



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:27 AM UTC

PDB ID : 6N8L / pdb_00006n8l
EMDB ID : EMD-0371
Title : Cryo-EM structure of early cytoplasmic-late (ECL) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.60 Å(reported)
Based on initial model : 3JCT

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

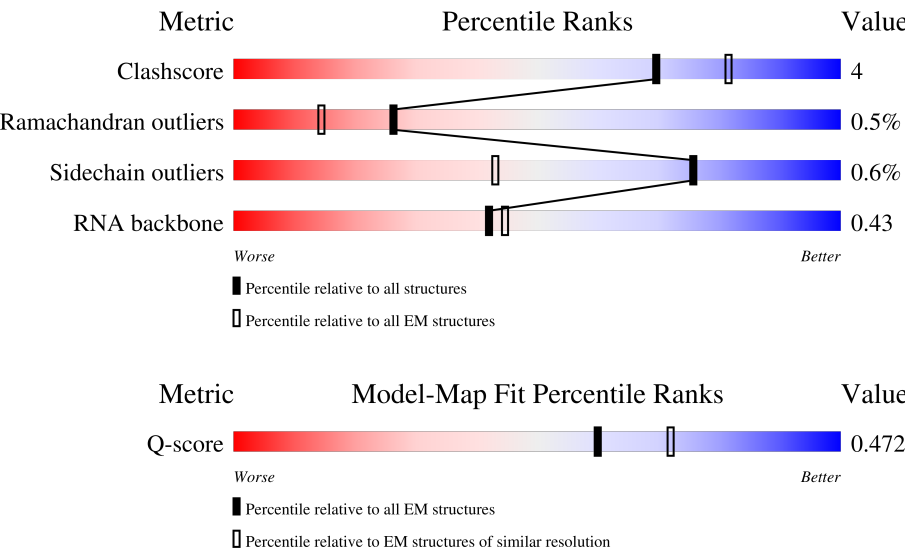
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



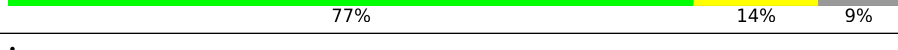
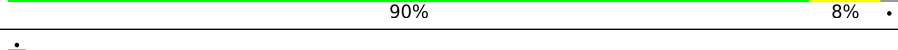
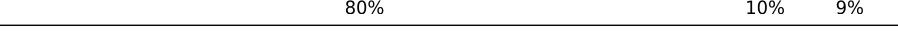
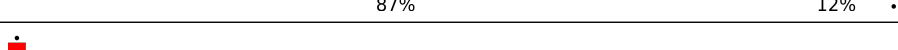
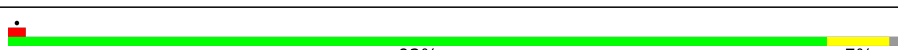
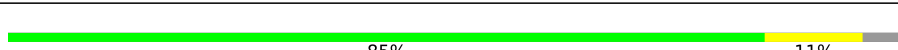
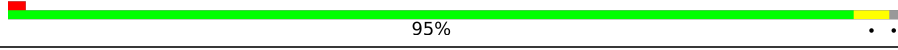
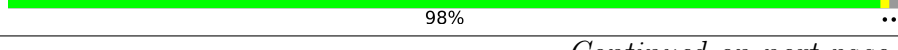
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	v	518	
2	s	217	
3	A	254	

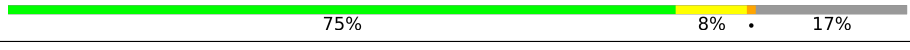
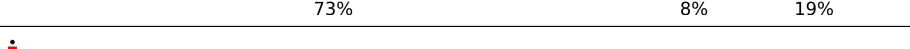
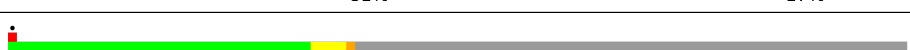
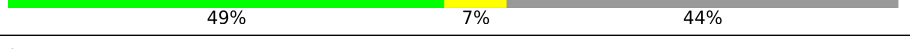
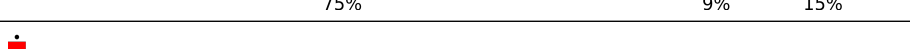
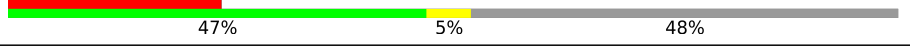
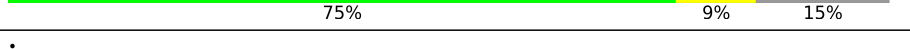
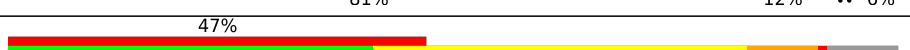
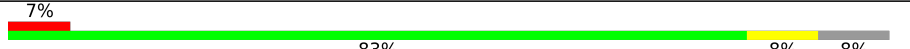
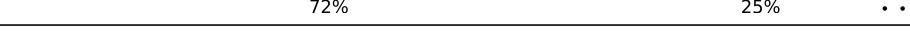
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Mol	Chain	Length	Quality of chain
4	a	149	
5	B	387	
6	b	647	
7	C	362	
8	c	105	
9	d	113	
10	E	176	
11	e	130	
12	F	244	
13	f	107	
14	G	256	
15	g	121	
16	I	166	
17	H	191	
18	h	120	
19	i	100	
20	j	88	
21	k	78	
22	L	199	
23	l	51	
24	M	138	
25	p	92	
26	N	204	
27	u	199	
28	O	199	

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Mol	Chain	Length	Quality of chain
29	P	184	
30	Q	186	
31	R	189	
32	S	172	
33	T	160	
34	U	121	
35	V	137	
36	W	236	
37	X	142	
38	Y	127	
39	y	245	
40	Z	136	
41	z	106	
42	D	297	
43	J	174	
44	q	106	
45	o	59	
46	1	3396	
47	2	121	
48	3	158	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 129926 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 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	362	Total	C	N	O	S	0	0
			2783	1770	472	522	19		

- Molecule 2 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	s	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 3 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	245	Total	C	N	O	S	0	0
			1863	1162	376	324	1		

- Molecule 4 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	94	Total	C	N	O	S	0	0
			742	484	131	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	248	Total	C	N	O	S	0	0
			1989	1222	372	387	8		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L30.

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

- Molecule 9 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	160	Total	C	N	O	S	0	0
			1270	818	229	222	1		

- Molecule 11 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 13 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 15 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1056	660	195	198	3		

- Molecule 17 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 18 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	96	Total	C	N	O	S	0	0
			743	465	148	128	2		

- Molecule 20 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	85	Total	C	N	O	S	0	0
			670	408	146	111	5		

- Molecule 21 is a protein called 60S ribosomal protein L38.

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

- Molecule 22 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	L	187	Total	C	N	O	0	0
			1491	929	306	256		

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 24 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 25 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 26 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 27 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	149	Total	C	N	O	S	0	0
			1256	788	252	207	9		

- Molecule 28 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	178	Total	C	N	O		0	0
			1409	876	281	252			

- Molecule 30 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	154	Total	C	N	O	S	0	0
			1191	753	231	205	2		

- Molecule 31 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	154	Total	C	N	O		0	0
			1241	772	262	207			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	170	Total	C	N	O	S	0	0
			1425	916	265	241	3		

- Molecule 33 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	61	Total	C	N	O	S	0	0
			476	295	95	85	1		

- Molecule 34 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	104	Total	C	N	O		0	0
			826	535	136	155			

- Molecule 35 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 36 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	W	133	Total	C	N	O	S	0	0
			1053	660	177	214	2		

- Molecule 37 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 38 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 39 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	y	225	Total	C	N	O	S	0	0
			1698	1054	295	343	6		

- Molecule 40 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 41 is a protein called UPF0642 protein YBL028C.

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

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	251	Total	C	N	O	S	0	0
			1983	1253	353	375	2		

- Molecule 43 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	J	164	Total	C	N	O	S	0	0
			1304	816	243	242	3		

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	97	Total	C	N	O	S	0	0
			783	493	158	127	5		

- Molecule 45 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	54	Total	C	N	O	0	0
			433	271	94	68		

- Molecule 46 is a RNA chain called *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	3201	Total	C	N	O	P	0	0
			68471	30584	12345	22341	3201		

- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

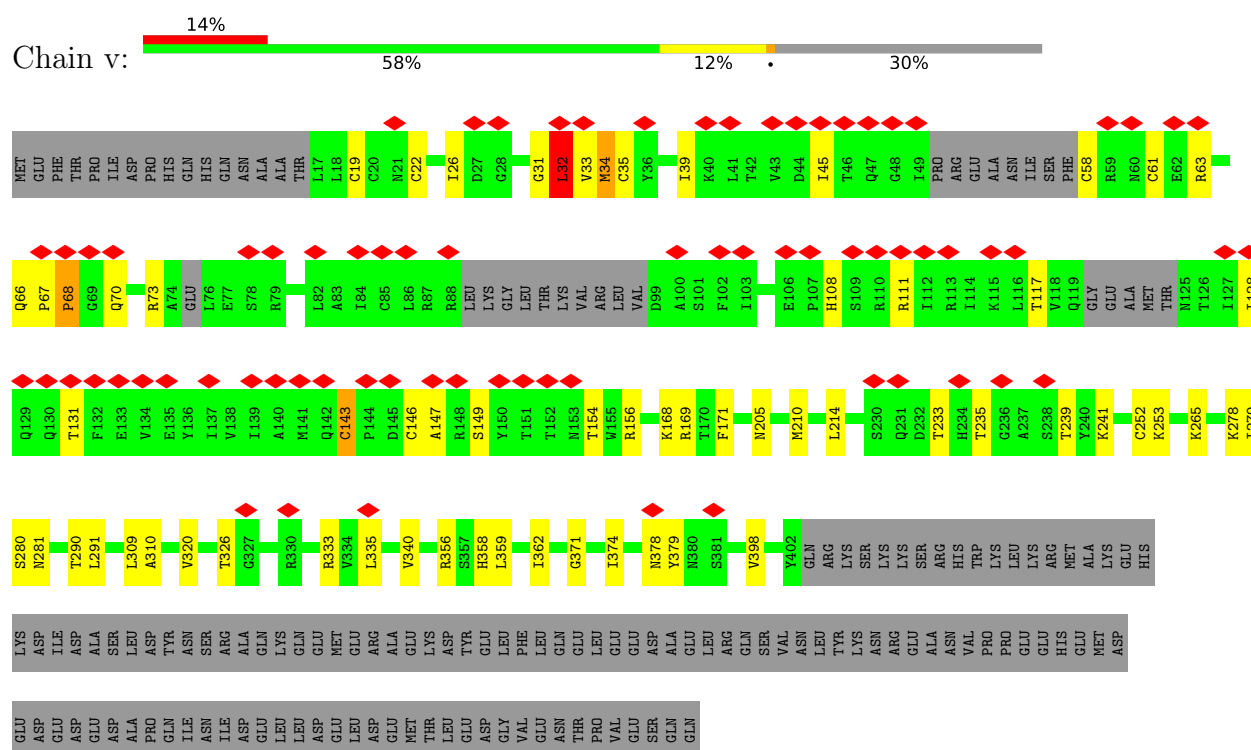
- Molecule 48 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

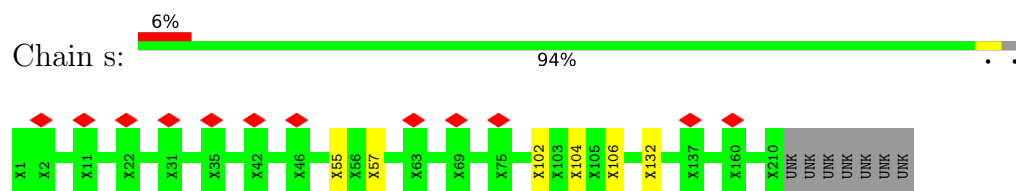
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

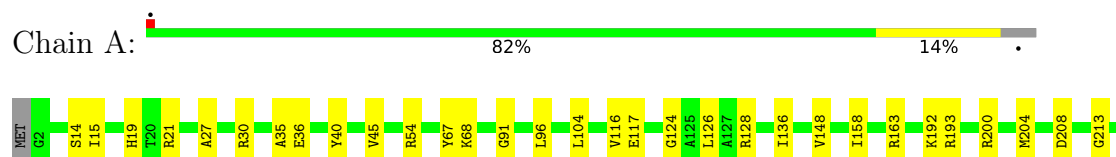
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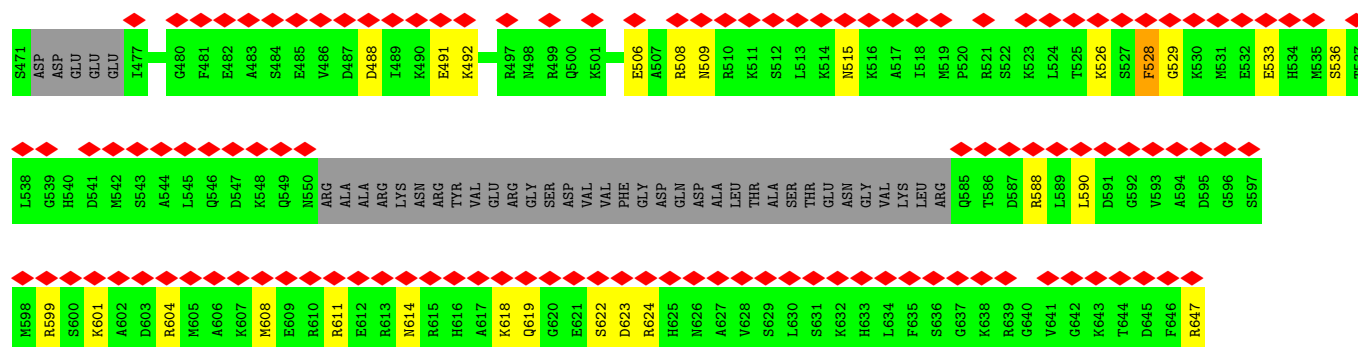


• Molecule 2: Ribosomal Protein uL1

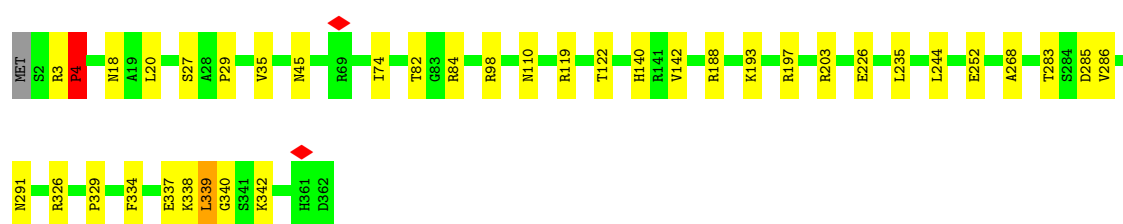
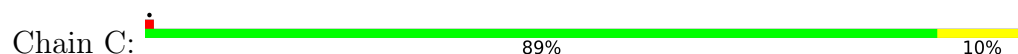


• Molecule 3: 60S ribosomal protein L2-A

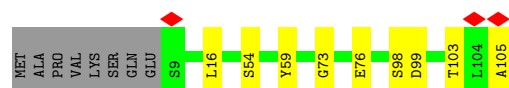
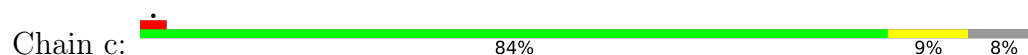




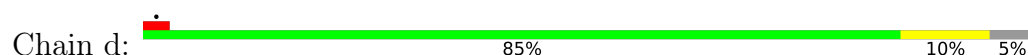
• Molecule 7: 60S ribosomal protein L4-A



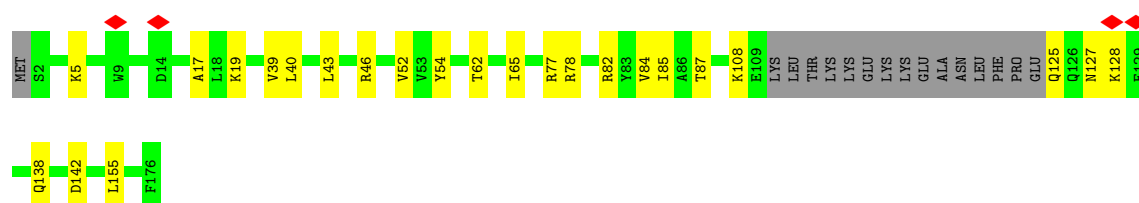
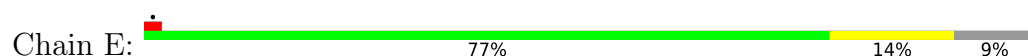
• Molecule 8: 60S ribosomal protein L30



• Molecule 9: 60S ribosomal protein L31-A



• Molecule 10: 60S ribosomal protein L6-A



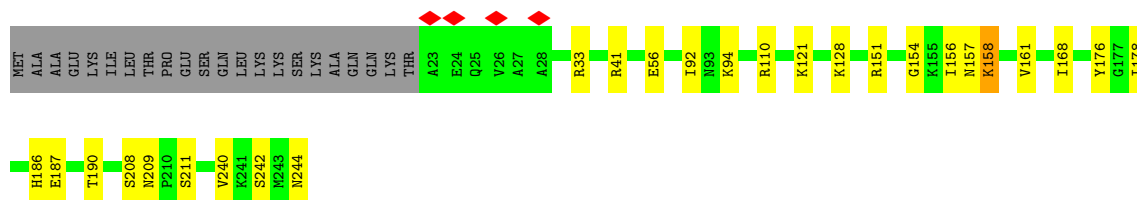
• Molecule 11: 60S ribosomal protein L32

Chain e:  90% 8%



- Molecule 12: 60S ribosomal protein L7-A

Chain F:  80% 10% 9%



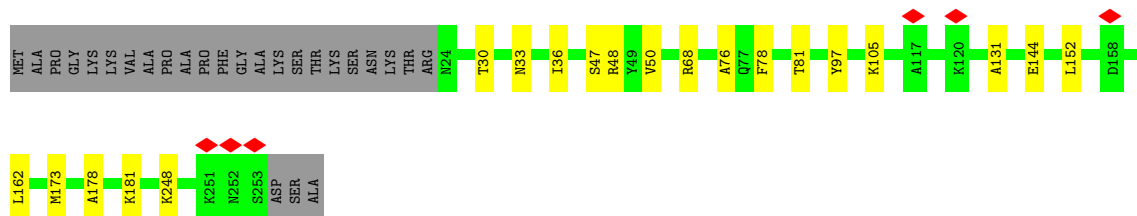
- Molecule 13: 60S ribosomal protein L33-A

Chain f:  87% 12%



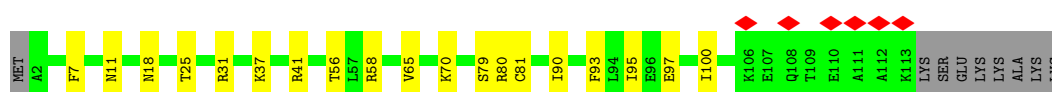
- Molecule 14: 60S ribosomal protein L8-A

Chain G:  82% 8% 10%



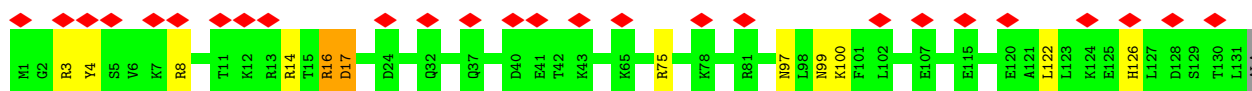
- Molecule 15: 60S ribosomal protein L34-A

Chain g:  5% 77% 16% 7%



- Molecule 16: Bud site selection protein 20

Chain I:  16% 72% 6% 21%



ASN VAL LYS THR THR GLU PRO THR LEU PRO TRP ALA ALA ASP ALA GLU ALA ASN THR ALA VAL THR GLU ALA GLU SER THR ALA SER ALA SER THR

- Molecule 17: 60S ribosomal protein L9-A

Chain H:  90% 8% ..



- Molecule 18: 60S ribosomal protein L35-A

Chain h:  92% 7% .



- Molecule 19: 60S ribosomal protein L36-A

Chain i:  85% 11% .



- Molecule 20: 60S ribosomal protein L37-A

Chain j:  88% 9% .



