



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:07 AM UTC

PDB ID : 6N8O / pdb_00006n8o
EMDB ID : EMD-0374
Title : Cryo-EM structure of Rpl10-inserted (RI) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.50 Å(reported)
Based on initial model : 5T62

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

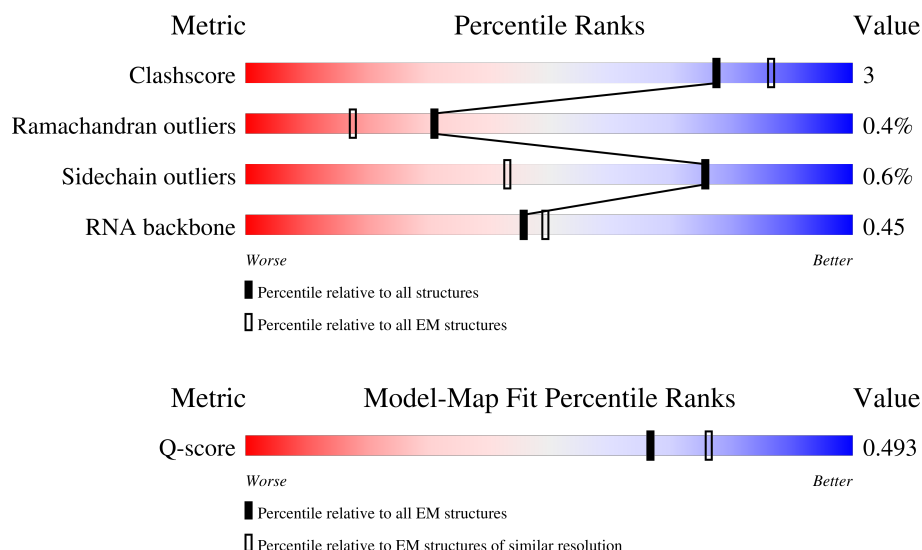
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



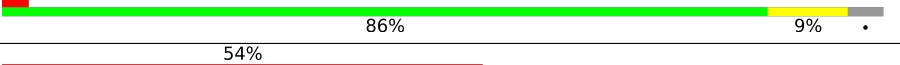
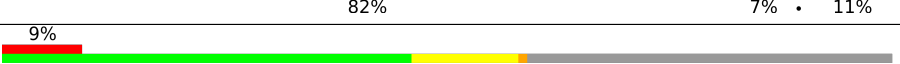
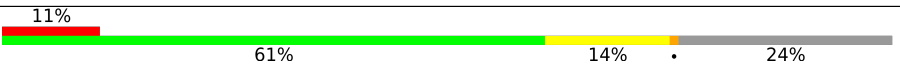
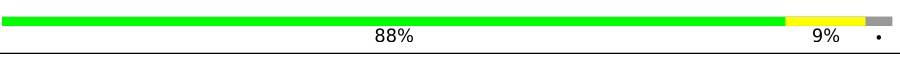
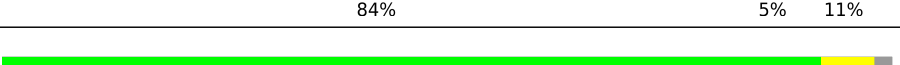
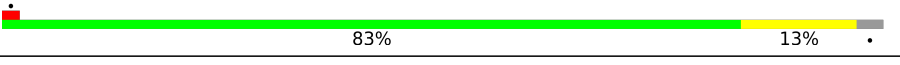
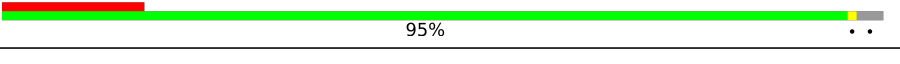
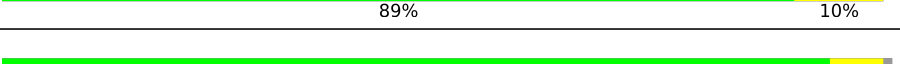
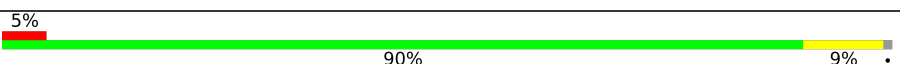
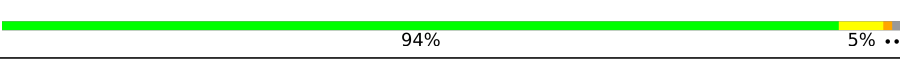
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	A	3396	 68% 23% 6%
2	B	121	 78% 22%
3	C	158	 78% 21%

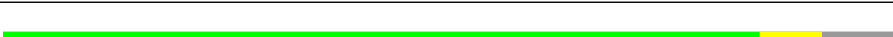
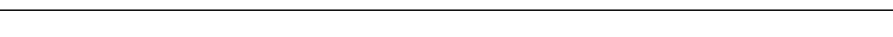
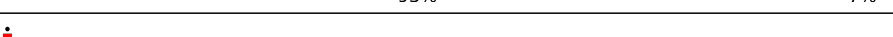
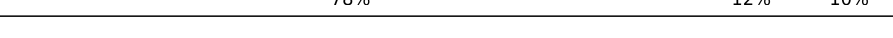
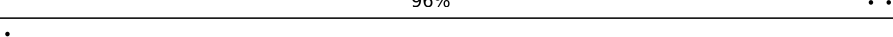
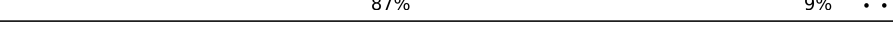
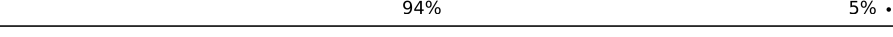
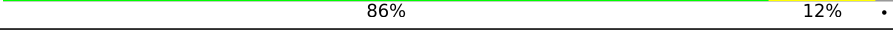
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Mol	Chain	Length	Quality of chain
4	Y	364	
5	X	245	
6	L	165	
7	W	640	
8	V	518	
9	D	254	
10	E	387	
11	F	362	
12	G	297	
13	H	176	
14	I	244	
15	J	256	
16	K	191	
17	Z	221	
18	M	174	
19	N	199	
20	O	138	
21	Q	106	
22	R	92	
23	S	217	
24	a	204	
25	b	199	
26	c	184	
27	d	186	
28	e	189	

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Mol	Chain	Length	Quality of chain
29	f	172	 91% 6% ...
30	g	160	 86% 13% .
31	h	121	 75% 5% 20%
32	i	137	 91% 5% . .
33	j	155	 37% . 61%
34	k	142	 76% 9% 15%
35	l	127	 92% 6% .
36	m	136	 86% 13% .
37	n	149	 82% 15% . .
38	o	59	 5% 92% 7% .
39	p	105	 85% 7% 9%
40	q	113	 88% 6% 5%
41	r	130	 90% 7% .
42	s	107	 93% 7% .
43	t	121	 78% 12% 10%
44	u	120	 96% . .
45	v	100	 87% 9% . .
46	w	88	 90% 5% . 5%
47	x	78	 94% 5% .
48	y	51	 86% 12% .
49	z	128	 34% 5% 60%

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 133453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3201	Total	C	N	O	P	0	0
			68470	30584	12346	22339	3201		

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called Tyrosine-protein phosphatase YVH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	128	Total	C	N	O	S	0	0
			991	625	179	179	8		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	234	Total	C	N	O	S	0	0
			1710	1063	294	346	7		

- Molecule 6 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	147	Total	C	N	O		0	0
			817	499	159	159			

- Molecule 7 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	377	Total	C	N	O	S	0	0
			2976	1905	516	548	7		

- Molecule 8 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	392	Total	C	N	O	S	0	0
			3034	1930	523	561	20		

- Molecule 9 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 10 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	384	Total	C	N	O	S	0	0
			3059	1940	582	529	8		

- Molecule 11 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 12 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	289	Total	C	N	O	S	0	0
			2315	1464	403	446	2		

- Molecule 13 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	155	Total	C	N	O	S	0	0
			1217	785	220	211	1		

- Molecule 14 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	220	Total	C	N	O	S	0	0
			1770	1143	322	304	1		

- Molecule 15 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	227	Total	C	N	O	S	0	0
			1762	1128	315	316	3		

- Molecule 16 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	201	Total	C	N	O	S	0	0
			1648	1050	309	284	5		

- Molecule 18 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 19 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	193	Total	C	N	O	S	0	0
			1539	959	314	266			

- Molecule 20 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 21 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 22 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	88	Total	C	N	O	S	0	0
			673	416	135	116	6		

- Molecule 23 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	210	Total	C	N	O	S	0	0
			1050	630	210	210			

- Molecule 24 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	183	Total	C	N	O	S	0	0
			1420	882	281	257			

- Molecule 27 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 28 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	151	Total	C	N	O	0	0
			1219	757	258	204		

- Molecule 29 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	159	Total	C	N	O	S	0
			1276	805	246	221	4	0

- Molecule 31 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	h	97	Total	C	N	O		0
			766	496	126	144		0

- Molecule 32 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	i	132	Total	C	N	O	S	0
			981	617	184	173	7	0

- Molecule 33 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	61	Total	C	N	O	S	0
			509	328	100	80	1	0

- Molecule 34 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	k	121	Total	C	N	O	S	0
			964	620	169	173	2	0

- Molecule 35 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 36 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 38 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 39 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 40 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	107	Total	C	N	O	S	0	0
			866	550	165	150	1		

- Molecule 41 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	126	Total	C	N	O	S	0	0
			1012	641	204	166	1		

- Molecule 42 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 44 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	98	Total	C	N	O	S	0	0
			753	471	150	130	2		

- Molecule 46 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 47 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	x	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 48 is a protein called 60S ribosomal protein L39.

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

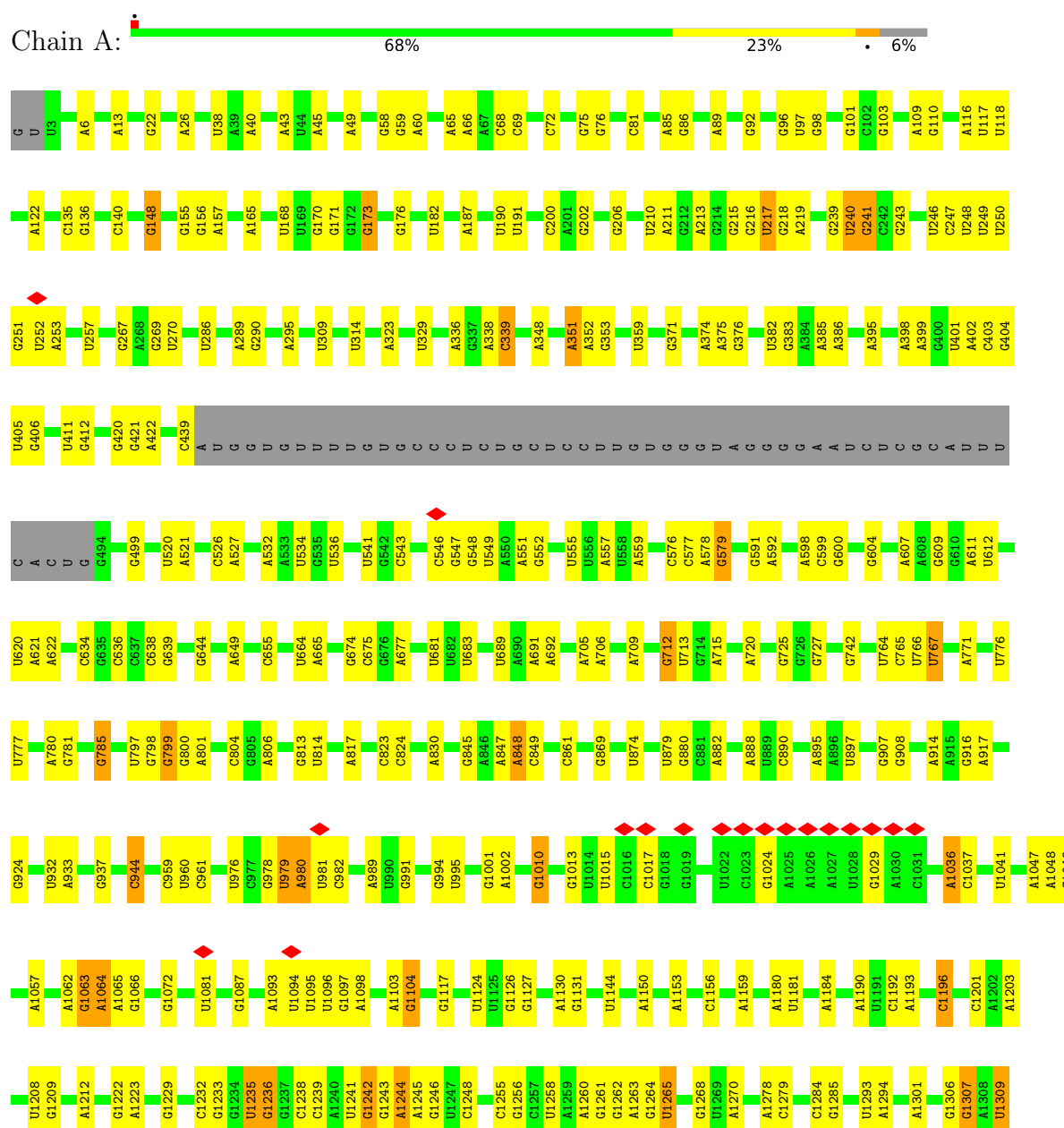
- Molecule 49 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	51	Total	C	N	O	S	0	0
			408	253	84	66	5		

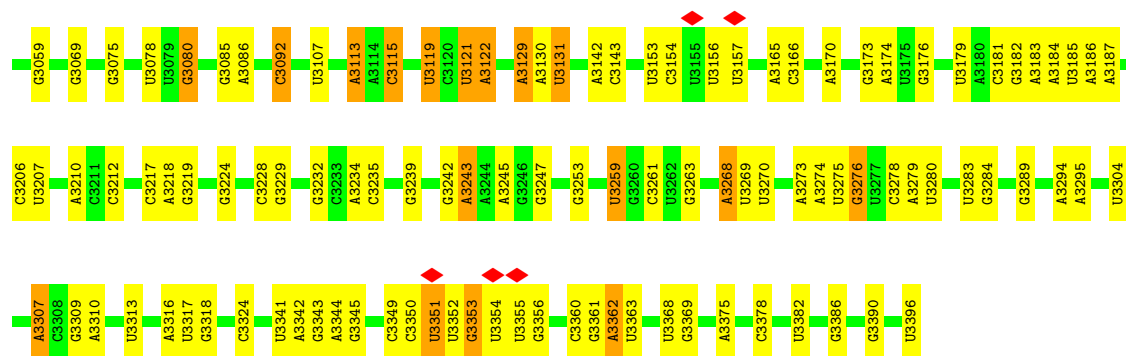
3 Residue-property plots

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

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







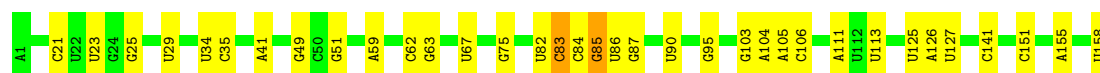
• Molecule 2: 5S rRNA

Chain B: 78% 22%



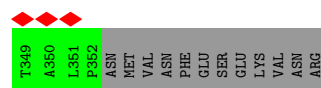
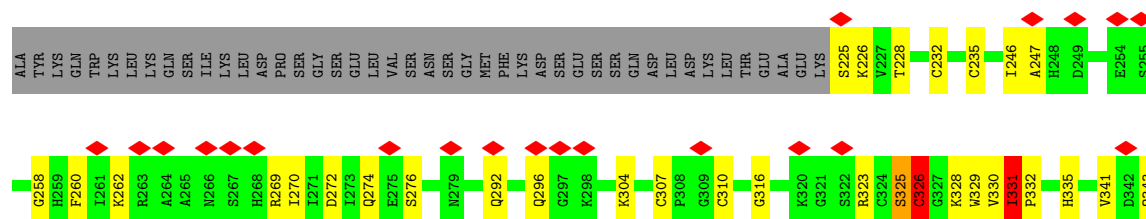
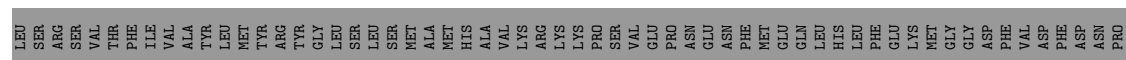
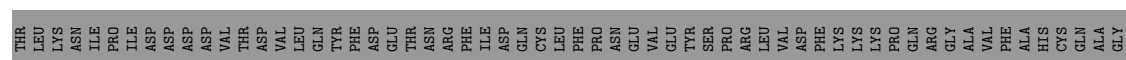
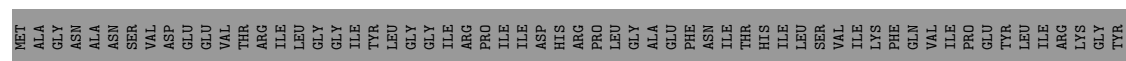
• Molecule 3: 5.8S rRNA

Chain C: 78% 21%



• Molecule 4: Tyrosine-protein phosphatase YVH1

Chain Y: 7% 26% 8% 65%

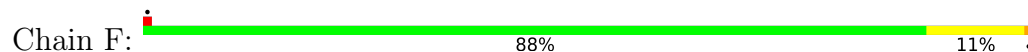
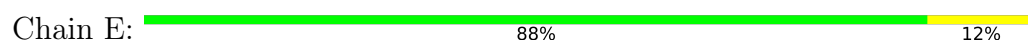
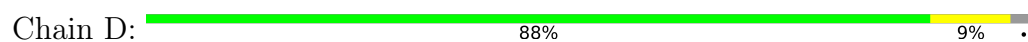


• Molecule 5: Eukaryotic translation initiation factor 6

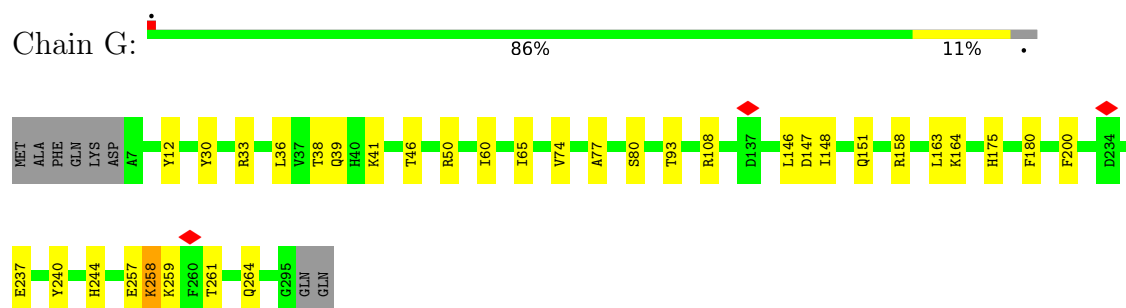
Chain X: 86% 9%



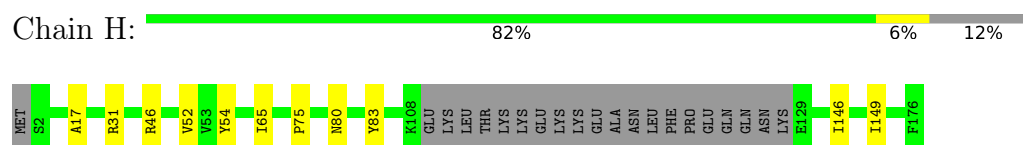
Chain V:



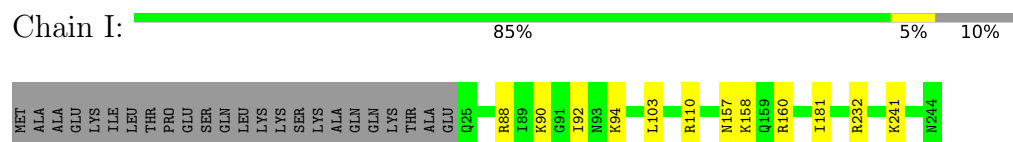
- Molecule 12: 60S ribosomal protein L5



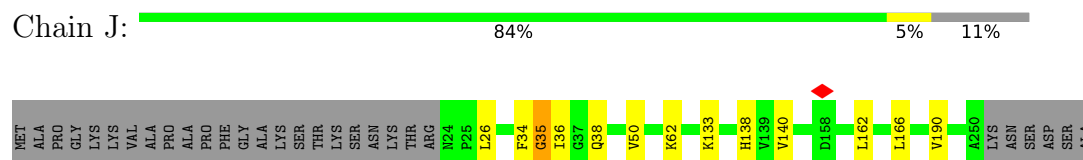
- Molecule 13: 60S ribosomal protein L6-A



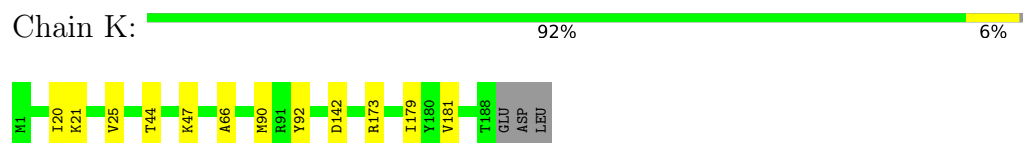
- Molecule 14: 60S ribosomal protein L7-A



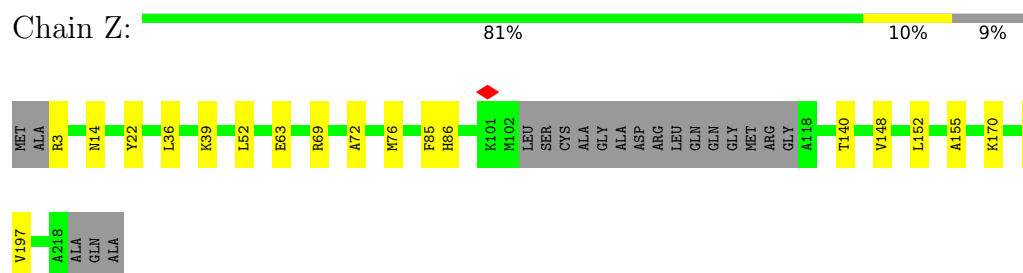
- Molecule 15: 60S ribosomal protein L8-A



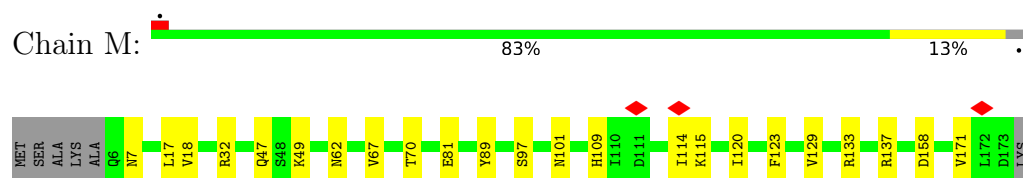
- Molecule 16: 60S ribosomal protein L9-A



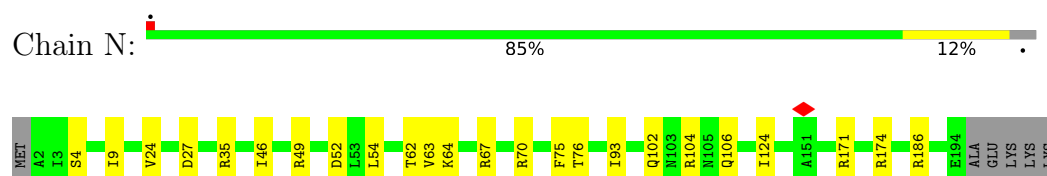
- Molecule 17: 60S ribosomal protein L10



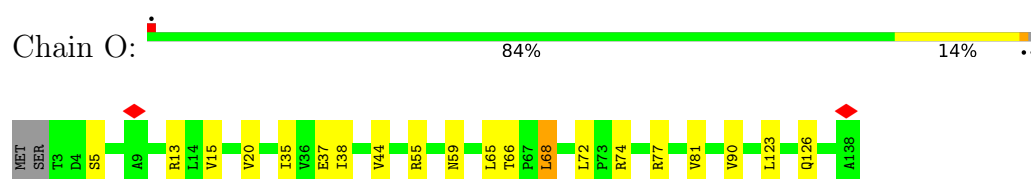
- Molecule 18: 60S ribosomal protein L11-A



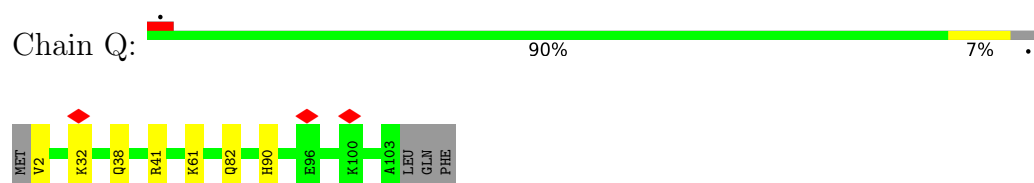
- Molecule 19: 60S ribosomal protein L13-A



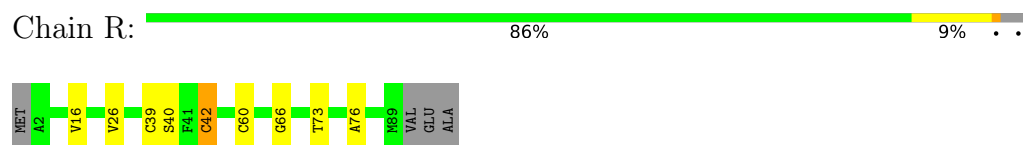
- Molecule 20: 60S ribosomal protein L14-A



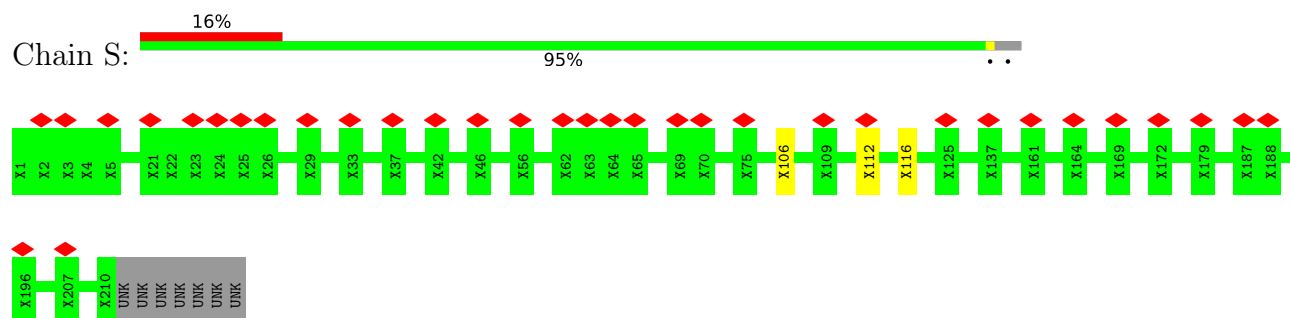
- Molecule 21: 60S ribosomal protein L42-A



- Molecule 22: 60S ribosomal protein L43-A



- Molecule 23: Ribosomal Protein uL1



- Molecule 24: 60S ribosomal protein L15-A

Chain a:  89% 10%

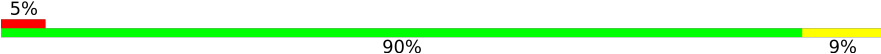


- Molecule 25: 60S ribosomal protein L16-A

Chain b:  93% 6%

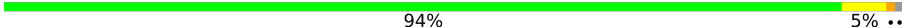


- Molecule 26: 60S ribosomal protein L17-A

Chain c:  5% 90% 9%



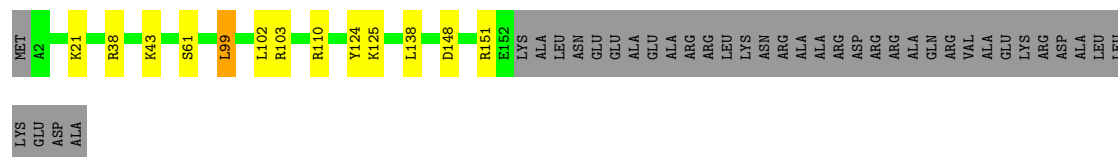
- Molecule 27: 60S ribosomal protein L18-A

Chain d:  94% 5%



- Molecule 28: 60S ribosomal protein L19-A

Chain e:  73% 6% 20%



- Molecule 29: 60S ribosomal protein L20-A

Chain f:  91% 6% ...



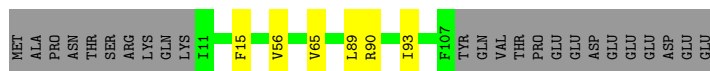
- Molecule 30: 60S ribosomal protein L21-A

Chain g:  86% 13%



- Molecule 31: 60S ribosomal protein L22-A

Chain h:  75% 5% 20%



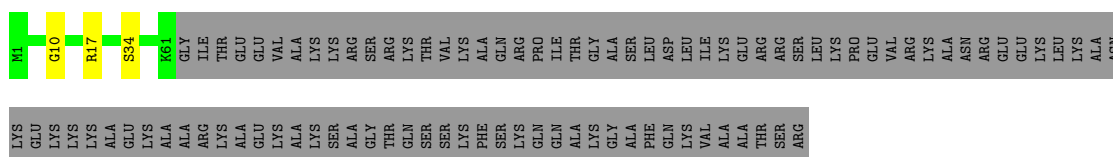
- Molecule 32: 60S ribosomal protein L23-A

Chain i:  91% 5% . .



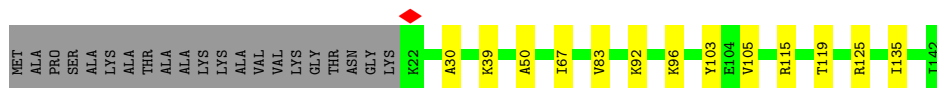
- Molecule 33: 60S ribosomal protein L24-A

Chain j:  37% 61%



- Molecule 34: 60S ribosomal protein L25

Chain k:  76% 9% 15%



- Molecule 35: 60S ribosomal protein L26-A

Chain l:  92% 6% .



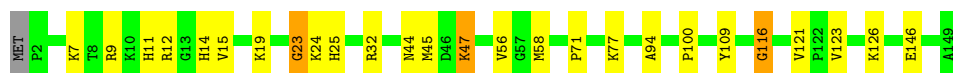
- Molecule 36: 60S ribosomal protein L27-A

Chain m:  86% 13% .

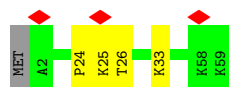
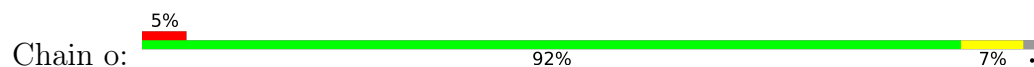


- Molecule 37: 60S ribosomal protein L28

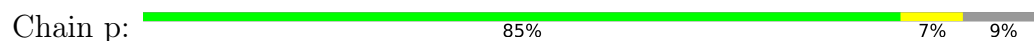
Chain n:  82% 15% . .



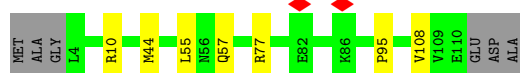
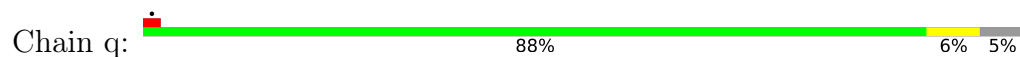
- Molecule 38: 60S ribosomal protein L29



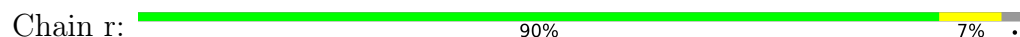
- Molecule 39: 60S ribosomal protein L30



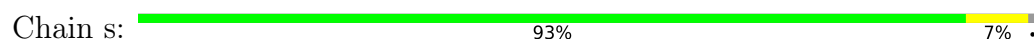
- Molecule 40: 60S ribosomal protein L31-A



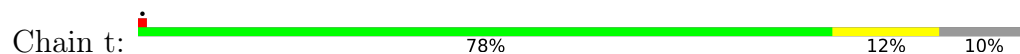
- Molecule 41: 60S ribosomal protein L32



- Molecule 42: 60S ribosomal protein L33-A



- Molecule 43: 60S ribosomal protein L34-A

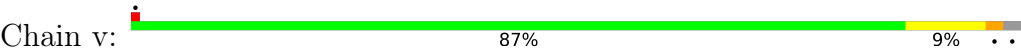


- Molecule 44: 60S ribosomal protein L35-A

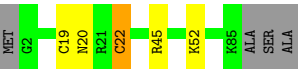
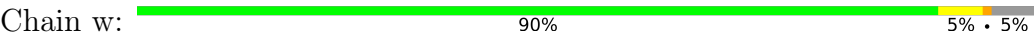




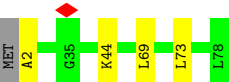
• Molecule 45: 60S ribosomal protein L36-A



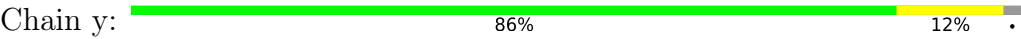
• Molecule 46: 60S ribosomal protein L37-A



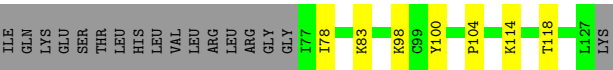
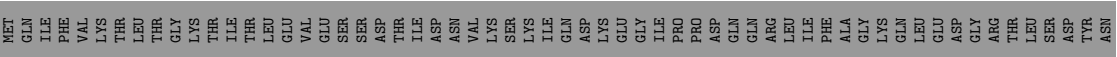
• Molecule 47: 60S ribosomal protein L38



• Molecule 48: 60S ribosomal protein L39



• Molecule 49: Ubiquitin-60S ribosomal protein L40



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112292	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	0.161	Depositor
Minimum map value	-0.089	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	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 ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/76644	0.36	6/119497 (0.0%)
2	B	0.31	0/2883	0.28	0/4491
3	C	0.36	0/3746	0.35	0/5832
4	Y	0.36	0/1016	1.05	7/1368 (0.5%)
5	X	0.30	0/1729	0.65	2/2355 (0.1%)
6	L	0.34	0/359	0.90	2/489 (0.4%)
7	W	0.31	0/3039	0.86	6/4124 (0.1%)
8	V	0.31	0/3093	0.77	6/4203 (0.1%)
9	D	0.39	0/1908	0.63	0/2564
10	E	0.38	0/3130	0.65	0/4206
11	F	0.36	0/2800	0.71	5/3790 (0.1%)
12	G	0.30	0/2364	0.66	4/3190 (0.1%)
13	H	0.31	0/1236	0.61	0/1661
14	I	0.35	0/1807	0.64	0/2432
15	J	0.32	0/1794	0.64	1/2425 (0.0%)
16	K	0.33	0/1514	0.65	0/2039
17	Z	0.29	0/1684	0.55	0/2259
18	M	0.27	0/1365	0.67	0/1831
19	N	0.34	0/1564	0.72	3/2102 (0.1%)
20	O	0.32	0/1068	0.58	0/1438
21	Q	0.33	0/831	0.64	0/1097
22	R	0.36	0/680	0.68	0/905
24	a	0.40	0/1757	0.62	0/2354
25	b	0.36	0/1585	0.60	0/2128
26	c	0.38	0/1443	0.68	0/1944
27	d	0.35	0/1465	0.65	0/1965
28	e	0.35	0/1236	0.62	0/1650
29	f	0.36	0/1468	0.65	3/1973 (0.2%)
30	g	0.35	0/1300	0.64	0/1743
31	h	0.29	0/781	0.63	0/1058
32	i	0.37	0/996	0.58	0/1340
33	j	0.32	0/521	0.56	0/691
34	k	0.34	0/979	0.59	0/1321
35	l	0.33	0/995	0.57	0/1329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
36	m	0.36	0/1118	0.67	0/1497
37	n	0.38	0/1204	0.81	6/1612 (0.4%)
38	o	0.32	0/473	0.82	2/629 (0.3%)
39	p	0.31	0/745	0.53	0/1001
40	q	0.39	0/880	0.63	0/1182
41	r	0.33	0/1033	0.62	0/1383
42	s	0.39	0/868	0.62	0/1168
43	t	0.39	0/871	0.65	1/1164 (0.1%)
44	u	0.32	0/978	0.64	0/1301
45	v	0.31	0/759	0.64	0/1009
46	w	0.41	0/680	0.75	0/901
47	x	0.30	0/614	0.56	0/822
48	y	0.38	0/443	0.66	0/588
49	z	0.31	0/414	0.61	0/551
All	All	0.35	0/141860	0.50	54/208602 (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
4	Y	0	3
5	X	0	1
7	W	0	10
8	V	0	2
10	E	0	1
11	F	0	2
14	I	0	2
15	J	0	2
16	K	0	1
18	M	0	2
23	S	0	1
29	f	0	2
37	n	0	3
38	o	0	1
44	u	0	1
All	All	0	34

