



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:37 PM UTC

PDB ID : 5T6R / pdb_00005t6r
EMDB ID : EMD-8368
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during 60S ribosome biogenesis: 60S-Nmd3 Complex
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.
Deposited on : 2016-09-01
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

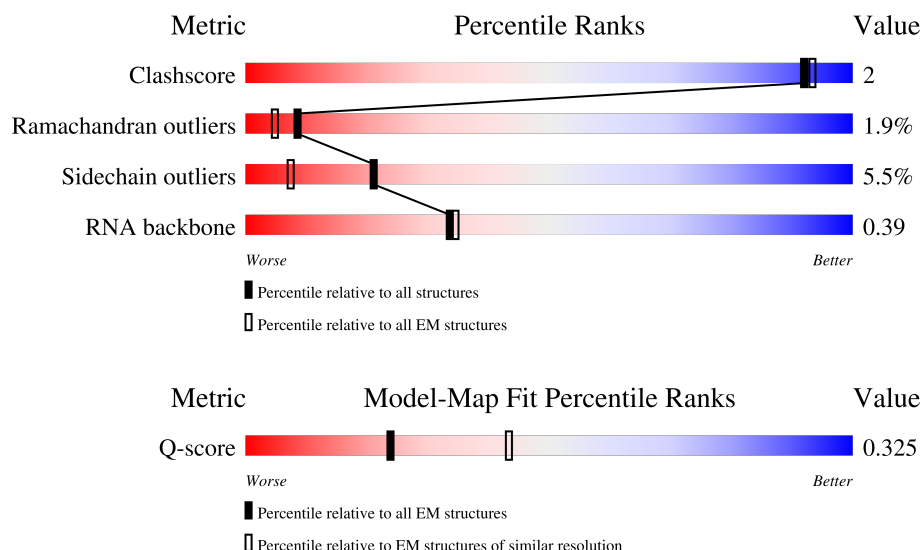
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

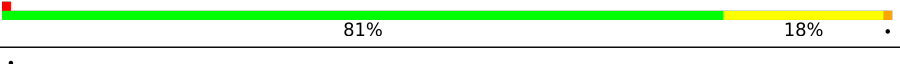
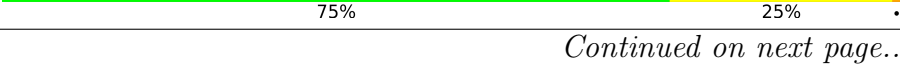
The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	3396	
2	B	121	
3	C	158	

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Mol	Chain	Length	Quality of chain
4	D	254	
5	E	387	
6	F	362	
7	G	297	
8	H	176	
9	I	244	
10	J	256	
11	K	191	
12	L	221	
13	M	174	
14	N	199	
15	O	138	
16	a	204	
17	b	199	
18	c	184	
19	d	186	
20	e	189	
21	f	172	
22	g	160	
23	h	121	
24	i	137	
25	j	155	
26	k	142	
27	l	127	
28	m	136	

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Mol	Chain	Length	Quality of chain
29	n	149	
30	o	59	
31	p	105	
32	q	113	
33	r	130	
34	s	107	
35	t	121	
36	u	120	
37	v	100	
38	w	88	
39	x	78	
40	y	51	
41	z	128	
42	Q	106	
43	R	92	
44	S	210	
45	V	917	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 126616 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 25S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3204	Total	C	N	O	P	0	0
			68535	30613	12358	22360	3204		

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

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 Ribosomal RNA.

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 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	50	Total	C	N	O	0	0
			406	258	77	71		

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	v	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 44 is a protein called Ribosomal Protein uL1.

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

- Molecule 45 is a protein called Maltose binding protein, 60S ribosomal export protein Nmd3 fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	251	Total	C	N	O	S	0	0
			1975	1263	333	372	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-396	ILE	THR	conflict	UNP A0A0F8NYV9
V	-15	HIS	-	linker	UNP A0A0F8NYV9
V	-14	HIS	-	linker	UNP A0A0F8NYV9
V	-13	HIS	-	linker	UNP A0A0F8NYV9
V	-12	HIS	-	linker	UNP A0A0F8NYV9
V	-11	HIS	-	linker	UNP A0A0F8NYV9
V	-10	HIS	-	linker	UNP A0A0F8NYV9
V	-9	HIS	-	linker	UNP A0A0F8NYV9
V	-8	HIS	-	linker	UNP A0A0F8NYV9
V	-7	HIS	-	linker	UNP A0A0F8NYV9
V	-6	HIS	-	linker	UNP A0A0F8NYV9
V	-5	GLU	-	linker	UNP A0A0F8NYV9
V	-4	ASN	-	linker	UNP A0A0F8NYV9
V	-3	LEU	-	linker	UNP A0A0F8NYV9
V	-2	TYR	-	linker	UNP A0A0F8NYV9
V	-1	PHE	-	linker	UNP A0A0F8NYV9
V	0	GLN	-	linker	UNP A0A0F8NYV9
V	1	GLY	-	linker	UNP A0A0F8NYV9

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

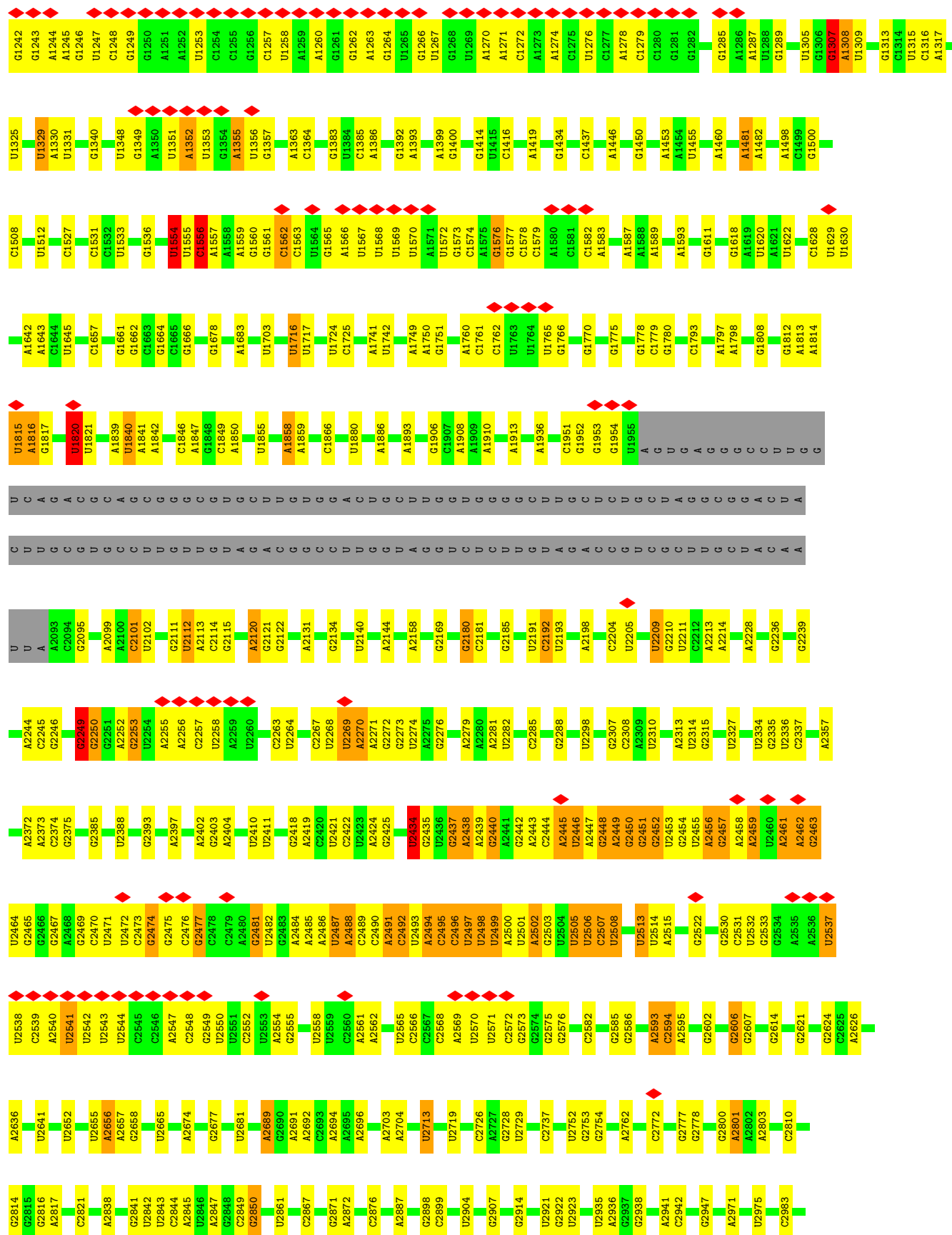
Mol	Chain	Residues	Atoms		AltConf
46	A	84	Total 84	Mg 84	0
46	C	1	Total 1	Mg 1	0
46	i	1	Total 1	Mg 1	0

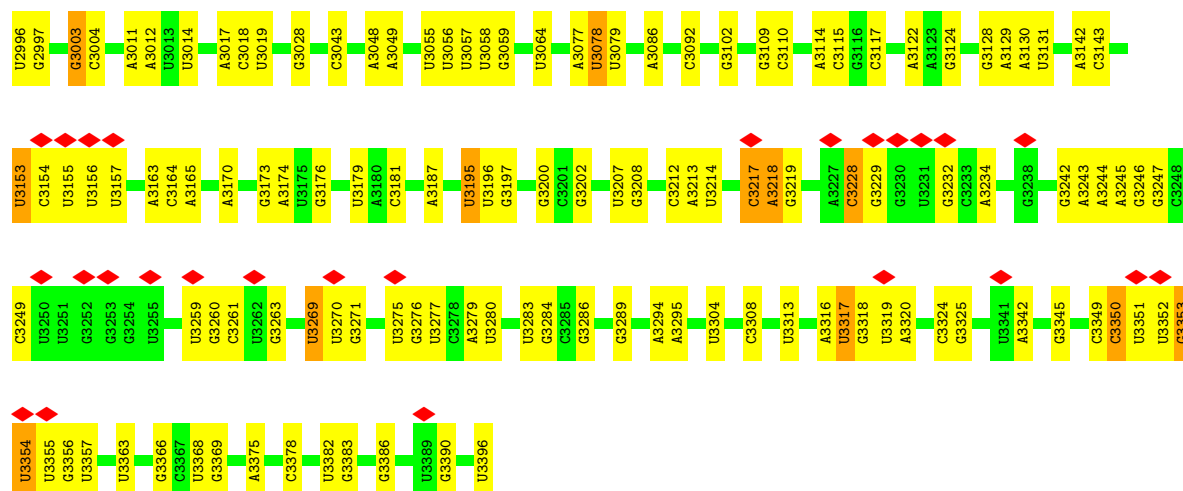
- Molecule 47 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
47	A	3	Total 3	K 3	0

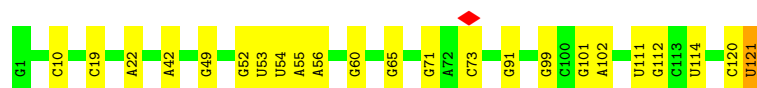
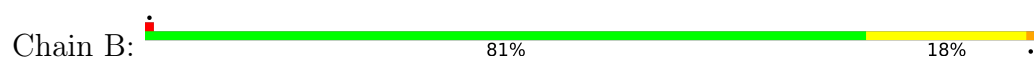
- Molecule 48 is water.