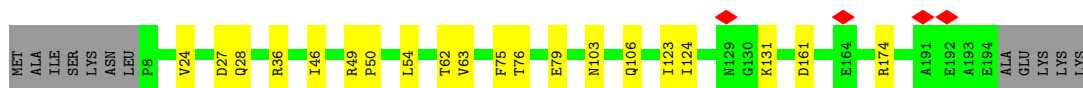
- Molecule 21: 60S ribosomal protein L38

Chain k:  88% 10% .



- Molecule 22: 60S ribosomal protein L13-A

Chain L:  84% 10% 6%

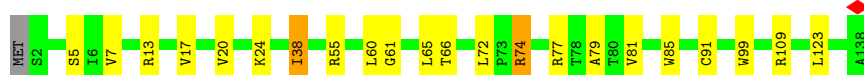
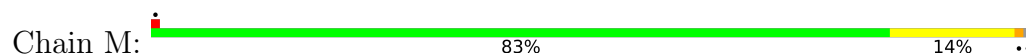


- Molecule 23: 60S ribosomal protein L39

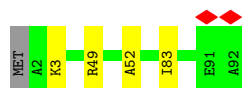
Chain l:  78% 20% .



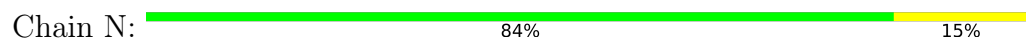
- Molecule 24: 60S ribosomal protein L14-A



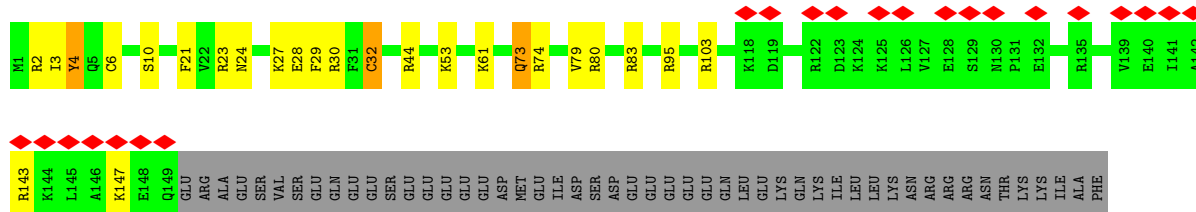
- Molecule 25: 60S ribosomal protein L43-A



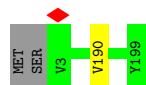
- Molecule 26: 60S ribosomal protein L15-A



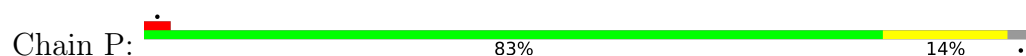
- Molecule 27: Ribosome biogenesis protein RLP24

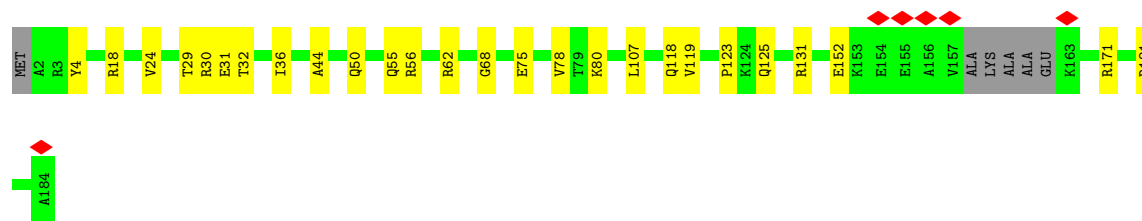


- Molecule 28: 60S ribosomal protein L16-A



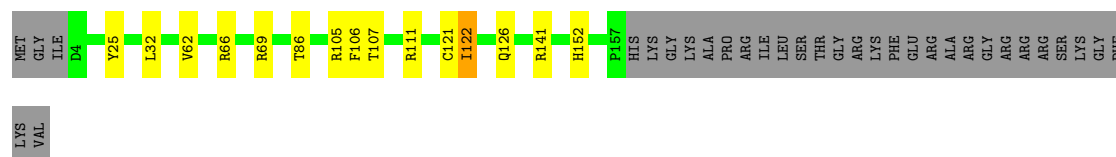
- Molecule 29: 60S ribosomal protein L17-A





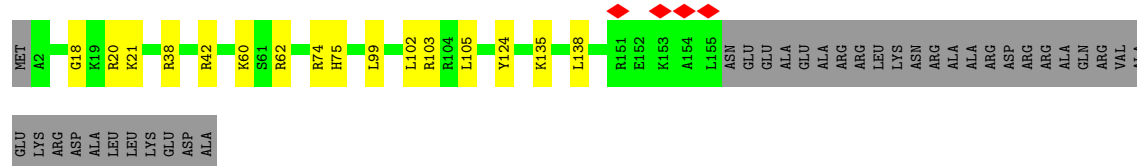
- Molecule 30: 60S ribosomal protein L18-A

Chain Q: 75% 8% 17%



- Molecule 31: 60S ribosomal protein L19-A

Chain R: 73% 8% 19%



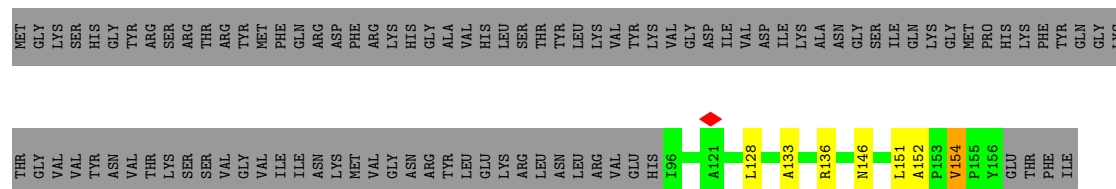
- Molecule 32: 60S ribosomal protein L20-A

Chain S: 81% 17% 2%



- Molecule 33: 60S ribosomal protein L21-A

Chain T: 34% 62% 4%



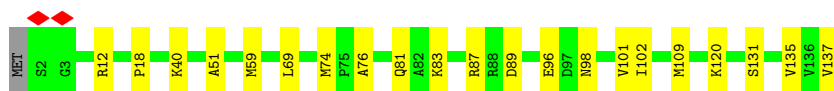
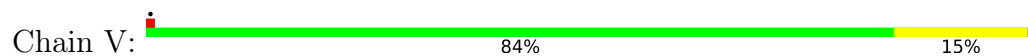
- Molecule 34: 60S ribosomal protein L22-A

Chain U: 80% 6% 14%

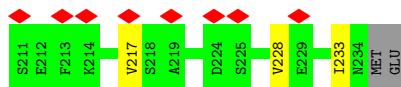
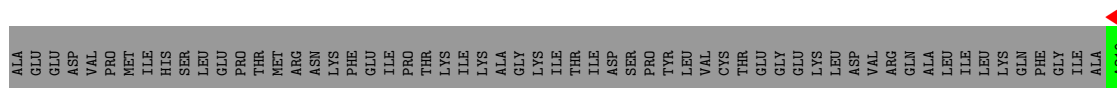
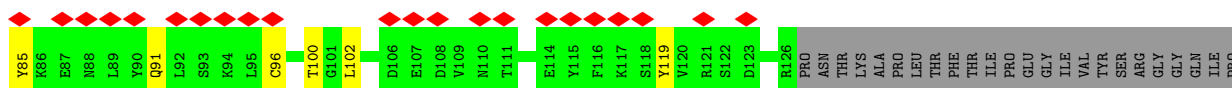




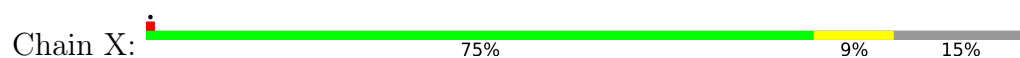
- Molecule 35: 60S ribosomal protein L23-A



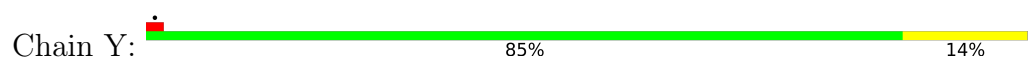
- Molecule 36: Ribosome assembly factor MRT4



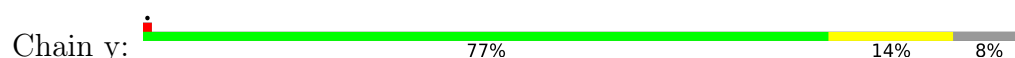
- Molecule 37: 60S ribosomal protein L25

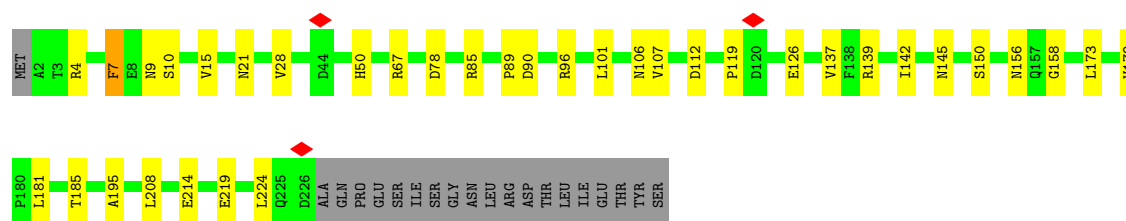


- Molecule 38: 60S ribosomal protein L26-A

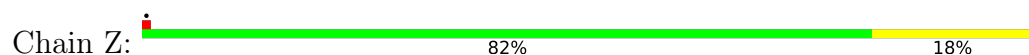


- Molecule 39: Eukaryotic translation initiation factor 6

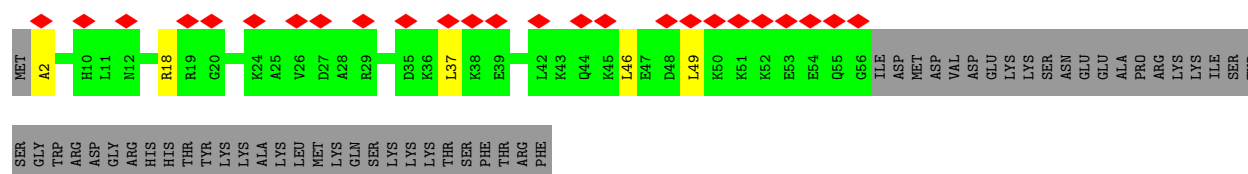




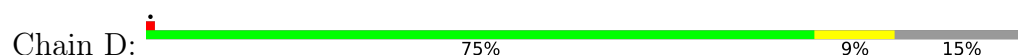
- Molecule 40: 60S ribosomal protein L27-A



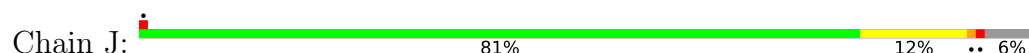
- Molecule 41: UPF0642 protein YBL028C



- Molecule 42: 60S ribosomal protein L5

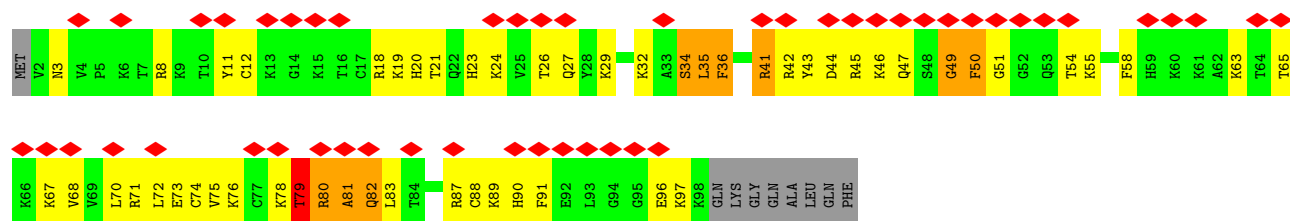


- Molecule 43: 60S ribosomal protein L11-A

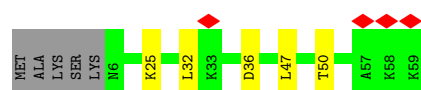
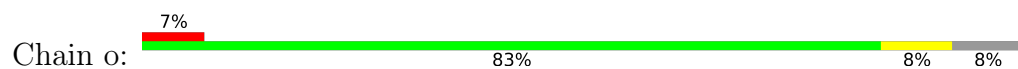


- Molecule 44: 60S ribosomal protein L42-A

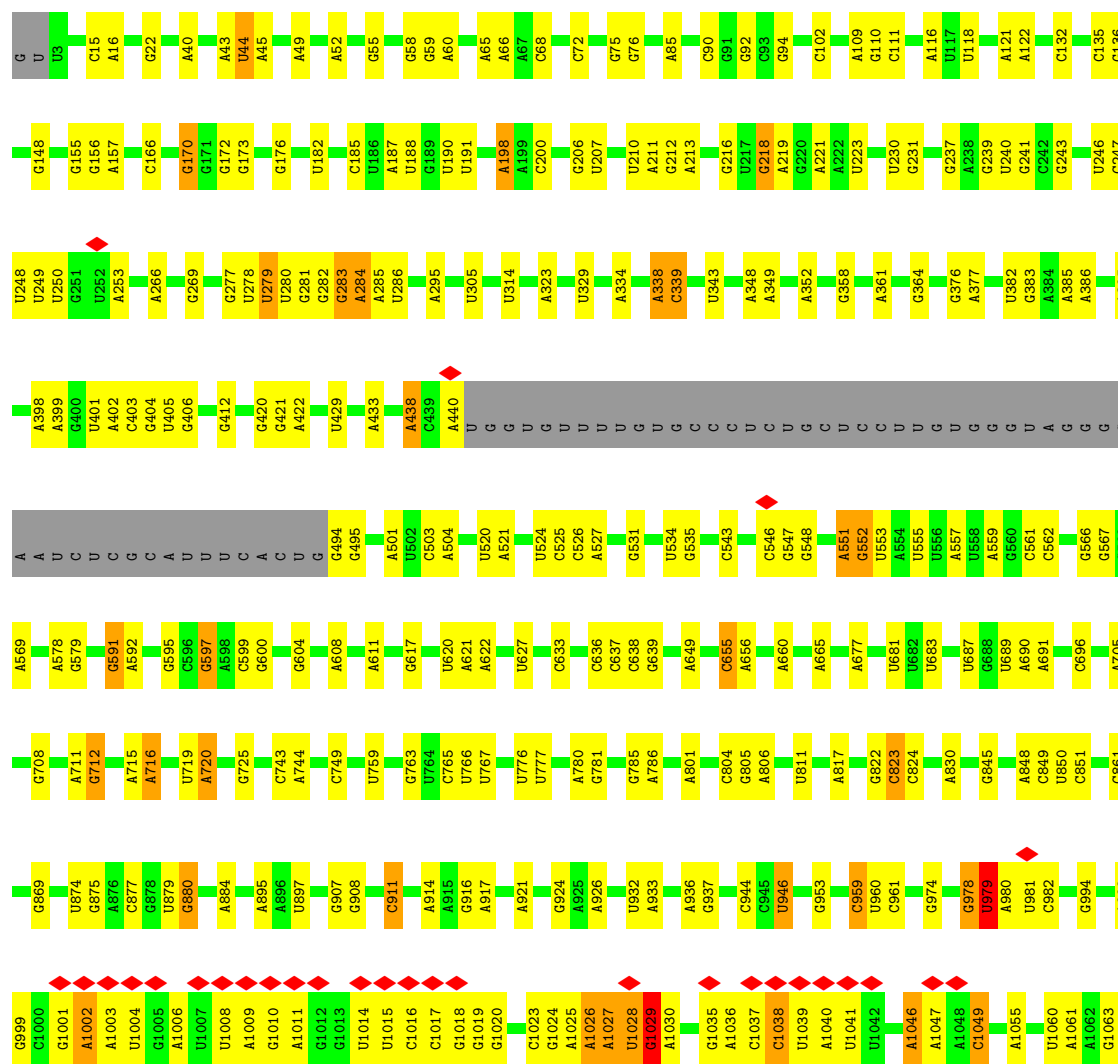




• Molecule 45: 60S ribosomal protein L29



• Molecule 46: *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	v	0.35	0/2831	0.78	5/3847 (0.1%)
3	A	0.42	0/1897	0.76	1/2550 (0.0%)
4	a	0.38	0/758	0.66	1/1023 (0.1%)
5	B	0.43	0/3152	0.82	4/4239 (0.1%)
6	b	0.26	0/2016	0.75	4/2692 (0.1%)
7	C	0.37	0/2801	0.70	4/3792 (0.1%)
8	c	0.33	0/751	0.60	0/1008
9	d	0.41	0/887	0.65	0/1191
10	E	0.31	0/1291	0.65	0/1735
11	e	0.34	0/1041	0.66	0/1394
12	F	0.37	0/1821	0.73	4/2451 (0.2%)
13	f	0.41	0/868	0.61	0/1168
14	G	0.36	0/1830	0.72	2/2469 (0.1%)
15	g	0.39	0/891	0.68	0/1191
16	I	0.25	0/1072	0.66	0/1440
17	H	0.32	0/1514	0.66	0/2039
18	h	0.34	0/978	0.63	0/1301
19	i	0.34	0/749	0.69	1/995 (0.1%)
20	j	0.41	0/685	0.74	0/908
21	k	0.36	0/618	0.64	0/826
22	L	0.37	0/1516	0.75	2/2037 (0.1%)
23	l	0.42	0/443	0.70	0/588
24	M	0.34	0/1074	0.62	0/1446
25	p	0.35	0/701	0.68	0/934
26	N	0.44	0/1757	0.71	0/2354
27	u	0.34	0/1278	0.78	1/1699 (0.1%)
28	O	0.38	0/1585	0.63	0/2128
29	P	0.39	0/1431	0.63	0/1921
30	Q	0.37	0/1211	0.66	0/1633
31	R	0.38	0/1258	0.68	0/1679
32	S	0.35	0/1460	0.68	4/1962 (0.2%)
33	T	0.30	0/483	0.68	0/650
34	U	0.28	0/843	0.66	0/1143
35	V	0.40	0/1018	0.65	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	W	0.23	0/1068	0.59	0/1442
37	X	0.35	0/974	0.62	0/1314
38	Y	0.35	0/1004	0.63	0/1341
39	y	0.30	0/1719	0.65	0/2340
40	Z	0.35	0/1118	0.67	0/1497
41	z	0.18	0/445	0.50	0/585
42	D	0.33	0/2023	0.69	0/2729
43	J	0.27	0/1324	0.78	3/1778 (0.2%)
44	q	0.53	0/795	1.10	3/1050 (0.3%)
45	o	0.37	0/444	0.68	0/592
46	1	0.36	0/76644	0.38	9/119495 (0.0%)
47	2	0.30	0/2883	0.29	0/4491
48	3	0.38	0/3724	0.37	0/5798
All	All	0.36	0/138674	0.52	48/204254 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	v	0	3
3	A	0	1
5	B	0	3
6	b	0	3
7	C	0	1
12	F	0	1
14	G	0	2
16	I	0	1
17	H	0	1
18	h	0	1
22	L	0	1
30	Q	0	1
32	S	0	2
33	T	0	1
38	Y	0	1
39	y	0	2
42	D	0	3
43	J	0	3
44	q	0	9
45	o	0	1
All	All	0	41