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	t	81	CYS	CA-CB-SG	8.03	132.87	114.40
11	F	182	LEU	N-CA-C	-7.87	105.65	114.62
12	G	257	GLU	CA-C-N	7.55	135.96	121.54
12	G	257	GLU	C-N-CA	7.55	135.96	121.54
37	n	47	LYS	CA-C-N	6.88	134.69	121.54
37	n	47	LYS	C-N-CA	6.88	134.69	121.54
7	W	337	ILE	CA-C-N	6.84	134.61	121.54
7	W	337	ILE	C-N-CA	6.84	134.61	121.54
19	N	93	ILE	N-CA-C	-6.64	106.53	112.90
38	o	24	PRO	CA-C-N	6.56	134.08	121.54
38	o	24	PRO	C-N-CA	6.56	134.08	121.54
4	Y	328	LYS	CA-C-N	6.50	133.96	121.54
4	Y	328	LYS	C-N-CA	6.50	133.96	121.54
12	G	258	LYS	CA-C-N	6.47	133.91	121.54
12	G	258	LYS	C-N-CA	6.47	133.91	121.54
4	Y	331	ILE	N-CA-C	-6.36	95.15	108.88
37	n	116	GLY	N-CA-C	6.23	127.95	113.18
8	V	348	VAL	CA-C-N	6.15	129.86	120.82
8	V	348	VAL	C-N-CA	6.15	129.86	120.82
4	Y	329	TRP	N-CA-C	-5.92	98.19	110.80
4	Y	326	CYS	CB-CA-C	-5.91	98.67	110.42
8	V	96	ARG	N-CA-C	5.83	117.89	110.61
8	V	95	VAL	N-CA-C	5.67	121.14	109.34
6	L	105	GLN	CA-C-N	5.65	128.12	120.38
6	L	105	GLN	C-N-CA	5.65	128.12	120.38
1	A	2513	U	P-O3'-C3'	5.63	128.65	120.20
4	Y	325	SER	CA-C-N	5.55	132.15	121.54
4	Y	325	SER	C-N-CA	5.55	132.15	121.54
8	V	44	ASP	CA-C-N	5.51	131.90	121.97
8	V	44	ASP	C-N-CA	5.51	131.90	121.97
1	A	1576	G	P-O3'-C3'	5.50	128.44	120.20
15	J	190	VAL	N-CA-C	-5.49	107.93	113.20
5	X	161	VAL	CA-C-N	5.48	128.01	120.39
5	X	161	VAL	C-N-CA	5.48	128.01	120.39
37	n	23	GLY	CA-C-N	5.46	131.97	121.54
37	n	23	GLY	C-N-CA	5.46	131.97	121.54
1	A	2541	U	P-O3'-C3'	5.45	128.38	120.20
29	f	23	LYS	CA-C-N	5.44	131.93	121.54
29	f	23	LYS	C-N-CA	5.44	131.93	121.54
7	W	363	SER	CA-C-N	5.35	128.58	120.13
7	W	363	SER	C-N-CA	5.35	128.58	120.13
37	n	47	LYS	CA-CB-CG	5.31	124.71	114.10
1	A	1815	U	P-O3'-C3'	5.26	128.08	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	979	U	P-O3'-C3'	5.22	128.03	120.20
19	N	75	PHE	CA-C-N	5.21	131.50	121.54
19	N	75	PHE	C-N-CA	5.21	131.50	121.54
7	W	306	LYS	CA-C-N	5.19	127.29	120.60
7	W	306	LYS	C-N-CA	5.19	127.29	120.60
1	A	1064	A	P-O3'-C3'	5.08	127.82	120.20
11	F	4	PRO	CA-C-N	5.08	131.24	121.54
11	F	4	PRO	C-N-CA	5.08	131.24	121.54
11	F	337	GLU	CA-C-N	5.06	131.21	121.54
11	F	337	GLU	C-N-CA	5.06	131.21	121.54
29	f	13	ARG	N-CA-CB	-5.04	101.98	110.49

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	E	346	THR	Peptide
11	F	338	LYS	Peptide
11	F	4	PRO	Peptide
14	I	157	ASN	Peptide
14	I	232	ARG	Peptide
15	J	34	PHE	Peptide
15	J	35	GLY	Peptide
16	K	21	LYS	Peptide
18	M	171	VAL	Peptide
18	M	7	ASN	Peptide
23	S	106	UNK	Peptide
8	V	15	ALA	Peptide
8	V	44	ASP	Peptide
7	W	134	LEU	Peptide
7	W	137	PRO	Peptide
7	W	142	TRP	Peptide
7	W	176	LEU	Peptide
7	W	337	ILE	Peptide
7	W	371	THR	Peptide
7	W	373	HIS	Peptide
7	W	441	ILE	Peptide
7	W	445	SER	Peptide
7	W	467	ALA	Peptide
5	X	7	PHE	Peptide
4	Y	325	SER	Peptide
4	Y	326	CYS	Peptide

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Mol	Chain	Res	Type	Group
4	Y	331	ILE	Peptide
29	f	12	ARG	Peptide
29	f	23	LYS	Peptide
37	n	116	GLY	Peptide
37	n	14	HIS	Peptide
37	n	23	GLY	Peptide
38	o	25	LYS	Peptide
44	u	83	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	68470	0	34406	222	0
2	B	2579	0	1304	8	0
3	C	3353	0	1695	7	0
4	Y	991	0	980	12	0
5	X	1710	0	1667	11	0
6	L	817	0	430	7	0
7	W	2976	0	2977	39	0
8	V	3034	0	3004	90	0
9	D	1874	0	1943	15	0
10	E	3059	0	3127	25	0
11	F	2748	0	2859	28	0
12	G	2315	0	2270	21	0
13	H	1217	0	1308	8	0
14	I	1770	0	1851	7	0
15	J	1762	0	1839	7	0
16	K	1493	0	1566	8	0
17	Z	1648	0	1687	11	0
18	M	1344	0	1370	12	0
19	N	1539	0	1597	15	0
20	O	1053	0	1149	12	0
21	Q	819	0	890	6	0
22	R	673	0	715	5	0
23	S	1050	0	236	1	0
24	a	1720	0	1779	17	0
25	b	1555	0	1659	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	c	1420	0	1437	10	0
27	d	1441	0	1543	8	0
28	e	1219	0	1301	11	0
29	f	1432	0	1470	7	0
30	g	1276	0	1323	15	0
31	h	766	0	782	4	0
32	i	981	0	1031	7	0
33	j	509	0	537	2	0
34	k	964	0	1025	10	0
35	l	984	0	1075	7	0
36	m	1092	0	1155	11	0
37	n	1173	0	1215	14	0
38	o	462	0	491	1	0
39	p	737	0	792	4	0
40	q	866	0	908	4	0
41	r	1012	0	1079	7	0
42	s	850	0	880	5	0
43	t	861	0	919	7	0
44	u	969	0	1078	2	0
45	v	753	0	826	7	0
46	w	665	0	668	5	0
47	x	608	0	671	4	0
48	y	436	0	475	4	0
49	z	408	0	446	5	0
All	All	133453	0	97435	616	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 3.