Mol	Chain	Residues	Atoms		AltConf
48	A	10	Total 10	O 10	0
48	c	1	Total 1	O 1	0
48	e	1	Total 1	O 1	0

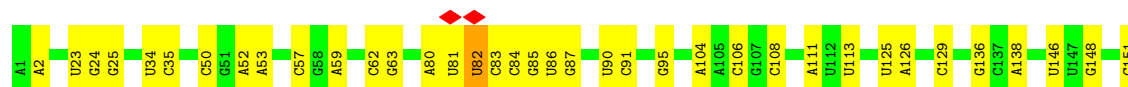
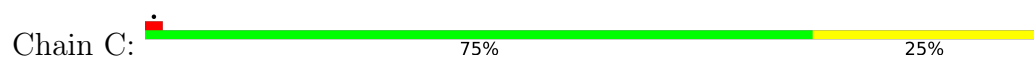




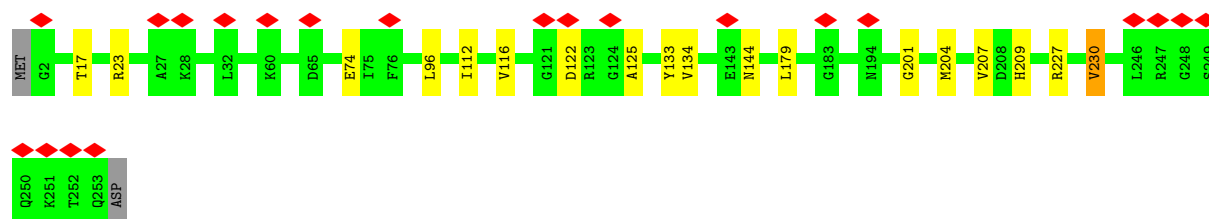
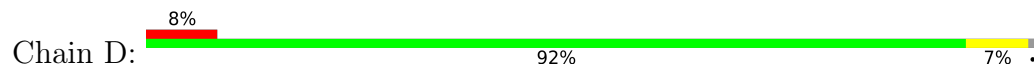
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 5.8S Ribosomal RNA

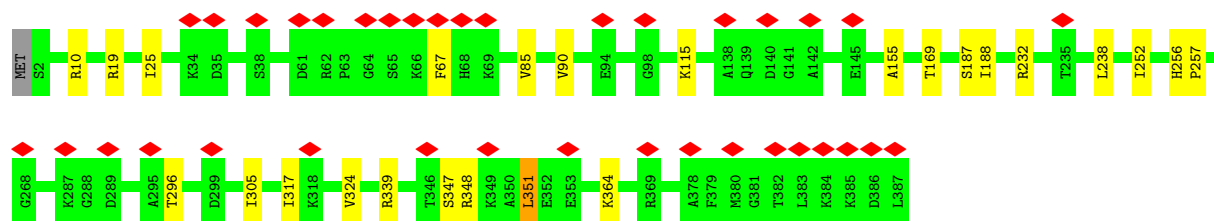


• Molecule 4: 60S ribosomal protein L2-A

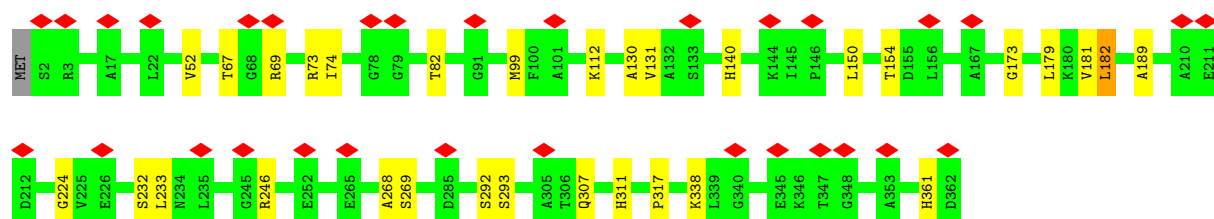
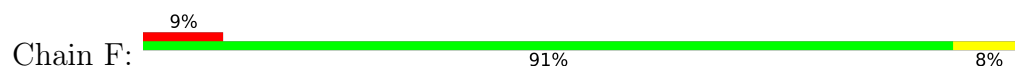


• Molecule 5: 60S ribosomal protein L3

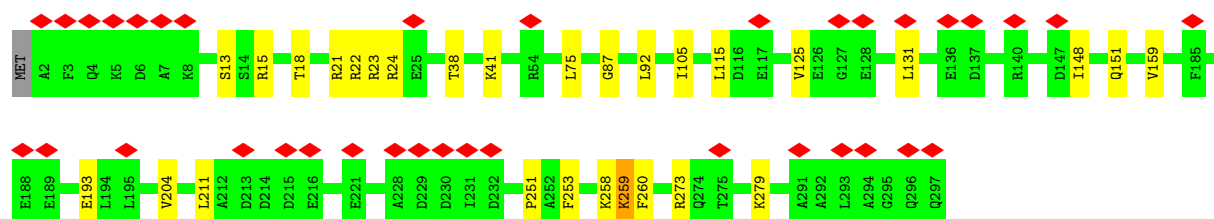
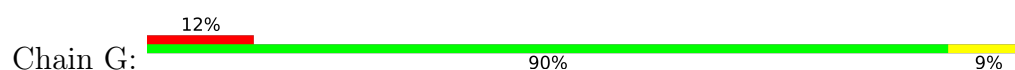




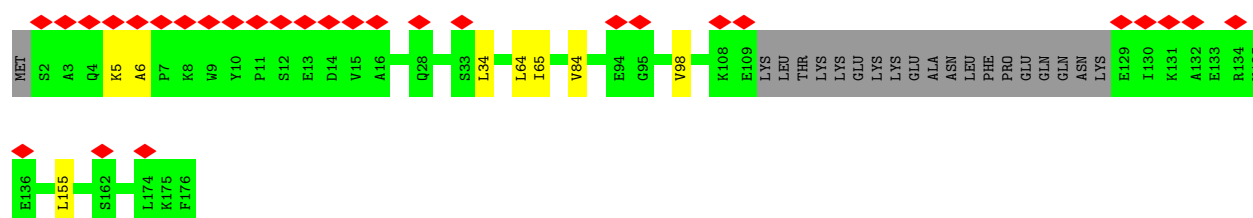
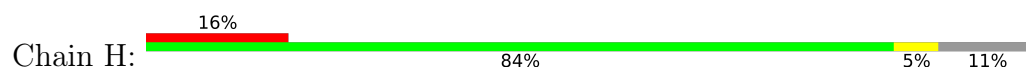
• Molecule 6: 60S ribosomal protein L4-A



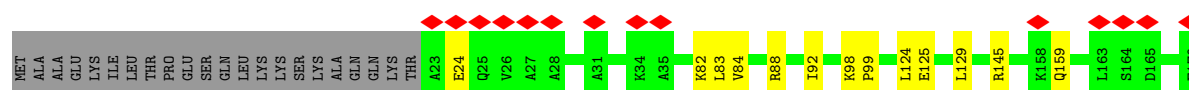
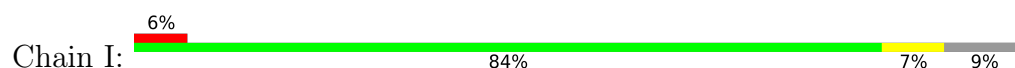
• Molecule 7: 60S ribosomal protein L5

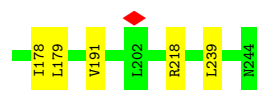


• Molecule 8: 60S ribosomal protein L6-A

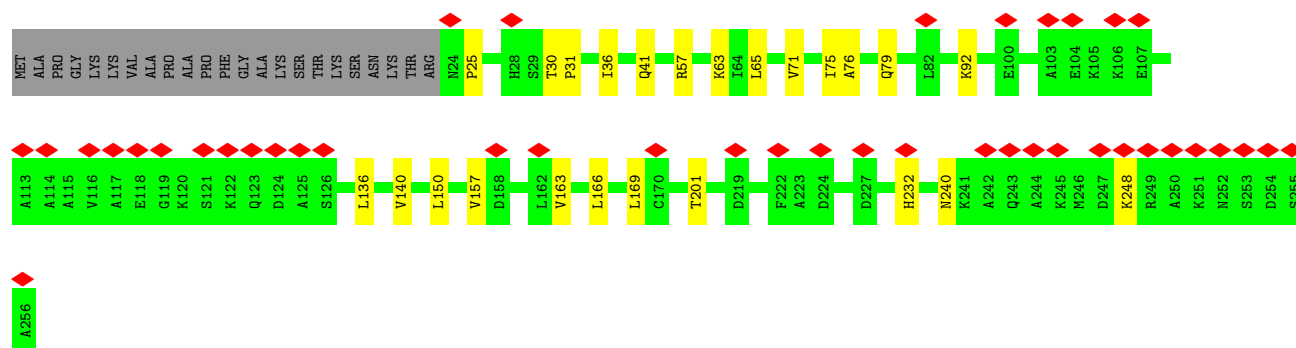
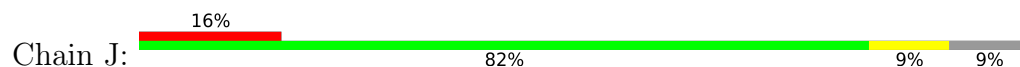


• Molecule 9: 60S ribosomal protein L7-A

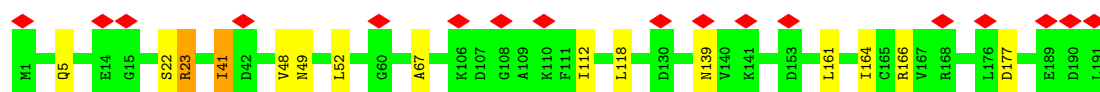
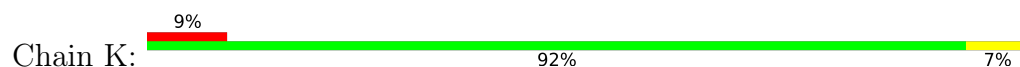