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	515	ASN	CA-C-N	-8.08	112.82	122.44
6	b	515	ASN	C-N-CA	-8.08	112.82	122.44
4	a	66	ALA	N-CA-C	-7.13	105.50	114.56
12	F	157	ASN	CA-C-N	7.10	135.09	121.54
12	F	157	ASN	C-N-CA	7.10	135.09	121.54
1	v	146	CYS	CA-CB-SG	6.75	129.91	114.40
43	J	154	THR	CA-C-N	6.58	134.12	121.54
43	J	154	THR	C-N-CA	6.58	134.12	121.54
46	1	2770	G	O5'-C5'-C4'	6.55	121.33	111.50
5	B	138	ALA	CA-C-N	6.48	130.54	120.82
5	B	138	ALA	C-N-CA	6.48	130.54	120.82
44	q	36	PHE	CA-C-O	-6.43	111.00	119.10
14	G	78	PHE	CA-C-N	5.96	132.92	121.54
14	G	78	PHE	C-N-CA	5.96	132.92	121.54
43	J	112	LEU	N-CA-C	-5.90	105.73	113.17
19	i	28	TYR	N-CA-C	-5.88	106.75	114.04
32	S	23	LYS	CA-C-N	5.86	132.73	121.54
32	S	23	LYS	C-N-CA	5.86	132.73	121.54
6	b	397	LYS	CA-C-N	5.72	132.47	121.54
6	b	397	LYS	C-N-CA	5.72	132.47	121.54
1	v	32	LEU	CA-C-N	5.71	132.24	121.97
1	v	32	LEU	C-N-CA	5.71	132.24	121.97
46	1	2541	U	P-O3'-C3'	5.65	128.67	120.20
44	q	82	GLN	N-CA-C	5.59	118.52	109.86
46	1	1576	G	P-O3'-C3'	5.52	128.48	120.20
22	L	75	PHE	CA-C-N	5.48	132.01	121.54
22	L	75	PHE	C-N-CA	5.48	132.01	121.54
46	1	1027	A	P-O3'-C3'	5.44	128.35	120.20
46	1	1815	U	P-O3'-C3'	5.40	128.30	120.20
46	1	1038	C	P-O3'-C3'	5.37	128.26	120.20
46	1	1029	G	P-O3'-C3'	5.30	128.15	120.20
44	q	80	ARG	N-CA-C	5.29	118.32	107.37
7	C	337	GLU	CA-C-N	5.29	131.64	121.54
7	C	337	GLU	C-N-CA	5.29	131.64	121.54
1	v	35	CYS	CA-CB-SG	5.28	126.55	114.40
46	1	979	U	P-O3'-C3'	5.26	128.09	120.20
3	A	218	HIS	N-CA-C	5.20	117.90	109.83
1	v	34	MET	CA-CB-CG	5.15	124.39	114.10
32	S	17	GLU	CA-C-N	5.14	131.35	121.54
32	S	17	GLU	C-N-CA	5.14	131.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	2770	G	C5'-C4'-C3'	5.14	123.70	116.00
12	F	176	TYR	CA-C-N	-5.12	111.37	121.41
12	F	176	TYR	C-N-CA	-5.12	111.37	121.41
7	C	4	PRO	CA-C-N	5.05	131.18	121.54
7	C	4	PRO	C-N-CA	5.05	131.18	121.54
27	u	32	CYS	CA-CB-SG	-5.04	102.81	114.40
5	B	4	ARG	CA-C-N	5.01	131.11	121.54
5	B	4	ARG	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	219	ILE	Peptide
5	B	221	THR	Peptide
5	B	33	PRO	Peptide
5	B	340	LYS	Peptide
7	C	4	PRO	Peptide
42	D	140	ARG	Peptide
42	D	257	GLU	Peptide
42	D	259	LYS	Peptide
12	F	158	LYS	Peptide
14	G	30	THR	Peptide
14	G	76	ALA	Peptide
17	H	21	LYS	Peptide
16	I	16	ARG	Peptide
43	J	153	LYS	Peptide
43	J	154	THR	Peptide
43	J	171	VAL	Peptide
22	L	131	LYS	Peptide
30	Q	152	HIS	Peptide
32	S	22	PRO	Peptide
32	S	23	LYS	Peptide
33	T	154	VAL	Peptide
38	Y	125	LYS	Peptide
6	b	438	GLY	Peptide
6	b	446	ASP	Peptide
6	b	528	PHE	Peptide
18	h	83	LYS	Peptide
45	o	25	LYS	Peptide
44	q	34	SER	Peptide
44	q	35	LEU	Peptide

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Mol	Chain	Res	Type	Group
44	q	41	ARG	Peptide
44	q	49	GLY	Peptide
44	q	50	PHE	Peptide
44	q	78	LYS	Peptide
44	q	79	THR	Peptide
44	q	81	ALA	Peptide
44	q	97	LYS	Peptide
1	v	278	LYS	Peptide
1	v	31	GLY	Peptide
1	v	32	LEU	Peptide
39	y	145	ASN	Peptide
39	y	7	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	v	2783	0	2750	40	0
2	s	1050	0	240	3	0
3	A	1863	0	1930	24	0
4	a	742	0	785	8	0
5	B	3081	0	3165	45	0
6	b	1989	0	1959	31	0
7	C	2749	0	2863	23	0
8	c	743	0	797	5	0
9	d	873	0	914	8	0
10	E	1270	0	1355	18	0
11	e	1020	0	1090	7	0
12	F	1784	0	1862	19	0
13	f	850	0	880	8	0
14	G	1798	0	1894	13	0
15	g	881	0	945	12	0
16	I	1056	0	1084	9	0
17	H	1493	0	1566	11	0
18	h	969	0	1078	7	0
19	i	743	0	822	7	0
20	j	670	0	675	7	0
21	k	612	0	682	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1491	0	1543	15	0
23	l	436	0	475	10	0
24	M	1059	0	1154	17	0
25	p	694	0	734	5	0
26	N	1720	0	1779	22	0
27	u	1256	0	1308	17	0
28	O	1555	0	1659	1	0
29	P	1409	0	1450	16	0
30	Q	1191	0	1265	9	0
31	R	1241	0	1330	13	0
32	S	1425	0	1466	18	0
33	T	476	0	499	6	0
34	U	826	0	843	4	0
35	V	1003	0	1048	16	0
36	W	1053	0	1001	11	0
37	X	959	0	1023	8	0
38	Y	993	0	1081	11	0
39	y	1698	0	1687	24	0
40	Z	1092	0	1155	19	0
41	z	444	0	478	4	0
42	D	1983	0	1937	16	0
43	J	1304	0	1318	11	0
44	q	783	0	853	46	0
45	o	433	0	455	3	0
46	1	68471	0	34407	288	0
47	2	2579	0	1304	15	0
48	3	3333	0	1685	15	0
All	All	129926	0	94273	707	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 4.