All (616) 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)
8:V:94:LYS:CE	8:V:97:LEU:HD21	1.32	1.54
8:V:94:LYS:NZ	8:V:97:LEU:HD21	1.24	1.52
8:V:94:LYS:NZ	8:V:97:LEU:CD2	2.05	1.19
8:V:94:LYS:CE	8:V:97:LEU:CD2	2.21	1.17
8:V:94:LYS:HE3	8:V:97:LEU:HD21	1.26	1.12
8:V:49:ILE:HA	8:V:90:LYS:HD2	1.30	1.11
8:V:95:VAL:CB	8:V:120:GLY:CA	2.30	1.10
8:V:94:LYS:HE3	8:V:97:LEU:CD2	1.80	1.08
8:V:90:LYS:HE2	8:V:90:LYS:HA	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:95:VAL:CB	8:V:120:GLY:HA3	1.88	1.02
8:V:94:LYS:HE3	8:V:97:LEU:CG	1.92	0.99
8:V:95:VAL:CB	8:V:120:GLY:H	1.74	0.99
8:V:95:VAL:CB	8:V:120:GLY:N	2.26	0.98
8:V:49:ILE:HG22	8:V:90:LYS:CD	1.95	0.95
8:V:96:ARG:O	8:V:97:LEU:C	2.14	0.90
8:V:94:LYS:HZ2	8:V:97:LEU:HD21	1.29	0.90
8:V:49:ILE:CA	8:V:90:LYS:HD2	2.03	0.86
8:V:94:LYS:HZ1	8:V:97:LEU:HD21	1.44	0.82
8:V:94:LYS:HZ1	8:V:97:LEU:CD2	1.96	0.78
8:V:96:ARG:O	8:V:98:VAL:N	2.20	0.75
8:V:49:ILE:HG22	8:V:90:LYS:HD3	1.66	0.75
4:Y:307:CYS:SG	4:Y:310:CYS:N	2.60	0.74
8:V:90:LYS:HA	8:V:90:LYS:CE	2.17	0.71
1:A:3274:A:H2'	26:c:171:ARG:HH12	1.57	0.70
8:V:89:LEU:C	8:V:89:LEU:HD13	2.17	0.70
8:V:94:LYS:HZ2	8:V:97:LEU:CD2	1.86	0.70
8:V:94:LYS:HE3	8:V:97:LEU:HG	1.73	0.70
8:V:89:LEU:HD13	8:V:89:LEU:O	1.92	0.70
8:V:49:ILE:CG2	8:V:90:LYS:HG3	2.24	0.67
43:t:44:CYS:SG	43:t:45:GLY:N	2.68	0.66
8:V:90:LYS:HE2	8:V:90:LYS:CA	2.17	0.66
18:M:47:GLN:HG2	18:M:67:VAL:HG12	1.78	0.66
8:V:94:LYS:CD	8:V:97:LEU:HD21	2.23	0.65
11:F:283:THR:HG22	11:F:285:ASP:H	1.61	0.64
7:W:205:VAL:HG13	7:W:213:PHE:HB2	1.79	0.64
8:V:49:ILE:HB	8:V:90:LYS:HG3	1.79	0.63
10:E:227:GLU:HG3	10:E:270:ARG:HE	1.64	0.63
1:A:2284:C:O2	8:V:205:ASN:ND2	2.32	0.63
26:c:126:ARG:NH2	26:c:140:GLU:OE2	2.32	0.63
10:E:232:ARG:NH1	10:E:269:GLN:O	2.32	0.63
19:N:46:ILE:HG22	19:N:49:ARG:HB2	1.80	0.62
28:e:103:ARG:NH1	28:e:124:TYR:OH	2.32	0.62
7:W:237:LYS:HB2	7:W:240:LEU:HD13	1.81	0.62
8:V:168:LYS:HB2	8:V:171:PHE:HB3	1.81	0.62
1:A:976:U:H5''	27:d:141:ARG:HH22	1.64	0.62
1:A:1255:C:H2'	1:A:1256:G:H8	1.63	0.62
1:A:1602:A:H5''	28:e:38:ARG:HG3	1.82	0.61
18:M:109:HIS:HD2	18:M:123:PHE:H	1.48	0.61
5:X:4:ARG:NH1	5:X:210:THR:O	2.33	0.61
12:G:261:THR:OG1	12:G:264:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:75:ILE:HG22	30:g:88:ARG:HG2	1.81	0.61
10:E:10:ARG:NH2	10:E:263:SER:O	2.33	0.61
6:L:28:UNK:O	6:L:31:UNK:N	2.34	0.60
10:E:57:VAL:HG22	10:E:73:VAL:HG12	1.83	0.60
8:V:56:SER:HB2	8:V:65:LEU:HB3	1.83	0.60
39:p:30:THR:HG22	39:p:91:SER:HB2	1.83	0.60
4:Y:228:THR:HG21	4:Y:343:GLN:HE21	1.67	0.60
9:D:117:GLU:HG2	9:D:124:GLY:H	1.66	0.60
19:N:24:VAL:HG12	24:a:199:LEU:HB2	1.82	0.60
4:Y:260:PHE:HB2	4:Y:274:GLN:HB2	1.84	0.60
1:A:804:C:OP1	11:F:98:ARG:NH2	2.34	0.60
15:J:35:GLY:HA3	15:J:38:GLN:HE21	1.67	0.60
8:V:19:CYS:SG	8:V:20:CYS:N	2.75	0.60
17:Z:36:LEU:HD11	17:Z:69:ARG:HD3	1.83	0.60
1:A:1208:U:O2	1:A:3115:C:N4	2.34	0.59
1:A:3343:G:H21	1:A:3362:A:H2	1.50	0.59
5:X:101:LEU:HA	32:i:135:VAL:HG22	1.84	0.59
1:A:2727:A:OP2	1:A:2728:G:N2	2.35	0.59
8:V:49:ILE:HG22	8:V:90:LYS:CG	2.32	0.59
29:f:23:LYS:O	30:g:146:ASN:ND2	2.35	0.59
1:A:2137:U:OP2	1:A:2142:A:N6	2.36	0.59
1:A:1363:A:OP1	14:I:160:ARG:NH1	2.35	0.59
12:G:50:ARG:NH1	12:G:147:ASP:OD2	2.36	0.58
8:V:49:ILE:CG2	8:V:90:LYS:CD	2.77	0.58
1:A:2908:G:O2'	49:z:114:LYS:NZ	2.36	0.58
34:k:115:ARG:NH1	34:k:119:THR:OG1	2.35	0.58
8:V:49:ILE:HG22	8:V:90:LYS:HD2	1.83	0.58
8:V:58:CYS:SG	8:V:61:CYS:N	2.66	0.58
25:b:10:ASP:HB2	25:b:117:ARG:HB3	1.85	0.58
1:A:1571:A:H2'	1:A:1572:U:H4'	1.86	0.58
12:G:93:THR:OG1	12:G:158:ARG:NH1	2.37	0.58
1:A:2227:C:OP1	21:Q:32:LYS:NZ	2.37	0.58
1:A:1724:U:O4	28:e:125:LYS:NZ	2.37	0.57
1:A:2948:C:OP1	10:E:244:ARG:NH2	2.37	0.57
1:A:767:U:H4'	19:N:186:ARG:HH12	1.70	0.57
18:M:133:ARG:NH2	18:M:158:ASP:OD2	2.37	0.57
19:N:64:LYS:O	19:N:67:ARG:NH1	2.37	0.57
14:I:88:ARG:NH1	14:I:90:LYS:O	2.37	0.57
8:V:94:LYS:HE3	8:V:97:LEU:CD1	2.34	0.57
20:O:72:LEU:HD11	20:O:81:VAL:HG22	1.86	0.57
1:A:2443:A:N6	1:A:2503:G:O6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:3:LYS:O	36:m:6:LYS:NZ	2.37	0.57
48:y:21:ARG:HH12	48:y:24:PRO:HG3	1.70	0.57
25:b:37:ARG:HH21	25:b:160:ARG:HH22	1.52	0.57
1:A:980:A:H2	1:A:1104:G:H21	1.52	0.57
30:g:17:ARG:NH1	30:g:45:ASN:OD1	2.37	0.57
1:A:2290:C:O2'	7:W:413:GLN:NE2	2.37	0.57
1:A:712:G:OP1	19:N:174:ARG:NH1	2.38	0.56
1:A:3186:A:N3	16:K:44:THR:OG1	2.37	0.56
14:I:88:ARG:HE	14:I:103:LEU:HD13	1.70	0.56
25:b:119:VAL:HG11	29:f:167:ARG:HE	1.70	0.56
28:e:102:LEU:HD22	28:e:138:LEU:HD13	1.86	0.56
2:B:8:G:OP2	12:G:30:TYR:OH	2.22	0.56
8:V:49:ILE:HB	8:V:90:LYS:CG	2.34	0.56
12:G:146:LEU:HG	12:G:163:LEU:HD12	1.87	0.56
7:W:314:GLU:HG2	7:W:315:GLU:H	1.70	0.56
20:O:13:ARG:NH1	20:O:65:LEU:O	2.38	0.56
40:q:55:LEU:HB2	40:q:95:PRO:HD3	1.88	0.56
24:a:73:ARG:HH21	24:a:92:LEU:HD21	1.71	0.56
12:G:65:ILE:HG22	12:G:74:VAL:HA	1.88	0.56
1:A:217:U:O2	35:l:103:LYS:NZ	2.37	0.56
8:V:49:ILE:CB	8:V:90:LYS:HG3	2.36	0.56
5:X:106:ASN:ND2	5:X:150:SER:OG	2.32	0.56
1:A:3042:U:OP2	1:A:3092:C:N4	2.39	0.56
7:W:217:ASP:OD1	7:W:220:ARG:NH2	2.39	0.56
8:V:16:THR:HG22	8:V:17:LEU:HD12	1.87	0.56
10:E:10:ARG:NH1	10:E:11:HIS:O	2.39	0.56
7:W:139:ARG:HH22	7:W:196:GLU:HB2	1.70	0.55
1:A:1521:G:O6	48:y:17:LYS:NZ	2.39	0.55
8:V:119:GLN:HA	8:V:129:GLN:HA	1.88	0.55
12:G:240:TYR:O	12:G:244:HIS:ND1	2.40	0.55
8:V:280:SER:OG	8:V:281:ASN:N	2.38	0.55
11:F:327:LEU:HD23	14:I:181:ILE:HG21	1.89	0.55
1:A:499:G:H5''	42:s:48:ARG:HH22	1.71	0.55
22:R:39:CYS:SG	22:R:40:SER:N	2.79	0.55
29:f:109:ASP:OD1	29:f:113:ARG:NH1	2.39	0.55
46:w:19:CYS:SG	46:w:22:CYS:N	2.78	0.55
1:A:674:G:OP1	11:F:31:ARG:NH1	2.38	0.55
1:A:3351:U:O2'	1:A:3353:G:N2	2.39	0.55
7:W:208:ARG:O	7:W:500:ASN:ND2	2.39	0.55
11:F:226:GLU:HB3	11:F:237:GLN:HE21	1.71	0.55
1:A:534:U:OP1	29:f:132:THR:OG1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:66:GLN:HB2	8:V:70:GLN:HB2	1.87	0.55
11:F:4:PRO:HD2	11:F:22:LEU:HD13	1.89	0.55
24:a:37:HIS:HE1	24:a:63:ARG:HH11	1.54	0.55
8:V:47:GLN:OE1	8:V:51:ARG:NH2	2.36	0.55
37:n:7:LYS:O	37:n:11:HIS:ND1	2.40	0.55
1:A:412:G:OP1	26:c:62:ARG:NH1	2.40	0.55
1:A:2450:G:H1	1:A:2497:U:H3	1.56	0.55
6:L:60:VAL:HB	6:L:80:LEU:HD11	1.89	0.55
1:A:1613:A:OP1	47:x:2:ALA:N	2.40	0.54
8:V:58:CYS:HB3	8:V:63:ARG:H	1.71	0.54
1:A:727:G:OP2	1:A:742:G:N2	2.40	0.54
15:J:162:LEU:HA	24:a:7:LEU:HD11	1.89	0.54
12:G:60:ILE:HB	12:G:80:SER:HB3	1.89	0.54
8:V:89:LEU:HD12	8:V:90:LYS:HE3	1.88	0.54
47:x:69:LEU:HD12	47:x:73:LEU:HD23	1.89	0.54
1:A:1156:C:OP2	14:I:94:LYS:NZ	2.41	0.54
11:F:237:GLN:O	11:F:246:ARG:NH1	2.41	0.54
12:G:77:ALA:O	12:G:108:ARG:NH1	2.41	0.54
8:V:102:PHE:HB3	8:V:114:ILE:HG13	1.90	0.54
11:F:338:LYS:O	11:F:340:GLY:N	2.41	0.54
21:Q:38:GLN:OE1	21:Q:41:ARG:NH2	2.40	0.54
26:c:109:ALA:HA	26:c:112:LEU:HD13	1.89	0.54
1:A:2440:G:N2	1:A:2508:U:O2	2.40	0.54
4:Y:304:LYS:HA	4:Y:316:GLY:HA2	1.89	0.54
36:m:121:ARG:NH2	36:m:127:ASN:OD1	2.34	0.54
10:E:368:GLY:O	33:j:17:ARG:NH1	2.37	0.54
1:A:2953:U:H2'	1:A:2954:U:H2'	1.90	0.54
7:W:430:LYS:NZ	7:W:453:ASP:O	2.40	0.54
1:A:2349:U:O2'	1:A:3307:A:N3	2.41	0.53
8:V:49:ILE:CB	8:V:90:LYS:HD2	2.38	0.53
9:D:136:ILE:HG12	9:D:148:VAL:HG12	1.91	0.53
12:G:41:LYS:NZ	30:g:30:TYR:O	2.39	0.53
16:K:47:LYS:NZ	20:O:5:SER:O	2.41	0.53
1:A:813:G:O2'	46:w:45:ARG:NH2	2.42	0.53
1:A:1547:G:OP1	24:a:108:ARG:NH2	2.41	0.53
10:E:53:MET:HG2	10:E:77:THR:HG22	1.91	0.53
1:A:1260:A:HO2'	1:A:1279:C:HO2'	1.56	0.53
1:A:2185:G:O2'	1:A:2314:U:OP2	2.25	0.53
1:A:3242:G:O6	10:E:150:ARG:NH1	2.40	0.53
3:C:141:C:O2	24:a:112:ASN:ND2	2.41	0.53
45:v:5:THR:HG23	45:v:12:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3049:A:O2'	10:E:364:LYS:NZ	2.41	0.53
7:W:242:THR:HG23	7:W:245:GLN:H	1.74	0.53
1:A:713:U:OP1	19:N:171:ARG:NH1	2.41	0.53
1:A:1408:G:OP1	41:r:33:ARG:NH2	2.40	0.53
1:A:2842:U:OP1	1:A:2898:G:N2	2.41	0.53
8:V:24:THR:OG1	8:V:35:CYS:SG	2.59	0.53
18:M:114:ILE:HG22	18:M:115:LYS:HG3	1.90	0.53
1:A:216:G:OP1	35:l:16:ARG:NH1	2.41	0.53
1:A:215:G:OP1	35:l:12:ARG:NH1	2.35	0.53
6:L:105:GLN:HA	6:L:143:UNK:HA	1.90	0.53
10:E:303:LYS:HD2	10:E:361:THR:HG21	1.91	0.53
36:m:23:VAL:HG12	36:m:45:GLY:HA3	1.91	0.53
1:A:38:U:H4'	37:n:32:ARG:HD2	1.91	0.53
1:A:609:G:OP2	11:F:315:LYS:NZ	2.41	0.53
8:V:253:LYS:NZ	8:V:277:SER:O	2.42	0.52
15:J:50:VAL:HG12	34:k:30:ALA:HA	1.92	0.52
29:f:42:TRP:HE1	29:f:58:ILE:HD11	1.73	0.52
6:L:76:SER:HA	6:L:80:LEU:HD12	1.91	0.52
8:V:49:ILE:HG22	8:V:90:LYS:HG3	1.91	0.52
1:A:1609:C:OP1	34:k:125:ARG:NH2	2.43	0.52
1:A:2176:U:OP1	9:D:54:ARG:NH2	2.37	0.52
1:A:2469:G:H1	1:A:2476:C:H42	1.58	0.52
32:i:69:LEU:HD12	32:i:74:MET:HE1	1.89	0.52
32:i:74:MET:HE3	32:i:102:ILE:HG21	1.91	0.52
48:y:28:ARG:NH1	48:y:36:ARG:O	2.42	0.52
30:g:89:LEU:HD23	30:g:91:LEU:HD21	1.92	0.52
1:A:171:G:N2	1:A:248:U:O2	2.43	0.52
1:A:845:G:N2	1:A:848:A:OP2	2.42	0.52
1:A:3276:G:O6	26:c:171:ARG:NH2	2.42	0.52
7:W:147:SER:HB2	7:W:150:GLN:H	1.74	0.52
30:g:18:ASP:HB2	30:g:21:LYS:HB2	1.93	0.52
7:W:182:GLU:O	7:W:188:TRP:NE1	2.39	0.51
1:A:1390:A:N6	1:A:1418:A:O2'	2.42	0.51
1:A:1307:G:OP1	25:b:59:ARG:NH1	2.43	0.51
1:A:1316:C:OP2	25:b:133:ARG:NE	2.43	0.51
17:Z:72:ALA:HB2	17:Z:155:ALA:HB2	1.92	0.51
1:A:69:C:OP1	24:a:178:HIS:ND1	2.32	0.51
1:A:1048:A:H2'	17:Z:22:TYR:HE2	1.75	0.51
1:A:2945:G:O2'	1:A:2948:C:OP2	2.28	0.51
7:W:491:TYR:HA	7:W:496:LEU:HB2	1.92	0.51
8:V:90:LYS:CE	8:V:90:LYS:CA	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:G:OP1	19:N:70:ARG:NH2	2.44	0.51
1:A:1261:G:O2'	1:A:1278:A:N1	2.44	0.51
7:W:462:VAL:O	7:W:466:ARG:N	2.44	0.51
8:V:144:PRO:HA	8:V:147:ALA:HB3	1.91	0.51
10:E:54:THR:OG1	10:E:360:ASP:O	2.27	0.51
19:N:4:SER:O	37:n:44:ASN:ND2	2.32	0.51
1:A:86:G:O2'	1:A:98:G:O6	2.28	0.51
1:A:1203:A:OP2	1:A:1301:A:N6	2.43	0.51
24:a:68:ARG:NH1	24:a:124:ASP:O	2.43	0.51
1:A:1506:A:H5''	1:A:1507:G:H5''	1.93	0.51
1:A:2375:G:O2'	1:A:2377:G:OP2	2.27	0.51
1:A:785:G:O6	37:n:77:LYS:NZ	2.43	0.51
1:A:2880:U:OP1	32:i:47:ASN:ND2	2.44	0.51
6:L:106:LEU:O	6:L:110:ILE:N	2.38	0.51
8:V:107:PRO:O	8:V:110:ARG:NH1	2.37	0.51
12:G:39:GLN:NE2	12:G:46:THR:O	2.43	0.51
1:A:1474:A:O2'	40:q:57:GLN:NE2	2.44	0.51
1:A:1150:A:O2'	42:s:21:ARG:NH2	2.41	0.50
1:A:2471:U:O2	1:A:2473:C:N4	2.44	0.50
1:A:1430:U:H2'	37:n:9:ARG:HH22	1.77	0.50
8:V:179:LEU:HA	8:V:184:HIS:HE1	1.76	0.50
31:h:56:VAL:HG22	31:h:65:VAL:HG22	1.93	0.50
40:q:44:MET:O	40:q:77:ARG:NH1	2.44	0.50
1:A:200:C:OP1	35:l:60:ARG:NH1	2.45	0.50
1:A:814:U:H5'	46:w:45:ARG:HH22	1.76	0.50
1:A:1830:G:H5''	34:k:92:LYS:HD2	1.93	0.50
7:W:205:VAL:HB	7:W:235:VAL:HG22	1.93	0.50
18:M:32:ARG:NH1	18:M:120:ILE:O	2.45	0.50
11:F:82:THR:HG23	11:F:84:ARG:H	1.75	0.50
17:Z:52:LEU:HD12	17:Z:152:LEU:HB3	1.94	0.50
1:A:2537:U:N3	1:A:2543:U:O4	2.44	0.50
1:A:2712:U:O2'	1:A:2743:A:O2'	2.29	0.50
1:A:3344:A:H2	1:A:3361:G:H21	1.57	0.50
34:k:103:TYR:HB3	34:k:135:ILE:HD11	1.93	0.50
1:A:289:A:O2'	24:a:93:LYS:O	2.29	0.50
1:A:665:A:OP1	24:a:203:ARG:NH1	2.44	0.50
1:A:1808:G:OP2	36:m:133:LYS:NZ	2.44	0.50
8:V:56:SER:H	8:V:87:ARG:HH12	1.59	0.50
9:D:92:LYS:HE3	9:D:93:LYS:HE2	1.94	0.50
11:F:187:LEU:HD11	11:F:193:LYS:HD3	1.93	0.50
20:O:15:VAL:HG23	20:O:35:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:A:H4'	34:k:39:LYS:HE3	1.92	0.50
1:A:2894:C:HO2'	1:A:3107:U:HO2'	1.59	0.50
8:V:94:LYS:NZ	8:V:97:LEU:HD22	2.19	0.50
18:M:49:LYS:HB3	18:M:62:ASN:HA	1.94	0.50
1:A:664:U:H5'	11:F:107:ARG:HA	1.93	0.50
1:A:1364:C:OP1	14:I:110:ARG:NH2	2.45	0.50
1:A:1580:A:OP2	1:A:2522:G:N2	2.45	0.50
5:X:116:LEU:HD22	5:X:140:GLN:HB3	1.92	0.50
1:A:405:U:O2'	1:A:1395:G:N2	2.44	0.50
1:A:1431:G:OP2	37:n:12:ARG:NH1	2.42	0.50
1:A:1899:G:O2'	1:A:2334:U:O4	2.29	0.50
4:Y:276:SER:HB3	4:Y:326:CYS:HA	1.93	0.50
7:W:181:PHE:HA	7:W:392:VAL:HG13	1.94	0.50
8:V:63:ARG:HD3	8:V:71:TRP:HB3	1.94	0.49
13:H:31:ARG:NH2	42:s:105:SER:O	2.45	0.49
24:a:42:PRO:HG3	24:a:61:ILE:HG13	1.93	0.49
1:A:3129:A:N6	1:A:3131:U:O2	2.45	0.49
8:V:95:VAL:CB	8:V:120:GLY:C	2.84	0.49
10:E:305:ILE:HD11	10:E:317:ILE:HG21	1.94	0.49
1:A:1126:G:OP2	17:Z:14:ASN:ND2	2.45	0.49
8:V:45:ILE:HG13	8:V:47:GLN:H	1.76	0.49
7:W:161:GLU:HG3	7:W:165:LYS:HE3	1.94	0.49
7:W:403:LEU:HB3	7:W:409:LEU:HD23	1.95	0.49
1:A:2457:G:H22	1:A:2487:U:H3	1.61	0.49
8:V:89:LEU:C	8:V:89:LEU:CD1	2.86	0.49
3:C:83:C:H1'	3:C:85:G:H21	1.77	0.49
7:W:318:LEU:HD13	7:W:320:LYS:HB2	1.95	0.49
7:W:336:LEU:HD13	7:W:384:MET:HB2	1.95	0.49
7:W:357:VAL:HA	7:W:379:LEU:HD22	1.95	0.49
7:W:203:GLN:HB2	7:W:233:LEU:HD23	1.94	0.49
8:V:49:ILE:CG2	8:V:90:LYS:CG	2.90	0.49
1:A:2196:C:H2'	1:A:2242:A:H61	1.77	0.49
15:J:26:LEU:HD11	36:m:123:GLN:HA	1.93	0.49
27:d:175:ALA:HB2	37:n:56:VAL:HG13	1.94	0.49
39:p:25:LEU:O	39:p:29:SER:OG	2.29	0.49
1:A:383:G:N2	1:A:386:A:OP2	2.43	0.49
1:A:1242:G:N2	1:A:1242:G:OP1	2.41	0.49
1:A:2688:U:OP1	12:G:12:TYR:OH	2.29	0.49
22:R:73:THR:HG23	22:R:76:ALA:H	1.78	0.49
1:A:348:A:N3	1:A:352:A:O2'	2.45	0.48
13:H:80:ASN:HB3	13:H:83:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:t:11:ASN:O	43:t:18:ASN:ND2	2.39	0.48
1:A:1863:G:N1	1:A:1866:C:OP2	2.46	0.48
1:A:1381:A:OP1	11:F:197:ARG:NH2	2.46	0.48
45:v:34:SER:HG	45:v:37:THR:H	1.57	0.48
1:A:1196:C:OP1	1:A:1309:U:O2'	2.29	0.48
1:A:1232:C:H2'	1:A:1233:G:H8	1.78	0.48
8:V:81:LEU:HD23	8:V:102:PHE:HD1	1.78	0.48
24:a:112:ASN:OD1	24:a:112:ASN:N	2.46	0.48
1:A:1489:A:OP2	1:A:1838:G:N1	2.37	0.48
1:A:526:C:N3	1:A:527:A:N6	2.60	0.48
1:A:3085:G:OP1	33:j:34:SER:OG	2.30	0.48
8:V:88:ARG:HH12	8:V:116:LEU:CD1	2.26	0.48
10:E:41:VAL:HG22	10:E:185:GLY:HA3	1.95	0.48
42:s:52:VAL:HG22	42:s:66:VAL:HG22	1.96	0.48
1:A:1127:G:N2	1:A:1130:A:OP2	2.40	0.48
11:F:3:ARG:HH12	11:F:24:ALA:HA	1.78	0.48
20:O:68:LEU:HD22	20:O:90:VAL:HG23	1.96	0.48
27:d:122:ILE:HG23	27:d:126:GLN:HB2	1.96	0.48
1:A:1385:C:OP1	11:F:141:ARG:NH1	2.37	0.48
1:A:1705:U:O2	1:A:1786:G:O2'	2.31	0.48
8:V:94:LYS:HE3	8:V:97:LEU:HD11	1.94	0.48
13:H:54:TYR:HA	13:H:65:ILE:HG22	1.94	0.48
3:C:41:A:N6	3:C:103:G:O2'	2.43	0.48
1:A:1235:U:H4'	1:A:1236:G:H5'	1.96	0.48
1:A:2964:G:N2	1:A:2967:A:OP2	2.47	0.48
1:A:2987:A:H5''	25:b:68:ARG:HH12	1.77	0.48
8:V:95:VAL:CB	8:V:120:GLY:O	2.62	0.48
16:K:90:MET:HG2	16:K:181:VAL:HA	1.96	0.48
20:O:37:GLU:OE2	20:O:74:ARG:NH2	2.46	0.48
37:n:71:PRO:HG2	37:n:109:TYR:HA	1.96	0.48
1:A:1720:U:OP1	28:e:110:ARG:NH1	2.47	0.47
1:A:3268:A:OP1	13:H:46:ARG:NH1	2.39	0.47
11:F:40:THR:O	11:F:44:LYS:NZ	2.41	0.47
15:J:62:LYS:HD3	24:a:29:GLU:HG3	1.96	0.47
27:d:71:LEU:HD13	27:d:99:THR:HG21	1.96	0.47
32:i:108:GLU:HA	32:i:128:ARG:HG3	1.96	0.47
34:k:50:ALA:HB1	44:u:66:VAL:HG11	1.94	0.47
1:A:634:C:H4'	41:r:47:ARG:HH12	1.78	0.47
1:A:2193:U:H5''	1:A:2194:G:H5'	1.96	0.47
9:D:180:LEU:HD11	22:R:26:VAL:HG21	1.96	0.47