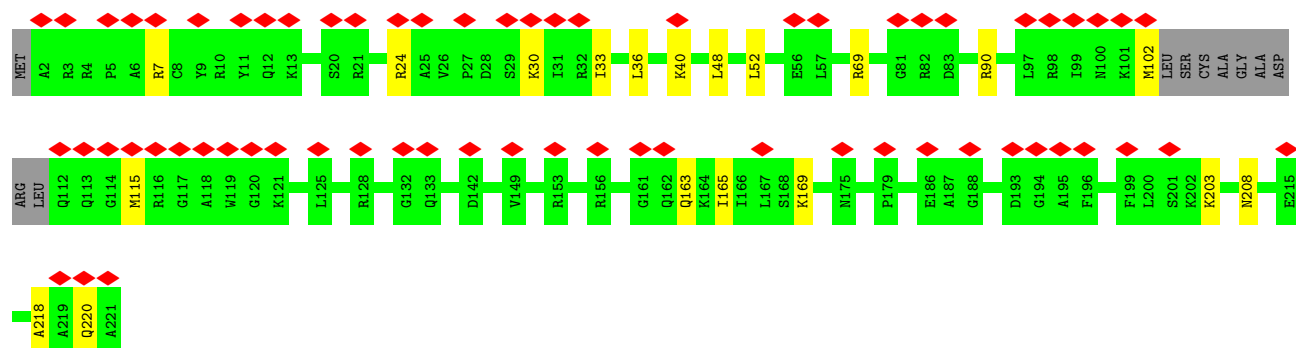
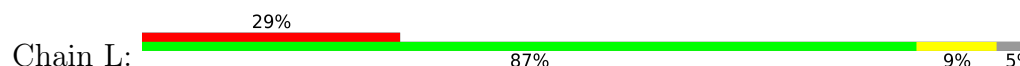
- Molecule 10: 60S ribosomal protein L8-A



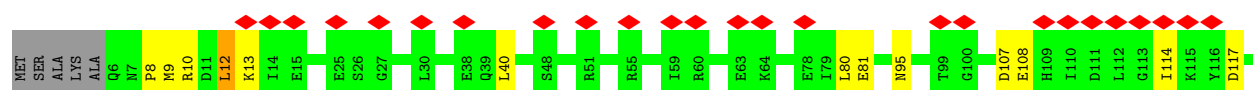
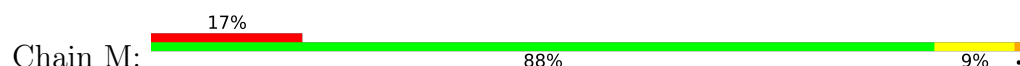
- Molecule 11: 60S ribosomal protein L9-A

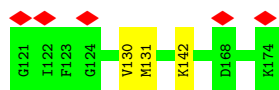


- Molecule 12: 60S ribosomal protein L10

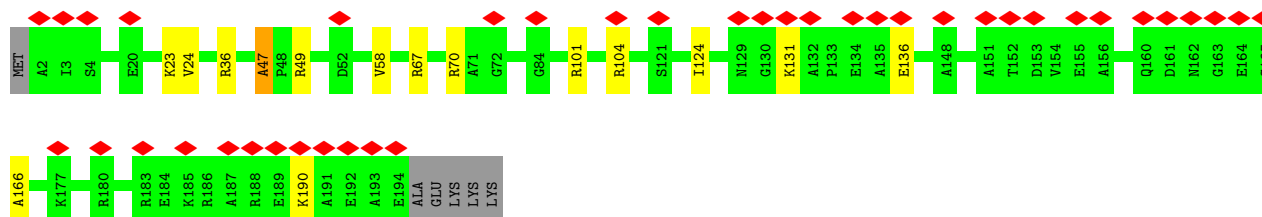
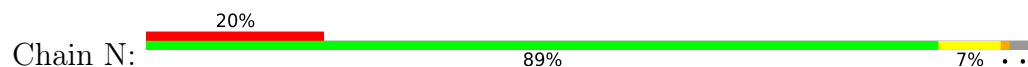


- Molecule 13: 60S ribosomal protein L11-A

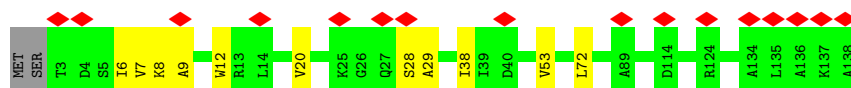




- Molecule 14: 60S ribosomal protein L13-A



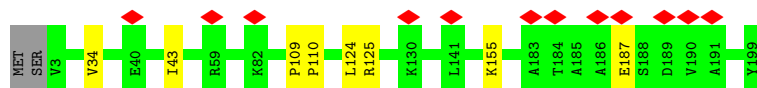
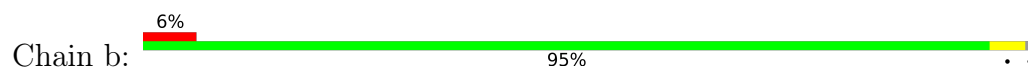
- Molecule 15: 60S ribosomal protein L14-A



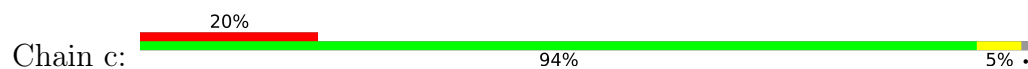
- Molecule 16: 60S ribosomal protein L15-A



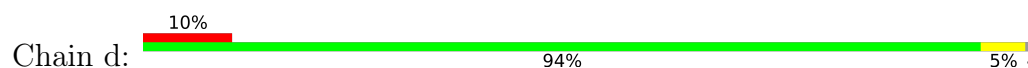
- Molecule 17: 60S ribosomal protein L16-A

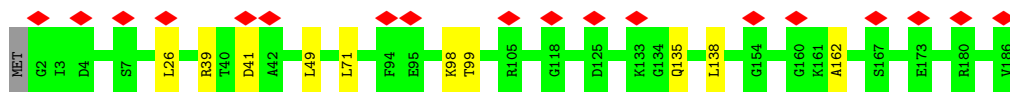


- Molecule 18: 60S ribosomal protein L17-A

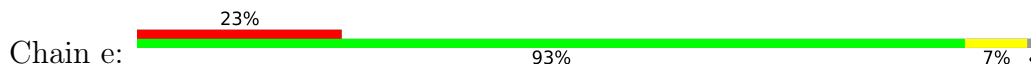


- Molecule 19: 60S ribosomal protein L18-A

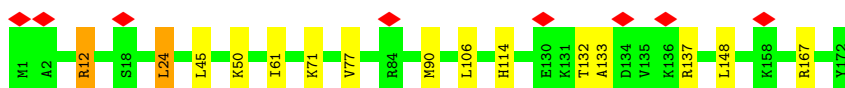
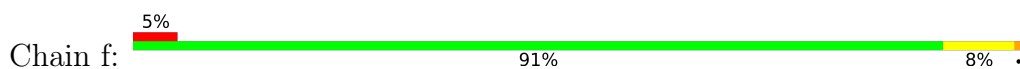




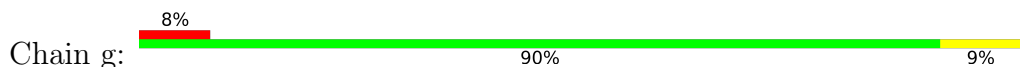
- Molecule 20: 60S ribosomal protein L19-A



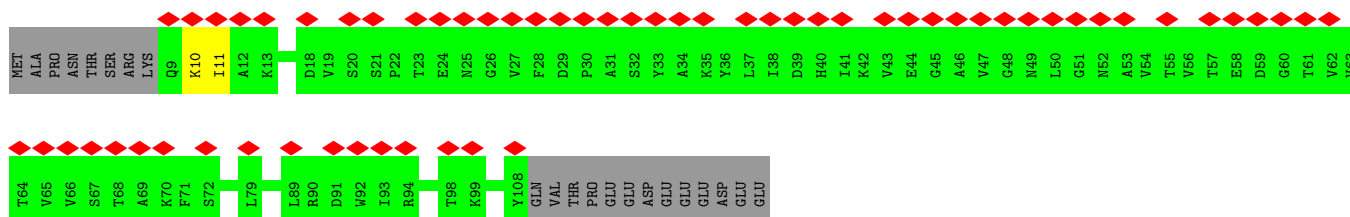
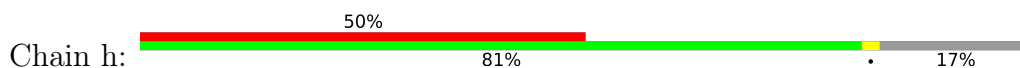
- Molecule 21: 60S ribosomal protein L20-A



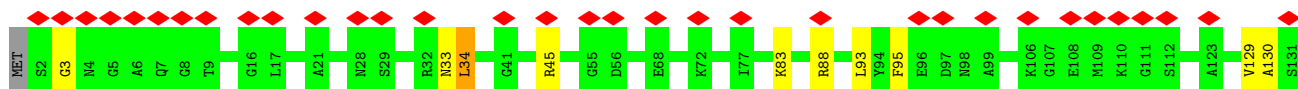
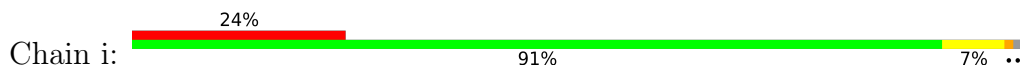
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 23: 60S ribosomal protein L22-A

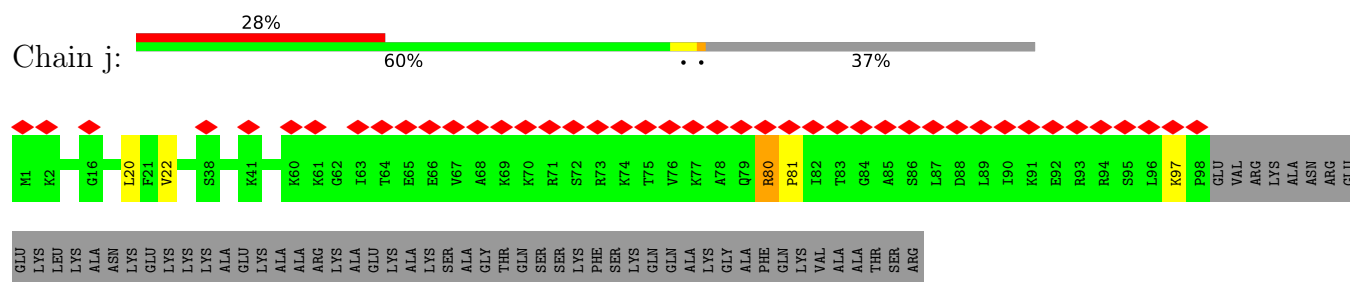


- Molecule 24: 60S ribosomal protein L23-A

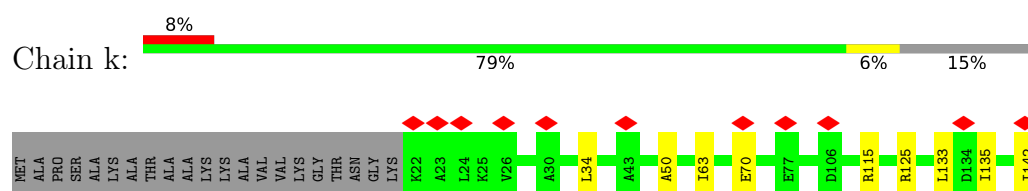




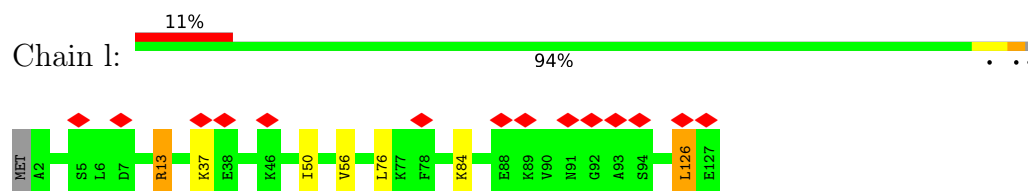
- Molecule 25: 60S ribosomal protein L24-A