All (707) 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)
46:1:2835:U:H3	46:1:2853:A:H61	1.37	0.72
46:1:2534:G:H1	46:1:2545:C:H42	1.39	0.70
25:p:49:ARG:HH21	25:p:52:ALA:HB2	1.57	0.69
10:E:125:GLN:HE21	10:E:125:GLN:HA	1.57	0.69
38:Y:55:GLU:HB2	38:Y:108:LYS:HB2	1.75	0.69
1:v:156:ARG:HH12	1:v:239:THR:HA	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:46:ILE:HG22	22:L:49:ARG:HB2	1.75	0.68
10:E:125:GLN:HA	10:E:125:GLN:NE2	2.10	0.67
1:v:378:ASN:HB2	44:q:89:LYS:HB2	1.77	0.66
44:q:18:ARG:NH2	46:1:759:U:OP2	2.29	0.66
46:1:1201:C:H42	46:1:2857:C:H5'	1.61	0.66
46:1:2469:G:H1	46:1:2476:C:H42	1.43	0.65
48:3:72:A:H61	48:3:79:A:H61	1.44	0.65
35:V:81:GLN:O	35:V:98:ASN:ND2	2.31	0.64
1:v:233:THR:HG21	46:1:2942:C:H42	1.63	0.64
20:j:52:LYS:HG2	20:j:55:ARG:HH21	1.62	0.64
39:y:119:PRO:O	39:y:139:ARG:NH2	2.30	0.64
43:J:47:GLN:HG2	43:J:67:VAL:HG12	1.80	0.64
1:v:378:ASN:HA	44:q:90:HIS:HB2	1.80	0.63
5:B:28:ARG:NH2	46:1:3140:G:N7	2.46	0.63
24:M:72:LEU:HD11	24:M:81:VAL:HG22	1.78	0.63
36:W:55:GLU:HA	36:W:58:THR:HG22	1.80	0.63
7:C:193:LYS:NZ	48:3:21:C:OP1	2.31	0.63
44:q:49:GLY:HA2	46:1:278:U:H3'	1.81	0.63
3:A:54:ARG:NH2	46:1:2176:U:OP1	2.31	0.63
13:f:99:ARG:NH1	46:1:3275:U:O2'	2.32	0.62
35:V:69:LEU:HD23	35:V:74:MET:HE1	1.81	0.62
15:g:90:ILE:HD12	40:Z:81:LEU:HD13	1.82	0.62
22:L:174:ARG:HH12	46:1:712:G:H5'	1.63	0.62
22:L:24:VAL:HG12	26:N:199:LEU:HB2	1.81	0.62
42:D:218:ARG:NH2	47:2:31:U:O2'	2.33	0.61
23:l:27:ILE:O	23:l:33:ASN:ND2	2.34	0.61
46:1:2404:A:H62	46:1:2872:A:H62	1.49	0.61
26:N:203:ARG:NH1	46:1:665:A:OP1	2.32	0.61
1:v:205:ASN:ND2	46:1:2284:C:O2	2.33	0.61
7:C:334:PHE:HA	7:C:339:LEU:HD12	1.82	0.61
41:z:2:ALA:N	46:1:3015:G:OP2	2.33	0.61
6:b:647:ARG:NH1	46:1:877:C:N3	2.49	0.60
36:W:54:GLN:NE2	46:1:1232:C:O2	2.33	0.60
12:F:121:LYS:HB2	33:T:133:ALA:HB3	1.84	0.60
26:N:5:LYS:NZ	46:1:266:A:OP1	2.35	0.60
25:p:49:ARG:NH2	46:1:1793:C:OP2	2.35	0.60
27:u:44:ARG:NH2	46:1:2111:G:N3	2.50	0.60
1:v:379:TYR:H	44:q:90:HIS:CD2	2.19	0.60
16:I:4:TYR:OH	16:I:8:ARG:NH2	2.34	0.60
40:Z:52:LYS:O	40:Z:65:ARG:NH1	2.35	0.60
44:q:70:LEU:HD22	44:q:83:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:73:LYS:NZ	32:S:97:VAL:O	2.34	0.60
46:1:358:G:N2	46:1:361:A:OP2	2.34	0.60
46:1:3346:U:H3	46:1:3359:A:H61	1.50	0.59
35:V:12:ARG:NH1	46:1:3092:C:O2	2.34	0.59
31:R:103:ARG:NH1	31:R:124:TYR:OH	2.35	0.59
46:1:999:G:N3	46:1:1002:A:N6	2.50	0.59
6:b:604:ARG:NH1	46:1:377:A:OP2	2.35	0.59
29:P:131:ARG:NH2	46:1:2356:A:N3	2.49	0.59
37:X:27:ARG:NH2	48:3:150:G:OP1	2.36	0.59
3:A:221:LYS:NZ	46:1:2965:U:O2	2.36	0.59
5:B:216:ASP:HB3	5:B:278:ILE:HA	1.84	0.59
9:d:31:ARG:NH2	46:1:1884:A:OP1	2.34	0.59
24:M:13:ARG:NH1	24:M:65:LEU:O	2.36	0.59
27:u:44:ARG:NH2	46:1:2111:G:O2'	2.35	0.59
44:q:42:ARG:HD2	44:q:46:LYS:HB2	1.84	0.59
3:A:230:VAL:HG23	46:1:2424:A:H61	1.68	0.59
3:A:117:GLU:HG2	3:A:124:GLY:H	1.67	0.59
7:C:291:ASN:ND2	46:1:1350:A:OP1	2.36	0.59
29:P:50:GLN:HB3	29:P:55:GLN:HB2	1.85	0.59
44:q:71:ARG:HH21	44:q:82:GLN:HE21	1.48	0.58
35:V:40:LYS:HZ2	35:V:59:MET:HE2	1.68	0.58
46:1:2117:A:HO2'	46:1:3080:G:HO2'	1.50	0.58
48:3:126:A:O2'	48:3:128:U:OP2	2.20	0.58
1:v:58:CYS:SG	1:v:143:CYS:N	2.67	0.58
14:G:48:ARG:NH1	46:1:2526:C:N3	2.51	0.58
27:u:74:ARG:HH21	39:y:96:ARG:HH11	1.50	0.58
31:R:60:LYS:NZ	46:1:1671:C:OP1	2.35	0.58
46:1:198:A:N3	46:1:218:G:O2'	2.36	0.58
46:1:2425:G:H1	46:1:2604:U:H3	1.50	0.58
32:S:42:TRP:HE1	32:S:58:ILE:HD11	1.68	0.58
3:A:192:LYS:HB3	3:A:193:ARG:HE	1.67	0.58
37:X:77:GLU:HG2	37:X:133:LEU:HD21	1.84	0.58
46:1:526:C:N3	46:1:527:A:N6	2.51	0.58
46:1:1004:U:H3	46:1:1046:A:H61	1.52	0.58
29:P:62:ARG:NH1	46:1:412:G:OP1	2.36	0.58
14:G:68:ARG:NH1	46:1:2514:U:OP2	2.37	0.58
5:B:266:ARG:NH2	46:1:2392:C:O2'	2.37	0.57
20:j:72:ARG:NH1	48:3:95:G:OP2	2.37	0.57
38:Y:16:ARG:NH1	46:1:216:G:OP1	2.35	0.57
40:Z:23:VAL:HG12	40:Z:45:GLY:HA3	1.84	0.57
22:L:28:GLN:HB3	26:N:201:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:124:LEU:HD22	33:T:154:VAL:HA	1.86	0.57
5:B:235:THR:HG21	5:B:249:VAL:HG22	1.86	0.57
22:L:27:ASP:HB3	48:3:29:U:H5''	1.86	0.57
46:1:978:G:O2'	46:1:979:U:O2	2.20	0.57
11:e:47:ARG:NH1	46:1:1147:G:OP1	2.35	0.57
14:G:144:GLU:HA	14:G:173:MET:HE2	1.86	0.57
15:g:11:ASN:O	15:g:18:ASN:ND2	2.37	0.57
36:W:54:GLN:NE2	46:1:1257:C:O2	2.38	0.57
4:a:71:PRO:HG2	4:a:109:TYR:HA	1.87	0.57
6:b:509:ASN:HA	9:d:61:LYS:HE3	1.86	0.57
39:y:126:GLU:OE1	39:y:139:ARG:NH1	2.38	0.57
34:U:77:LYS:NZ	46:1:1678:G:OP2	2.36	0.57
42:D:93:THR:O	42:D:158:ARG:NH2	2.37	0.57
47:2:77:G:N2	47:2:102:A:OP2	2.36	0.57
6:b:614:ASN:O	29:P:125:GLN:NE2	2.37	0.57
44:q:67:LYS:HG2	46:1:2792:A:H2'	1.87	0.57
46:1:2818:U:O2'	46:1:2870:C:N4	2.38	0.57
31:R:74:ARG:NH1	46:1:1942:U:OP2	2.38	0.56
39:y:158:GLY:HA2	39:y:179:VAL:HB	1.87	0.56
46:1:2137:U:OP2	46:1:2142:A:N6	2.38	0.56
13:f:21:ARG:O	46:1:633:C:O2'	2.23	0.56
46:1:1103:A:N6	46:1:1363:A:O2'	2.38	0.56
5:B:308:MET:HE2	46:1:3329:U:H5''	1.86	0.56
24:M:79:ALA:HB2	46:1:525:C:H5''	1.87	0.56
31:R:38:ARG:HG3	46:1:1602:A:H5''	1.87	0.56
7:C:98:ARG:NH2	46:1:804:C:OP1	2.38	0.56
1:v:333:ARG:HH12	1:v:362:ILE:HG23	1.71	0.56
3:A:35:ALA:HA	14:G:36:ILE:HD11	1.88	0.56
46:1:3352:U:H4'	46:1:3353:G:H5'	1.86	0.56
7:C:329:PRO:HB3	12:F:41:ARG:HH21	1.71	0.56
31:R:42:ARG:NH2	46:1:1600:U:OP1	2.39	0.56
39:y:106:ASN:ND2	39:y:150:SER:OG	2.39	0.56
46:1:566:G:H2'	46:1:567:G:H8	1.71	0.56
1:v:58:CYS:HB3	1:v:61:CYS:HB2	1.87	0.56
10:E:46:ARG:NH2	46:1:3268:A:OP1	2.39	0.56
22:L:36:ARG:NH2	46:1:687:U:OP2	2.38	0.56
29:P:171:ARG:NH2	46:1:3274:A:N7	2.54	0.56
41:z:18:ARG:NH2	46:1:3100:U:OP1	2.39	0.56
46:1:1222:G:O2'	46:1:1285:G:N1	2.38	0.56
40:Z:54:THR:H	40:Z:57:HIS:HD2	1.54	0.56
26:N:73:ARG:HH21	26:N:92:LEU:HD22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Z:15:ARG:HD2	40:Z:79:HIS:HD2	1.71	0.56
7:C:338:LYS:O	7:C:340:GLY:N	2.39	0.55
42:D:146:LEU:HD22	42:D:163:LEU:HD12	1.87	0.55
46:1:3155:U:H5'	46:1:3156:U:H4'	1.86	0.55
18:h:59:ASN:ND2	48:3:97:A:O2'	2.39	0.55
19:i:34:SER:OG	19:i:37:THR:N	2.35	0.55
44:q:65:THR:OG1	46:1:2794:G:OP2	2.23	0.55
30:Q:86:THR:HG22	30:Q:105:ARG:HB2	1.89	0.55
44:q:82:GLN:HB2	46:1:2790:A:H2	1.69	0.55
12:F:128:LYS:HE3	47:2:99:G:H4'	1.89	0.55
36:W:45:LEU:HD12	36:W:48:VAL:HG11	1.88	0.55
1:v:359:LEU:HD22	1:v:362:ILE:HD11	1.89	0.55
6:b:619:GLN:HG3	23:l:46:ARG:HH21	1.72	0.55
6:b:459:GLU:HB3	27:u:103:ARG:HH22	1.71	0.55
7:C:188:ARG:NH1	46:1:1382:G:OP2	2.40	0.55
11:e:42:VAL:HG12	11:e:52:GLN:HE21	1.72	0.55
24:M:85:TRP:NE1	24:M:91:CYS:SG	2.80	0.55
44:q:49:GLY:N	46:1:278:U:OP2	2.39	0.55
16:l:17:ASP:OD2	27:u:23:ARG:NH1	2.40	0.55
18:h:85:THR:OG1	48:3:36:G:OP2	2.24	0.55
36:W:217:VAL:HG12	36:W:233:ILE:HD11	1.88	0.55
39:y:101:LEU:HD13	39:y:107:VAL:HG21	1.89	0.55
15:g:41:ARG:HD2	15:g:56:THR:HG21	1.89	0.55
44:q:26:THR:N	44:q:71:ARG:O	2.39	0.55
32:S:115:ARG:NH2	46:1:1320:C:O2	2.39	0.55
35:V:120:LYS:HB2	35:V:137:VAL:HG22	1.89	0.55
5:B:227:GLU:HG2	5:B:270:ARG:HE	1.72	0.54
6:b:390:PRO:O	6:b:395:ARG:NH1	2.39	0.54
11:e:101:SER:HB3	46:1:1389:G:H5''	1.89	0.54
42:D:15:ARG:NH1	46:1:2689:A:OP1	2.40	0.54
6:b:601:LYS:NZ	46:1:377:A:OP1	2.40	0.54
8:c:54:SER:OG	46:1:2552:C:N4	2.40	0.54
35:V:12:ARG:HH12	46:1:3092:C:H1'	1.72	0.54
15:g:37:LYS:NZ	46:1:1591:G:OP1	2.39	0.54
1:v:108:HIS:HB2	46:1:2839:G:H21	1.72	0.54
10:E:82:ARG:NH2	46:1:501:A:OP1	2.40	0.54
26:N:42:PRO:HG3	26:N:61:ILE:HG13	1.89	0.54
6:b:448:GLU:HB2	6:b:451:ALA:HB3	1.88	0.54
7:C:119:ARG:NH2	46:1:696:C:OP2	2.40	0.54
14:G:33:ASN:ND2	46:1:2549:G:N7	2.55	0.54
24:M:74:ARG:NH2	46:1:534:U:O4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:54:TYR:HA	10:E:65:ILE:HG22	1.89	0.54
46:1:1635:G:N2	46:1:1638:A:OP2	2.34	0.54
46:1:2457:G:N1	46:1:2461:A:OP1	2.38	0.54
46:1:1060:U:H2'	46:1:1061:A:H8	1.73	0.54
1:v:291:LEU:HD11	1:v:358:HIS:HB3	1.90	0.54
46:1:68:C:N4	46:1:314:U:O2'	2.40	0.54
46:1:1551:C:O2'	46:1:2170:U:O2'	2.26	0.54
23:l:2:ALA:N	46:1:1493:G:O6	2.41	0.53
44:q:11:TYR:HA	44:q:20:HIS:HA	1.89	0.53
46:1:3129:A:N6	46:1:3131:U:O2	2.41	0.53
5:B:214:MET:O	5:B:341:SER:OG	2.26	0.53
7:C:283:THR:HG22	7:C:285:ASP:H	1.74	0.53
17:H:47:LYS:HD3	24:M:5:SER:HB2	1.89	0.53
3:A:21:ARG:HD3	46:1:824:C:H5''	1.91	0.53
5:B:215:ILE:HD13	5:B:338:LEU:HD12	1.90	0.53
46:1:90:C:O2'	46:1:282:G:OP1	2.26	0.53
46:1:708:G:N2	46:1:711:A:OP2	2.41	0.53
46:1:1489:A:OP2	46:1:1838:G:N1	2.37	0.53
39:y:126:GLU:HG3	39:y:137:VAL:HG11	1.89	0.53
17:H:20:ILE:HG21	17:H:45:PHE:HD2	1.72	0.53
24:M:109:ARG:NH1	46:1:3210:A:OP1	2.39	0.53
46:1:1551:C:HO2'	46:1:2170:U:HO2'	1.55	0.53
10:E:40:LEU:HD13	10:E:84:VAL:HG11	1.91	0.53
34:U:21:SER:O	34:U:25:ASN:ND2	2.42	0.53
39:y:28:VAL:HG12	39:y:50:HIS:HB3	1.90	0.53
41:z:46:LEU:HD23	41:z:49:LEU:HD12	1.90	0.53
1:v:169:ARG:HH21	1:v:253:LYS:HD3	1.73	0.53
10:E:43:LEU:HD11	10:E:85:ILE:HG13	1.91	0.53
14:G:47:SER:OG	46:1:2585:G:O6	2.25	0.53
32:S:109:ASP:OD1	32:S:113:ARG:NH1	2.42	0.53
38:Y:122:LYS:HG2	46:1:185:C:H5''	1.91	0.53
43:J:15:GLU:HB3	43:J:130:VAL:HG13	1.89	0.53
46:1:1055:A:N3	47:2:81:U:O2'	2.41	0.53
35:V:76:ALA:HA	35:V:102:ILE:HA	1.90	0.53
3:A:68:LYS:NZ	46:1:1580:A:OP1	2.42	0.53
46:1:44:U:O4	46:1:94:G:N2	2.40	0.53
5:B:216:ASP:OD1	5:B:216:ASP:N	2.41	0.53
6:b:588:ARG:HB3	23:l:21:ARG:HH21	1.73	0.53
44:q:41:ARG:HG3	46:1:283:G:H5''	1.91	0.53
46:1:877:C:HO2'	46:1:880:G:HO2'	1.57	0.53
32:S:44:PHE:HE1	32:S:122:HIS:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:139:ARG:NH2	22:L:161:ASP:OD2	2.42	0.52
6:b:622:SER:OG	23:l:46:ARG:NH1	2.42	0.52
43:J:109:HIS:HD2	43:J:123:PHE:H	1.57	0.52
1:v:63:ARG:HE	1:v:73:ARG:HE	1.57	0.52
3:A:136:ILE:HG13	3:A:148:VAL:HG12	1.91	0.52
20:j:52:LYS:NZ	46:1:364:G:OP2	2.41	0.52
22:L:79:GLU:OE2	22:L:103:ASN:ND2	2.41	0.52
38:Y:126:LEU:HD12	38:Y:127:GLU:HG2	1.91	0.52
15:g:79:SER:OG	15:g:80:ARG:NH1	2.42	0.52
5:B:317:ILE:O	5:B:319:ASN:N	2.43	0.52
6:b:608:MET:SD	6:b:611:ARG:NH1	2.75	0.52
18:h:91:ALA:O	26:N:143:ARG:NH2	2.43	0.52
9:d:55:LEU:HB2	9:d:95:PRO:HD3	1.91	0.52
26:N:37:HIS:HE1	26:N:63:ARG:HH11	1.58	0.52
43:J:96:PHE:HB2	43:J:156:LYS:HE3	1.91	0.52
44:q:23:HIS:HB3	44:q:72:LEU:HB3	1.92	0.52
46:1:845:G:N2	46:1:848:A:OP2	2.43	0.52
1:v:111:ARG:NH1	46:1:2849:C:O2'	2.29	0.52
6:b:392:ASP:HB3	6:b:395:ARG:HD3	1.92	0.52
11:e:118:LYS:NZ	46:1:438:A:OP1	2.39	0.52
12:F:178:ILE:HD11	12:F:187:GLU:HG3	1.90	0.52
5:B:303:LYS:HD2	5:B:361:THR:HG21	1.92	0.52
31:R:62:ARG:NH1	46:1:3068:U:OP2	2.37	0.52
32:S:132:THR:OG1	46:1:534:U:OP1	2.28	0.52
36:W:42:VAL:HG12	36:W:102:LEU:HG	1.92	0.52
7:C:3:ARG:NH2	7:C:27:SER:OG	2.43	0.52
7:C:326:ARG:NH1	46:1:608:A:O3'	2.43	0.52
37:X:68:THR:HA	37:X:73:MET:HE1	1.92	0.52
42:D:71:GLY:O	47:2:7:G:O2'	2.21	0.52
46:1:2471:U:O4	46:1:2474:G:N2	2.42	0.52
31:R:102:LEU:HD22	31:R:138:LEU:HD13	1.92	0.51
1:v:210:MET:HE2	1:v:214:LEU:HD11	1.91	0.51
8:c:103:THR:HG22	8:c:105:ALA:H	1.74	0.51
14:G:162:LEU:HA	26:N:7:LEU:HD11	1.90	0.51
42:D:65:ILE:HG12	42:D:74:VAL:HG22	1.92	0.51
46:1:1189:C:N4	46:1:1316:C:OP2	2.43	0.51
46:1:2116:G:OP1	46:1:2118:C:N4	2.43	0.51
18:h:48:ARG:HH12	48:3:48:A:H5''	1.75	0.51
35:V:87:ARG:HH22	35:V:137:VAL:HG13	1.76	0.51
26:N:155:VAL:HG12	46:1:58:G:H4'	1.93	0.51
27:u:2:ARG:O	27:u:4:TYR:N	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:290:THR:HA	1:v:335:LEU:HD11	1.92	0.51
29:P:30:ARG:NH1	29:P:31:GLU:OE2	2.41	0.51
37:X:100:LYS:NZ	37:X:106:ASP:OD1	2.44	0.51
3:A:67:TYR:OH	46:1:2525:G:N7	2.42	0.51
5:B:57:VAL:HG23	5:B:357:LYS:HB3	1.92	0.51
46:1:1203:A:N3	46:1:2855:U:O2'	2.40	0.51
42:D:77:ALA:O	42:D:108:ARG:NH1	2.44	0.51
5:B:74:GLU:OE2	5:B:283:TYR:OH	2.23	0.51
5:B:90:VAL:HG22	5:B:104:THR:HG22	1.93	0.51
5:B:226:PHE:O	46:1:1886:A:O2'	2.29	0.51
17:H:16:VAL:HG12	17:H:29:GLY:HA3	1.93	0.51
35:V:74:MET:HE3	35:V:102:ILE:HG21	1.93	0.51
46:1:2185:G:O2'	46:1:2314:U:OP2	2.29	0.51
5:B:10:ARG:NH1	5:B:11:HIS:O	2.44	0.50
23:l:21:ARG:HH22	23:l:24:PRO:HG3	1.75	0.50
25:p:3:LYS:NZ	46:1:850:U:OP1	2.42	0.50
32:S:57:GLU:OE1	33:T:136:ARG:NH1	2.44	0.50
46:1:1562:C:O2'	46:1:1563:C:O4'	2.29	0.50
4:a:112:ILE:HB	4:a:130:VAL:HG12	1.92	0.50
5:B:33:PRO:HG3	5:B:342:LEU:HA	1.93	0.50
14:G:81:THR:HG21	14:G:181:LYS:HE3	1.93	0.50
19:i:5:THR:HG23	19:i:12:ASN:HB2	1.93	0.50
44:q:79:THR:N	46:1:2771:U:OP2	2.40	0.50
17:H:89:LYS:HG2	17:H:145:VAL:HG22	1.92	0.50
19:i:59:ASP:O	19:i:63:ASN:ND2	2.45	0.50
32:S:9:VAL:HG22	32:S:61:ILE:HG22	1.94	0.50
8:c:73:GLY:N	8:c:76:GLU:OE2	2.44	0.50
29:P:56:ARG:NH1	29:P:75:GLU:OE2	2.45	0.50
18:h:118:ILE:HG12	22:L:123:ILE:HG22	1.92	0.50
29:P:107:LEU:HD23	29:P:152:GLU:HG3	1.92	0.50
39:y:9:ASN:ND2	46:1:3018:C:OP1	2.38	0.50
44:q:63:LYS:HB3	46:1:2794:G:H5''	1.94	0.50
27:u:10:SER:HB2	27:u:53:LYS:HB2	1.94	0.50
46:1:1203:A:OP2	46:1:1301:A:N6	2.43	0.50
5:B:325:LYS:NZ	46:1:3096:C:O3'	2.45	0.50
10:E:138:GLN:NE2	10:E:142:ASP:OD2	2.39	0.50
13:f:14:LEU:HD11	13:f:31:LYS:HB2	1.93	0.50
15:g:93:PHE:HZ	40:Z:83:THR:HG23	1.76	0.50
43:J:133:ARG:NH2	43:J:158:ASP:OD2	2.44	0.50
44:q:42:ARG:HD3	44:q:45:ARG:HB3	1.92	0.50
5:B:62:ARG:NH1	46:1:3039:C:OP1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:108:LYS:NZ	46:1:617:G:OP1	2.43	0.50
13:f:57:LYS:NZ	46:1:433:A:OP2	2.41	0.50
15:g:58:ARG:NH2	46:1:1592:G:OP1	2.45	0.50
24:M:20:VAL:O	24:M:66:THR:OG1	2.28	0.50
24:M:77:ARG:NH1	46:1:524:U:OP1	2.40	0.50
46:1:2452:G:O2'	46:1:2496:C:N4	2.44	0.50
1:v:111:ARG:HH12	46:1:2849:C:HO2'	1.54	0.49
6:b:427:TRP:HB3	27:u:83:ARG:HD2	1.94	0.49
47:2:7:G:H2'	47:2:8:G:H8	1.77	0.49
4:a:104:THR:HG21	4:a:112:ILE:HD11	1.94	0.49
12:F:110:ARG:NH1	46:1:1364:C:OP1	2.44	0.49
13:f:49:ILE:HG12	13:f:100:ILE:HG13	1.93	0.49
19:i:68:ARG:NH2	46:1:2218:G:OP1	2.45	0.49
46:1:503:C:H2'	46:1:504:A:H8	1.77	0.49
27:u:80:ARG:NH2	39:y:90:ASP:OD1	2.45	0.49
35:V:135:VAL:HG22	39:y:101:LEU:HA	1.95	0.49
38:Y:13:ARG:NH1	48:3:24:G:N7	2.60	0.49
39:y:112:ASP:OD2	39:y:156:ASN:ND2	2.41	0.49
44:q:32:LYS:HG3	44:q:34:SER:H	1.77	0.49
46:1:3179:U:O4	46:1:3208:G:N2	2.40	0.49
44:q:8:ARG:HD3	44:q:72:LEU:HD11	1.94	0.49
46:1:946:U:O2	46:1:1374:G:N2	2.46	0.49
46:1:998:A:O2'	47:2:103:A:N3	2.45	0.49
11:e:2:ALA:O	11:e:90:LYS:NZ	2.42	0.49
36:W:96:CYS:HB2	36:W:100:THR:HG21	1.93	0.49
4:a:126:LYS:HG2	4:a:146:GLU:HB2	1.95	0.49
6:b:618:LYS:HG3	6:b:623:ASP:HB3	1.93	0.49
12:F:41:ARG:NH1	46:1:597:G:OP1	2.37	0.49
39:y:85:ARG:NH1	39:y:89:PRO:O	2.46	0.49
46:1:1816:A:H2'	46:1:1817:G:H8	1.78	0.49
26:N:112:ASN:N	26:N:112:ASN:OD1	2.45	0.49
40:Z:51:LEU:HB2	40:Z:65:ARG:HD2	1.94	0.49
9:d:86:LYS:HD3	9:d:87:ASN:HB2	1.95	0.49
37:X:105:VAL:HG21	37:X:135:ILE:HD12	1.92	0.49
46:1:1246:G:O2'	46:1:1264:G:OP2	2.30	0.49
2:s:106:UNK:O	2:s:132:UNK:N	2.46	0.49
7:C:342:LYS:NZ	12:F:56:GLU:OE1	2.42	0.49
27:u:24:ASN:ND2	35:V:96:GLU:OE1	2.45	0.49
1:v:310:ALA:HB2	1:v:379:TYR:HE1	1.78	0.49
13:f:52:VAL:HG22	13:f:66:VAL:HG22	1.95	0.49
19:i:18:THR:HG23	22:L:106:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:96:ARG:HH21	26:N:100:ALA:HB1	1.78	0.48
46:1:1562:C:H42	46:1:1578:C:H42	1.61	0.48
47:2:3:U:OP1	47:2:59:U:O2'	2.30	0.48
3:A:104:LEU:HD22	3:A:158:ILE:HD11	1.94	0.48
43:J:142:LYS:NZ	46:1:2664:C:OP2	2.47	0.48
46:1:1899:G:O2'	46:1:2334:U:O4	2.24	0.48
20:j:66:TYR:OH	20:j:73:ARG:NH2	2.45	0.48
44:q:34:SER:O	44:q:36:PHE:N	2.46	0.48
10:E:5:LYS:HD3	46:1:1423:C:H4'	1.94	0.48
30:Q:122:ILE:HG23	30:Q:126:GLN:HB2	1.94	0.48
11:e:104:ASN:ND2	46:1:1389:G:OP1	2.43	0.48
46:1:2094:C:H2'	46:1:2095:G:H8	1.79	0.48
10:E:52:VAL:HG11	10:E:65:ILE:HD13	1.95	0.48
24:M:17:VAL:HG21	24:M:74:ARG:HB3	1.94	0.48
24:M:60:LEU:HD13	32:S:152:LEU:HD11	1.96	0.48
26:N:36:ILE:HG12	26:N:64:VAL:HG23	1.95	0.48
31:R:20:ARG:NH1	46:1:1874:A:N7	2.62	0.48
12:F:186:HIS:O	12:F:190:THR:OG1	2.28	0.48
24:M:24:LYS:NZ	24:M:61:GLY:O	2.38	0.48
31:R:20:ARG:HG3	31:R:21:LYS:HG2	1.95	0.48
46:1:494:G:OP2	46:1:494:G:N2	2.36	0.48
17:H:92:TYR:HB3	17:H:179:ILE:HG12	1.95	0.48
40:Z:133:LYS:NZ	46:1:1808:G:OP2	2.47	0.48
46:1:405:U:O2'	46:1:1395:G:N2	2.47	0.48
46:1:1134:G:O2'	46:1:2642:A:N3	2.38	0.48
46:1:1350:A:H2'	46:1:1351:U:H3'	1.95	0.48
46:1:2945:G:O2'	46:1:2948:C:OP2	2.25	0.48
5:B:76:VAL:HG21	5:B:323:MET:HE3	1.96	0.47
29:P:78:VAL:HG12	29:P:80:LYS:H	1.79	0.47
39:y:7:PHE:O	39:y:10:SER:N	2.45	0.47
46:1:2373:A:N7	46:1:2867:C:O2'	2.47	0.47
32:S:43:TYR:OH	47:2:96:U:OP1	2.26	0.47
35:V:18:PRO:HA	35:V:51:ALA:HA	1.95	0.47
39:y:78:ASP:OD1	39:y:96:ARG:NH2	2.33	0.47
35:V:131:SER:O	39:y:106:ASN:ND2	2.47	0.47
46:1:1255:C:H2'	46:1:1256:G:H8	1.78	0.47
46:1:2450:G:H1	46:1:2497:U:H3	1.62	0.47
6:b:418:ASP:HA	6:b:428:LYS:HD3	1.95	0.47
18:h:75:TYR:HB3	37:X:46:TYR:HD1	1.78	0.47
44:q:41:ARG:HB2	44:q:44:ASP:HB2	1.96	0.47
10:E:128:LYS:NZ	46:1:3271:G:O6	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:12:CYS:N	44:q:19:LYS:O	2.37	0.47
44:q:21:THR:HB	44:q:76:LYS:HD2	1.96	0.47
46:1:188:U:O2'	46:1:207:U:O2	2.33	0.47
1:v:309:LEU:HD11	1:v:379:TYR:HB3	1.95	0.47
36:W:91:GLN:HB2	36:W:228:VAL:HG21	1.95	0.47
44:q:27:GLN:HB3	44:q:29:LYS:HE2	1.96	0.47
32:S:23:LYS:O	33:T:146:ASN:ND2	2.48	0.47
38:Y:70:ILE:HG13	38:Y:82:VAL:HG22	1.95	0.47
42:D:95:TRP:NE1	42:D:157:ALA:O	2.44	0.47
1:v:66:GLN:HG2	1:v:68:PRO:HD2	1.95	0.47
36:W:55:GLU:OE2	36:W:119:TYR:OH	2.29	0.47
39:y:4:ARG:HB3	39:y:208:LEU:HD23	1.95	0.47
46:1:1195:A:O2'	46:1:1320:C:OP1	2.32	0.47
11:e:123:LYS:HA	11:e:126:LEU:HB3	1.97	0.47
12:F:94:LYS:NZ	46:1:1156:C:OP2	2.43	0.47
46:1:2991:A:O2'	46:1:3309:G:N7	2.47	0.47
5:B:137:TYR:CZ	5:B:144:ILE:HG13	2.50	0.47
27:u:61:LYS:NZ	46:1:3366:G:OP1	2.48	0.47
46:1:348:A:N3	46:1:352:A:O2'	2.47	0.47
5:B:110:LEU:O	5:B:115:LYS:NZ	2.48	0.46
46:1:52:A:N3	46:1:811:U:O2'	2.48	0.46
1:v:143:CYS:O	1:v:147:ALA:N	2.49	0.46
7:C:35:VAL:HG21	7:C:244:LEU:HD21	1.97	0.46
10:E:17:ALA:O	46:1:591:G:O2'	2.33	0.46
15:g:65:VAL:O	15:g:70:LYS:NZ	2.47	0.46
46:1:2964:G:N2	46:1:2967:A:OP2	2.48	0.46
5:B:166:ILE:HD11	5:B:171:LEU:HD22	1.98	0.46
17:H:44:THR:OG1	46:1:3186:A:N3	2.43	0.46
27:u:143:ARG:O	27:u:147:LYS:N	2.45	0.46
1:v:265:LYS:NZ	46:1:2235:C:O2'	2.46	0.46
17:H:20:ILE:HB	24:M:7:VAL:HG22	1.97	0.46
26:N:112:ASN:ND2	48:3:141:C:O2	2.48	0.46
44:q:3:ASN:ND2	44:q:96:GLU:O	2.48	0.46
46:1:805:G:H2'	46:1:936:A:H61	1.80	0.46
46:1:2168:A:N6	46:1:2170:U:O2	2.49	0.46
12:F:151:ARG:HH22	46:1:1334:U:H4'	1.80	0.46
39:y:15:VAL:HG23	39:y:195:ALA:HB1	1.97	0.46
39:y:219:GLU:HG3	39:y:224:LEU:HB2	1.96	0.46
46:1:2249:G:N2	46:1:2268:U:O2	2.49	0.46
1:v:280:SER:OG	1:v:281:ASN:N	2.48	0.46
1:v:326:THR:HG21	1:v:356:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:234:LYS:NZ	46:1:2162:U:OP1	2.39	0.46
10:E:62:THR:HG21	10:E:78:ARG:HH11	1.80	0.46
46:1:1268:G:O2'	46:1:1269:U:O2	2.33	0.46
5:B:187:SER:OG	5:B:190:GLU:OE1	2.27	0.46
5:B:255:TRP:NE1	46:1:2395:G:OP1	2.48	0.46
5:B:274:SER:O	5:B:275:ARG:NH1	2.49	0.46
6:b:488:ASP:OD2	6:b:492:LYS:NZ	2.41	0.46
26:N:64:VAL:HG11	26:N:102:ALA:HB1	1.98	0.46
42:D:22:ARG:HE	42:D:27:LYS:HB2	1.81	0.46
46:1:638:C:N4	46:1:639:G:O6	2.49	0.46
46:1:1278:A:H1'	46:1:1279:C:H5'	1.98	0.46
46:1:2660:G:OP1	46:1:2750:U:O2'	2.34	0.46
46:1:2947:G:OP1	46:1:2982:A:N6	2.41	0.46
5:B:66:LYS:O	5:B:70:ARG:NH2	2.48	0.46
6:b:364:ALA:HB3	39:y:181:LEU:H	1.80	0.46
6:b:374:ARG:NH1	39:y:156:ASN:OD1	2.49	0.46
12:F:208:SER:OG	12:F:209:ASN:N	2.49	0.46
13:f:16:TYR:OH	13:f:89:LEU:O	2.30	0.46
46:1:170:G:N1	46:1:249:U:O2	2.48	0.46
46:1:279:U:H2'	46:1:280:U:C2	2.51	0.46
46:1:1303:A:N3	46:1:2885:C:O2'	2.44	0.46
44:q:58:PHE:CE2	44:q:63:LYS:HE3	2.50	0.46
1:v:156:ARG:HA	1:v:241:LYS:HG3	1.98	0.45
3:A:96:LEU:HD23	25:p:83:ILE:HG23	1.98	0.45
5:B:187:SER:O	5:B:190:GLU:N	2.40	0.45
15:g:7:PHE:HE2	46:1:1856:C:H1'	1.80	0.45
16:I:75:ARG:HH22	46:1:2112:U:H2'	1.80	0.45
20:j:14:LYS:HD3	23:l:51:ILE:HD11	1.99	0.45
46:1:1227:C:N4	46:1:1282:G:O6	2.50	0.45
46:1:1609:C:N4	46:1:1610:G:O6	2.49	0.45
6:b:508:ARG:HH12	46:1:3073:A:H1'	1.81	0.45
44:q:81:ALA:HA	46:1:2769:A:N3	2.31	0.45
46:1:1233:G:H1	46:1:1255:C:H42	1.63	0.45
5:B:69:LYS:HE2	6:b:416:LEU:HG	1.98	0.45
44:q:82:GLN:NE2	46:1:2791:G:H21	2.15	0.45
46:1:2839:G:N2	46:1:2850:G:O2'	2.50	0.45
7:C:122:THR:HG22	7:C:235:LEU:HB2	1.98	0.45
40:Z:67:LYS:NZ	46:1:1630:U:OP1	2.43	0.45
44:q:54:THR:O	46:1:44:U:O2'	2.20	0.45
46:1:2452:G:H1'	46:1:2496:C:H42	1.81	0.45
21:k:69:LEU:HD12	21:k:73:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:21:PHE:HD2	27:u:29:PHE:HD2	1.65	0.45
46:1:2272:G:N2	46:1:2272:G:OP2	2.50	0.45
46:1:2280:A:N6	46:1:2282:U:O2'	2.49	0.45
48:3:81:U:H1'	48:3:82:U:H3'	1.99	0.45
30:Q:62:VAL:HG13	30:Q:66:ARG:HD2	1.99	0.45
40:Z:15:ARG:HD2	40:Z:79:HIS:CD2	2.49	0.45
46:1:1025:A:H4'	46:1:1026:A:H5''	1.99	0.45
46:1:1150:A:N6	46:1:2369:G:O2'	2.49	0.45
29:P:29:THR:HA	29:P:32:THR:HG22	1.99	0.45
3:A:27:ALA:O	3:A:128:ARG:NH2	2.50	0.45
12:F:33:ARG:NH2	46:1:595:G:OP1	2.50	0.45
15:g:25:THR:HG21	15:g:31:ARG:HD2	1.98	0.45
22:L:62:THR:HG1	46:1:102:C:HO2'	1.65	0.45
32:S:170:THR:OG1	32:S:171:PHE:N	2.41	0.45
39:y:185:THR:OG1	39:y:214:GLU:OE2	2.30	0.45
46:1:531:G:H1	46:1:561:C:H42	1.65	0.45
10:E:77:ARG:NH2	46:1:3273:A:OP2	2.50	0.45
24:M:55:ARG:HH12	24:M:77:ARG:HA	1.81	0.45
7:C:20:LEU:HD11	7:C:252:GLU:HG3	1.99	0.45
42:D:261:THR:HG1	42:D:264:GLN:H	1.62	0.45
3:A:30:ARG:O	3:A:163:ARG:NH1	2.41	0.44
5:B:95:THR:HG22	46:1:3243:A:H4'	1.98	0.44
34:U:18:ASP:HB3	34:U:104:ARG:HB3	1.99	0.44
38:Y:74:TYR:OH	48:3:75:G:OP2	2.32	0.44
40:Z:54:THR:OG1	40:Z:55:LYS:N	2.50	0.44
46:1:1376:C:O2'	46:1:1408:G:O2'	2.30	0.44
46:1:1565:G:N1	46:1:1573:G:O6	2.50	0.44
30:Q:69:ARG:HH22	46:1:720:A:H5'	1.82	0.44
40:Z:103:GLN:HG3	40:Z:106:GLN:HB2	1.98	0.44
17:H:90:MET:HE2	17:H:179:ILE:HG22	1.98	0.44
29:P:118:GLN:HE22	46:1:412:G:H21	1.65	0.44
31:R:18:GLY:HA3	46:1:1874:A:H5''	1.99	0.44
6:b:488:ASP:HA	6:b:491:GLU:HB2	2.00	0.44
6:b:506:GLU:HA	9:d:97:LEU:HD13	1.99	0.44
39:y:142:ILE:HG13	39:y:173:LEU:HD11	2.00	0.44
46:1:1028:U:H4'	46:1:1029:G:H3'	1.99	0.44
10:E:19:LYS:HG3	46:1:591:G:H1'	2.00	0.44
20:j:45:ARG:NH2	46:1:361:A:O3'	2.49	0.44
36:W:57:ARG:NH2	46:1:1258:U:O5'	2.50	0.44
5:B:19:ARG:N	46:1:2990:G:OP1	2.50	0.44
5:B:93:VAL:HG23	5:B:102:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:97:ASN:HB3	16:I:100:LYS:HB3	1.99	0.44
35:V:81:GLN:HG2	35:V:83:LYS:H	1.81	0.44
44:q:68:VAL:HG13	44:q:91:PHE:HB2	1.99	0.44
7:C:82:THR:HG23	7:C:84:ARG:H	1.82	0.44
16:I:4:TYR:HE2	46:1:2113:A:H5''	1.82	0.44
30:Q:106:PHE:CE2	30:Q:121:CYS:HB2	2.52	0.44
44:q:43:TYR:HA	44:q:47:GLN:HB2	2.00	0.44
46:1:2312:A:O2'	46:1:2315:G:N3	2.42	0.44
46:1:2618:G:OP1	46:1:2644:C:O2'	2.31	0.44
23:l:10:LYS:NZ	46:1:1834:U:OP2	2.44	0.44
26:N:18:VAL:HG13	26:N:19:LEU:HD12	1.98	0.44
34:U:19:VAL:HG12	34:U:105:LEU:HD13	1.99	0.44
5:B:242:THR:HG23	46:1:2948:C:H4'	1.99	0.44
7:C:197:ARG:HH12	46:1:338:A:H4'	1.83	0.44
14:G:248:LYS:NZ	46:1:2528:G:O3'	2.50	0.44
45:o:47:LEU:HA	45:o:50:THR:HG22	1.98	0.44
46:1:1188:U:OP1	46:1:1210:U:O2'	2.31	0.44
29:P:68:GLY:HA3	46:1:2350:C:H5''	2.00	0.43
43:J:137:ARG:NH1	47:2:28:C:OP1	2.49	0.43
44:q:45:ARG:HD2	46:1:283:G:OP1	2.18	0.43
44:q:87:ARG:NH2	46:1:2761:G:H2'	2.33	0.43
45:o:32:LEU:HD12	46:1:749:C:H5''	2.00	0.43
46:1:1003:A:N1	46:1:1049:C:O2'	2.47	0.43
46:1:2443:A:N6	46:1:2503:G:O6	2.50	0.43
35:V:101:VAL:HB	35:V:109:MET:HE1	1.99	0.43
46:1:339:C:OP1	46:1:1380:G:O2'	2.37	0.43
12:F:92:ILE:HD12	12:F:92:ILE:HA	1.79	0.43
15:g:97:GLU:OE2	40:Z:84:ARG:NE	2.41	0.43
46:1:1863:G:N1	46:1:1866:C:OP2	2.51	0.43
1:v:45:ILE:HG21	1:v:128:ILE:HG21	2.00	0.43
1:v:149:SER:HA	1:v:154:THR:HG22	2.01	0.43
6:b:624:ARG:NH1	23:l:41:ARG:O	2.48	0.43
10:E:127:ASN:OD1	29:P:181:ARG:NH1	2.51	0.43
18:h:77:PRO:HG2	37:X:50:ALA:HB2	2.00	0.43
30:Q:107:THR:O	30:Q:111:ARG:N	2.48	0.43
38:Y:32:SER:HA	38:Y:49:PRO:HA	1.99	0.43
3:A:40:TYR:N	46:1:2550:U:O4	2.48	0.43
4:a:117:ARG:NH1	46:1:716:A:N1	2.67	0.43
43:J:94:ARG:O	43:J:96:PHE:N	2.51	0.43
46:1:383:G:N2	46:1:386:A:OP2	2.38	0.43
1:v:235:THR:HG22	46:1:2922:G:H1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:45:ASN:HA	7:C:110:ASN:HD22	1.83	0.43
8:c:59:TYR:HE1	40:Z:82:PRO:HD2	1.84	0.43
38:Y:51:ARG:HG2	38:Y:52:ARG:H	1.83	0.43
38:Y:60:ARG:NH1	46:1:200:C:OP1	2.52	0.43
44:q:82:GLN:HB2	46:1:2790:A:C2	2.52	0.43
46:1:1816:A:H2'	46:1:1817:G:C8	2.53	0.43
46:1:1822:C:H2'	46:1:1823:A:H8	1.82	0.43
9:d:48:ASP:H	9:d:86:LYS:HE3	1.83	0.43
13:f:6:ARG:NH1	13:f:8:TYR:O	2.52	0.43
19:i:9:ILE:HD12	22:L:174:ARG:HE	1.83	0.43
20:j:5:THR:O	46:1:1851:G:N2	2.40	0.43
43:J:20:ASN:HB3	43:J:126:ASP:HB2	2.00	0.43
1:v:34:MET:HG3	1:v:39:ILE:HB	2.01	0.43
5:B:219:ALA:HB2	5:B:336:VAL:HG12	2.01	0.43
14:G:97:TYR:HB3	14:G:131:ALA:HA	2.01	0.43
35:V:89:ASP:OD1	35:V:89:ASP:N	2.43	0.43
46:1:959:C:O2	46:1:2614:G:O2'	2.33	0.43
46:1:1268:G:N2	46:1:1269:U:O4	2.51	0.43
27:u:6:CYS:HB2	27:u:32:CYS:HB3	1.56	0.43
29:P:123:PRO:HG3	48:3:14:C:H5''	2.00	0.43
40:Z:17:ARG:HG3	46:1:1639:C:N4	2.33	0.43
45:o:36:ASP:OD1	46:1:2737:C:O2'	2.32	0.43
6:b:385:LEU:HD11	6:b:396:ARG:HH12	1.84	0.42
16:I:3:ARG:NH1	46:1:1910:A:O3'	2.42	0.42
32:S:78:TRP:HB3	32:S:124:LEU:HD12	2.01	0.42
46:1:2103:U:H2'	46:1:2104:A:C8	2.54	0.42
47:2:60:G:H2'	47:2:61:G:H8	1.83	0.42
3:A:200:ARG:NH2	46:1:2186:U:OP2	2.52	0.42
5:B:119:TYR:HE1	46:1:3295:A:H5'	1.84	0.42
10:E:39:VAL:O	10:E:87:THR:OG1	2.35	0.42
14:G:152:LEU:HD23	14:G:178:ALA:HB3	2.01	0.42
46:1:627:U:H4'	46:1:1399:A:H1'	2.00	0.42
46:1:1192:C:N4	46:1:1302:A:OP2	2.52	0.42
46:1:2452:G:H2'	46:1:2462:A:C8	2.54	0.42
5:B:53:MET:HB2	46:1:3049:A:H5''	2.01	0.42
12:F:154:GLY:O	12:F:161:VAL:N	2.50	0.42
42:D:22:ARG:NH1	47:2:6:C:OP2	2.52	0.42
43:J:109:HIS:CD2	43:J:123:PHE:H	2.35	0.42
44:q:41:ARG:C	44:q:44:ASP:H	2.27	0.42
46:1:1785:U:H2'	46:1:1786:G:C8	2.54	0.42
1:v:66:GLN:HB3	1:v:70:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:55:UNK:O	2:s:57:UNK:N	2.53	0.42
5:B:47:LEU:HD12	5:B:335:ILE:HD11	2.00	0.42
16:I:14:ARG:NH1	16:I:16:ARG:O	2.50	0.42
33:T:152:ALA:O	33:T:154:VAL:N	2.52	0.42
46:1:1675:G:H2'	46:1:1676:A:H8	1.84	0.42
6:b:406:ASN:OD1	6:b:406:ASN:N	2.52	0.42
6:b:526:LYS:HG3	6:b:528:PHE:H	1.85	0.42
17:H:18:VAL:HG12	17:H:27:VAL:HG22	2.02	0.42
25:p:49:ARG:HE	25:p:52:ALA:HA	1.84	0.42
32:S:83:SER:OG	32:S:84:ARG:N	2.51	0.42
46:1:1900:A:H61	46:1:1908:A:H61	1.67	0.42
47:2:96:U:H2'	47:2:97:A:H8	1.85	0.42
12:F:151:ARG:NH2	46:1:1334:U:O3'	2.53	0.42
40:Z:54:THR:H	40:Z:57:HIS:CD2	2.36	0.42
42:D:163:LEU:HD21	42:D:175:HIS:CG	2.54	0.42
1:v:117:THR:HA	1:v:131:THR:HA	2.01	0.42
6:b:533:GLU:O	6:b:536:SER:OG	2.31	0.42
7:C:140:HIS:O	7:C:142:VAL:N	2.53	0.42
46:1:2901:G:O2'	46:1:3024:A:N1	2.52	0.42
1:v:19:CYS:HB2	1:v:34:MET:HA	2.01	0.42
5:B:92:TYR:HB2	5:B:157:VAL:HG23	2.01	0.42
22:L:174:ARG:NH1	46:1:712:G:OP1	2.52	0.42
43:J:154:THR:OG1	43:J:155:THR:N	2.52	0.42
6:b:457:GLU:OE2	27:u:95:ARG:NE	2.43	0.42
6:b:458:GLU:HB3	6:b:462:LYS:NZ	2.35	0.42
39:y:21:ASN:HB2	39:y:67:ARG:HB3	2.02	0.42
4:a:77:LYS:O	4:a:79:TRP:N	2.53	0.42
5:B:37:ARG:HH12	5:B:188:ILE:HG23	1.85	0.42
14:G:105:LYS:NZ	46:1:121:A:O2'	2.41	0.42
15:g:80:ARG:HB3	15:g:81:CYS:H	1.78	0.42
32:S:25:PHE:HD1	33:T:151:LEU:HD21	1.84	0.42
46:1:3322:A:H2'	46:1:3323:A:C8	2.55	0.42
3:A:116:VAL:HG13	3:A:126:LEU:HB2	2.02	0.41
5:B:216:ASP:OD2	5:B:339:ARG:NH1	2.53	0.41
24:M:123:LEU:HD22	28:O:190:VAL:HG23	2.02	0.41
26:N:108:ARG:NH2	46:1:1547:G:OP1	2.39	0.41
38:Y:86:THR:HG22	38:Y:96:PRO:HA	2.01	0.41
1:v:33:VAL:HG12	1:v:34:MET:HG2	2.02	0.41
3:A:14:SER:OG	46:1:911:C:OP1	2.28	0.41
3:A:204:MET:HB3	3:A:208:ASP:HB2	2.01	0.41
12:F:156:ILE:HD11	12:F:168:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:36:PHE:CD1	46:1:284:A:H5'	2.55	0.41
46:1:551:A:HO2'	46:1:552:G:H8	1.68	0.41
1:v:168:LYS:HB3	1:v:171:PHE:HB3	2.02	0.41
1:v:169:ARG:HD3	1:v:252:CYS:HB3	2.02	0.41
2:s:102:UNK:O	2:s:104:UNK:N	2.54	0.41
3:A:36:GLU:HG3	3:A:91:GLY:HA2	2.02	0.41
5:B:194:TRP:HE1	41:z:37:LEU:HD21	1.85	0.41
23:l:11:GLN:NE2	48:3:45:C:O2'	2.53	0.41
31:R:105:LEU:HD12	31:R:135:LYS:HE3	2.02	0.41
46:1:1524:A:O2'	46:1:1526:U:OP2	2.29	0.41
1:v:371:GLY:HA2	1:v:398:VAL:HG23	2.02	0.41
4:a:148:ILE:H	4:a:148:ILE:HG13	1.71	0.41
16:l:122:LEU:O	16:l:126:HIS:N	2.50	0.41
24:M:66:THR:HG22	24:M:99:TRP:HZ3	1.85	0.41
31:R:62:ARG:HH12	46:1:3067:C:H3'	1.85	0.41
46:1:637:C:OP1	46:1:2377:G:N2	2.45	0.41
46:1:2570:U:H4'	46:1:2571:U:H2'	2.02	0.41
5:B:252:ILE:HG22	46:1:2394:G:H5'	2.01	0.41
5:B:254:ALA:O	46:1:2394:G:O2'	2.38	0.41
7:C:18:ASN:ND2	7:C:252:GLU:OE2	2.54	0.41
44:q:55:LYS:HA	44:q:55:LYS:HD3	1.87	0.41
46:1:655:C:H2'	46:1:656:A:C8	2.55	0.41
5:B:215:ILE:HD11	5:B:324:VAL:HG21	2.02	0.41
46:1:1228:C:H2'	46:1:1229:G:H8	1.85	0.41
1:v:320:VAL:HA	1:v:340:VAL:HG23	2.02	0.41
3:A:19:HIS:HD2	46:1:823:C:H4'	1.85	0.41
21:k:40:GLN:HE21	21:k:55:VAL:HG13	1.85	0.41
44:q:24:LYS:O	44:q:73:GLU:N	2.38	0.41
46:1:2261:G:H3'	46:1:2262:A:H4'	2.02	0.41
1:v:111:ARG:HH22	46:1:2849:C:H4'	1.85	0.41
12:F:211:SER:H	12:F:242:SER:HB2	1.86	0.41
30:Q:141:ARG:NH2	46:1:743:C:N3	2.61	0.41
32:S:71:LYS:NZ	46:1:562:C:O3'	2.53	0.41
36:W:31:ARG:HH21	36:W:85:TYR:HB2	1.86	0.41
7:C:203:ARG:NH1	7:C:226:GLU:OE2	2.54	0.41
9:d:46:THR:OG1	9:d:86:LYS:NZ	2.46	0.41
12:F:158:LYS:HD3	12:F:158:LYS:HA	1.91	0.41
17:H:21:LYS:HG3	17:H:22:SER:H	1.86	0.41
26:N:85:THR:HG21	44:q:51:GLY:H	1.85	0.41
26:N:114:ARG:HD3	26:N:137:PRO:HG3	2.03	0.41
29:P:36:ILE:HD11	29:P:44:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:3007:U:H2'	46:1:3008:A:H8	1.85	0.41
7:C:29:PRO:HB3	30:Q:25:TYR:HE2	1.86	0.41
40:Z:32:GLY:HA2	40:Z:40:HIS:CE1	2.55	0.41
44:q:50:PHE:H	46:1:279:U:P	2.44	0.41
44:q:71:ARG:HD2	44:q:82:GLN:HG2	2.02	0.41
6:b:590:LEU:HD13	6:b:599:ARG:HD3	2.03	0.40
19:i:9:ILE:HD13	22:L:174:ARG:HH21	1.86	0.40
26:N:110:ALA:HB1	26:N:113:LEU:HD23	2.03	0.40
31:R:75:HIS:ND1	46:1:1940:G:OP1	2.54	0.40
42:D:48:LYS:HD3	42:D:48:LYS:HA	1.87	0.40
46:1:3177:G:O2'	46:1:3179:U:OP1	2.34	0.40
14:G:50:VAL:HG12	37:X:30:ALA:HA	2.03	0.40
21:k:32:ASN:OD1	21:k:35:GLY:HA3	2.21	0.40
21:k:45:VAL:HG23	21:k:52:TYR:HB2	2.03	0.40
29:P:4:TYR:HE1	29:P:18:ARG:HD2	1.86	0.40
42:D:22:ARG:NE	42:D:27:LYS:HE3	2.36	0.40
42:D:158:ARG:NH2	47:2:47:C:OP2	2.52	0.40
44:q:74:CYS:SG	44:q:75:VAL:N	2.94	0.40
44:q:80:ARG:HB3	46:1:2769:A:C8	2.56	0.40
44:q:81:ALA:N	46:1:2769:A:H2'	2.37	0.40
46:1:2418:G:OP2	46:1:2606:G:N2	2.53	0.40
46:1:3163:A:N6	46:1:3288:G:O6	2.54	0.40
16:I:99:ASN:HD22	27:u:73:GLN:NE2	2.19	0.40
17:H:170:LYS:HB3	17:H:175:PHE:HD2	1.86	0.40
46:1:221:A:O2'	46:1:223:U:OP2	2.32	0.40
5:B:136:LYS:HE3	5:B:144:ILE:HD11	2.03	0.40
9:d:75:ILE:HG12	9:d:93:VAL:HG22	2.04	0.40
12:F:240:VAL:O	12:F:244:ASN:N	2.51	0.40
22:L:49:ARG:HA	22:L:50:PRO:HD3	1.86	0.40
26:N:27:VAL:HG23	26:N:129:TYR:HE2	1.86	0.40
27:u:28:GLU:OE1	27:u:30:ARG:NH2	2.50	0.40
40:Z:33:SER:OG	40:Z:34:LYS:N	2.54	0.40
46:1:15:C:H2'	46:1:16:A:H8	1.87	0.40
46:1:1228:C:H2'	46:1:1229:G:C8	2.57	0.40
46:1:1941:C:H4'	46:1:3362:A:H1'	2.03	0.40
1:v:66:GLN:HA	1:v:67:PRO:HD3	1.92	0.40
3:A:15:ILE:HB	46:1:822:G:H1'	2.03	0.40
3:A:204:MET:O	3:A:213:GLY:N	2.54	0.40
7:C:286:VAL:HG13	30:Q:32:LEU:HD12	2.02	0.40
8:c:98:SER:OG	8:c:99:ASP:N	2.55	0.40
24:M:38:ILE:HD13	32:S:148:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:122:ASN:HB3	26:N:129:TYR:HD2	1.86	0.40
40:Z:135:ARG:HH22	46:1:1807:G:H5''	1.86	0.40
42:D:84:PRO:HB3	42:D:89:THR:HG22	2.03	0.40
47:2:60:G:H2'	47:2:61:G:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	352/518 (68%)	305 (87%)	44 (12%)	3 (1%)	14	46
3	A	243/254 (96%)	217 (89%)	25 (10%)	1 (0%)	30	61
4	a	92/149 (62%)	84 (91%)	6 (6%)	2 (2%)	5	30
5	B	384/387 (99%)	343 (89%)	38 (10%)	3 (1%)	16	49
6	b	242/647 (37%)	226 (93%)	13 (5%)	3 (1%)	10	41
7	C	359/362 (99%)	325 (90%)	31 (9%)	3 (1%)	16	49
8	c	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
9	d	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
10	E	156/176 (89%)	148 (95%)	8 (5%)	0	100	100
11	e	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
12	F	220/244 (90%)	197 (90%)	23 (10%)	0	100	100
13	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
14	G	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
15	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
16	I	129/166 (78%)	116 (90%)	12 (9%)	1 (1%)	16	49
17	H	186/191 (97%)	168 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	h	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
19	i	94/100 (94%)	87 (93%)	7 (7%)	0	100	100
20	j	83/88 (94%)	76 (92%)	7 (8%)	0	100	100
21	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
22	L	185/199 (93%)	163 (88%)	21 (11%)	1 (0%)	24	57
23	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
24	M	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
25	p	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
26	N	201/204 (98%)	186 (92%)	15 (8%)	0	100	100
27	u	147/199 (74%)	137 (93%)	7 (5%)	3 (2%)	6	32
28	O	195/199 (98%)	190 (97%)	5 (3%)	0	100	100
29	P	174/184 (95%)	169 (97%)	5 (3%)	0	100	100
30	Q	152/186 (82%)	141 (93%)	11 (7%)	0	100	100
31	R	152/189 (80%)	145 (95%)	7 (5%)	0	100	100
32	S	168/172 (98%)	149 (89%)	16 (10%)	3 (2%)	6	34
33	T	59/160 (37%)	54 (92%)	5 (8%)	0	100	100
34	U	102/121 (84%)	94 (92%)	8 (8%)	0	100	100
35	V	134/137 (98%)	129 (96%)	5 (4%)	0	100	100
36	W	129/236 (55%)	126 (98%)	3 (2%)	0	100	100
37	X	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
38	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
39	y	223/245 (91%)	211 (95%)	12 (5%)	0	100	100
40	Z	133/136 (98%)	117 (88%)	16 (12%)	0	100	100
41	z	53/106 (50%)	53 (100%)	0	0	100	100
42	D	245/297 (82%)	225 (92%)	17 (7%)	3 (1%)	10	41
43	J	162/174 (93%)	141 (87%)	17 (10%)	4 (2%)	4	28
44	q	95/106 (90%)	76 (80%)	18 (19%)	1 (1%)	11	43
45	o	52/59 (88%)	48 (92%)	4 (8%)	0	100	100
All	All	6774/8171 (83%)	6248 (92%)	495 (7%)	31 (0%)	26	57

