100	 0.4020
i	 0.3450	 0.0510
j	 0.2500	 0.0620
k	 0.0280	 0.1500
l	 0.5140	 0.3440
m	 0.1180	 -0.0010
n	 0.2750	 0.0470
o	 0.7820	 0.3540



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Chain	Atom inclusion	Q-score
p	 0.8100	 0.3480
q	 0.8170	 0.3840
r	 0.7390	 0.3070
s	 0.1260	 0.0060
u	 0.2390	 -0.0540
v	 0.7310	 0.3520
w	 0.7940	 0.3490
x	 0.1280	 0.0260
y	 0.2260	 0.0240
z	 0.7600	 0.3430