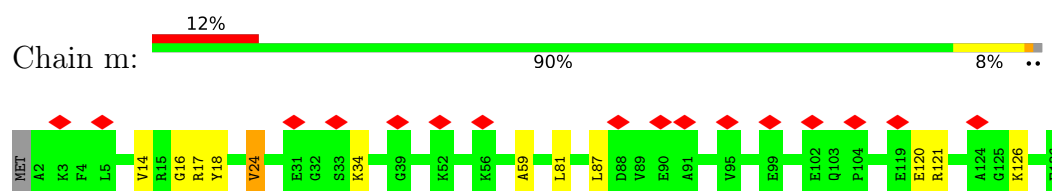
- Molecule 26: 60S ribosomal protein L25



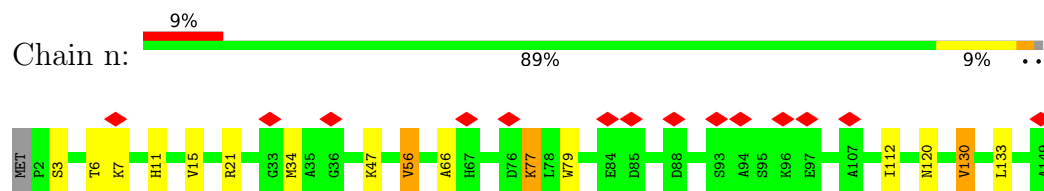
- Molecule 27: 60S ribosomal protein L26-A



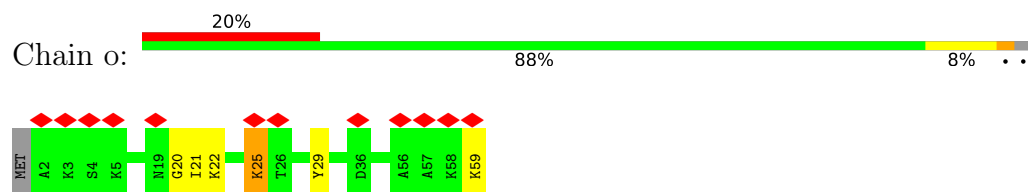
- Molecule 28: 60S ribosomal protein L27-A



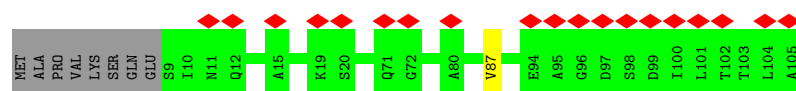
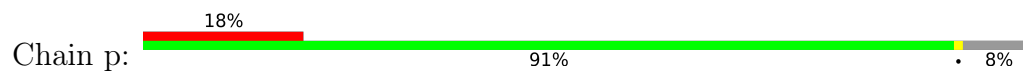
- Molecule 29: 60S ribosomal protein L28



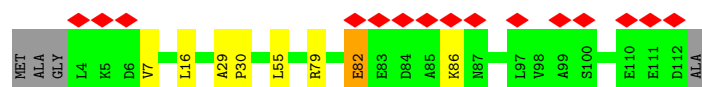
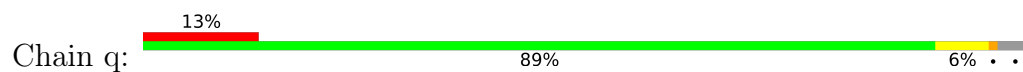
- Molecule 30: 60S ribosomal protein L29



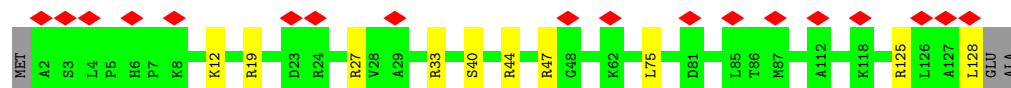
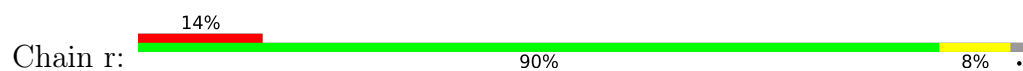
- Molecule 31: 60S ribosomal protein L30



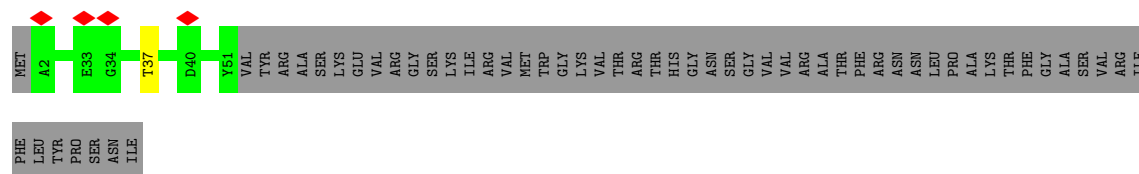
- Molecule 32: 60S ribosomal protein L31-A



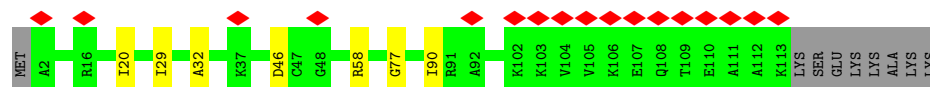
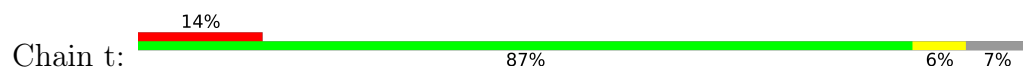
- Molecule 33: 60S ribosomal protein L32



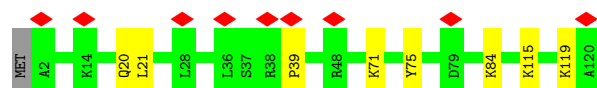
- Molecule 34: 60S ribosomal protein L33-A



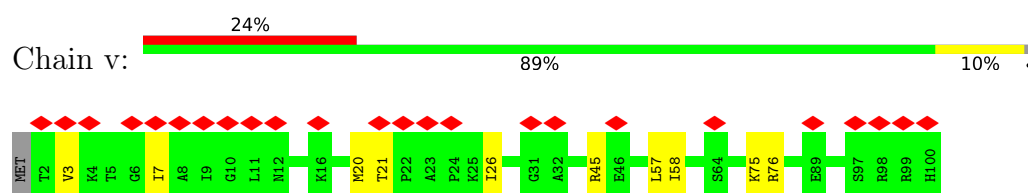
- Molecule 35: 60S ribosomal protein L34-A



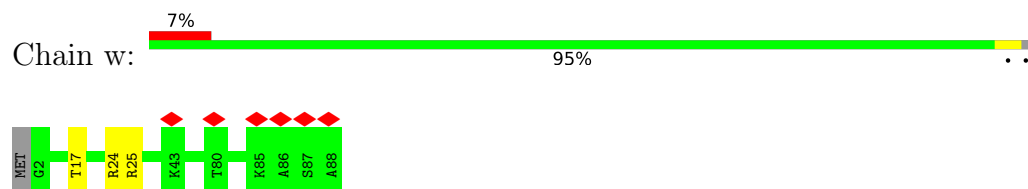
- Molecule 36: 60S ribosomal protein L35-A



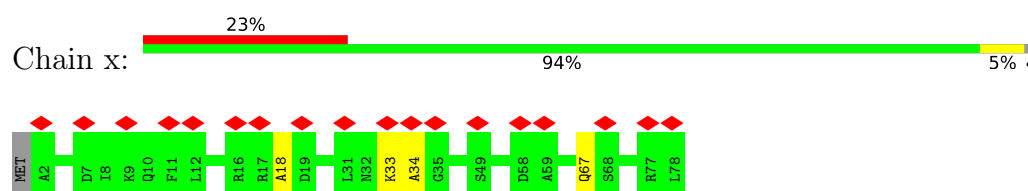
- Molecule 37: 60S ribosomal protein L36-A



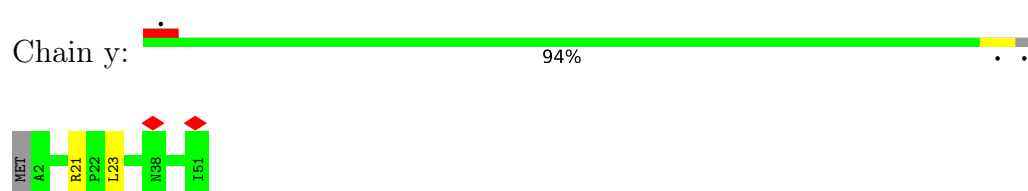
- Molecule 38: 60S ribosomal protein L37-A



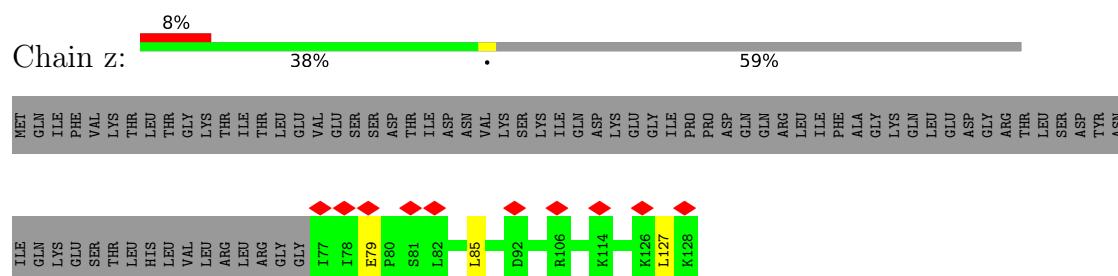
- Molecule 39: 60S ribosomal protein L38