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	339	LEU
27	u	3	ILE
43	J	95	ASN
16	I	17	ASP
22	L	63	VAL
42	D	140	ARG
43	J	154	THR
43	J	155	THR
3	A	219	ILE
4	a	78	LEU
5	B	34	LYS
6	b	398	LEU
7	C	4	PRO
27	u	73	GLN
43	J	172	LEU
4	a	77	LYS
27	u	4	TYR
32	S	13	ARG
32	S	24	LEU
1	v	32	LEU
1	v	279	ILE
6	b	397	LYS
6	b	529	GLY
42	D	258	LYS
44	q	35	LEU
7	C	268	ALA
32	S	23	LYS
1	v	68	PRO
5	B	188	ILE
5	B	239	PRO
42	D	141	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	v	309/467 (66%)	305 (99%)	4 (1%)	61 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	188/196 (96%)	186 (99%)	2 (1%)	65	74
4	a	77/119 (65%)	76 (99%)	1 (1%)	61	72
5	B	322/323 (100%)	318 (99%)	4 (1%)	63	73
6	b	211/573 (37%)	210 (100%)	1 (0%)	81	80
7	C	288/289 (100%)	287 (100%)	1 (0%)	86	83
8	c	81/88 (92%)	80 (99%)	1 (1%)	63	73
9	d	94/97 (97%)	94 (100%)	0	100	100
10	E	137/153 (90%)	136 (99%)	1 (1%)	76	78
11	e	109/111 (98%)	109 (100%)	0	100	100
12	F	186/205 (91%)	186 (100%)	0	100	100
13	f	90/91 (99%)	90 (100%)	0	100	100
14	G	189/208 (91%)	189 (100%)	0	100	100
15	g	95/103 (92%)	93 (98%)	2 (2%)	47	65
16	I	116/141 (82%)	116 (100%)	0	100	100
17	H	168/171 (98%)	168 (100%)	0	100	100
18	h	104/105 (99%)	104 (100%)	0	100	100
19	i	78/82 (95%)	77 (99%)	1 (1%)	61	72
20	j	69/71 (97%)	69 (100%)	0	100	100
21	k	68/69 (99%)	68 (100%)	0	100	100
22	L	147/159 (92%)	144 (98%)	3 (2%)	48	66
23	l	45/46 (98%)	45 (100%)	0	100	100
24	M	108/109 (99%)	106 (98%)	2 (2%)	50	67
25	p	71/72 (99%)	71 (100%)	0	100	100
26	N	175/176 (99%)	174 (99%)	1 (1%)	78	79
27	u	132/180 (73%)	130 (98%)	2 (2%)	57	70
28	O	160/162 (99%)	160 (100%)	0	100	100
29	P	143/146 (98%)	141 (99%)	2 (1%)	59	71
30	Q	126/151 (83%)	125 (99%)	1 (1%)	73	77
31	R	127/154 (82%)	126 (99%)	1 (1%)	73	77
32	S	154/156 (99%)	153 (99%)	1 (1%)	78	79
33	T	50/137 (36%)	49 (98%)	1 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	U	91/107 (85%)	91 (100%)	0	100	100
35	V	104/105 (99%)	104 (100%)	0	100	100
36	W	113/213 (53%)	113 (100%)	0	100	100
37	X	104/118 (88%)	103 (99%)	1 (1%)	68	75
38	Y	109/110 (99%)	109 (100%)	0	100	100
39	y	192/211 (91%)	192 (100%)	0	100	100
40	Z	115/116 (99%)	115 (100%)	0	100	100
41	z	48/95 (50%)	48 (100%)	0	100	100
42	D	203/245 (83%)	202 (100%)	1 (0%)	81	80
43	J	140/150 (93%)	139 (99%)	1 (1%)	76	78
44	q	84/91 (92%)	82 (98%)	2 (2%)	43	63
45	o	43/47 (92%)	43 (100%)	0	100	100
All	All	5763/6918 (83%)	5726 (99%)	37 (1%)	76	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	v	22	CYS
1	v	26	ILE
1	v	143	CYS
1	v	374	ILE
3	A	45	VAL
3	A	219	ILE
4	a	78	LEU
5	B	79	VAL
5	B	85	VAL
5	B	168	LYS
5	B	229	VAL
6	b	445	LEU
7	C	74	ILE
8	c	16	LEU
10	E	155	LEU
15	g	95	ILE
15	g	100	ILE
19	i	60	LEU
22	L	54	LEU
22	L	76	THR
22	L	124	ILE