21:Q:38:GLN:HA	21:Q:41:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:123:LEU:HD22	25:b:190:VAL:HG23	1.94	0.47
26:c:64:ASN:O	26:c:80:LYS:NZ	2.43	0.47
45:v:57:LEU:HD12	45:v:90:MET:HG3	1.95	0.47
7:W:170:GLN:HA	7:W:176:LEU:HD21	1.96	0.47
12:G:164:LYS:HB2	12:G:180:PHE:HE1	1.79	0.47
1:A:944:C:O2'	41:r:33:ARG:NH1	2.48	0.47
1:A:2446:U:O4	1:A:2447:A:N6	2.47	0.47
1:A:1264:G:N2	1:A:1265:U:O4	2.41	0.47
1:A:1293:U:O4	1:A:1294:A:N6	2.48	0.47
1:A:1635:G:N2	1:A:1638:A:OP2	2.39	0.47
1:A:3022:G:O2'	1:A:3031:G:O6	2.27	0.47
12:G:36:LEU:HB3	12:G:50:ARG:HD3	1.96	0.47
1:A:2415:C:OP1	9:D:2:GLY:N	2.48	0.47
3:C:75:G:OP2	35:l:74:TYR:OH	2.32	0.47
11:F:264:SER:OG	11:F:265:GLU:N	2.48	0.47
11:F:334:PHE:HA	11:F:339:LEU:HD12	1.96	0.47
35:l:56:VAL:HG11	35:l:104:LEU:HD13	1.97	0.47
8:V:186:ASP:OD2	8:V:206:HIS:ND1	2.48	0.47
17:Z:39:LYS:HA	17:Z:86:HIS:CD2	2.50	0.47
8:V:49:ILE:CG2	8:V:90:LYS:HD2	2.43	0.46
1:A:1565:G:N2	1:A:1575:A:N3	2.63	0.46
5:X:206:THR:OG1	5:X:207:GLY:N	2.48	0.46
1:A:89:A:N7	27:d:171:LYS:NZ	2.63	0.46
1:A:339:C:OP1	1:A:1380:G:O2'	2.33	0.46
1:A:3182:G:OP1	25:b:117:ARG:NH2	2.49	0.46
1:A:3268:A:H1'	13:H:75:PRO:HG3	1.97	0.46
9:D:36:GLU:OE1	9:D:163:ARG:NH1	2.48	0.46
28:e:148:ASP:OD1	28:e:151:ARG:NH2	2.43	0.46
1:A:591:G:O2'	13:H:17:ALA:O	2.32	0.46
1:A:1682:U:O4	31:h:90:ARG:NH1	2.48	0.46
1:A:1747:G:H21	47:x:2:ALA:HB1	1.81	0.46
1:A:2467:G:H21	1:A:2488:A:H62	1.64	0.46
1:A:2666:C:OP2	1:A:2687:G:N1	2.43	0.46
8:V:156:ARG:HA	8:V:241:LYS:HG3	1.98	0.46
26:c:50:GLN:HB3	26:c:55:GLN:HB2	1.98	0.46
1:A:289:A:H2'	1:A:290:G:H8	1.79	0.46
1:A:2415:C:H5'	9:D:207:VAL:HG12	1.98	0.46
11:F:302:ALA:HA	27:d:39:ARG:HH12	1.81	0.46
1:A:1807:G:H5''	36:m:135:ARG:HH22	1.81	0.46
4:Y:316:GLY:H	4:Y:335:HIS:CE1	2.33	0.46
8:V:49:ILE:CB	8:V:90:LYS:CG	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:325:SER:HA	8:V:336:ALA:HA	1.98	0.46
13:H:146:ILE:HD13	13:H:149:ILE:HD12	1.97	0.46
16:K:20:ILE:HG12	16:K:25:VAL:HG22	1.97	0.46
17:Z:182:LEU:HD22	17:Z:185:ARG:HH11	1.81	0.46
19:N:106:GLN:HB3	45:v:18:THR:HG23	1.98	0.46
37:n:100:PRO:HG2	37:n:123:VAL:HG12	1.98	0.46
8:V:108:HIS:O	8:V:110:ARG:NH2	2.49	0.46
5:X:99:GLU:OE2	5:X:125:THR:OG1	2.23	0.45
8:V:117:THR:HG22	8:V:119:GLN:HB2	1.97	0.45
36:m:57:HIS:HB3	36:m:61:LYS:HB2	1.99	0.45
49:z:98:LYS:HD3	49:z:118:THR:HG21	1.98	0.45
1:A:2899:C:O2'	1:A:2901:G:OP2	2.31	0.45
7:W:454:ILE:H	7:W:454:ILE:HG13	1.56	0.45
11:F:206:LEU:HD11	11:F:237:GLN:HG2	1.98	0.45
1:A:148:G:OP2	24:a:4:TYR:OH	2.23	0.45
1:A:1392:G:O2'	1:A:1417:G:N1	2.41	0.45
1:A:2950:G:OP2	1:A:2950:G:N2	2.42	0.45
2:B:87:G:H1	2:B:94:C:H42	1.64	0.45
18:M:81:GLU:OE2	18:M:89:TYR:OH	2.33	0.45
1:A:2899:C:N3	16:K:173:ARG:NH1	2.60	0.45
1:A:3041:U:OP1	32:i:12:ARG:NH1	2.47	0.45
11:F:7:THR:OG1	11:F:147:GLU:OE2	2.31	0.45
12:G:200:PHE:HB3	12:G:237:GLU:HG3	1.99	0.45
31:h:89:LEU:HB3	31:h:93:ILE:HD12	1.98	0.45
1:A:173:G:N1	1:A:246:U:O2	2.50	0.45
1:A:1477:A:OP1	1:A:3075:G:O2'	2.33	0.45
1:A:3069:G:O2'	28:e:61:SER:OG	2.33	0.45
9:D:243:THR:OG1	9:D:244:GLY:N	2.49	0.45
26:c:107:LEU:HD23	26:c:152:GLU:HG3	1.98	0.45
43:t:66:SER:OG	43:t:67:LYS:N	2.50	0.45
1:A:1013:G:O6	1:A:1036:A:N6	2.50	0.45
1:A:3119:U:H4'	49:z:104:PRO:HG2	1.98	0.45
10:E:188:ILE:HG22	10:E:191:LYS:HD2	1.97	0.45
1:A:800:G:O6	11:F:104:LYS:NZ	2.39	0.45
1:A:1677:G:H21	1:A:1755:C:HO2'	1.62	0.45
3:C:21:C:OP1	11:F:193:LYS:NZ	2.39	0.45
3:C:29:U:H5''	19:N:27:ASP:HB3	1.99	0.45
16:K:90:MET:HE2	16:K:179:ILE:HG22	1.99	0.45
17:Z:170:LYS:HD3	17:Z:175:ASN:HA	1.97	0.45
28:e:99:LEU:HD11	28:e:103:ARG:HH21	1.81	0.45
42:s:14:LEU:HD11	42:s:31:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:v:70:ARG:O	45:v:74:LYS:N	2.50	0.45
1:A:89:A:OP1	27:d:170:ARG:NH2	2.50	0.45
4:Y:232:CYS:HA	4:Y:341:VAL:HG23	1.99	0.45
12:G:163:LEU:HD21	12:G:175:HIS:CG	2.52	0.45
26:c:56:ARG:NH1	26:c:75:GLU:OE2	2.48	0.45
43:t:41:ARG:HG2	43:t:56:THR:HG21	1.98	0.45
49:z:78:ILE:HG21	49:z:83:LYS:HE3	1.98	0.45
1:A:68:C:N4	1:A:314:U:O2'	2.50	0.45
1:A:351:A:N6	48:y:37:TYR:O	2.44	0.45
1:A:591:G:N2	1:A:612:U:OP1	2.38	0.45
1:A:2117:A:O2'	1:A:3080:G:O2'	2.29	0.45
8:V:50:PRO:HD2	8:V:90:LYS:HG2	1.99	0.45
17:Z:3:ARG:NH2	17:Z:63:GLU:OE2	2.50	0.45
34:k:105:VAL:HG21	34:k:135:ILE:HD12	1.97	0.45
1:A:1243:G:N2	1:A:1270:A:O2'	2.40	0.45
1:A:2307:G:O2'	1:A:2310:U:OP2	2.35	0.45
1:A:2991:A:O2'	1:A:3309:G:N7	2.50	0.45
4:Y:258:GLY:O	4:Y:276:SER:OG	2.32	0.45
6:L:109:ILE:O	6:L:113:UNK:N	2.50	0.45
15:J:133:LYS:HD3	15:J:138:HIS:HE1	1.82	0.45
19:N:9:ILE:HD11	37:n:45:MET:HE1	1.97	0.45
30:g:14:MET:HE1	30:g:55:LYS:HB2	1.99	0.45
1:A:2768:U:O2'	21:Q:82:GLN:NE2	2.50	0.44
19:N:52:ASP:OD1	19:N:52:ASP:N	2.51	0.44
21:Q:2:VAL:N	21:Q:90:HIS:O	2.50	0.44
32:i:102:ILE:H	32:i:102:ILE:HG13	1.58	0.44
36:m:54:THR:OG1	36:m:55:LYS:N	2.49	0.44
1:A:845:G:O2'	1:A:847:A:N7	2.35	0.44
7:W:246:ARG:HB2	7:W:312:GLN:HE21	1.83	0.44
8:V:88:ARG:HH12	8:V:116:LEU:HD11	1.82	0.44
1:A:240:U:H4'	1:A:241:G:H5'	2.00	0.44
1:A:824:C:H5''	9:D:21:ARG:HD3	1.99	0.44
1:A:2712:U:HO2'	1:A:2743:A:HO2'	1.58	0.44
7:W:139:ARG:NH1	7:W:196:GLU:OE1	2.42	0.44
1:A:309:U:OP1	45:v:84:LYS:NZ	2.47	0.44
1:A:2424:A:H61	9:D:230:VAL:HG11	1.81	0.44
8:V:79:ARG:HD3	8:V:82:LEU:HD22	1.99	0.44
12:G:148:ILE:HG12	12:G:151:GLN:HB3	2.00	0.44
18:M:18:VAL:HG22	18:M:70:THR:HG22	2.00	0.44
39:p:57:GLU:OE2	39:p:69:TYR:OH	2.28	0.44
1:A:638:C:N4	1:A:639:G:O6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:G:OP1	43:t:58:ARG:NH2	2.51	0.44
1:A:2631:U:OP2	30:g:4:SER:OG	2.34	0.44
37:n:126:LYS:HG2	37:n:146:GLU:HB2	1.99	0.44
1:A:69:C:O2'	1:A:101:G:O2'	2.36	0.44
1:A:1624:G:O2'	1:A:1643:A:N1	2.49	0.44
1:A:2895:G:O2'	49:z:100:TYR:O	2.26	0.44
1:A:3166:C:H42	1:A:3284:G:H1	1.65	0.44
4:Y:225:SER:OG	4:Y:226:LYS:N	2.50	0.44
1:A:2249:G:N2	1:A:2268:U:O2	2.51	0.44
7:W:246:ARG:HA	7:W:249:TRP:HB2	2.00	0.44
9:D:80:GLU:HG3	22:R:66:GLY:HA2	2.00	0.44
15:J:140:VAL:HG22	15:J:166:LEU:HD21	1.99	0.44
2:B:7:G:OP1	12:G:33:ARG:NH1	2.50	0.44
3:C:83:C:N3	35:l:52:ARG:NH2	2.66	0.44
7:W:236:ASN:HB3	7:W:263:TYR:CZ	2.53	0.44
30:g:17:ARG:HG2	30:g:22:HIS:HA	1.98	0.44
1:A:1765:U:H5'	28:e:43:LYS:HZ3	1.83	0.43
13:H:52:VAL:HG11	13:H:65:ILE:HD13	1.99	0.43
37:n:94:ALA:HB2	37:n:121:VAL:HG22	2.00	0.43
1:A:1062:A:H5''	1:A:1063:G:H5'	2.00	0.43
7:W:207:ALA:HA	7:W:210:PRO:HG3	2.00	0.43
18:M:109:HIS:CD2	18:M:123:PHE:H	2.31	0.43
36:m:24:VAL:HG11	36:m:87:LEU:HD23	2.00	0.43
7:W:411:ILE:HA	7:W:414:LEU:HD23	1.99	0.43
40:q:10:ARG:HG3	40:q:108:VAL:HA	2.00	0.43
44:u:13:SER:OG	44:u:14:LYS:N	2.51	0.43
1:A:371:G:N1	1:A:374:A:OP2	2.45	0.43
1:A:1597:C:H5'	1:A:1696:A:H1'	2.01	0.43
1:A:1873:U:OP1	28:e:21:LYS:NZ	2.49	0.43
1:A:3261:C:OP1	20:O:126:GLN:NE2	2.42	0.43
2:B:44:C:H2'	2:B:45:A:H8	1.84	0.43
8:V:94:LYS:CE	8:V:97:LEU:HD11	2.48	0.43
8:V:326:THR:HG21	8:V:356:ARG:HH22	1.83	0.43
11:F:3:ARG:HH22	11:F:24:ALA:HB2	1.83	0.43
18:M:97:SER:OG	18:M:101:ASN:N	2.45	0.43
20:O:20:VAL:O	20:O:66:THR:OG1	2.30	0.43
1:A:2483:G:H21	1:A:2485:A:H8	1.66	0.43
4:Y:292:GLN:HE21	4:Y:296:GLN:HG2	1.83	0.43
10:E:56:ILE:HD11	10:E:356:LEU:HD13	2.00	0.43
45:v:74:LYS:HD2	45:v:80:PHE:HD1	1.84	0.43
1:A:1447:G:N7	26:c:25:SER:OG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3121:U:H1'	1:A:3122:A:H5''	1.99	0.43
43:t:29:ILE:HD11	43:t:31:ARG:HH21	1.82	0.43
1:A:3183:A:H2'	1:A:3184:A:H8	1.84	0.43
10:E:317:ILE:O	10:E:319:ASN:N	2.51	0.43
18:M:17:LEU:HD13	18:M:129:VAL:HG22	1.99	0.43
10:E:140:ASP:OD1	10:E:140:ASP:N	2.51	0.43
30:g:88:ARG:NH2	38:o:33:LYS:O	2.52	0.43
46:w:19:CYS:SG	46:w:20:ASN:N	2.92	0.43
1:A:1783:U:H2'	1:A:1784:G:C8	2.54	0.42
8:V:192:GLU:HA	8:V:197:LEU:HA	2.01	0.42
17:Z:76:MET:HE3	17:Z:148:VAL:HG22	2.00	0.42
1:A:576:C:OP1	14:I:241:LYS:NZ	2.36	0.42
2:B:96:U:OP1	29:f:43:TYR:OH	2.31	0.42
30:g:79:MET:HB3	30:g:84:TYR:CE1	2.54	0.42
31:h:15:PHE:HB2	31:h:65:VAL:HB	2.01	0.42
36:m:46:ILE:HA	36:m:70:PRO:HA	2.00	0.42
1:A:2329:C:H4'	7:W:473:GLN:HG2	2.02	0.42
8:V:321:LEU:HD12	8:V:339:THR:HG22	2.01	0.42
1:A:2290:C:H1'	7:W:413:GLN:HE22	1.84	0.42
1:A:3243:A:H4'	10:E:95:THR:HG22	2.02	0.42
11:F:64:SER:HA	11:F:75:PRO:HA	2.02	0.42
1:A:58:G:H4'	24:a:155:VAL:HG12	2.01	0.42
1:A:882:A:OP1	1:A:1847:A:N6	2.40	0.42
1:A:1616:U:O2	1:A:1829:G:N2	2.51	0.42
1:A:2168:A:N6	1:A:2170:U:O2	2.52	0.42
17:Z:85:PHE:HA	17:Z:140:THR:HG22	2.00	0.42
1:A:664:U:O2	1:A:799:G:N2	2.52	0.42
1:A:797:U:H2'	1:A:798:G:H8	1.84	0.42
1:A:989:A:O2'	30:g:104:GLU:OE1	2.38	0.42
1:A:2157:G:H4'	1:A:2158:A:H5'	2.00	0.42
1:A:2786:G:N2	37:n:58:MET:SD	2.81	0.42
30:g:51:GLY:HA3	30:g:92:ARG:HG3	2.01	0.42
1:A:1306:G:N2	1:A:1307:G:N7	2.62	0.42
1:A:1638:A:H5'	36:m:15:ARG:HD3	2.01	0.42
1:A:2149:A:N6	1:A:2187:G:O2'	2.47	0.42
1:A:2947:G:N2	1:A:2948:C:O2	2.53	0.42
8:V:359:LEU:HD22	8:V:362:ILE:HD11	2.00	0.42
20:O:55:ARG:HH12	20:O:77:ARG:HA	1.83	0.42
2:B:28:C:OP1	18:M:137:ARG:NH1	2.51	0.42
8:V:279:ILE:HD12	8:V:279:ILE:HA	1.89	0.42
9:D:134:VAL:HG12	9:D:150:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:262:TRP:HB3	11:F:276:LEU:HD11	2.02	0.42
7:W:428:ILE:HD11	7:W:496:LEU:HB3	2.02	0.42
1:A:2252:A:H61	1:A:2264:U:H3	1.68	0.41
2:B:38:U:N3	2:B:41:G:OP2	2.52	0.41
5:X:62:MET:HE3	5:X:73:PRO:HG3	2.01	0.41
8:V:49:ILE:HA	8:V:90:LYS:CD	2.23	0.41
8:V:345:ASP:HA	8:V:348:VAL:HG12	2.02	0.41
10:E:43:LEU:HD23	10:E:181:ILE:HG21	2.02	0.41
11:F:110:ASN:HD22	24:a:201:ARG:HB3	1.85	0.41
16:K:92:TYR:HB2	16:K:142:ASP:HB3	2.00	0.41
1:A:1578:C:O2'	1:A:1649:U:OP1	2.38	0.41
1:A:2844:C:N3	4:Y:269:ARG:NH2	2.67	0.41
2:B:119:U:O5'	12:G:258:LYS:NZ	2.53	0.41
1:A:1404:G:N2	1:A:1407:A:OP2	2.47	0.41
7:W:190:GLN:HE21	7:W:374:PHE:HB3	1.84	0.41
8:V:25:PRO:HB2	8:V:26:ILE:HD12	2.02	0.41
12:G:38:THR:HG22	30:g:30:TYR:HB3	2.02	0.41
19:N:102:GLN:HB2	19:N:104:ARG:HH11	1.85	0.41
25:b:26:GLN:HB2	25:b:33:ILE:HD11	2.02	0.41
30:g:68:THR:OG1	30:g:69:LYS:N	2.50	0.41
34:k:96:LYS:HE3	34:k:96:LYS:HB2	1.90	0.41
1:A:1236:G:N2	1:A:1244:A:OP1	2.45	0.41
5:X:15:VAL:HA	5:X:61:ARG:HG2	2.01	0.41
7:W:427:ARG:O	7:W:428:ILE:HG13	2.20	0.41
7:W:465:ALA:HB2	7:W:483:ALA:HB2	2.02	0.41
1:A:3259:U:H5''	1:A:3261:C:H5	1.84	0.41
5:X:97:VAL:HG12	5:X:99:GLU:HG2	2.01	0.41
7:W:403:LEU:HD22	7:W:408:VAL:HG11	2.02	0.41
5:X:151:TYR:HE1	5:X:192:VAL:HG22	1.85	0.41
6:L:28:UNK:O	6:L:29:UNK:C	2.68	0.41
10:E:86:VAL:HG22	10:E:162:VAL:HG12	2.02	0.41
12:G:30:TYR:HD1	12:G:30:TYR:HA	1.78	0.41
1:A:577:C:O2'	1:A:579:G:OP1	2.37	0.41
8:V:380:ASN:O	21:Q:61:LYS:NZ	2.41	0.41
1:A:1794:G:H4'	9:D:191:LEU:HD12	2.03	0.41
27:d:152:HIS:ND1	27:d:162:ALA:O	2.45	0.41
39:p:27:TYR:O	39:p:30:THR:OG1	2.35	0.41
1:A:353:G:O6	46:w:52:LYS:NZ	2.42	0.41
1:A:1184:A:H5''	20:O:59:ASN:HD22	1.86	0.41
8:V:81:LEU:HD22	8:V:114:ILE:HD11	2.02	0.41
8:V:143:CYS:O	8:V:146:CYS:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:67:PHE:HD1	10:E:70:ARG:HG2	1.84	0.41
23:S:112:UNK:O	23:S:116:UNK:N	2.54	0.41
1:A:267:G:H21	24:a:50:ARG:HB2	1.86	0.41
1:A:1388:U:O2'	41:r:99:ASN:O	2.34	0.41
1:A:2940:A:OP2	10:E:2:SER:N	2.55	0.41
7:W:338:ASN:HB3	7:W:384:MET:HE2	2.03	0.41
10:E:223:GLY:HA2	10:E:271:GLY:HA3	2.03	0.41
11:F:150:LEU:HD21	11:F:172:VAL:HG11	2.03	0.41
22:R:42:CYS:HB3	22:R:60:CYS:HB3	1.54	0.41
37:n:19:LYS:HB3	37:n:25:HIS:HB2	2.02	0.41
1:A:1751:G:O6	47:x:44:LYS:NZ	2.36	0.40
1:A:2505:U:O2	1:A:2506:U:N3	2.33	0.40
4:Y:262:LYS:HB3	4:Y:272:ASP:HB2	2.03	0.40
7:W:507:ASP:OD1	7:W:507:ASP:N	2.54	0.40
10:E:215:ILE:HD13	10:E:282:ILE:HD11	2.03	0.40
34:k:67:ILE:HD12	34:k:83:VAL:HG12	2.03	0.40
1:A:1010:G:N2	1:A:1041:U:O2	2.49	0.40
1:A:2174:G:P	9:D:193:ARG:HH11	2.44	0.40
19:N:35:ARG:HH11	19:N:35:ARG:HD2	1.77	0.40
19:N:62:THR:O	19:N:64:LYS:N	2.54	0.40
41:r:3:SER:HB3	41:r:71:HIS:CE1	2.56	0.40
41:r:76:VAL:HG21	41:r:82:LEU:HD23	2.02	0.40
1:A:411:U:H2'	1:A:412:G:C8	2.57	0.40
1:A:1778:G:O2'	1:A:1780:G:OP2	2.32	0.40
43:t:44:CYS:SG	43:t:46:ASP:N	2.87	0.40
1:A:1723:A:OP2	28:e:103:ARG:NH2	2.55	0.40
1:A:3113:A:O2'	16:K:66:ALA:O	2.37	0.40
1:A:3283:U:H2'	1:A:3284:G:H8	1.87	0.40
5:X:88:LEU:HD23	5:X:92:VAL:HG11	2.02	0.40
7:W:200:LEU:HB3	7:W:339:ILE:HG22	2.03	0.40
20:O:38:ILE:HG22	20:O:44:VAL:HG12	2.03	0.40
29:f:90:MET:HE1	29:f:114:HIS:CE1	2.56	0.40
41:r:100:ILE:HB	41:r:105:ARG:HE	1.86	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	
4	Y	126/364 (35%)	99 (79%)	23 (18%)	4 (3%)	3	24
5	X	230/245 (94%)	222 (96%)	8 (4%)	0	100	100
6	L	53/165 (32%)	48 (91%)	5 (9%)	0	100	100
7	W	373/640 (58%)	313 (84%)	53 (14%)	7 (2%)	6	33
8	V	388/518 (75%)	332 (86%)	52 (13%)	4 (1%)	12	44
9	D	244/254 (96%)	227 (93%)	17 (7%)	0	100	100
10	E	382/387 (99%)	357 (94%)	24 (6%)	1 (0%)	36	67
11	F	359/362 (99%)	328 (91%)	28 (8%)	3 (1%)	16	49
12	G	287/297 (97%)	266 (93%)	20 (7%)	1 (0%)	36	67
13	H	151/176 (86%)	144 (95%)	7 (5%)	0	100	100
14	I	218/244 (89%)	204 (94%)	13 (6%)	1 (0%)	24	57
15	J	225/256 (88%)	215 (96%)	9 (4%)	1 (0%)	30	62
16	K	186/191 (97%)	173 (93%)	13 (7%)	0	100	100
17	Z	197/221 (89%)	187 (95%)	10 (5%)	0	100	100
18	M	166/174 (95%)	153 (92%)	13 (8%)	0	100	100
19	N	191/199 (96%)	170 (89%)	20 (10%)	1 (0%)	24	57
20	O	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
21	Q	100/106 (94%)	93 (93%)	7 (7%)	0	100	100
22	R	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
24	a	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
25	b	195/199 (98%)	187 (96%)	8 (4%)	0	100	100
26	c	181/184 (98%)	167 (92%)	14 (8%)	0	100	100
27	d	183/186 (98%)	174 (95%)	9 (5%)	0	100	100
28	e	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
29	f	168/172 (98%)	156 (93%)	10 (6%)	2 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	g	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
31	h	95/121 (78%)	89 (94%)	6 (6%)	0	100	100
32	i	130/137 (95%)	127 (98%)	3 (2%)	0	100	100
33	j	59/155 (38%)	56 (95%)	2 (3%)	1 (2%)	7	35
34	k	119/142 (84%)	110 (92%)	9 (8%)	0	100	100
35	l	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
36	m	133/136 (98%)	119 (90%)	14 (10%)	0	100	100
37	n	146/149 (98%)	129 (88%)	14 (10%)	3 (2%)	5	31
38	o	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	34
39	p	94/105 (90%)	90 (96%)	4 (4%)	0	100	100
40	q	105/113 (93%)	96 (91%)	9 (9%)	0	100	100
41	r	124/130 (95%)	120 (97%)	4 (3%)	0	100	100
42	s	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
43	t	107/121 (88%)	101 (94%)	6 (6%)	0	100	100
44	u	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
45	v	96/100 (96%)	86 (90%)	9 (9%)	1 (1%)	12	44
46	w	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
47	x	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
48	y	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
49	z	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
All	All	7192/8490 (85%)	6643 (92%)	518 (7%)	31 (0%)	31	62