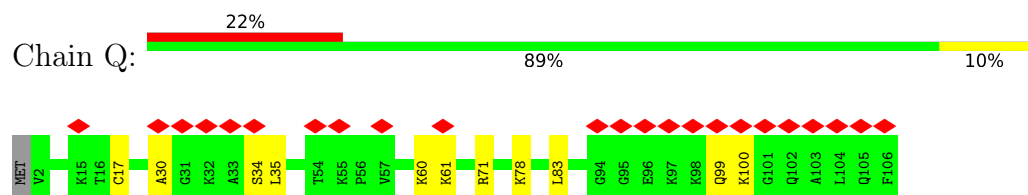
- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 42: 60S ribosomal protein L42-A



- Molecule 43: 60S ribosomal protein L43-A



LEU	LYS	V334	
TYR	SER	L335	
LYS	LYS	A336	
ASN	LYS	D337	
ARG	SER	A338	
GLU	ARG	R342	
GLU	ARG		
ASN	HIS		
ASN	TRP	D345	
VAL	LYS	L346	
PRO	LEU	G347	
PRO	LYS	V348	
GLU	ARG	V349	
GLU	MET	N349	
HIS	ALA	D350	
HIS	ALA		
GLU	LYS		
MET	GLU	V355	
ASP	HIS	R356	
GLU	LYS	S357	
ASP	ASP	H358	
GLU	ILE	L359	
ASP	ASP	G360	
GLU	ALA	G361	
ASP	SER	L362	
ALA	LEU	C363	
PRO	PRO	H364	
GLN	GLN	T364	
ILE	ASN	A365	
ASN	SER	G366	
ILE	ARG	D367	
ASP	ALA	S368	
GLU	LYS	V369	
LEU	GLN	N370	
LEU	GLN	G371	
ASP	GLU	T372	
GLU	MET	F373	
LEU	GLU	L374	
ASP	ARG	A375	
GLU	ALA	N376	
MET	GLU		
THR	LYS		
LEU	ASP	D382	
LEU	ASP	L383	
ASP	LEU	F384	
GLY	LEU	D385	
VAL	PHE	G386	
GLU	LEU	L387	
ASN	GLN	N388	
THR	GLU	L389	
PRO	LEU		
VAL	GLU	D390	
GLU	GLU	V391	
SER	ASP	V392	
GLN	ALA	P393	
GLN	GLU	D394	
	LEU	V395	
	ARG	V396	
	GLN	L397	
	SER	V398	
	VAL	K399	
	ASN	K400	
		L401	
		T397	
		GLN	
		ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/76717	0.68	48/119611 (0.0%)
2	B	0.38	0/2883	0.65	0/4491
3	C	0.37	0/3746	0.65	1/5832 (0.0%)
4	D	0.53	0/1948	0.75	0/2617
5	E	0.53	0/3146	0.74	0/4228
6	F	0.54	0/2800	0.78	0/3790
7	G	0.54	0/2425	0.76	0/3271
8	H	0.54	0/1260	0.73	0/1694
9	I	0.54	0/1821	0.79	0/2451
10	J	0.56	0/1836	0.84	2/2481 (0.1%)
11	K	0.53	0/1539	0.72	0/2073
12	L	0.53	0/1741	0.71	0/2335
13	M	0.56	0/1374	0.80	0/1842
14	N	0.56	0/1568	0.85	2/2106 (0.1%)
15	O	0.54	0/1068	0.81	0/1438
16	a	0.54	0/1757	0.80	0/2354
17	b	0.54	0/1585	0.82	3/2128 (0.1%)
18	c	0.53	0/1443	0.79	0/1944
19	d	0.55	0/1465	0.75	0/1965
20	e	0.53	0/1538	0.82	0/2050
21	f	0.50	0/1481	0.73	0/1990
22	g	0.53	0/1300	0.72	0/1743
23	h	0.57	0/812	0.72	0/1099
24	i	0.55	0/1018	0.75	0/1369
25	j	0.53	0/712	0.93	2/958 (0.2%)
26	k	0.52	0/979	0.72	0/1321
27	l	0.55	0/1004	0.73	0/1341
28	m	0.52	0/1118	0.75	0/1497
29	n	0.51	0/1204	0.74	0/1612
30	o	0.55	0/473	0.80	0/629
31	p	0.54	0/751	0.75	0/1008
32	q	0.50	0/890	0.72	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	r	0.53	0/1041	0.71	0/1394
34	s	0.48	0/414	0.70	0/556
35	t	0.53	0/890	0.74	0/1189
36	u	0.56	0/978	0.81	0/1301
37	v	0.59	0/778	0.85	0/1034
38	w	0.54	0/696	0.74	0/923
39	x	0.53	0/618	0.71	0/826
40	y	0.53	0/443	0.74	0/588
41	z	0.58	0/423	0.77	0/562
42	Q	0.51	0/860	0.73	0/1136
43	R	0.54	0/701	0.80	0/934
45	V	0.60	0/2015	1.21	6/2738 (0.2%)
All	All	0.45	0/135259	0.72	64/199645 (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
30	o	0	1