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Mol	Chain	Res	Type
24	M	38	ILE
24	M	74	ARG
26	N	183	THR
27	u	27	LYS
27	u	79	VAL
29	P	24	VAL
29	P	119	VAL
30	Q	122	ILE
31	R	99	LEU
32	S	45	LEU
33	T	128	LEU
37	X	38	LEU
42	D	105	ILE
43	J	12	LEU
44	q	79	THR
44	q	88	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	v	163	GLN
1	v	167	HIS
1	v	349	ASN
4	a	120	ASN
5	B	177	HIS
5	B	231	HIS
6	b	365	GLN
6	b	384	ASN
6	b	413	ASN
6	b	415	ASN
6	b	470	ASN
6	b	500	GLN
6	b	509	ASN
6	b	626	ASN
7	C	221	ASN
9	d	57	GLN
9	d	87	ASN
10	E	125	GLN
12	F	81	HIS
12	F	244	ASN
14	G	85	ASN
14	G	221	ASN

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Mol	Chain	Res	Type
14	G	240	ASN
15	g	69	HIS
16	I	67	HIS
16	I	73	HIS
16	I	99	ASN
16	I	103	ASN
16	I	106	GLN
17	H	157	ASN
17	H	183	HIS
18	h	59	ASN
20	j	57	HIS
21	k	40	GLN
22	L	12	ASN
22	L	99	HIS
22	L	120	GLN
23	l	11	GLN
23	l	20	ASN
23	l	25	GLN
24	M	27	GLN
24	M	41	GLN
26	N	37	HIS
27	u	24	ASN
27	u	45	ASN
29	P	96	GLN
29	P	97	ASN
29	P	118	GLN
29	P	145	HIS
30	Q	5	HIS
30	Q	9	GLN
30	Q	10	HIS
31	R	150	GLN
32	S	122	HIS
32	S	157	GLN
33	T	103	GLN
33	T	131	GLN
34	U	49	ASN
35	V	7	GLN
35	V	98	ASN
36	W	54	GLN
36	W	74	GLN
36	W	223	ASN
36	W	232	ASN

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Mol	Chain	Res	Type
38	Y	4	GLN
38	Y	42	GLN
39	y	50	HIS
39	y	79	GLN
39	y	106	ASN
39	y	140	GLN
39	y	145	ASN
39	y	162	HIS
39	y	178	GLN
41	z	44	GLN
42	D	45	ASN
42	D	57	ASN
43	J	43	GLN
43	J	95	ASN
43	J	109	HIS
44	q	82	GLN
44	q	90	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	1	3198/3396 (94%)	722 (22%)	39 (1%)
47	2	120/121 (99%)	15 (12%)	0
48	3	156/158 (98%)	28 (17%)	2 (1%)
All	All	3474/3675 (94%)	765 (22%)	41 (1%)

All (765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	1	22	G
46	1	40	A
46	1	43	A
46	1	44	U
46	1	45	A
46	1	49	A
46	1	55	G
46	1	59	G
46	1	60	A
46	1	65	A
46	1	66	A
46	1	72	C

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Mol	Chain	Res	Type
46	1	75	G
46	1	76	G
46	1	85	A
46	1	92	G
46	1	109	A
46	1	110	G
46	1	111	C
46	1	116	A
46	1	118	U
46	1	122	A
46	1	132	C
46	1	135	C
46	1	136	G
46	1	148	G
46	1	155	G
46	1	156	G
46	1	157	A
46	1	166	C
46	1	170	G
46	1	172	G
46	1	173	G
46	1	176	G
46	1	182	U
46	1	187	A
46	1	190	U
46	1	191	U
46	1	198	A
46	1	206	G
46	1	210	U
46	1	211	A
46	1	212	G
46	1	213	A
46	1	218	G
46	1	219	A
46	1	230	U
46	1	231	G
46	1	237	G
46	1	240	U
46	1	241	G
46	1	243	G
46	1	246	U
46	1	247	C

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Mol	Chain	Res	Type
46	1	248	U
46	1	250	U
46	1	253	A
46	1	269	G
46	1	277	G
46	1	279	U
46	1	281	G
46	1	283	G
46	1	284	A
46	1	285	A
46	1	286	U
46	1	295	A
46	1	305	U
46	1	323	A
46	1	329	U
46	1	334	A
46	1	338	A
46	1	339	C
46	1	343	U
46	1	349	A
46	1	376	G
46	1	382	U
46	1	385	A
46	1	395	A
46	1	398	A
46	1	399	A
46	1	401	U
46	1	402	A
46	1	403	C
46	1	404	G
46	1	406	G
46	1	420	G
46	1	421	G
46	1	422	A
46	1	429	U
46	1	438	A
46	1	440	A
46	1	495	G
46	1	520	U
46	1	521	A
46	1	535	G
46	1	543	C

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Mol	Chain	Res	Type
46	1	546	C
46	1	547	G
46	1	548	G
46	1	551	A
46	1	552	G
46	1	553	U
46	1	555	U
46	1	557	A
46	1	559	A
46	1	569	A
46	1	578	A
46	1	579	G
46	1	591	G
46	1	592	A
46	1	597	G
46	1	600	G
46	1	604	G
46	1	611	A
46	1	620	U
46	1	621	A
46	1	622	A
46	1	636	C
46	1	649	A
46	1	655	C
46	1	660	A
46	1	677	A
46	1	681	U
46	1	683	U
46	1	689	U
46	1	690	A
46	1	691	A
46	1	705	A
46	1	712	G
46	1	715	A
46	1	716	A
46	1	719	U
46	1	720	A
46	1	725	G
46	1	744	A
46	1	763	G
46	1	765	C
46	1	766	U

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Mol	Chain	Res	Type
46	1	767	U
46	1	776	U
46	1	777	U
46	1	780	A
46	1	781	G
46	1	785	G
46	1	786	A
46	1	801	A
46	1	806	A
46	1	817	A
46	1	823	C
46	1	830	A
46	1	849	C
46	1	851	C
46	1	861	C
46	1	869	G
46	1	874	U
46	1	875	G
46	1	879	U
46	1	880	G
46	1	884	A
46	1	895	A
46	1	897	U
46	1	907	G
46	1	908	G
46	1	911	C
46	1	914	A
46	1	916	G
46	1	917	A
46	1	921	A
46	1	924	G
46	1	926	A
46	1	932	U
46	1	933	A
46	1	937	G
46	1	944	C
46	1	946	U
46	1	953	G
46	1	959	C
46	1	960	U
46	1	961	C
46	1	974	G

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Mol	Chain	Res	Type
46	1	978	G
46	1	979	U
46	1	980	A
46	1	981	U
46	1	982	C
46	1	994	G
46	1	1001	G
46	1	1002	A
46	1	1006	A
46	1	1008	U
46	1	1009	A
46	1	1010	G
46	1	1011	A
46	1	1014	U
46	1	1015	U
46	1	1016	C
46	1	1017	C
46	1	1018	G
46	1	1019	G
46	1	1020	G
46	1	1023	C
46	1	1024	G
46	1	1026	A
46	1	1027	A
46	1	1028	U
46	1	1029	G
46	1	1030	A
46	1	1035	G
46	1	1036	A
46	1	1037	C
46	1	1038	C
46	1	1039	U
46	1	1040	A
46	1	1041	U
46	1	1046	A
46	1	1047	A
46	1	1049	C
46	1	1063	G
46	1	1064	A
46	1	1065	A
46	1	1081	U
46	1	1082	U

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Mol	Chain	Res	Type
46	1	1087	G
46	1	1093	A
46	1	1094	U
46	1	1095	U
46	1	1097	G
46	1	1098	A
46	1	1103	A
46	1	1104	G
46	1	1109	U
46	1	1111	U
46	1	1117	G
46	1	1124	U
46	1	1131	G
46	1	1140	G
46	1	1143	A
46	1	1153	A
46	1	1159	A
46	1	1161	G
46	1	1178	G
46	1	1180	A
46	1	1181	U
46	1	1190	A
46	1	1192	C
46	1	1193	A
46	1	1195	A
46	1	1196	C
46	1	1201	C
46	1	1208	U
46	1	1212	A
46	1	1213	G
46	1	1217	A
46	1	1219	C
46	1	1220	U
46	1	1221	A
46	1	1222	G
46	1	1227	C
46	1	1235	U
46	1	1236	G
46	1	1237	G
46	1	1238	C
46	1	1239	C
46	1	1241	U

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Mol	Chain	Res	Type
46	1	1243	G
46	1	1244	A
46	1	1245	A
46	1	1246	G
46	1	1248	C
46	1	1249	G
46	1	1252	A
46	1	1253	U
46	1	1254	C
46	1	1258	U
46	1	1262	G
46	1	1263	A
46	1	1264	G
46	1	1265	U
46	1	1268	G
46	1	1270	A
46	1	1271	A
46	1	1272	C
46	1	1278	A
46	1	1279	C
46	1	1285	G
46	1	1286	A
46	1	1287	A
46	1	1292	C
46	1	1295	G
46	1	1305	U
46	1	1307	G
46	1	1309	U
46	1	1313	G
46	1	1316	C
46	1	1325	U
46	1	1330	A
46	1	1331	U
46	1	1332	A
46	1	1348	U
46	1	1349	G
46	1	1350	A
46	1	1351	U
46	1	1352	A
46	1	1353	U
46	1	1356	U
46	1	1386	A

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Mol	Chain	Res	Type
46	1	1391	C
46	1	1392	G
46	1	1399	A
46	1	1400	G
46	1	1408	G
46	1	1416	C
46	1	1419	A
46	1	1430	U
46	1	1434	G
46	1	1437	C
46	1	1443	G
46	1	1445	U
46	1	1446	A
46	1	1450	G
46	1	1455	U
46	1	1475	A
46	1	1480	G
46	1	1481	A
46	1	1482	A
46	1	1484	U
46	1	1492	G
46	1	1496	C
46	1	1503	A
46	1	1508	C
46	1	1512	U
46	1	1533	U
46	1	1536	G
46	1	1537	A
46	1	1546	A
46	1	1547	G
46	1	1555	U
46	1	1556	C
46	1	1557	A
46	1	1559	A
46	1	1561	G
46	1	1562	C
46	1	1563	C
46	1	1565	G
46	1	1567	U
46	1	1568	U
46	1	1569	U
46	1	1570	U

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Mol	Chain	Res	Type
46	1	1572	U
46	1	1574	C
46	1	1576	G
46	1	1577	G
46	1	1579	C
46	1	1580	A
46	1	1581	C
46	1	1582	C
46	1	1583	A
46	1	1587	A
46	1	1589	A
46	1	1590	G
46	1	1593	A
46	1	1619	A
46	1	1620	U
46	1	1628	C
46	1	1629	U
46	1	1632	A
46	1	1633	C
46	1	1636	U
46	1	1642	A
46	1	1643	A
46	1	1645	U
46	1	1649	U
46	1	1656	A
46	1	1657	C
46	1	1662	G
46	1	1677	G
46	1	1682	U
46	1	1683	A
46	1	1696	A
46	1	1702	U
46	1	1711	C
46	1	1716	U
46	1	1717	U
46	1	1724	U
46	1	1725	C
46	1	1736	G
46	1	1741	A
46	1	1742	U
46	1	1749	A
46	1	1750	A