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	135	ILE
8	V	95	VAL
8	V	97	LEU
11	F	339	LEU
12	G	259	LYS
38	o	26	THR
4	Y	247	ALA
4	Y	326	CYS
7	W	442	GLN
15	J	36	ILE

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Mol	Chain	Res	Type
19	N	63	VAL
29	f	13	ARG
37	n	24	LYS
8	V	68	PRO
11	F	5	GLN
14	I	158	LYS
29	f	24	LEU
4	Y	323	ARG
7	W	338	ASN
10	E	347	SER
11	F	4	PRO
37	n	15	VAL
37	n	47	LYS
7	W	241	LEU
7	W	395	ASN
7	W	443	THR
8	V	45	ILE
45	v	34	SER
7	W	337	ILE
33	j	10	GLY
4	Y	246	ILE

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	
4	Y	110/323 (34%)	105 (96%)	5 (4%)	24	50
5	X	186/211 (88%)	185 (100%)	1 (0%)	81	80
6	L	30/65 (46%)	30 (100%)	0	100	100
7	W	317/555 (57%)	314 (99%)	3 (1%)	70	76
8	V	332/467 (71%)	331 (100%)	1 (0%)	86	83
9	D	189/196 (96%)	187 (99%)	2 (1%)	65	74
10	E	317/323 (98%)	315 (99%)	2 (1%)	78	79
11	F	288/289 (100%)	287 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	G	238/245 (97%)	238 (100%)	0	100	100
13	H	131/153 (86%)	131 (100%)	0	100	100
14	I	185/205 (90%)	184 (100%)	1 (0%)	81	80
15	J	182/208 (88%)	182 (100%)	0	100	100
16	K	168/171 (98%)	168 (100%)	0	100	100
17	Z	175/187 (94%)	174 (99%)	1 (1%)	78	79
18	M	146/150 (97%)	146 (100%)	0	100	100
19	N	153/159 (96%)	150 (98%)	3 (2%)	48	67
20	O	107/109 (98%)	106 (99%)	1 (1%)	70	76
21	Q	87/91 (96%)	87 (100%)	0	100	100
22	R	69/72 (96%)	67 (97%)	2 (3%)	37	60
24	a	175/176 (99%)	174 (99%)	1 (1%)	78	79
25	b	160/162 (99%)	160 (100%)	0	100	100
26	c	140/146 (96%)	138 (99%)	2 (1%)	59	71
27	d	150/151 (99%)	149 (99%)	1 (1%)	76	78
28	e	125/154 (81%)	124 (99%)	1 (1%)	73	77
29	f	155/156 (99%)	154 (99%)	1 (1%)	78	79
30	g	136/137 (99%)	136 (100%)	0	100	100
31	h	84/107 (78%)	84 (100%)	0	100	100
32	i	102/105 (97%)	101 (99%)	1 (1%)	68	75
33	j	54/129 (42%)	54 (100%)	0	100	100
34	k	104/118 (88%)	104 (100%)	0	100	100
35	l	108/110 (98%)	108 (100%)	0	100	100
36	m	115/116 (99%)	115 (100%)	0	100	100
37	n	118/119 (99%)	118 (100%)	0	100	100
38	o	46/47 (98%)	46 (100%)	0	100	100
39	p	81/88 (92%)	81 (100%)	0	100	100
40	q	92/97 (95%)	92 (100%)	0	100	100
41	r	108/111 (97%)	108 (100%)	0	100	100
42	s	90/91 (99%)	90 (100%)	0	100	100
43	t	94/103 (91%)	92 (98%)	2 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	u	104/105 (99%)	104 (100%)	0	100	100
45	v	78/82 (95%)	77 (99%)	1 (1%)	61	72
46	w	69/71 (97%)	68 (99%)	1 (1%)	59	71
47	x	67/69 (97%)	67 (100%)	0	100	100
48	y	45/46 (98%)	45 (100%)	0	100	100
49	z	46/116 (40%)	46 (100%)	0	100	100
All	All	6056/7091 (85%)	6022 (99%)	34 (1%)	76	79

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

Mol	Chain	Res	Type
4	Y	235	CYS
4	Y	270	ILE
4	Y	330	VAL
4	Y	331	ILE
4	Y	332	PRO
5	X	142	ILE
7	W	136	VAL
7	W	237	LYS
7	W	454	ILE
8	V	127	ILE
9	D	88	ILE
9	D	101	VAL
10	E	79	VAL
10	E	104	THR
11	F	74	ILE
14	I	92	ILE
17	Z	197	VAL
19	N	54	LEU
19	N	76	THR
19	N	124	ILE
20	O	68	LEU
22	R	16	VAL
22	R	42	CYS
24	a	183	THR
26	c	114	VAL
26	c	119	VAL
27	d	122	ILE
28	e	99	LEU
29	f	24	LEU

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Mol	Chain	Res	Type
32	i	102	ILE
43	t	47	CYS
43	t	95	ILE
45	v	57	LEU
46	w	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
4	Y	274	GLN
4	Y	292	GLN
4	Y	318	ASN
4	Y	335	HIS
4	Y	343	GLN
5	X	156	ASN
5	X	162	HIS
7	W	170	GLN
7	W	231	ASN
7	W	323	ASN
7	W	375	GLN
7	W	406	ASN
7	W	413	GLN
7	W	458	GLN
8	V	11	HIS
8	V	21	ASN
8	V	66	GLN
8	V	153	ASN
8	V	231	GLN
8	V	358	HIS
8	V	364	HIS
9	D	139	HIS
9	D	140	ASN
9	D	209	HIS
9	D	216	HIS
9	D	218	HIS
10	E	224	HIS
10	E	243	HIS
10	E	293	ASN
11	F	9	HIS
11	F	43	ASN
11	F	45	ASN
11	F	110	ASN

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Mol	Chain	Res	Type
11	F	221	ASN
11	F	296	GLN
12	G	264	GLN
13	H	167	ASN
14	I	64	GLN
14	I	93	ASN
14	I	112	ASN
14	I	244	ASN
15	J	24	ASN
15	J	38	GLN
15	J	95	ASN
15	J	243	GLN
16	K	58	HIS
16	K	64	HIS
16	K	125	ASN
17	Z	14	ASN
17	Z	55	ASN
17	Z	86	HIS
17	Z	123	HIS
18	M	109	HIS
19	N	99	HIS
20	O	41	GLN
20	O	62	GLN
21	Q	82	GLN
22	R	25	GLN
24	a	37	HIS
24	a	70	ASN
25	b	55	HIS
25	b	193	GLN
26	c	28	ASN
27	d	5	HIS
29	f	8	GLN
29	f	88	HIS
30	g	22	HIS
30	g	131	GLN
30	g	146	ASN
31	h	87	ASN
32	i	98	ASN
33	j	58	HIS
35	l	110	HIS
36	m	57	HIS
36	m	123	GLN

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Mol	Chain	Res	Type
37	n	14	HIS
37	n	74	ASN
37	n	120	ASN
40	q	17	HIS
40	q	57	GLN
41	r	20	HIS
41	r	49	ASN
41	r	71	HIS
41	r	104	ASN
43	t	83	ASN
44	u	108	GLN
46	w	57	HIS
46	w	76	ASN
47	x	67	GLN
48	y	43	ASN
49	z	90	ASN
49	z	117	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3198/3396 (94%)	642 (20%)	33 (1%)
2	B	120/121 (99%)	16 (13%)	0
3	C	157/158 (99%)	28 (17%)	1 (0%)
All	All	3475/3675 (94%)	686 (19%)	34 (0%)

All (686) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	A
1	A	22	G
1	A	26	A
1	A	40	A
1	A	43	A
1	A	45	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	72	C

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Mol	Chain	Res	Type
1	A	75	G
1	A	76	G
1	A	81	C
1	A	85	A
1	A	92	G
1	A	96	G
1	A	97	U
1	A	109	A
1	A	110	G
1	A	116	A
1	A	117	U
1	A	118	U
1	A	122	A
1	A	135	C
1	A	136	G
1	A	140	C
1	A	148	G
1	A	155	G
1	A	156	G
1	A	157	A
1	A	165	A
1	A	168	U
1	A	170	G
1	A	173	G
1	A	176	G
1	A	182	U
1	A	187	A
1	A	190	U
1	A	191	U
1	A	202	G
1	A	206	G
1	A	210	U
1	A	211	A
1	A	213	A
1	A	217	U
1	A	218	G
1	A	219	A
1	A	240	U
1	A	241	G
1	A	243	G
1	A	247	C
1	A	249	U

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Mol	Chain	Res	Type
1	A	250	U
1	A	251	G
1	A	252	U
1	A	253	A
1	A	257	U
1	A	269	G
1	A	270	U
1	A	286	U
1	A	295	A
1	A	323	A
1	A	329	U
1	A	336	A
1	A	338	A
1	A	339	C
1	A	351	A
1	A	359	U
1	A	375	A
1	A	376	G
1	A	382	U
1	A	385	A
1	A	395	A
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	406	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	439	C
1	A	520	U
1	A	521	A
1	A	532	A
1	A	536	U
1	A	541	U
1	A	543	C
1	A	546	C
1	A	547	G
1	A	548	G
1	A	549	U

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Mol	Chain	Res	Type
1	A	551	A
1	A	552	G
1	A	555	U
1	A	557	A
1	A	559	A
1	A	578	A
1	A	579	G
1	A	592	A
1	A	598	A
1	A	600	G
1	A	604	G
1	A	607	A
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	636	C
1	A	644	G
1	A	649	A
1	A	655	C
1	A	675	C
1	A	677	A
1	A	681	U
1	A	683	U
1	A	689	U
1	A	691	A
1	A	692	A
1	A	705	A
1	A	706	A
1	A	709	A
1	A	712	G
1	A	715	A
1	A	720	A
1	A	725	G
1	A	764	U
1	A	765	C
1	A	766	U
1	A	767	U
1	A	771	A
1	A	776	U
1	A	777	U
1	A	780	A

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Mol	Chain	Res	Type
1	A	781	G
1	A	785	G
1	A	799	G
1	A	801	A
1	A	806	A
1	A	817	A
1	A	823	C
1	A	830	A
1	A	848	A
1	A	849	C
1	A	861	C
1	A	869	G
1	A	874	U
1	A	879	U
1	A	880	G
1	A	888	A
1	A	890	C
1	A	895	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	924	G
1	A	932	U
1	A	933	A
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	961	C
1	A	978	G
1	A	979	U
1	A	980	A
1	A	981	U
1	A	982	C
1	A	991	G
1	A	994	G
1	A	995	U
1	A	1001	G
1	A	1002	A

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Mol	Chain	Res	Type
1	A	1010	G
1	A	1015	U
1	A	1017	C
1	A	1024	G
1	A	1029	G
1	A	1036	A
1	A	1037	C
1	A	1047	A
1	A	1049	C
1	A	1057	A
1	A	1063	G
1	A	1064	A
1	A	1065	A
1	A	1066	G
1	A	1072	G
1	A	1081	U
1	A	1087	G
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1117	G
1	A	1124	U
1	A	1131	G
1	A	1144	U
1	A	1153	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1190	A
1	A	1192	C
1	A	1193	A
1	A	1196	C
1	A	1201	C
1	A	1209	G
1	A	1212	A
1	A	1222	G
1	A	1223	A

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Mol	Chain	Res	Type
1	A	1229	G
1	A	1235	U
1	A	1236	G
1	A	1238	C
1	A	1239	C
1	A	1241	U
1	A	1242	G
1	A	1244	A
1	A	1245	A
1	A	1246	G
1	A	1248	C
1	A	1258	U
1	A	1262	G
1	A	1263	A
1	A	1265	U
1	A	1268	G
1	A	1285	G
1	A	1307	G
1	A	1309	U
1	A	1313	G
1	A	1316	C
1	A	1317	A
1	A	1330	A
1	A	1345	G
1	A	1349	G
1	A	1350	A
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1418	A
1	A	1419	A
1	A	1430	U
1	A	1434	G
1	A	1437	C
1	A	1446	A

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Mol	Chain	Res	Type
1	A	1450	G
1	A	1455	U
1	A	1466	G
1	A	1475	A
1	A	1481	A
1	A	1484	U
1	A	1496	C
1	A	1503	A
1	A	1508	C
1	A	1523	U
1	A	1546	A
1	A	1555	U
1	A	1556	C
1	A	1557	A
1	A	1560	G
1	A	1561	G
1	A	1562	C
1	A	1563	C
1	A	1564	U
1	A	1566	A
1	A	1567	U
1	A	1568	U
1	A	1569	U
1	A	1570	U
1	A	1572	U
1	A	1573	G
1	A	1575	A
1	A	1576	G
1	A	1577	G
1	A	1579	C
1	A	1580	A
1	A	1582	C
1	A	1583	A
1	A	1587	A
1	A	1589	A
1	A	1593	A
1	A	1603	A
1	A	1605	A
1	A	1618	G
1	A	1619	A
1	A	1621	A
1	A	1629	U

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Mol	Chain	Res	Type
1	A	1642	A
1	A	1643	A
1	A	1645	U
1	A	1657	C
1	A	1662	G
1	A	1677	G
1	A	1683	A
1	A	1716	U
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1735	G
1	A	1741	A
1	A	1742	U
1	A	1743	G
1	A	1749	A
1	A	1750	A
1	A	1751	G
1	A	1759	C
1	A	1760	A
1	A	1762	C
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1780	G
1	A	1790	G
1	A	1792	C
1	A	1797	A
1	A	1814	A
1	A	1816	A
1	A	1817	G
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1842	A
1	A	1849	C
1	A	1850	A
1	A	1866	C
1	A	1867	A
1	A	1880	U
1	A	1893	A
1	A	1904	C

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Mol	Chain	Res	Type
1	A	1906	G
1	A	1908	A
1	A	1918	C
1	A	1930	A
1	A	1952	G
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2113	A
1	A	2121	G
1	A	2122	G
1	A	2131	A
1	A	2139	A
1	A	2158	A
1	A	2169	G
1	A	2175	U
1	A	2184	U
1	A	2185	G
1	A	2187	G
1	A	2188	A
1	A	2192	C
1	A	2205	U
1	A	2209	U
1	A	2210	G
1	A	2244	A
1	A	2249	G
1	A	2250	G
1	A	2253	G
1	A	2254	U
1	A	2255	A
1	A	2256	A
1	A	2260	U
1	A	2261	G
1	A	2262	A
1	A	2265	C
1	A	2267	C
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2273	G
1	A	2281	A