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	V	386	GLY	CA-C-N	26.92	157.70	122.16
45	V	386	GLY	C-N-CA	26.92	157.70	122.16
45	V	386	GLY	O-C-N	-16.17	101.67	122.70
25	j	80	ARG	CA-C-N	10.69	133.20	119.84
25	j	80	ARG	C-N-CA	10.69	133.20	119.84
1	A	1307	G	C2'-C3'-O3'	10.43	125.14	109.50
1	A	65	A	C4'-C3'-O3'	8.47	122.10	109.40
1	A	3078	U	C4'-C3'-O3'	8.38	121.97	109.40
1	A	2249	G	C2'-C3'-O3'	8.37	126.26	113.70
1	A	979	U	C2'-C3'-O3'	8.31	121.97	109.50
1	A	3218	A	C4'-C3'-O3'	8.03	121.44	109.40
1	A	3269	U	C4'-C3'-O3'	7.87	121.21	109.40
1	A	2513	U	C4'-C3'-O3'	7.82	121.13	109.40
17	b	110	PRO	N-CA-C	7.79	120.20	110.70
10	J	30	THR	CA-C-N	7.76	129.54	119.84
10	J	30	THR	C-N-CA	7.76	129.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1576	G	C2'-C3'-O3'	7.71	121.06	109.50
45	V	398	VAL	N-CA-C	7.68	118.47	110.72
45	V	391	TYR	N-CA-C	-7.38	104.12	113.72
1	A	1716	U	C2'-C3'-O3'	7.33	120.49	109.50
1	A	2496	C	C4'-C3'-O3'	7.25	120.28	109.40
1	A	169	U	C4'-C3'-O3'	7.22	120.24	109.40
1	A	1329	U	C4'-C3'-O3'	7.11	120.06	109.40
1	A	916	G	C2'-C3'-O3'	-7.02	103.17	113.70
1	A	3317	U	C4'-C3'-O3'	6.94	119.81	109.40
1	A	1554	U	C4'-C3'-O3'	6.84	119.66	109.40
1	A	1097	G	C2'-C3'-O3'	6.75	119.62	109.50
1	A	3195	U	C4'-C3'-O3'	6.67	119.41	109.40
1	A	2541	U	C2'-C3'-O3'	6.56	119.34	109.50
1	A	1820	U	C4'-C3'-O3'	6.55	119.22	109.40
1	A	3228	C	C4'-C3'-O3'	6.52	119.17	109.40
1	A	2593	A	C4'-C3'-O3'	6.49	119.14	109.40
1	A	2209	U	C2'-C3'-O3'	6.45	119.17	109.50
45	V	261	LYS	N-CA-C	6.29	117.80	111.07
1	A	1815	U	C2'-C3'-O3'	6.27	118.91	109.50
1	A	873	C	C2'-C3'-O3'	-6.22	104.37	113.70
1	A	2101	C	C2'-C3'-O3'	6.21	118.81	109.50
1	A	3353	G	C4'-C3'-O3'	6.09	118.53	109.40
1	A	3003	G	C2'-C3'-O3'	6.07	122.80	113.70
1	A	2112	U	C2'-C3'-O3'	5.96	118.43	109.50
1	A	2537	U	C2'-C3'-O3'	5.92	118.38	109.50
17	b	109	PRO	CA-C-N	5.72	126.27	120.38
17	b	109	PRO	C-N-CA	5.72	126.27	120.38
1	A	1064	A	C2'-C3'-O3'	5.65	117.97	109.50
1	A	1352	A	C2'-C3'-O3'	5.65	117.97	109.50
1	A	2269	U	C2'-C3'-O3'	5.63	117.94	109.50
14	N	47	ALA	CA-C-N	-5.63	113.96	120.04
14	N	47	ALA	C-N-CA	-5.63	113.96	120.04
1	A	1355	A	C2'-C3'-O3'	5.62	117.92	109.50
1	A	1103	A	C2'-C3'-O3'	5.58	117.86	109.50
1	A	1196	C	C2'-C3'-O3'	5.54	117.81	109.50
3	C	82	U	C2'-C3'-O3'	5.53	122.00	113.70
1	A	1562	C	C4'-C3'-O3'	5.51	117.67	109.40
1	A	2269	U	C4'-C3'-O3'	5.50	117.65	109.40
1	A	2434	U	C2'-C3'-O3'	5.34	117.51	109.50
1	A	599	C	C2'-C3'-O3'	5.31	121.67	113.70
1	A	1355	A	C4'-C3'-O3'	5.29	117.34	109.40
1	A	1329	U	C2'-C3'-O3'	5.14	117.20	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1097	G	C4'-C3'-O3'	5.11	117.06	109.40
1	A	1556	C	C4'-C3'-O3'	5.11	117.06	109.40
1	A	3350	C	C2'-C3'-O3'	5.10	121.35	113.70
1	A	599	C	C3'-C2'-O2'	5.06	118.29	110.70
1	A	1064	A	C4'-C3'-O3'	5.04	116.95	109.40
1	A	1816	A	C2'-C3'-O3'	5.03	121.24	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	o	20	GLY	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	A	68535	0	34437	207	0
2	B	2579	0	1304	1	0
3	C	3353	0	1695	1	0
4	D	1914	0	1981	5	0
5	E	3075	0	3142	5	0
6	F	2748	0	2859	1	0
7	G	2375	0	2325	2	0
8	H	1239	0	1326	0	0
9	I	1784	0	1862	1	0
10	J	1804	0	1877	3	0
11	K	1518	0	1587	3	0
12	L	1705	0	1736	11	0
13	M	1353	0	1383	1	0
14	N	1543	0	1608	1	0
15	O	1053	0	1149	1	0
16	a	1720	0	1779	2	0
17	b	1555	0	1659	0	0
18	c	1420	0	1437	1	0
19	d	1441	0	1543	1	0
20	e	1521	0	1617	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	f	1445	0	1487	5	0
22	g	1276	0	1323	1	0
23	h	796	0	812	0	0
24	i	1003	0	1048	11	0
25	j	699	0	640	2	0
26	k	964	0	1025	0	0
27	l	993	0	1081	1	0
28	m	1092	0	1155	3	0
29	n	1173	0	1215	5	0
30	o	462	0	491	0	0
31	p	743	0	797	0	0
32	q	876	0	912	1	0
33	r	1020	0	1090	0	0
34	s	406	0	416	0	0
35	t	880	0	945	2	0
36	u	969	0	1078	0	0
37	v	771	0	849	0	0
38	w	681	0	687	0	0
39	x	612	0	682	0	0
40	y	436	0	475	0	0
41	z	417	0	459	0	0
42	Q	847	0	918	0	0
43	R	694	0	738	0	0
44	S	1050	0	247	2	0
45	V	1975	0	1984	72	0
46	A	84	0	0	0	0
46	C	1	0	0	0	0
46	i	1	0	0	0	0
47	A	3	0	0	0	0
48	A	10	0	0	2	0
48	c	1	0	0	0	0
48	e	1	0	0	0	0
All	All	126616	0	90860	320	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 2.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2434:U:O4	1:A:2595:A:N1	1.60	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:102:MET:CG	45:V:152:THR:HA	1.58	1.32
12:L:102:MET:HG3	45:V:152:THR:CA	1.63	1.28
45:V:388:ASN:O	45:V:390:ASP:N	1.73	1.21
1:A:2410:U:O4	1:A:2801:A:N1	1.87	1.06
1:A:2461:A:C4	1:A:2485:A:C2	2.45	1.04
1:A:2490:C:C2	1:A:2491:A:N6	2.28	1.02
1:A:1453:A:H61	1:A:1840:U:H3	1.07	1.02
1:A:2469:G:C6	1:A:2470:C:N4	2.32	0.97
1:A:2449:A:N1	1:A:2498:U:O2	1.97	0.97
1:A:2482:U:O4	1:A:2486:A:N6	1.98	0.96
1:A:2434:U:O4	1:A:2595:A:C2	2.19	0.95
1:A:78:U:H3	1:A:325:A:H61	1.08	0.95
1:A:2440:G:N2	1:A:2508:U:O2	2.00	0.95
1:A:2463:G:N2	1:A:2493:U:N3	2.15	0.95
1:A:2448:G:O6	1:A:2498:U:C2	2.20	0.94
1:A:2490:C:O2	1:A:2491:A:N7	2.01	0.94
1:A:2922:G:O6	45:V:235:THR:OG1	1.85	0.94
1:A:2636:A:H61	1:A:2641:U:H3	1.05	0.94
1:A:2448:G:C2	1:A:2499:U:O2	2.21	0.93
1:A:1190:A:H61	1:A:1315:U:H3	1.15	0.93
45:V:389:ILE:HG22	45:V:389:ILE:O	1.67	0.92
1:A:2461:A:C5	1:A:2485:A:C2	2.58	0.92
1:A:2448:G:O6	1:A:2498:U:O2	1.91	0.89
45:V:337:ASP:OD2	45:V:356:ARG:HG3	1.70	0.89
1:A:3077:A:N6	48:A:3501:HOH:O	2.04	0.89
1:A:1554:U:H3	1:A:1559:A:H61	1.14	0.89
12:L:102:MET:HG3	45:V:152:THR:HA	0.87	0.87
1:A:2450:G:N1	1:A:2497:U:N3	2.21	0.87
1:A:2450:G:H1	1:A:2497:U:H3	1.23	0.85
1:A:2658:G:N2	1:A:2713:U:O2	2.08	0.85
45:V:367:ASP:CG	45:V:400:LYS:NZ	2.35	0.84
1:A:2507:C:H5''	1:A:2507:C:H6	1.43	0.83
45:V:367:ASP:CG	45:V:400:LYS:HZ2	1.85	0.83
1:A:2463:G:N2	1:A:2493:U:C4	2.47	0.82
1:A:2636:A:N6	1:A:2641:U:H3	1.79	0.80
12:L:102:MET:CB	45:V:152:THR:HA	2.10	0.80
24:i:130:ALA:HA	24:i:133:SER:OG	1.80	0.80
1:A:2449:A:C2	1:A:2498:U:O2	2.36	0.79
1:A:2636:A:N1	1:A:2641:U:O4	2.16	0.79
45:V:372:TYR:CE1	45:V:398:VAL:HG21	2.20	0.77
1:A:78:U:O4	1:A:324:A:N1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:372:TYR:CE1	45:V:398:VAL:CG2	2.68	0.77
1:A:2445:A:N3	1:A:2502:A:C2	2.53	0.77
1:A:2469:G:C5	1:A:2470:C:N4	2.52	0.77
1:A:1554:U:H3	1:A:1559:A:N6	1.82	0.76
1:A:2876:C:H4'	45:V:233:THR:HB	1.67	0.76
45:V:368:SER:O	45:V:401:LEU:C	2.28	0.76
1:A:1190:A:N1	1:A:1315:U:O4	2.19	0.75
1:A:1453:A:N6	1:A:1840:U:H3	1.84	0.75
1:A:2448:G:N1	1:A:2499:U:C2	2.54	0.75
1:A:2449:A:C6	1:A:2498:U:O2	2.39	0.75
1:A:2469:G:N1	1:A:2470:C:N4	2.33	0.75
1:A:2249:G:C8	1:A:2272:G:C8	2.74	0.75
1:A:2437:G:C6	1:A:2438:A:C6	2.73	0.75
1:A:1481:A:O2'	1:A:1858:A:H1'	1.87	0.75
45:V:367:ASP:OD2	45:V:400:LYS:NZ	2.19	0.75
1:A:2439:A:C2	1:A:2440:G:C5	2.75	0.74
1:A:2451:G:H21	1:A:2495:C:N4	1.85	0.74
1:A:2463:G:N2	1:A:2493:U:H3	1.83	0.74
1:A:2493:U:C4	1:A:2494:A:C4	2.75	0.74
1:A:1188:U:O4	1:A:1317:A:N1	2.21	0.74
1:A:2410:U:O4	1:A:2801:A:C2	2.40	0.74
1:A:2490:C:H1'	1:A:2491:A:N7	2.03	0.74
1:A:78:U:H3	1:A:325:A:N6	1.84	0.74
1:A:2488:A:OP2	1:A:2490:C:N4	2.21	0.73
1:A:2253:G:O6	1:A:2263:C:N4	2.22	0.73
1:A:3064:U:O4	48:A:3501:HOH:O	2.07	0.73
1:A:2463:G:C2	1:A:2493:U:O4	2.43	0.72
45:V:372:TYR:HE1	45:V:398:VAL:CG2	2.03	0.71
1:A:1190:A:N6	1:A:1315:U:H3	1.86	0.71
1:A:1453:A:N1	1:A:1840:U:O4	2.25	0.70
1:A:2461:A:C5	1:A:2485:A:N1	2.60	0.69
1:A:2410:U:H3	1:A:2801:A:H61	1.39	0.69
1:A:2470:C:H1'	1:A:2489:C:O4'	1.92	0.68
1:A:2482:U:C4	1:A:2486:A:N6	2.59	0.68
45:V:323:VAL:HG13	45:V:336:ALA:HB1	1.76	0.68
1:A:2447:A:N1	1:A:2499:U:O4	2.27	0.68
1:A:2447:A:C2	1:A:2500:A:C2	2.82	0.68
1:A:2469:G:C2	1:A:2470:C:N4	2.62	0.67
1:A:2440:G:C2	1:A:2508:U:O2	2.47	0.66
1:A:78:U:O4	1:A:325:A:N1	2.28	0.66
1:A:2450:G:N2	1:A:2497:U:C2	2.62	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:261:LYS:O	45:V:265:LYS:HG3	1.96	0.66
45:V:401:LEU:HD13	45:V:401:LEU:O	1.96	0.66
1:A:2624:G:OP1	45:V:162:ARG:HD3	1.96	0.66
45:V:389:ILE:O	45:V:389:ILE:CG2	2.40	0.66
45:V:350:ASP:OD2	45:V:350:ASP:N	2.27	0.65
45:V:401:LEU:O	45:V:401:LEU:HD22	1.96	0.65
1:A:2490:C:N3	1:A:2491:A:N6	2.42	0.65
45:V:231:GLN:O	45:V:231:GLN:HG3	1.97	0.64
12:L:102:MET:HG3	45:V:152:THR:N	2.12	0.64
1:A:2437:G:C6	1:A:2438:A:C5	2.86	0.64
1:A:2448:G:N1	1:A:2499:U:O2	2.30	0.63
1:A:2249:G:N7	1:A:2272:G:C4	2.67	0.63
1:A:2469:G:H2'	1:A:2470:C:C6	2.35	0.62
45:V:373:PHE:HD1	45:V:395:VAL:HG22	1.64	0.62
45:V:342:ARG:HB2	45:V:345:ASP:HB2	1.80	0.62
45:V:369:VAL:HG12	45:V:400:LYS:HA	1.81	0.62
5:E:67:PHE:CE1	24:i:88:ARG:HB2	2.35	0.62
1:A:2493:U:C5	1:A:2494:A:C8	2.89	0.61
45:V:362:ILE:O	45:V:362:ILE:HG13	2.00	0.61
45:V:392:VAL:HG13	45:V:393:PRO:HD2	1.82	0.61
1:A:2452:G:N2	1:A:2462:A:C8	2.68	0.60
45:V:348:VAL:O	45:V:349:ASN:CB	2.49	0.60
1:A:2445:A:C2	1:A:2502:A:N1	2.69	0.60
1:A:2469:G:H2'	1:A:2470:C:C5	2.36	0.60
1:A:2463:G:N2	1:A:2464:U:C2	2.70	0.60
45:V:388:ASN:C	45:V:390:ASP:N	2.58	0.60
1:A:640:U:OP1	29:n:21:ARG:NH2	2.35	0.59
1:A:2461:A:C4	1:A:2485:A:H2	2.17	0.59
1:A:2439:A:C2	1:A:2440:G:C4	2.91	0.59
1:A:2656:A:N1	1:A:2713:U:O4	2.36	0.59
1:A:2450:G:N1	1:A:2497:U:C4	2.70	0.59
1:A:78:U:H3	1:A:324:A:N6	2.01	0.59
1:A:2449:A:N1	1:A:2498:U:C2	2.71	0.59
45:V:387:LEU:HD13	45:V:392:VAL:HG22	1.85	0.59
1:A:167:U:O2	1:A:256:G:N2	2.36	0.58
45:V:291:LEU:HD11	45:V:358:HIS:CB	2.34	0.58
1:A:324:A:C6	1:A:325:A:N6	2.72	0.58
1:A:2492:C:H2'	1:A:2493:U:C5	2.38	0.58
1:A:2445:A:C4	1:A:2502:A:N1	2.72	0.58
45:V:401:LEU:C	45:V:401:LEU:HD22	2.29	0.58
1:A:2451:G:N2	1:A:2495:C:N4	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:392:VAL:CG1	45:V:393:PRO:HD2	2.34	0.57
1:A:1661:G:H2'	1:A:1662:G:C8	2.39	0.57
1:A:2507:C:H6	1:A:2507:C:C5'	2.13	0.57
1:A:2445:A:C2	1:A:2502:A:C2	2.92	0.57
1:A:2253:G:C2	1:A:2264:U:C2	2.93	0.56
1:A:2482:U:H3	1:A:2486:A:H61	1.52	0.56
1:A:2446:U:H2'	1:A:2447:A:C8	2.40	0.56
1:A:2448:G:C6	1:A:2499:U:C2	2.94	0.56
1:A:2437:G:C5	1:A:2438:A:C5	2.94	0.56
1:A:2448:G:N2	1:A:2499:U:O2	2.39	0.56
1:A:103:G:OP1	14:N:70:ARG:NH2	2.39	0.56
45:V:162:ARG:NH2	45:V:193:ALA:HB3	2.21	0.55
1:A:2437:G:O6	1:A:2438:A:C6	2.59	0.55
1:A:2445:A:N3	1:A:2502:A:N1	2.55	0.55