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Mol	Chain	Res	Type
46	1	1751	G
46	1	1760	A
46	1	1762	C
46	1	1765	U
46	1	1766	G
46	1	1770	G
46	1	1772	U
46	1	1775	G
46	1	1780	G
46	1	1785	U
46	1	1790	G
46	1	1797	A
46	1	1813	A
46	1	1814	A
46	1	1816	A
46	1	1817	G
46	1	1820	U
46	1	1821	U
46	1	1839	A
46	1	1842	A
46	1	1844	C
46	1	1849	C
46	1	1850	A
46	1	1867	A
46	1	1880	U
46	1	1886	A
46	1	1893	A
46	1	1905	G
46	1	1906	G
46	1	1951	C
46	1	1952	G
46	1	1953	G
46	1	1954	G
46	1	2100	A
46	1	2101	C
46	1	2102	U
46	1	2111	G
46	1	2112	U
46	1	2119	A
46	1	2121	G
46	1	2122	G
46	1	2131	A

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Mol	Chain	Res	Type
46	1	2139	A
46	1	2140	U
46	1	2142	A
46	1	2158	A
46	1	2160	G
46	1	2169	G
46	1	2171	G
46	1	2176	U
46	1	2184	U
46	1	2186	U
46	1	2188	A
46	1	2205	U
46	1	2209	U
46	1	2210	G
46	1	2244	A
46	1	2249	G
46	1	2250	G
46	1	2252	A
46	1	2259	A
46	1	2260	U
46	1	2261	G
46	1	2262	A
46	1	2263	C
46	1	2265	C
46	1	2267	C
46	1	2268	U
46	1	2269	U
46	1	2270	A
46	1	2273	G
46	1	2281	A
46	1	2282	U
46	1	2287	C
46	1	2288	G
46	1	2298	U
46	1	2306	C
46	1	2307	G
46	1	2308	C
46	1	2309	A
46	1	2310	U
46	1	2313	A
46	1	2314	U
46	1	2315	G

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Mol	Chain	Res	Type
46	1	2330	C
46	1	2334	U
46	1	2335	G
46	1	2336	U
46	1	2337	C
46	1	2361	A
46	1	2363	A
46	1	2373	A
46	1	2374	C
46	1	2375	G
46	1	2385	G
46	1	2388	U
46	1	2393	G
46	1	2397	A
46	1	2398	A
46	1	2401	A
46	1	2402	A
46	1	2403	G
46	1	2404	A
46	1	2411	U
46	1	2435	G
46	1	2437	G
46	1	2440	G
46	1	2442	G
46	1	2448	G
46	1	2450	G
46	1	2452	G
46	1	2453	U
46	1	2454	G
46	1	2455	U
46	1	2458	A
46	1	2459	A
46	1	2460	U
46	1	2464	U
46	1	2468	A
46	1	2470	C
46	1	2472	U
46	1	2474	G
46	1	2476	C
46	1	2477	G
46	1	2484	A
46	1	2486	A

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Mol	Chain	Res	Type
46	1	2487	U
46	1	2495	C
46	1	2496	C
46	1	2497	U
46	1	2498	U
46	1	2499	U
46	1	2501	U
46	1	2502	A
46	1	2503	G
46	1	2505	U
46	1	2506	U
46	1	2508	U
46	1	2514	U
46	1	2522	G
46	1	2531	C
46	1	2533	G
46	1	2537	U
46	1	2538	U
46	1	2539	C
46	1	2540	A
46	1	2541	U
46	1	2542	U
46	1	2544	U
46	1	2547	A
46	1	2549	G
46	1	2550	U
46	1	2552	C
46	1	2555	G
46	1	2561	A
46	1	2566	C
46	1	2567	C
46	1	2569	A
46	1	2570	U
46	1	2571	U
46	1	2572	C
46	1	2573	G
46	1	2577	C
46	1	2585	G
46	1	2593	A
46	1	2594	C
46	1	2600	C
46	1	2606	G

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Mol	Chain	Res	Type
46	1	2607	G
46	1	2614	G
46	1	2626	A
46	1	2635	A
46	1	2648	G
46	1	2652	U
46	1	2656	A
46	1	2657	A
46	1	2674	A
46	1	2677	G
46	1	2678	A
46	1	2688	U
46	1	2689	A
46	1	2691	A
46	1	2694	A
46	1	2696	A
46	1	2703	A
46	1	2704	A
46	1	2705	A
46	1	2719	U
46	1	2726	C
46	1	2728	G
46	1	2729	U
46	1	2742	C
46	1	2753	G
46	1	2755	C
46	1	2762	A
46	1	2768	U
46	1	2769	A
46	1	2770	G
46	1	2771	U
46	1	2772	C
46	1	2777	G
46	1	2778	G
46	1	2794	G
46	1	2796	G
46	1	2799	A
46	1	2800	G
46	1	2801	A
46	1	2802	A
46	1	2803	A
46	1	2804	A

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Mol	Chain	Res	Type
46	1	2810	C
46	1	2814	G
46	1	2816	G
46	1	2817	A
46	1	2828	G
46	1	2838	A
46	1	2842	U
46	1	2843	U
46	1	2844	C
46	1	2845	A
46	1	2850	G
46	1	2871	G
46	1	2872	A
46	1	2875	U
46	1	2876	C
46	1	2887	A
46	1	2899	C
46	1	2904	U
46	1	2914	G
46	1	2923	U
46	1	2924	U
46	1	2928	C
46	1	2933	A
46	1	2935	U
46	1	2936	A
46	1	2941	A
46	1	2951	G
46	1	2971	A
46	1	2978	U
46	1	2983	C
46	1	2996	U
46	1	2997	G
46	1	3011	A
46	1	3012	A
46	1	3021	A
46	1	3028	G
46	1	3056	U
46	1	3059	G
46	1	3080	G
46	1	3086	A
46	1	3092	C
46	1	3099	C

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Mol	Chain	Res	Type
46	1	3108	G
46	1	3109	G
46	1	3115	C
46	1	3119	U
46	1	3129	A
46	1	3130	A
46	1	3131	U
46	1	3142	A
46	1	3143	C
46	1	3148	U
46	1	3150	A
46	1	3153	U
46	1	3155	U
46	1	3156	U
46	1	3157	U
46	1	3164	C
46	1	3165	A
46	1	3168	A
46	1	3170	A
46	1	3173	G
46	1	3174	A
46	1	3175	U
46	1	3176	G
46	1	3179	U
46	1	3180	A
46	1	3181	C
46	1	3187	A
46	1	3196	U
46	1	3207	U
46	1	3209	A
46	1	3210	A
46	1	3217	C
46	1	3218	A
46	1	3219	G
46	1	3229	G
46	1	3239	G
46	1	3242	G
46	1	3243	A
46	1	3245	A
46	1	3247	G
46	1	3259	U
46	1	3260	G

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Mol	Chain	Res	Type
46	1	3263	G
46	1	3268	A
46	1	3270	U
46	1	3275	U
46	1	3276	G
46	1	3279	A
46	1	3280	U
46	1	3281	U
46	1	3289	G
46	1	3294	A
46	1	3295	A
46	1	3304	U
46	1	3308	C
46	1	3313	U
46	1	3316	A
46	1	3317	U
46	1	3318	G
46	1	3319	U
46	1	3320	A
46	1	3341	U
46	1	3345	G
46	1	3347	A
46	1	3350	C
46	1	3351	U
46	1	3352	U
46	1	3354	U
46	1	3355	U
46	1	3356	G
46	1	3357	U
46	1	3360	C
46	1	3363	U
46	1	3368	U
46	1	3369	G
46	1	3375	A
46	1	3378	C
46	1	3382	U
46	1	3386	G
46	1	3396	U
47	2	10	C
47	2	22	A
47	2	49	G
47	2	53	U

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Mol	Chain	Res	Type
47	2	54	U
47	2	65	G
47	2	73	C
47	2	74	C
47	2	76	A
47	2	102	A
47	2	109	G
47	2	112	G
47	2	114	U
47	2	120	C
47	2	121	U
48	3	23	U
48	3	25	G
48	3	34	U
48	3	35	C
48	3	39	G
48	3	51	G
48	3	59	A
48	3	62	C
48	3	63	G
48	3	80	A
48	3	81	U
48	3	82	U
48	3	83	C
48	3	84	C
48	3	86	U
48	3	87	G
48	3	90	U
48	3	91	C
48	3	95	G
48	3	104	A
48	3	106	C
48	3	111	A
48	3	113	U
48	3	125	U
48	3	126	A
48	3	138	A
48	3	148	G
48	3	155	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	1	239	G
46	1	283	G
46	1	285	A
46	1	547	G
46	1	599	C
46	1	916	G
46	1	979	U
46	1	1027	A
46	1	1029	G
46	1	1038	C
46	1	1064	A
46	1	1097	G
46	1	1103	A
46	1	1352	A
46	1	1355	A
46	1	1554	U
46	1	1576	G
46	1	1716	U
46	1	1815	U
46	1	1816	A
46	1	2101	C
46	1	2209	U
46	1	2249	G
46	1	2258	U
46	1	2264	U
46	1	2266	U
46	1	2454	G
46	1	2501	U
46	1	2513	U
46	1	2537	U
46	1	2541	U
46	1	2593	A
46	1	2769	A
46	1	2770	G
46	1	2815	G
46	1	3218	A
46	1	3228	C
46	1	3269	U
46	1	3353	G
48	3	82	U
48	3	85	G

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](#)

There are no chain breaks in this entry.

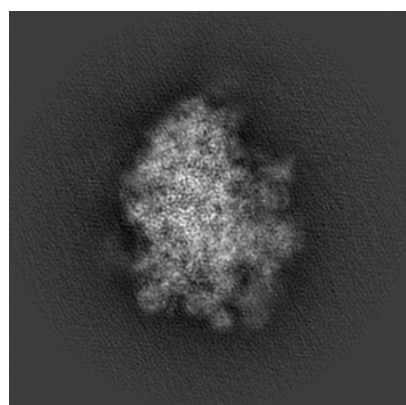
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0371. These allow visual inspection of the internal detail of the map and identification of artifacts.

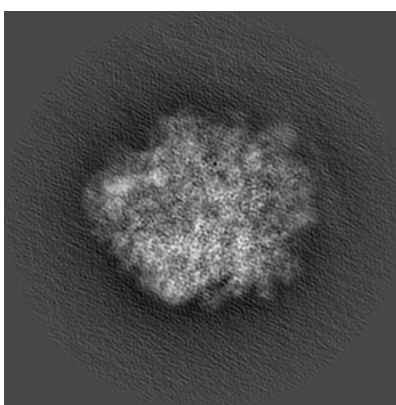
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

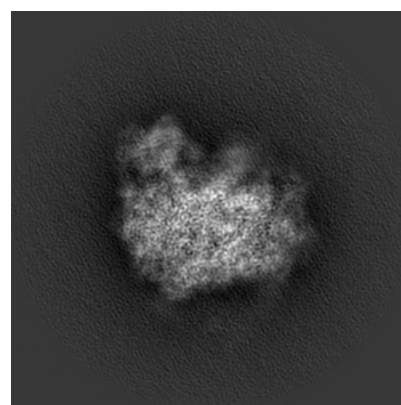
6.1.1 Primary map



X



Y

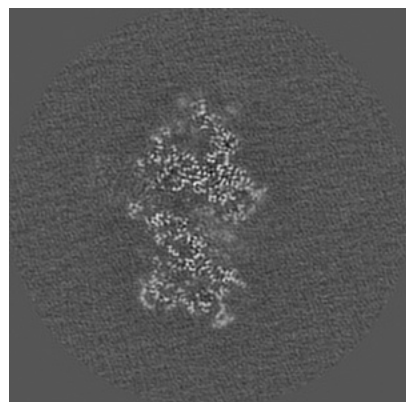


Z

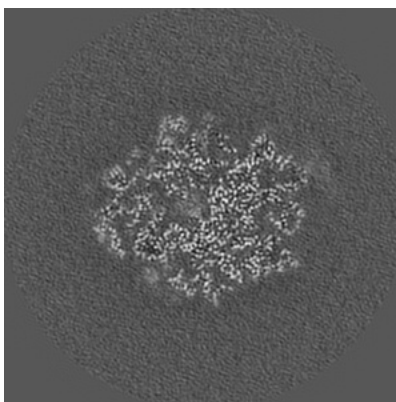
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

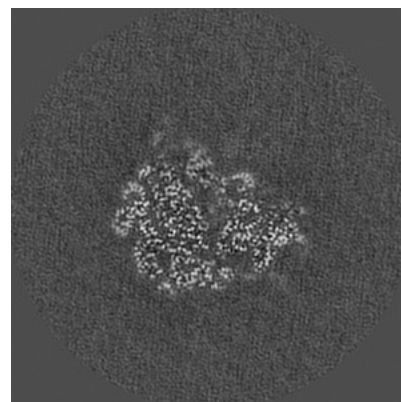
6.2.1 Primary map



X Index: 192



Y Index: 192

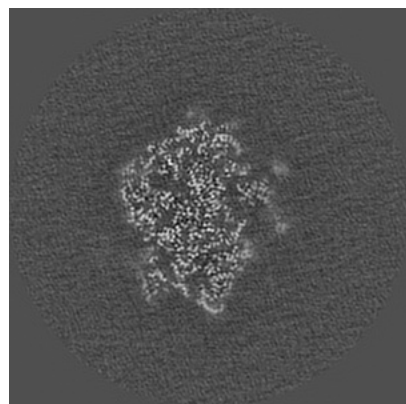


Z Index: 192

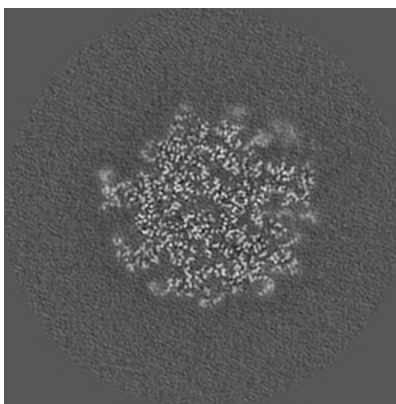
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

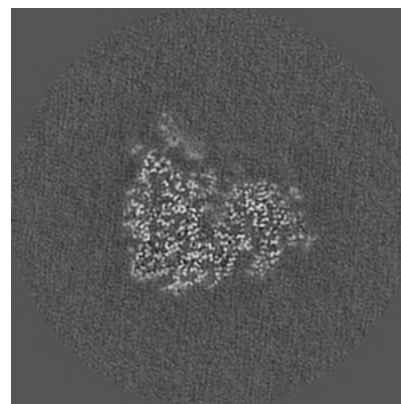
6.3.1 Primary map



X Index: 166



Y Index: 173

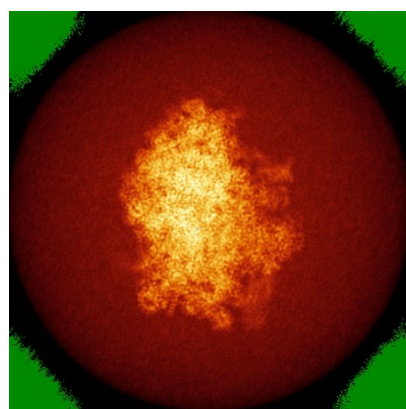


Z Index: 184

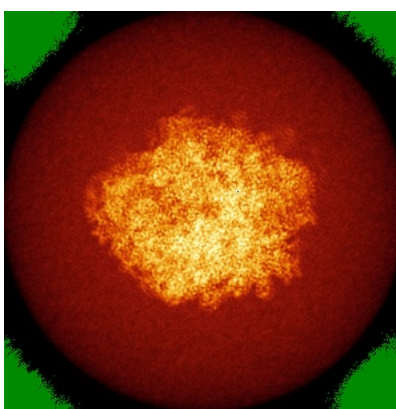
The images above show the largest variance slices of the map in three orthogonal directions.

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

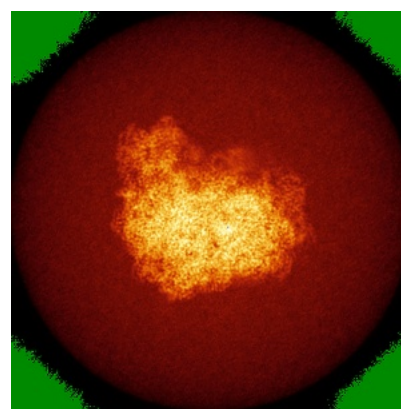
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