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Mol	Chain	Res	Type
1	A	2282	U
1	A	2288	G
1	A	2298	U
1	A	2306	C
1	A	2307	G
1	A	2308	C
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2317	A
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2372	A
1	A	2374	C
1	A	2375	G
1	A	2376	G
1	A	2385	G
1	A	2388	U
1	A	2393	G
1	A	2397	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2415	C
1	A	2435	G
1	A	2437	G
1	A	2440	G
1	A	2450	G
1	A	2451	G
1	A	2452	G
1	A	2453	U
1	A	2454	G
1	A	2457	G
1	A	2458	A
1	A	2459	A
1	A	2461	A
1	A	2462	A
1	A	2463	G
1	A	2465	G

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Mol	Chain	Res	Type
1	A	2468	A
1	A	2472	U
1	A	2474	G
1	A	2476	C
1	A	2477	G
1	A	2485	A
1	A	2488	A
1	A	2490	C
1	A	2495	C
1	A	2496	C
1	A	2497	U
1	A	2498	U
1	A	2499	U
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2506	U
1	A	2508	U
1	A	2509	U
1	A	2514	U
1	A	2515	A
1	A	2531	C
1	A	2533	G
1	A	2537	U
1	A	2538	U
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2549	G
1	A	2550	U
1	A	2552	C
1	A	2554	A
1	A	2561	A
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2576	G
1	A	2577	C

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Mol	Chain	Res	Type
1	A	2580	A
1	A	2582	C
1	A	2585	G
1	A	2593	A
1	A	2594	C
1	A	2600	C
1	A	2602	G
1	A	2606	G
1	A	2607	G
1	A	2611	U
1	A	2614	G
1	A	2628	A
1	A	2629	U
1	A	2648	G
1	A	2652	U
1	A	2656	A
1	A	2657	A
1	A	2663	G
1	A	2674	A
1	A	2677	G
1	A	2689	A
1	A	2691	A
1	A	2694	A
1	A	2696	A
1	A	2703	A
1	A	2704	A
1	A	2705	A
1	A	2713	U
1	A	2714	G
1	A	2719	U
1	A	2728	G
1	A	2729	U
1	A	2742	C
1	A	2753	G
1	A	2755	C
1	A	2777	G
1	A	2778	G
1	A	2796	G
1	A	2797	C
1	A	2799	A
1	A	2800	G
1	A	2801	A

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Mol	Chain	Res	Type
1	A	2803	A
1	A	2804	A
1	A	2810	C
1	A	2814	G
1	A	2817	A
1	A	2842	U
1	A	2845	A
1	A	2847	A
1	A	2850	G
1	A	2853	A
1	A	2860	U
1	A	2867	C
1	A	2869	U
1	A	2871	G
1	A	2872	A
1	A	2875	U
1	A	2887	A
1	A	2898	G
1	A	2904	U
1	A	2914	G
1	A	2923	U
1	A	2928	C
1	A	2933	A
1	A	2935	U
1	A	2936	A
1	A	2941	A
1	A	2951	G
1	A	2955	U
1	A	2971	A
1	A	2983	C
1	A	2996	U
1	A	2997	G
1	A	3011	A
1	A	3012	A
1	A	3014	U
1	A	3021	A
1	A	3022	G
1	A	3028	G
1	A	3059	G
1	A	3078	U
1	A	3080	G
1	A	3086	A

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Mol	Chain	Res	Type
1	A	3092	C
1	A	3113	A
1	A	3115	C
1	A	3119	U
1	A	3122	A
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3153	U
1	A	3154	C
1	A	3156	U
1	A	3157	U
1	A	3165	A
1	A	3170	A
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3185	U
1	A	3187	A
1	A	3206	C
1	A	3207	U
1	A	3210	A
1	A	3212	C
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3224	G
1	A	3229	G
1	A	3232	G
1	A	3234	A
1	A	3235	C
1	A	3239	G
1	A	3243	A
1	A	3245	A
1	A	3247	G
1	A	3253	G
1	A	3259	U
1	A	3263	G

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Mol	Chain	Res	Type
1	A	3268	A
1	A	3269	U
1	A	3270	U
1	A	3273	A
1	A	3275	U
1	A	3276	G
1	A	3278	C
1	A	3279	A
1	A	3280	U
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3307	A
1	A	3310	A
1	A	3313	U
1	A	3316	A
1	A	3317	U
1	A	3318	G
1	A	3324	C
1	A	3341	U
1	A	3342	A
1	A	3345	G
1	A	3349	C
1	A	3350	C
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3354	U
1	A	3355	U
1	A	3356	G
1	A	3360	C
1	A	3362	A
1	A	3363	U
1	A	3368	U
1	A	3369	G
1	A	3375	A
1	A	3378	C
1	A	3382	U
1	A	3386	G
1	A	3390	G
1	A	3396	U

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Mol	Chain	Res	Type
2	B	10	C
2	B	22	A
2	B	24	A
2	B	31	U
2	B	49	G
2	B	54	U
2	B	65	G
2	B	70	U
2	B	71	G
2	B	73	C
2	B	74	C
2	B	76	A
2	B	102	A
2	B	112	G
2	B	118	A
2	B	121	U
3	C	23	U
3	C	25	G
3	C	34	U
3	C	35	C
3	C	49	G
3	C	51	G
3	C	59	A
3	C	62	C
3	C	63	G
3	C	67	U
3	C	82	U
3	C	83	C
3	C	84	C
3	C	86	U
3	C	87	G
3	C	90	U
3	C	95	G
3	C	104	A
3	C	105	A
3	C	106	C
3	C	111	A
3	C	113	U
3	C	125	U
3	C	126	A
3	C	127	U
3	C	151	C

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Mol	Chain	Res	Type
3	C	155	A
3	C	158	U

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	239	G
1	A	547	G
1	A	599	C
1	A	916	G
1	A	979	U
1	A	1064	A
1	A	1097	G
1	A	1103	A
1	A	1222	G
1	A	1241	U
1	A	1284	C
1	A	1554	U
1	A	1576	G
1	A	1716	U
1	A	1815	U
1	A	1816	A
1	A	2101	C
1	A	2112	U
1	A	2209	U
1	A	2249	G
1	A	2264	U
1	A	2266	U
1	A	2501	U
1	A	2513	U
1	A	2537	U
1	A	2541	U
1	A	2593	A
1	A	3121	U
1	A	3218	A
1	A	3228	C
1	A	3269	U
1	A	3317	U
1	A	3353	G
3	C	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.

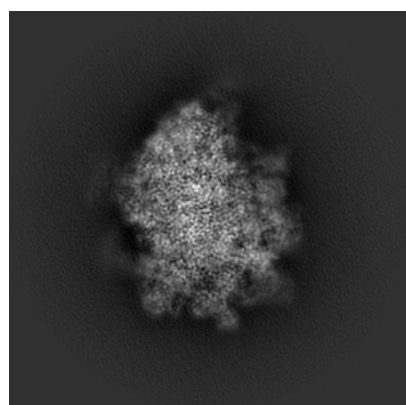
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0374. These allow visual inspection of the internal detail of the map and identification of artifacts.

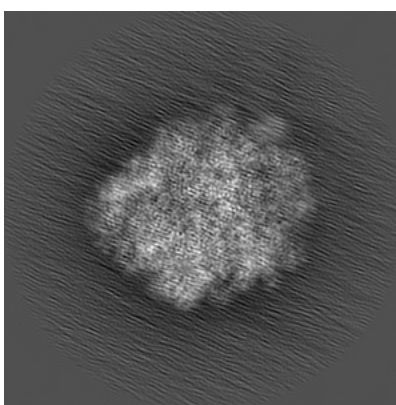
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

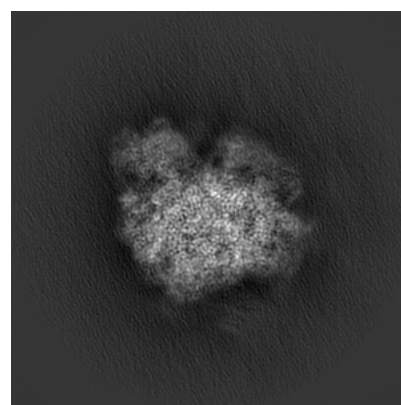
6.1.1 Primary map



X



Y

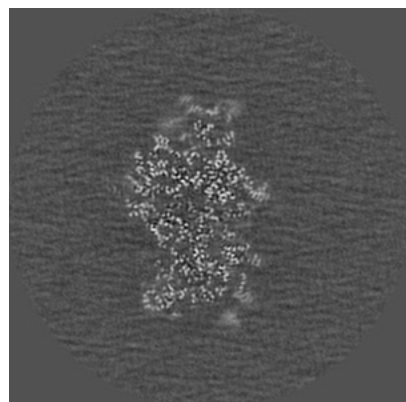


Z

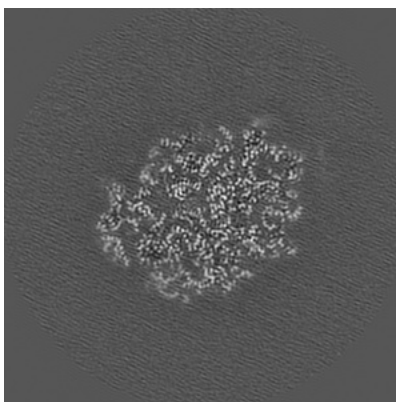
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

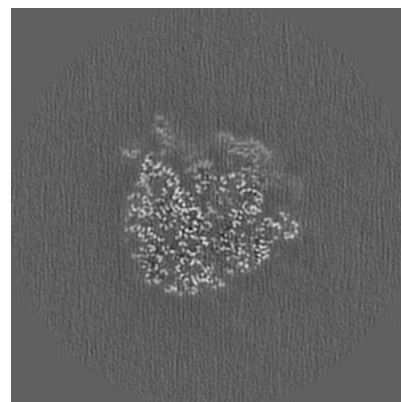
6.2.1 Primary map



X Index: 192



Y Index: 192

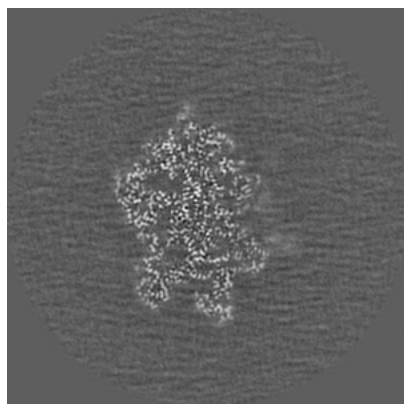


Z Index: 192

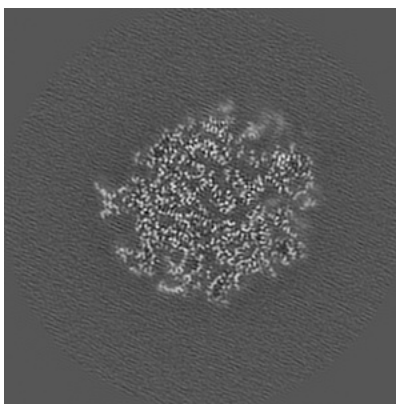
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

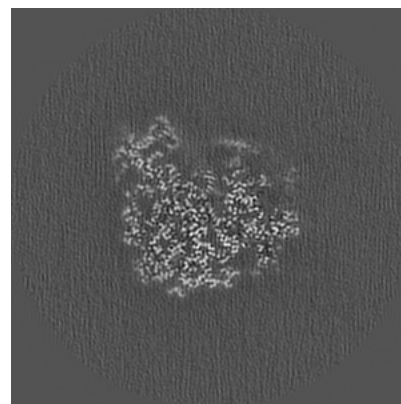
6.3.1 Primary map



X Index: 172



Y Index: 177

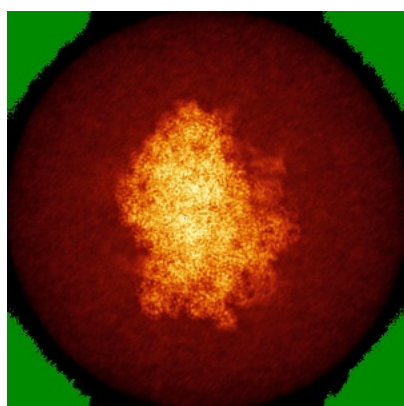


Z Index: 185

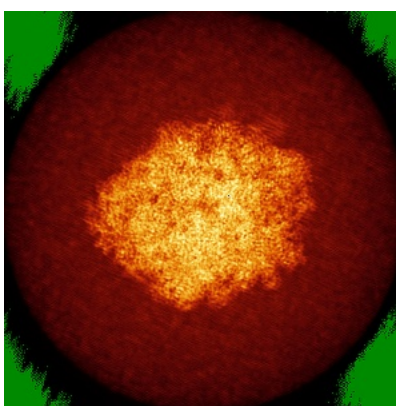
The images above show the largest variance slices of the map in three orthogonal directions.

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

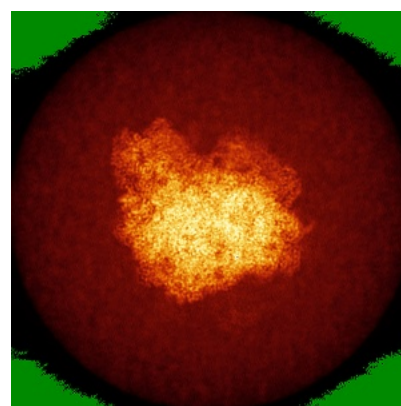
6.4.1 Primary map



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.

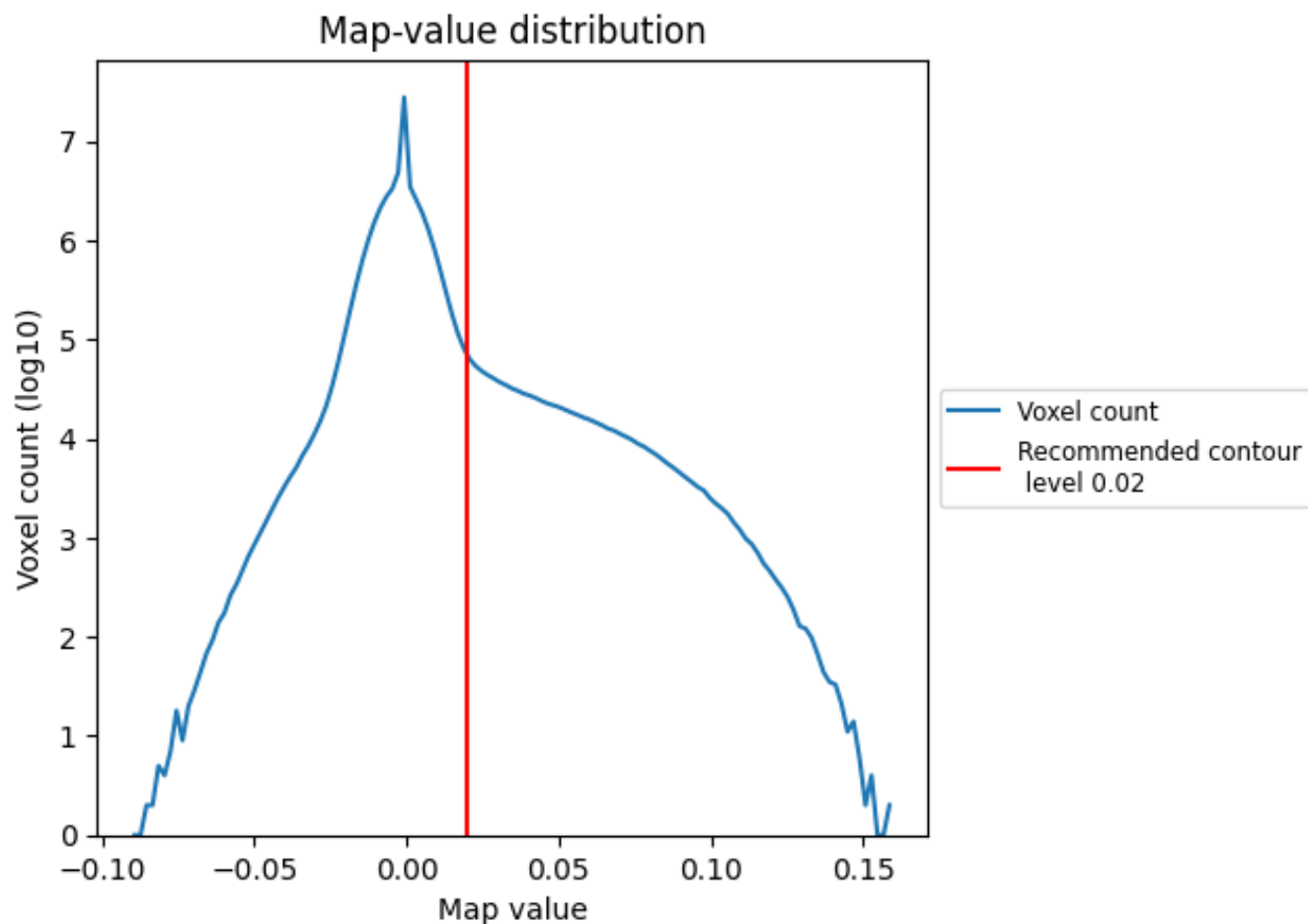
6.6 Mask visualisation

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

7 Map analysis [i](#)

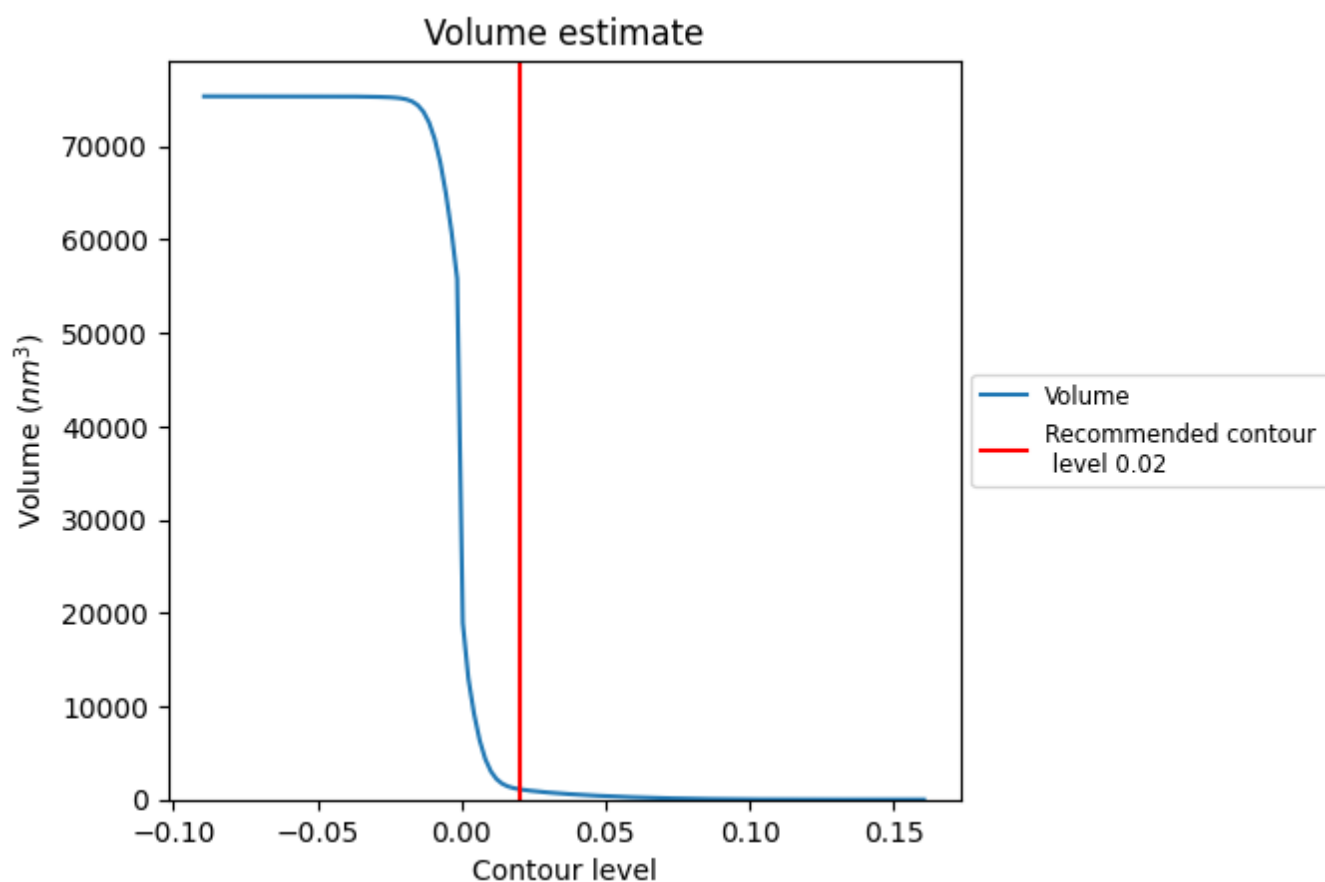
This section contains the results of statistical analysis of the map.