1:A:2457:G:N2	1:A:2486:A:C2	2.74	0.55
45:V:318:PHE:CE2	45:V:342:ARG:HG2	2.41	0.55
45:V:388:ASN:HB3	45:V:391:TYR:HB2	1.88	0.55
1:A:2490:C:O2	1:A:2491:A:C5	2.59	0.54
1:A:324:A:N6	1:A:325:A:N6	2.55	0.54
19:d:71:LEU:HD13	19:d:99:THR:HG21	1.89	0.54
45:V:372:TYR:HE1	45:V:398:VAL:HG21	1.62	0.54
1:A:1820:U:O4'	1:A:1820:U:O2	2.25	0.54
1:A:2469:G:C4	1:A:2470:C:N4	2.75	0.54
1:A:2499:U:C4	1:A:2500:A:C5	2.96	0.54
1:A:662:U:H2'	1:A:663:C:C6	2.43	0.54
1:A:2469:G:C2	1:A:2470:C:C4	2.96	0.54
1:A:160:G:N2	1:A:262:U:O2	2.41	0.53
1:A:2249:G:H2'	1:A:2250:G:H8	1.73	0.53
1:A:78:U:N3	1:A:324:A:N6	2.57	0.53
1:A:2271:A:N7	1:A:2272:G:C6	2.76	0.53
12:L:102:MET:CG	45:V:152:THR:CA	2.43	0.53
1:A:1556:C:O2	1:A:1556:C:O4'	2.25	0.53
1:A:2493:U:H3'	1:A:2494:A:O4'	2.09	0.53
45:V:261:LYS:NZ	45:V:265:LYS:HD3	2.23	0.53
1:A:2499:U:O4	1:A:2500:A:C6	2.62	0.53
1:A:2507:C:H5''	1:A:2507:C:C6	2.34	0.53
2:B:121:U:O2	2:B:121:U:O4'	2.27	0.53
45:V:348:VAL:O	45:V:349:ASN:HB3	2.09	0.53
24:i:129:VAL:O	24:i:133:SER:OG	2.24	0.53
1:A:2456:A:H2'	1:A:2457:G:O4'	2.09	0.53
1:A:2445:A:C2	1:A:2502:A:C6	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3217:C:O2	1:A:3217:C:C2'	2.57	0.52
1:A:2449:A:C6	1:A:2498:U:C2	2.98	0.52
1:A:2410:U:C4	1:A:2801:A:N1	2.72	0.52
1:A:2490:C:C1'	1:A:2491:A:N7	2.72	0.52
15:O:38:ILE:HD11	21:f:148:LEU:HD23	1.92	0.52
24:i:93:LEU:HB2	25:j:20:LEU:HD22	1.92	0.52
1:A:2470:C:C4	1:A:2471:U:O4	2.62	0.52
1:A:3153:U:O4'	1:A:3153:U:O2	2.28	0.52
12:L:102:MET:C	45:V:154:THR:HG23	2.36	0.51
1:A:2438:A:H2'	1:A:2439:A:H8	1.76	0.51
1:A:2624:G:OP1	45:V:162:ARG:CD	2.58	0.51
4:D:201:GLY:HA2	4:D:204:MET:HE2	1.93	0.51
12:L:102:MET:HB2	45:V:152:THR:HA	1.91	0.51
1:A:2507:C:C5'	1:A:2507:C:C6	2.93	0.50
1:A:2438:A:H2'	1:A:2439:A:C8	2.47	0.50
1:A:3043:C:OP1	24:i:45:ARG:NE	2.44	0.50
1:A:2440:G:N2	1:A:2508:U:C2	2.78	0.50
1:A:1573:G:N3	1:A:1573:G:H2'	2.27	0.50
35:t:20:ILE:HD12	35:t:32:ALA:HB1	1.94	0.50
1:A:2463:G:C2	1:A:2493:U:C4	2.97	0.50
5:E:67:PHE:CE2	24:i:88:ARG:HD3	2.47	0.50
1:A:2470:C:O4'	1:A:2489:C:H1'	2.12	0.50
1:A:3354:U:O2	1:A:3354:U:O4'	2.29	0.50
5:E:67:PHE:CD2	24:i:88:ARG:HD3	2.46	0.50
1:A:2481:G:H2'	1:A:2482:U:C4	2.48	0.49
1:A:2270:A:N6	1:A:2271:A:C6	2.81	0.49
1:A:2481:G:H2'	1:A:2482:U:C5	2.48	0.49
7:G:148:ILE:HG13	7:G:159:VAL:HG11	1.95	0.49
1:A:2505:U:H1'	1:A:2506:U:N3	2.28	0.48
1:A:2463:G:N2	1:A:2493:U:O4	2.45	0.48
1:A:324:A:C6	1:A:325:A:C6	3.02	0.48
12:L:102:MET:O	45:V:154:THR:CG2	2.62	0.48
45:V:355:VAL:HG21	45:V:395:VAL:O	2.12	0.48
1:A:2448:G:C6	1:A:2499:U:N3	2.82	0.48
1:A:2461:A:N9	1:A:2485:A:H2	2.11	0.48
10:J:71:VAL:HG12	16:a:21:PHE:CZ	2.49	0.48
24:i:132:ASN:N	24:i:132:ASN:ND2	2.60	0.48
1:A:2469:G:C4	1:A:2470:C:C5	3.02	0.47
1:A:2267:C:H2'	1:A:2268:U:C6	2.49	0.47
1:A:2505:U:H1'	1:A:2506:U:H3	1.79	0.47
1:A:2506:U:C3'	1:A:2506:U:C6	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2439:A:N1	1:A:2440:G:C6	2.82	0.47
5:E:67:PHE:CZ	24:i:88:ARG:HB2	2.50	0.47
7:G:38:THR:HG22	22:g:30:TYR:HB3	1.95	0.47
45:V:174:LEU:O	45:V:178:ILE:HG22	2.15	0.47
45:V:290:THR:O	45:V:291:LEU:C	2.57	0.47
1:A:2249:G:C4	1:A:2250:G:C8	3.03	0.47
24:i:33:ASN:C	24:i:34:LEU:HD23	2.40	0.47
45:V:218:VAL:HG22	45:V:219:PRO:HD2	1.96	0.46
45:V:387:LEU:HD13	45:V:392:VAL:CG2	2.46	0.46
1:A:2493:U:C4	1:A:2494:A:C5	3.03	0.46
1:A:3018:C:H2'	1:A:3019:U:C6	2.50	0.46
29:n:3:SER:O	29:n:6:THR:HG22	2.16	0.46
45:V:317:GLU:HA	45:V:370:MET:HE3	1.96	0.46
45:V:399:LYS:O	45:V:400:LYS:O	2.33	0.46
29:n:7:LYS:O	29:n:11:HIS:ND1	2.49	0.46
12:L:102:MET:C	45:V:154:THR:CG2	2.89	0.46
44:S:187:UNK:O	44:S:188:UNK:CB	2.63	0.46
1:A:2476:C:H2'	1:A:2477:G:H4'	1.98	0.45
1:A:1103:A:N6	1:A:1363:A:O2'	2.49	0.45
1:A:2467:G:O5'	1:A:2467:G:H8	1.99	0.45
1:A:2253:G:N1	1:A:2264:U:C4	2.84	0.45
45:V:162:ARG:HH22	45:V:193:ALA:HB3	1.82	0.45
1:A:2506:U:H3'	1:A:2507:C:H5''	1.98	0.45
45:V:323:VAL:CG1	45:V:336:ALA:HB1	2.46	0.45
1:A:2236:G:O2'	45:V:269:ASN:HB2	2.17	0.45
1:A:2437:G:H2'	1:A:2438:A:C8	2.52	0.45
45:V:364:HIS:CB	45:V:367:ASP:OD2	2.64	0.45
16:a:93:LYS:O	16:a:94:TYR:CB	2.65	0.45
1:A:2249:G:C5	1:A:2250:G:N7	2.85	0.44
1:A:2689:A:H2'	1:A:2689:A:N3	2.32	0.44
45:V:280:SER:OG	45:V:281:ASN:N	2.49	0.44
1:A:2253:G:C6	1:A:2264:U:C4	3.05	0.44
1:A:2493:U:O4	1:A:2494:A:C5	2.70	0.44
11:K:41:ILE:HD11	11:K:67:ALA:HB1	1.99	0.44
1:A:2270:A:C6	1:A:2271:A:C6	3.05	0.44
1:A:2270:A:C5	1:A:2271:A:C5	3.06	0.44
1:A:1307:G:O2'	1:A:1308:A:OP2	2.31	0.44
1:A:2452:G:O2'	1:A:2462:A:OP2	2.31	0.44
1:A:2180:G:H2'	1:A:2181:C:C6	2.52	0.44
1:A:2922:G:C6	45:V:235:THR:OG1	2.55	0.44
45:V:261:LYS:HZ1	45:V:265:LYS:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2439:A:C8	1:A:2439:A:O5'	2.71	0.44
4:D:112:ILE:HG23	4:D:133:TYR:HB2	1.99	0.44
1:A:2461:A:N9	1:A:2485:A:C2	2.81	0.43
1:A:3214:U:O2	1:A:3214:U:O4'	2.33	0.43
1:A:2838:A:N6	1:A:2850:G:O2'	2.50	0.43
3:C:25:G:N7	27:l:13:ARG:NH2	2.65	0.43
6:F:181:VAL:HG11	6:F:224:GLY:HA3	2.00	0.43
1:A:1913:A:N3	1:A:2120:A:H2'	2.32	0.43
21:f:77:VAL:HG11	21:f:106:LEU:HD13	2.00	0.43
9:I:98:LYS:HB3	9:I:99:PRO:HD3	2.01	0.43
1:A:2506:U:H3'	1:A:2506:U:H6	1.84	0.43
28:m:24:VAL:HG11	28:m:87:LEU:HD23	2.00	0.43
1:A:706:A:H2'	1:A:707:U:O4'	2.17	0.43
1:A:3277:U:O2	1:A:3277:U:O4'	2.34	0.43
32:q:29:ALA:HB3	32:q:30:PRO:HD3	2.01	0.43
45:V:291:LEU:HD23	45:V:334:VAL:HG11	1.51	0.43
1:A:2439:A:N1	1:A:2440:G:C5	2.87	0.43
1:A:2606:G:H2'	1:A:2606:G:N3	2.34	0.43
1:A:2469:G:O6	1:A:2474:G:N1	2.51	0.42
29:n:112:ILE:HB	29:n:130:VAL:HG12	2.01	0.42
1:A:2459:A:N1	1:A:2487:U:C2	2.87	0.42
4:D:204:MET:HE3	4:D:209:HIS:HB2	2.01	0.42
12:L:36:LEU:HD11	12:L:69:ARG:HD3	2.00	0.42
28:m:81:LEU:HD11	35:t:90:ILE:HD13	2.00	0.42
45:V:371:GLY:HA3	45:V:397:LEU:HA	2.01	0.42
45:V:155:TRP:CZ3	45:V:158:THR:OG1	2.72	0.42
20:e:130:ASN:O	20:e:132:PHE:N	2.53	0.42
29:n:77:LYS:O	29:n:79:TRP:N	2.53	0.42
1:A:2270:A:N6	1:A:2271:A:N1	2.68	0.42
1:A:2470:C:N4	1:A:2474:G:H22	2.18	0.42
1:A:2439:A:H8	1:A:2439:A:O5'	2.03	0.42
1:A:2446:U:H2'	1:A:2447:A:H8	1.84	0.42
1:A:2493:U:H2'	1:A:2494:A:O4'	2.19	0.42
1:A:1554:U:O4	1:A:1559:A:N1	2.52	0.42
1:A:2499:U:C5	1:A:2500:A:N7	2.88	0.42
10:J:140:VAL:HG22	10:J:166:LEU:HD21	2.01	0.42
1:A:2213:A:H2'	1:A:2214:A:C8	2.55	0.42
18:c:29:THR:HG21	18:c:146:ILE:HD11	2.01	0.42
1:A:2437:G:C5	1:A:2438:A:N7	2.89	0.41
45:V:388:ASN:C	45:V:388:ASN:HD22	2.26	0.41
1:A:2461:A:N7	1:A:2485:A:N1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:ILE:O	10:J:76:ALA:HB3	2.20	0.41
21:f:12:ARG:HB3	21:f:24:LEU:HD23	2.00	0.41
21:f:132:THR:O	21:f:133:ALA:HB3	2.21	0.41
1:A:78:U:C4	1:A:325:A:N1	2.88	0.41
1:A:436:A:H2'	1:A:437:G:O4'	2.20	0.41
13:M:12:LEU:HD12	13:M:131:MET:HE3	2.02	0.41
45:V:384:PHE:O	45:V:387:LEU:HB2	2.20	0.41
1:A:1188:U:C4	1:A:1317:A:N1	2.89	0.41
1:A:3017:A:C6	1:A:3018:C:C4	3.08	0.41
28:m:16:GLY:O	28:m:18:TYR:N	2.53	0.41
1:A:2424:A:N1	4:D:230:VAL:HG11	2.36	0.41
45:V:355:VAL:HG22	45:V:356:ARG:O	2.20	0.41
1:A:1793:C:C4	4:D:179:LEU:HD11	2.55	0.41
1:A:2410:U:H3	1:A:2801:A:N6	2.11	0.41
1:A:2456:A:O2'	1:A:2457:G:C4'	2.69	0.41
5:E:256:HIS:HA	5:E:257:PRO:C	2.44	0.41
11:K:112:ILE:HD13	11:K:161:LEU:HD12	2.03	0.41
11:K:22:SER:OG	11:K:23:ARG:N	2.42	0.41
45:V:265:LYS:HB3	45:V:265:LYS:HE3	1.72	0.41
45:V:291:LEU:HD11	45:V:358:HIS:HB2	2.01	0.41
1:A:2493:U:C3'	1:A:2494:A:O4'	2.69	0.41
24:i:95:PHE:CE1	25:j:22:VAL:HG11	2.56	0.41
45:V:367:ASP:CB	45:V:400:LYS:NZ	2.84	0.41
1:A:2249:G:C8	1:A:2272:G:N7	2.90	0.40
1:A:2191:U:H2'	1:A:2192:C:O4'	2.21	0.40
1:A:2490:C:OP1	44:S:204:UNK:O	2.38	0.40
1:A:2469:G:C4	1:A:2470:C:C4	3.10	0.40
1:A:2485:A:H8	1:A:2485:A:O5'	2.05	0.40
1:A:527:A:N6	1:A:566:G:C6	2.90	0.40
1:A:2594:C:C5	1:A:2595:A:C2	3.09	0.40
21:f:90:MET:HE1	21:f:114:HIS:NE2	2.36	0.40
45:V:218:VAL:HG22	45:V:219:PRO:CD	2.52	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	D	250/254 (98%)	228 (91%)	20 (8%)	2 (1%)	16	52
5	E	384/387 (99%)	343 (89%)	34 (9%)	7 (2%)	6	33
6	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	2	18
7	G	294/297 (99%)	267 (91%)	19 (6%)	8 (3%)	4	26
8	H	152/176 (86%)	137 (90%)	12 (8%)	3 (2%)	6	32
9	I	220/244 (90%)	203 (92%)	14 (6%)	3 (1%)	9	39
10	J	231/256 (90%)	202 (87%)	24 (10%)	5 (2%)	5	29
11	K	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
12	L	207/221 (94%)	187 (90%)	17 (8%)	3 (1%)	9	39
13	M	167/174 (96%)	145 (87%)	15 (9%)	7 (4%)	2	18
14	N	191/199 (96%)	170 (89%)	19 (10%)	2 (1%)	12	47
15	O	134/138 (97%)	125 (93%)	5 (4%)	4 (3%)	3	23
16	a	201/204 (98%)	189 (94%)	9 (4%)	3 (2%)	8	38
17	b	195/199 (98%)	187 (96%)	7 (4%)	1 (0%)	24	62
18	c	181/184 (98%)	161 (89%)	20 (11%)	0	100	100
19	d	183/186 (98%)	169 (92%)	11 (6%)	3 (2%)	7	37
20	e	186/189 (98%)	175 (94%)	7 (4%)	4 (2%)	5	29
21	f	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	10	42
22	g	157/160 (98%)	142 (90%)	12 (8%)	3 (2%)	6	32
23	h	98/121 (81%)	84 (86%)	13 (13%)	1 (1%)	12	47
24	i	134/137 (98%)	126 (94%)	7 (5%)	1 (1%)	18	54
25	j	96/155 (62%)	83 (86%)	10 (10%)	3 (3%)	3	23
26	k	119/142 (84%)	111 (93%)	7 (6%)	1 (1%)	16	52
27	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	7	37
28	m	133/136 (98%)	113 (85%)	18 (14%)	2 (2%)	8	38
29	n	146/149 (98%)	125 (86%)	16 (11%)	5 (3%)	3	21
30	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	1	16
31	p	95/105 (90%)	89 (94%)	6 (6%)	0	100	100
32	q	107/113 (95%)	98 (92%)	7 (6%)	2 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	r	125/130 (96%)	115 (92%)	8 (6%)	2 (2%)	7	37
34	s	48/107 (45%)	46 (96%)	2 (4%)	0	100	100
35	t	110/121 (91%)	105 (96%)	3 (3%)	2 (2%)	6	33
36	u	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	4	26
37	v	97/100 (97%)	88 (91%)	7 (7%)	2 (2%)	5	30
38	w	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
39	x	75/78 (96%)	68 (91%)	4 (5%)	3 (4%)	2	19
40	y	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
41	z	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6	32
42	Q	103/106 (97%)	88 (85%)	11 (11%)	4 (4%)	2	19
43	R	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	V	249/917 (27%)	222 (89%)	20 (8%)	7 (3%)	4	25
All	All	6355/7475 (85%)	5756 (91%)	479 (8%)	120 (2%)	8	32