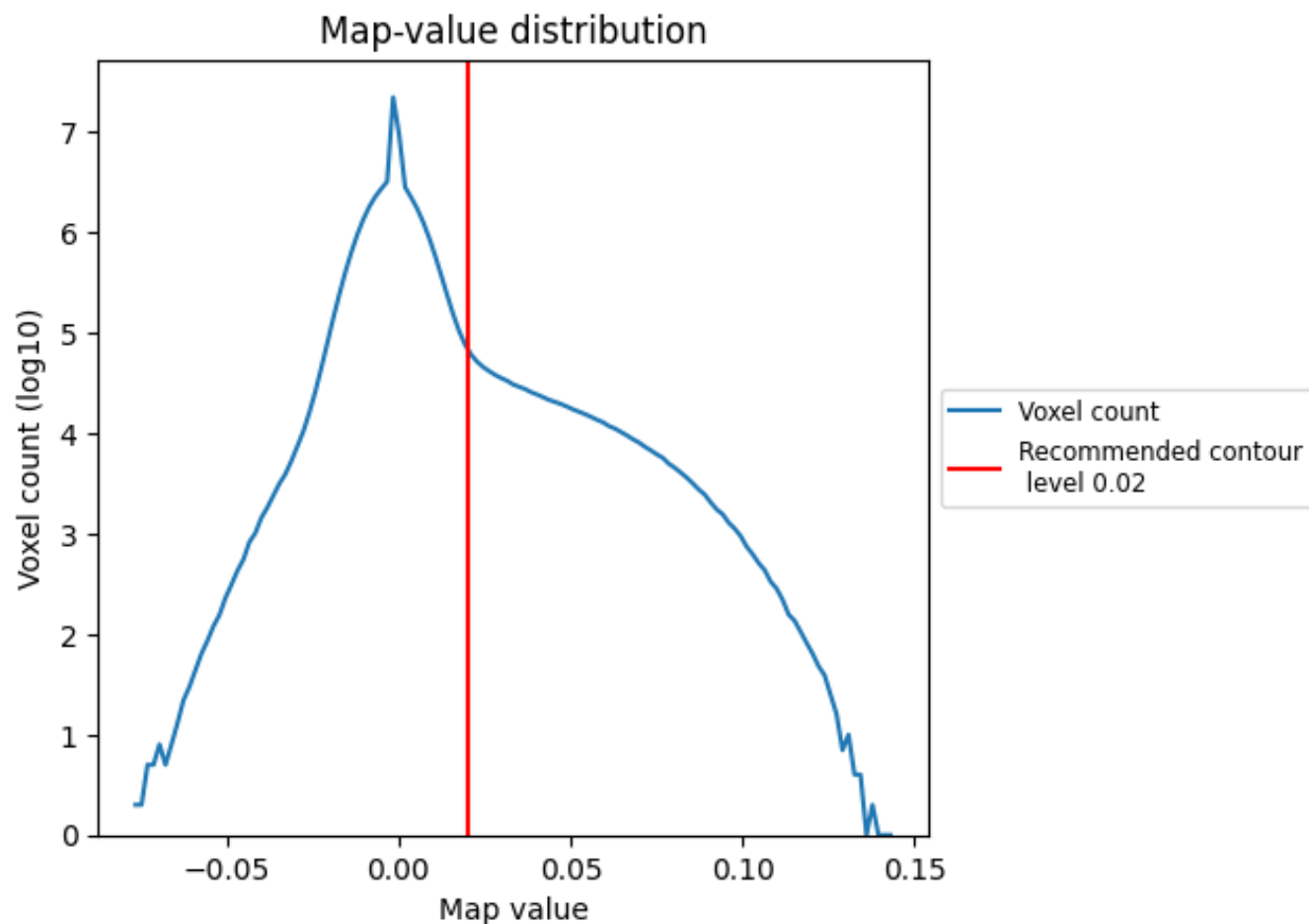
6.6 Mask visualisation

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

7 Map analysis [i](#)

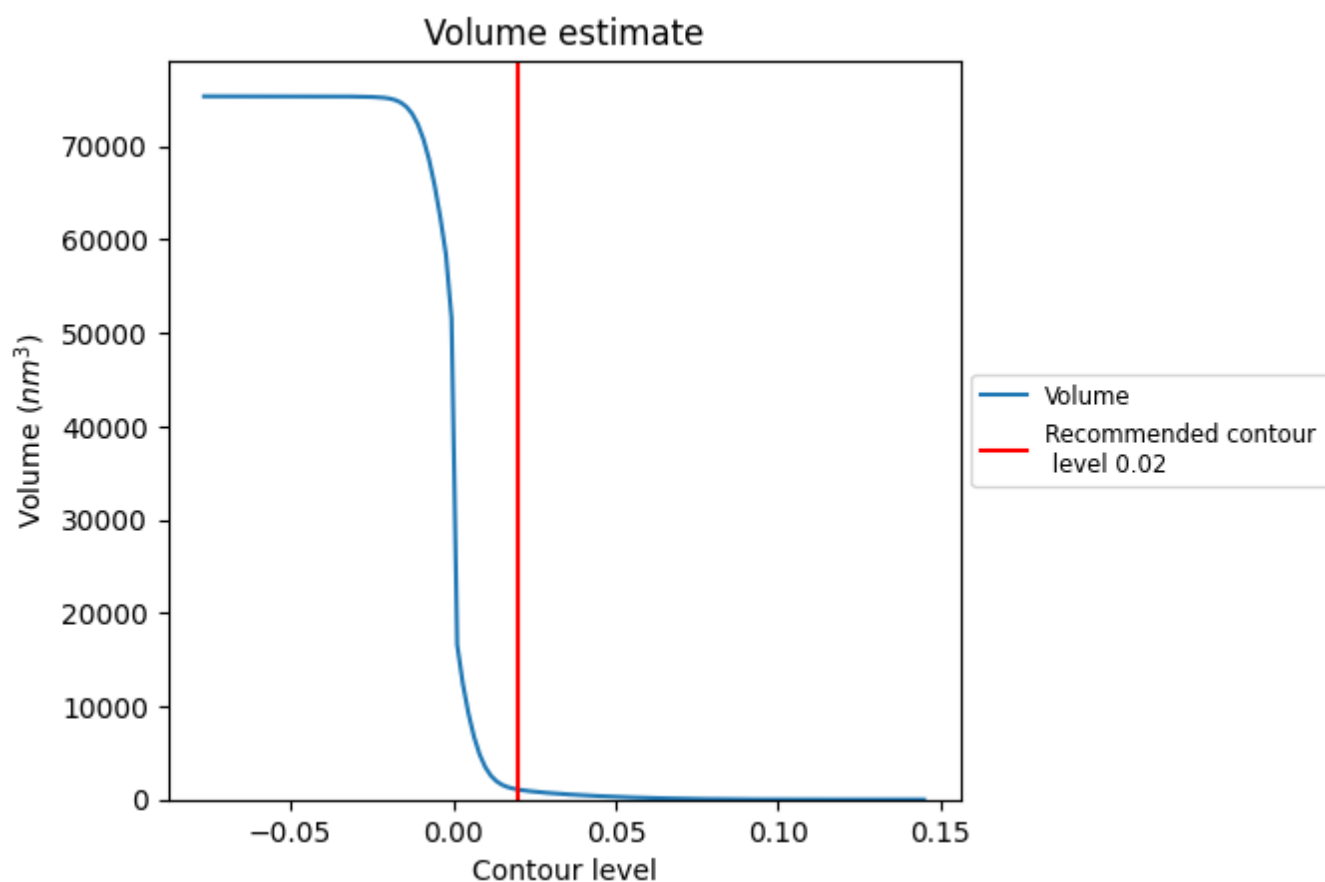
This section contains the results of statistical analysis of the map.

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.

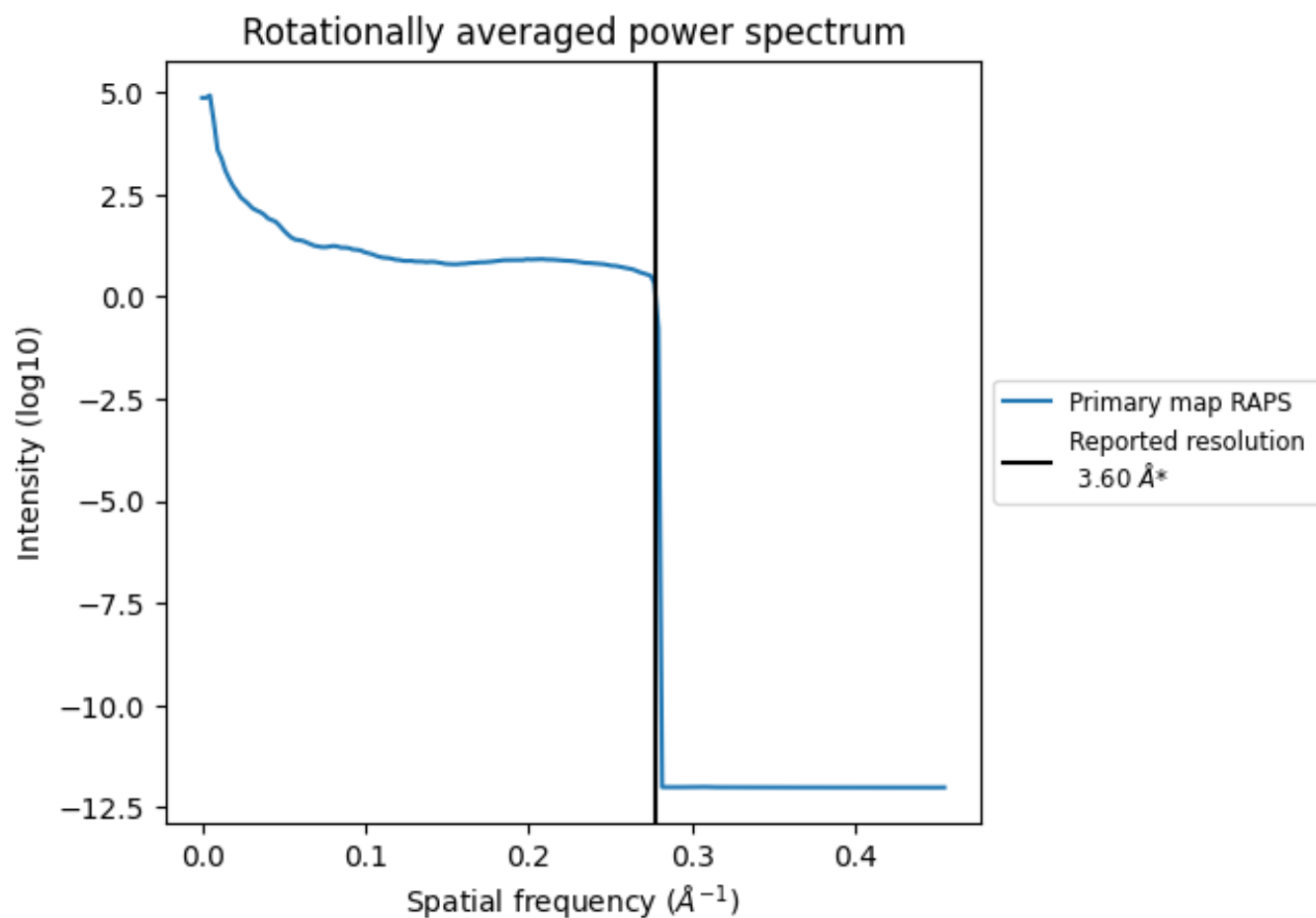
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1076 nm³; this corresponds to an approximate mass of 972 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

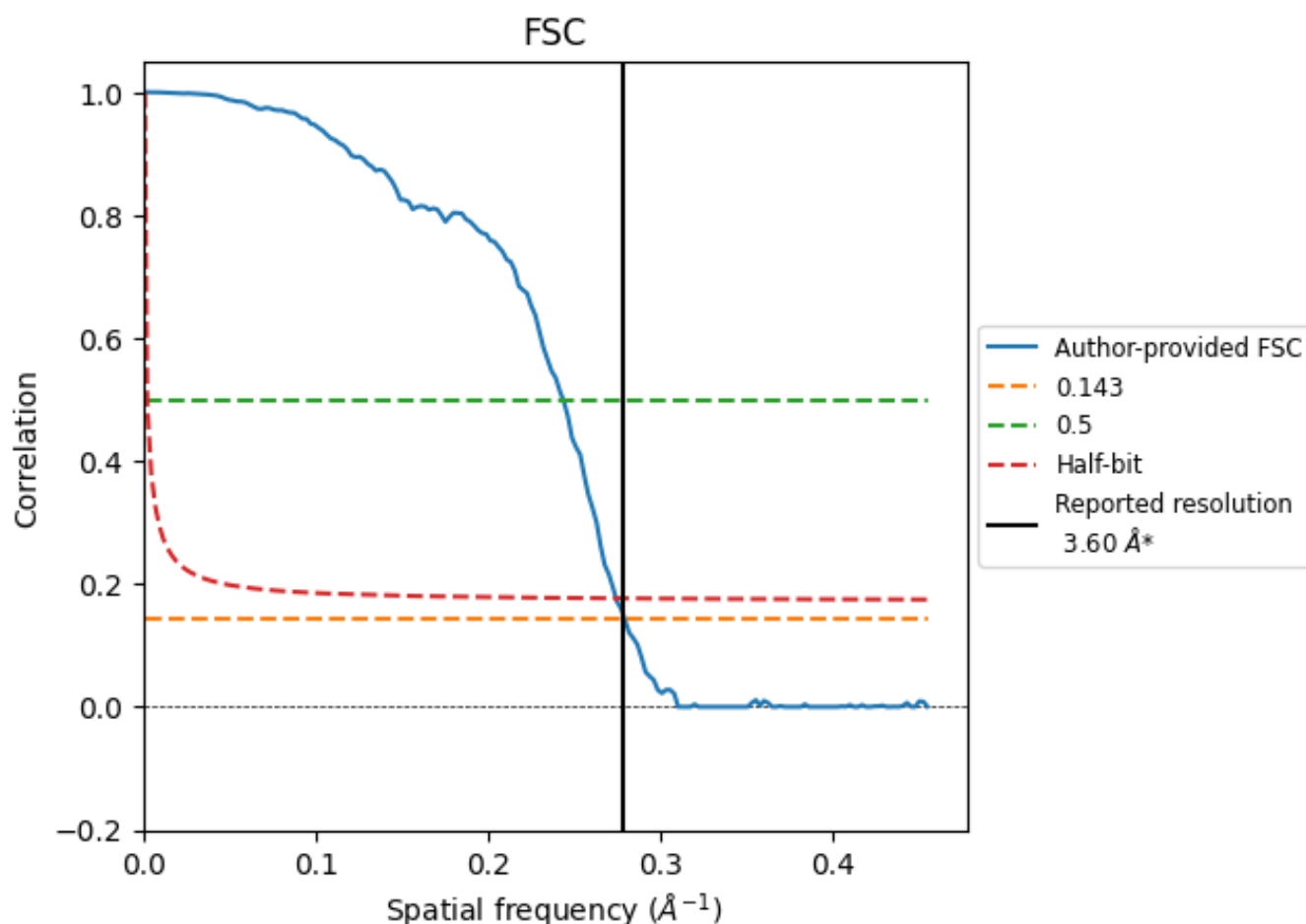


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

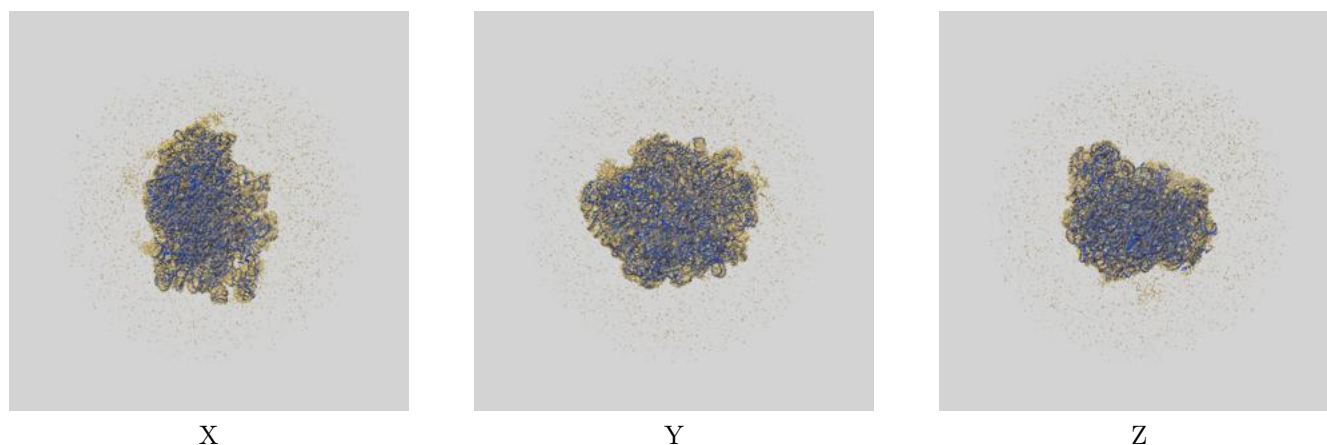
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.11	3.65
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

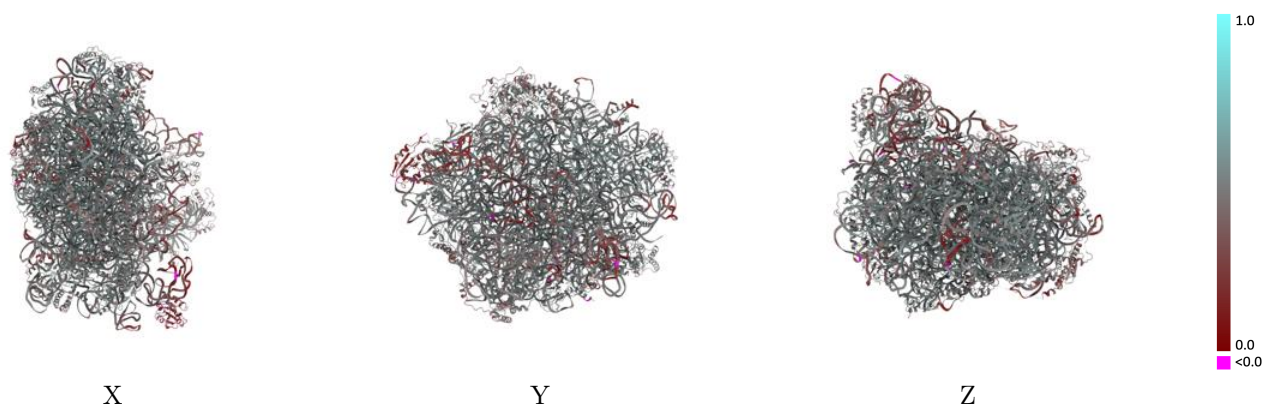
This section contains information regarding the fit between EMDB map EMD-0371 and PDB model 6N8L. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



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

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

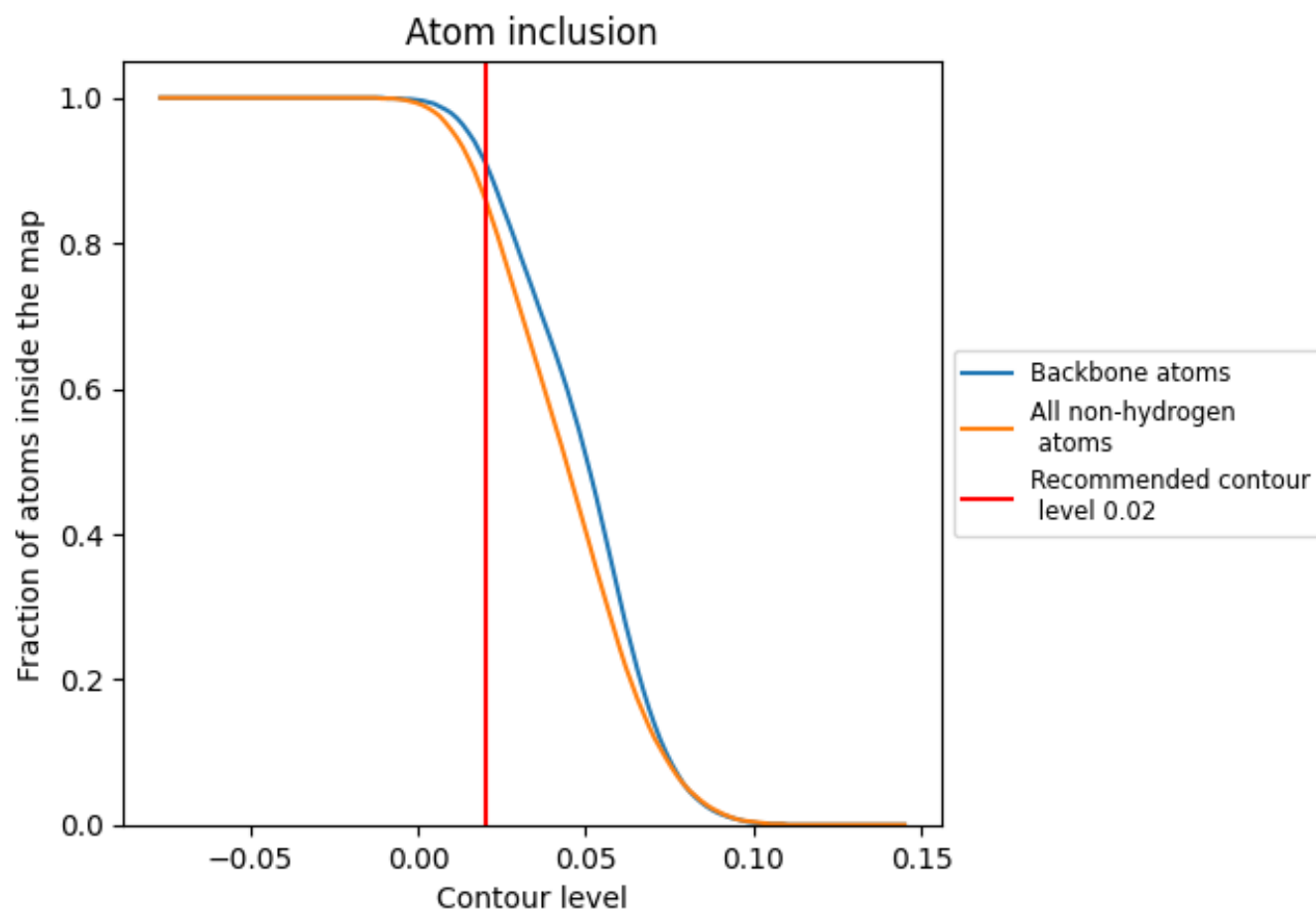


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4720
1	 0.9180	 0.4740
2	 0.9620	 0.4790
3	 0.9550	 0.4970
A	 0.8590	 0.5240
B	 0.8510	 0.5050
C	 0.8370	 0.5050
D	 0.8250	 0.4450
E	 0.7980	 0.4730
F	 0.8380	 0.4930
G	 0.8300	 0.4780
H	 0.8310	 0.4790
I	 0.5740	 0.4450
J	 0.7510	 0.4120
L	 0.8500	 0.4950
M	 0.8370	 0.4800
N	 0.8690	 0.5260
O	 0.8530	 0.5110
P	 0.8240	 0.5010
Q	 0.8530	 0.5040
R	 0.8390	 0.4980
S	 0.8210	 0.4960
T	 0.7750	 0.4230
U	 0.7800	 0.4170
V	 0.7960	 0.5020
W	 0.4710	 0.2330
X	 0.8360	 0.5020
Y	 0.8450	 0.5010
Z	 0.8270	 0.4950
a	 0.8420	 0.4950
b	 0.3890	 0.3710
c	 0.8250	 0.4680
d	 0.8280	 0.5000
e	 0.8260	 0.5170
f	 0.8540	 0.5260



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Chain	Atom inclusion	Q-score
g	 0.7970	 0.5000
h	 0.8320	 0.4920
i	 0.8430	 0.4850
j	 0.8870	 0.5350
k	 0.7600	 0.4660
l	 0.8530	 0.5220
o	 0.7990	 0.4720
p	 0.8190	 0.5090
q	 0.4150	 0.1540
s	 0.8420	 0.4070
u	 0.6980	 0.4340
v	 0.6310	 0.4180
y	 0.7810	 0.4540
z	 0.4170	 0.3790