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.

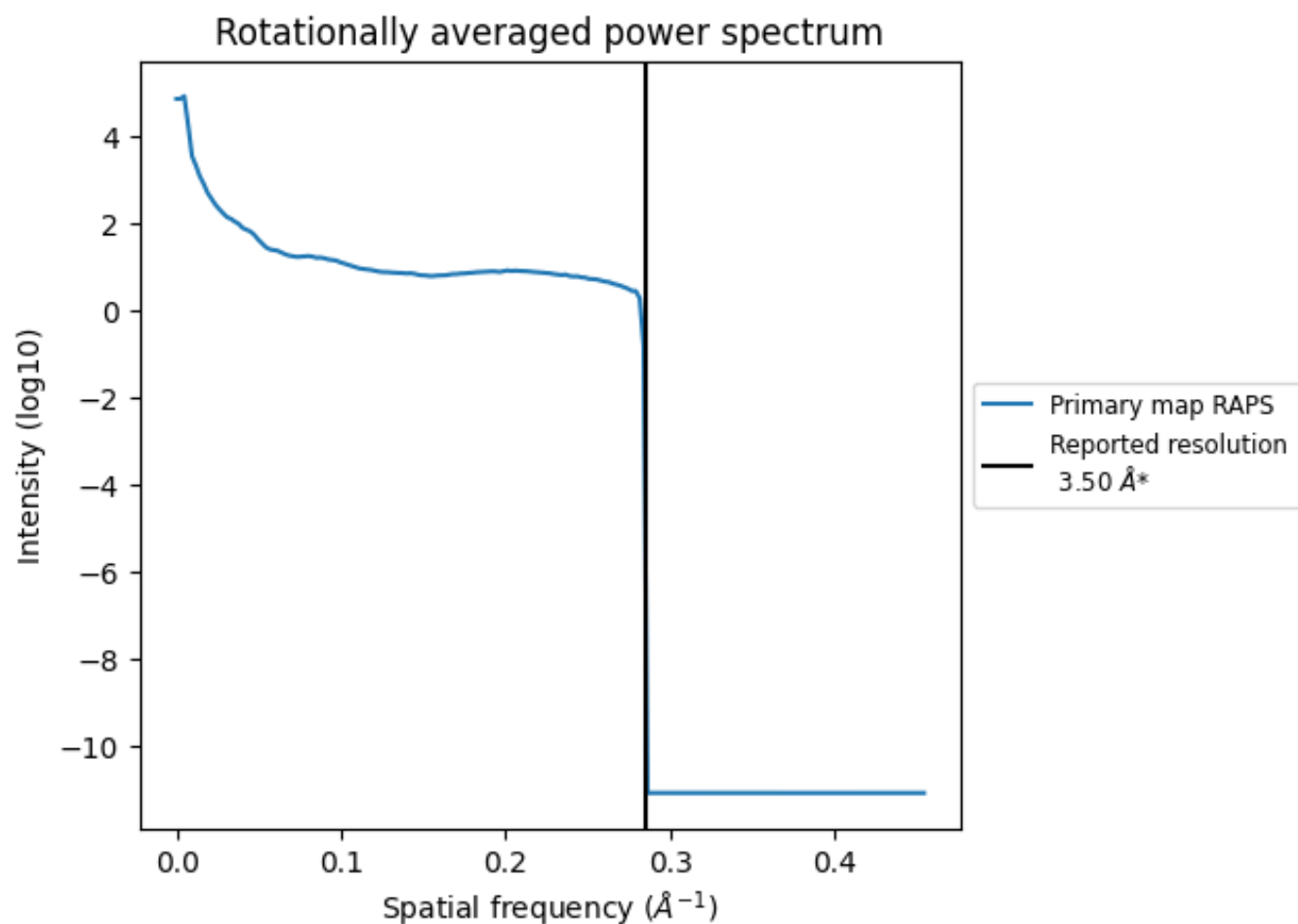
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1114 nm³; this corresponds to an approximate mass of 1006 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 ⓘ

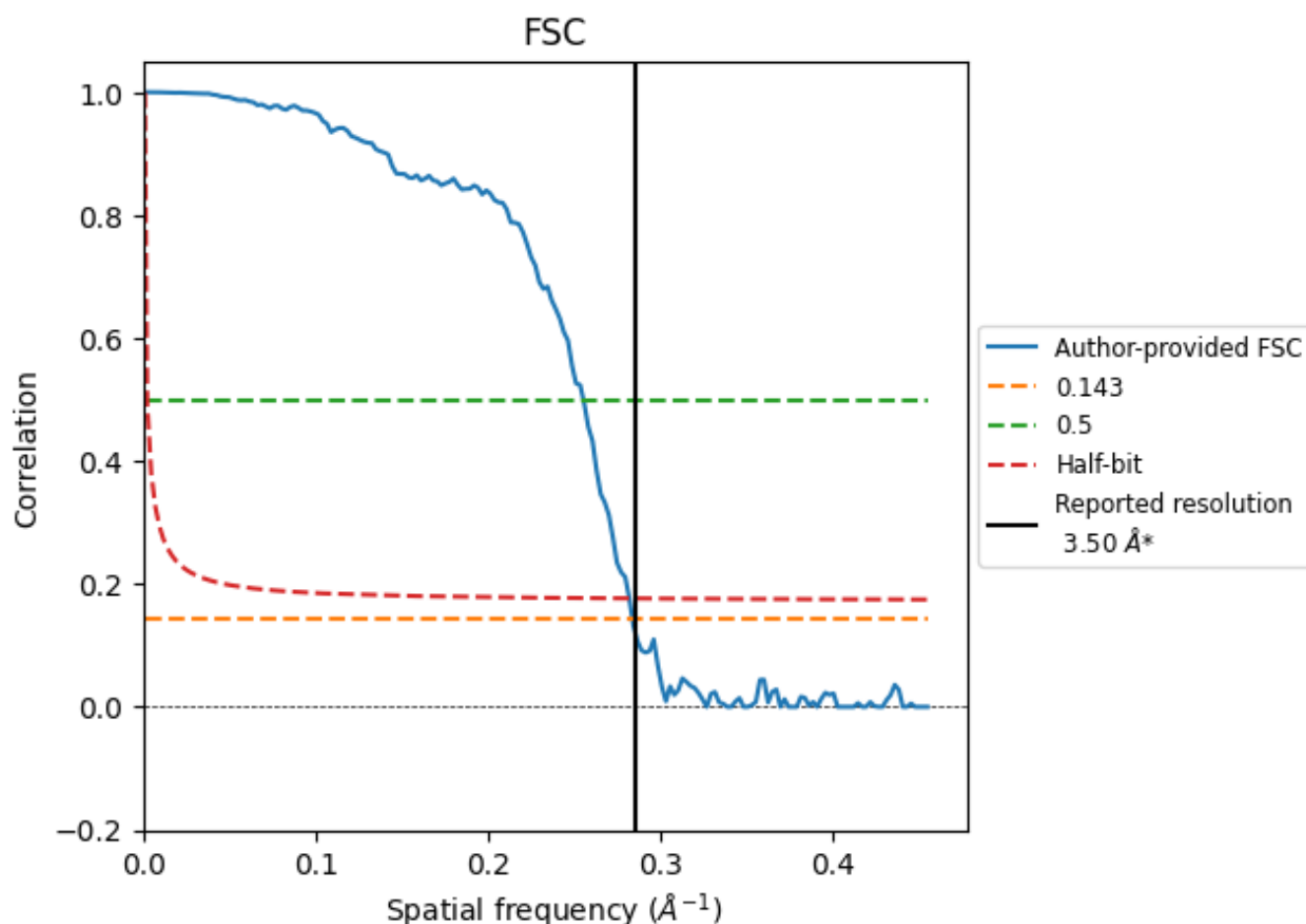


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	3.92	3.55
Unmasked-calculated*	-	-	-

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

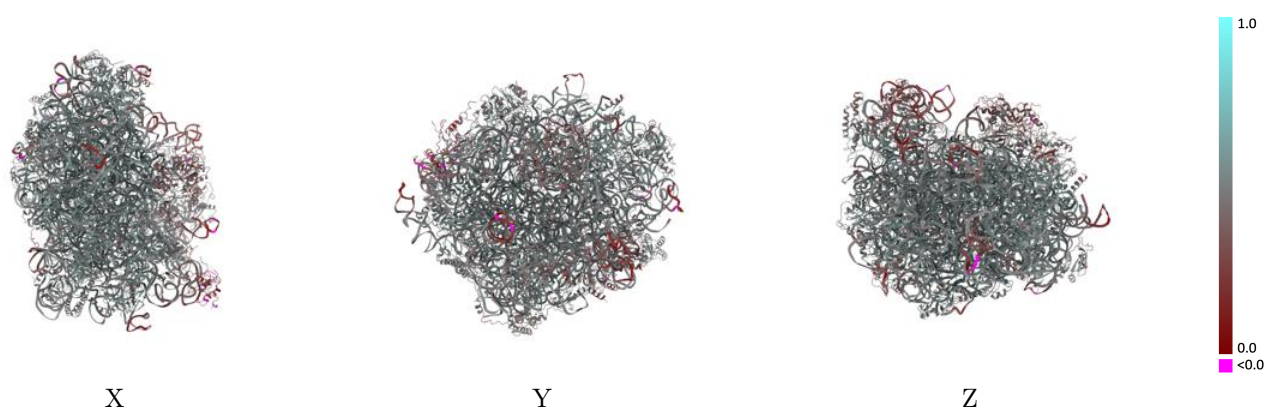
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0374 and PDB model 6N8O. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

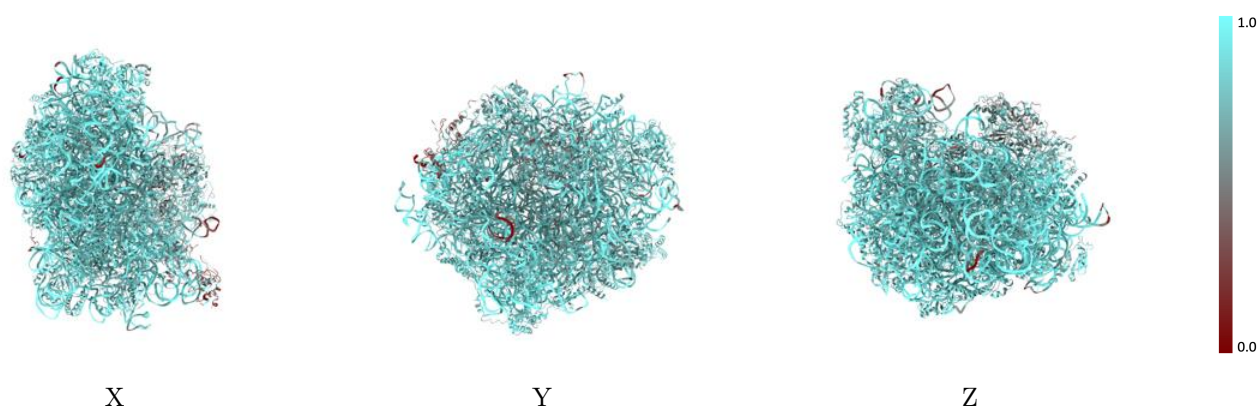
This section was not generated.

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



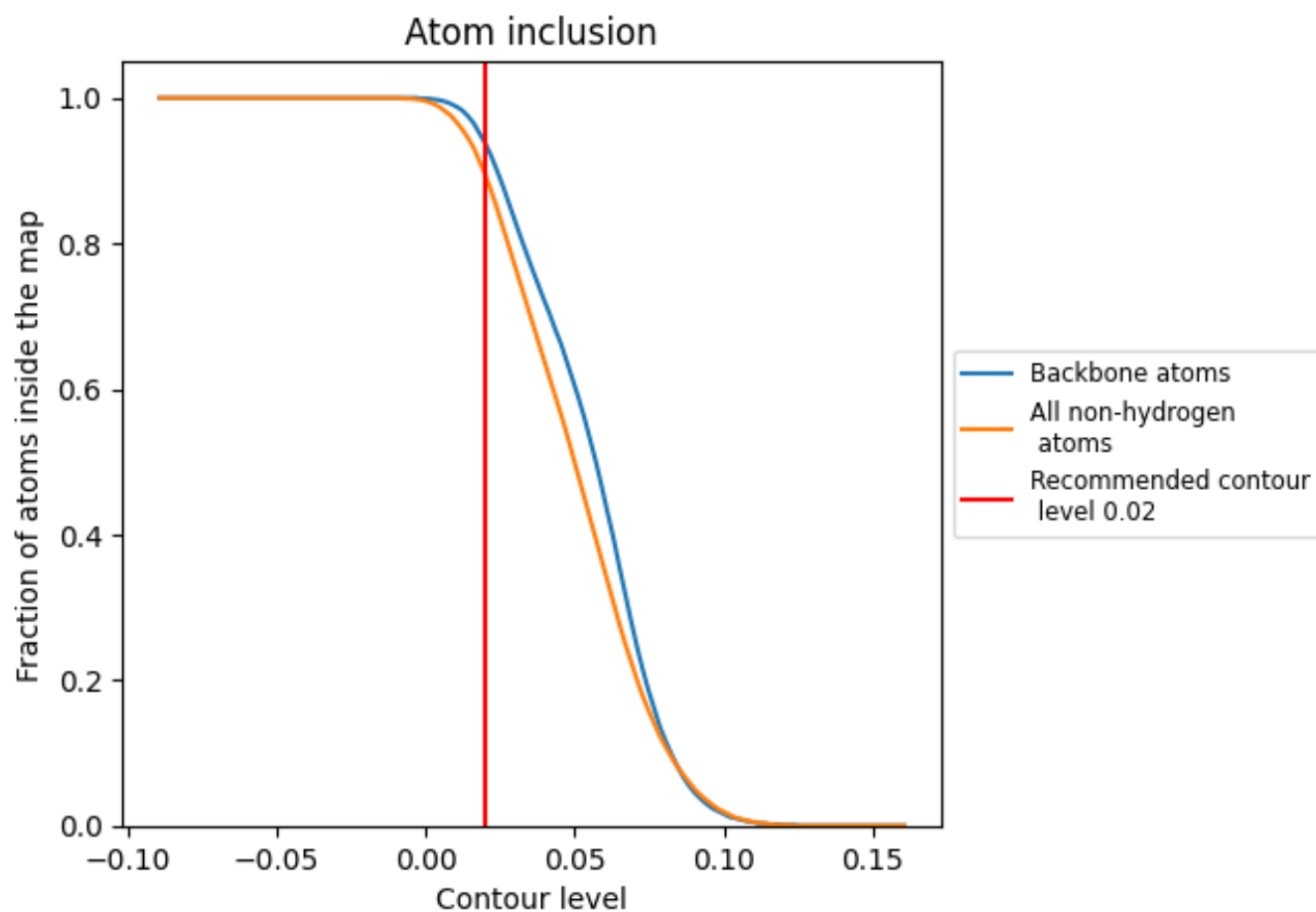
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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	 0.8940	 0.4930
A	 0.9460	 0.4950
B	 0.9710	 0.4980
C	 0.9610	 0.5030
D	 0.8810	 0.5360
E	 0.8830	 0.5230
F	 0.8620	 0.5110
G	 0.8500	 0.4670
H	 0.8490	 0.5020
I	 0.8630	 0.5040
J	 0.8700	 0.4960
K	 0.8660	 0.5120
L	 0.3830	 0.2450
M	 0.8010	 0.4380
N	 0.8600	 0.4980
O	 0.8760	 0.5080
Q	 0.8230	 0.5140
R	 0.8780	 0.5250
S	 0.7520	 0.3650
V	 0.6640	 0.4270
W	 0.6450	 0.3660
X	 0.7910	 0.4810
Y	 0.5990	 0.4140
Z	 0.8220	 0.4930
a	 0.8860	 0.5340
b	 0.8680	 0.5220
c	 0.8470	 0.5140
d	 0.8570	 0.5180
e	 0.8790	 0.5190
f	 0.8620	 0.5140
g	 0.8560	 0.5140
h	 0.8500	 0.4830
i	 0.8300	 0.5330
j	 0.8580	 0.5130
k	 0.8570	 0.5050



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Chain	Atom inclusion	Q-score
l	 0.8580	 0.5100
m	 0.8810	 0.5010
n	 0.8870	 0.5330
o	 0.8250	 0.4920
p	 0.8510	 0.4870
q	 0.8440	 0.5060
r	 0.8530	 0.5270
s	 0.8830	 0.5370
t	 0.8410	 0.5310
u	 0.8860	 0.5130
v	 0.8450	 0.4930
w	 0.9060	 0.5420
x	 0.8030	 0.4790
y	 0.8630	 0.5300
z	 0.8580	 0.5200