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	292	SER
9	I	178	ILE
10	J	31	PRO
10	J	157	VAL
14	N	47	ALA
16	a	94	TYR
20	e	131	ALA
22	g	124	VAL
25	j	81	PRO
42	Q	30	ALA
45	V	185	VAL
45	V	389	ILE
45	V	400	LYS
4	D	144	ASN
5	E	347	SER
5	E	348	ARG
5	E	351	LEU
6	F	130	ALA
6	F	131	VAL
6	F	182	LEU
6	F	293	SER

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Mol	Chain	Res	Type
7	G	87	GLY
8	H	98	VAL
9	I	159	GLN
10	J	36	ILE
10	J	79	GLN
13	M	10	ARG
13	M	95	ASN
15	O	8	LYS
19	d	41	ASP
25	j	97	LYS
27	l	84	LYS
29	n	77	LYS
45	V	390	ASP
5	E	187	SER
6	F	140	HIS
6	F	173	GLY
6	F	233	LEU
6	F	268	ALA
6	F	269	SER
7	G	258	LYS
7	G	259	LYS
7	G	260	PHE
8	H	5	LYS
10	J	25	PRO
12	L	24	ARG
13	M	114	ILE
15	O	9	ALA
15	O	29	ALA
17	b	187	GLU
19	d	98	LYS
21	f	24	LEU
22	g	159	PHE
26	k	50	ALA
28	m	17	ARG
29	n	66	ALA
30	o	25	LYS
33	r	40	SER
35	t	46	ASP
36	u	84	LYS
39	x	18	ALA
39	x	33	LYS
42	Q	34	SER

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Mol	Chain	Res	Type
45	V	194	LYS
6	F	338	LYS
7	G	21	ARG
12	L	218	ALA
13	M	8	PRO
13	M	9	MET
13	M	117	ASP
14	N	166	ALA
19	d	162	ALA
20	e	53	LYS
20	e	178	ALA
21	f	167	ARG
28	m	59	ALA
32	q	82	GLU
33	r	12	LYS
37	v	3	VAL
39	x	34	ALA
41	z	79	GLU
42	Q	17	CYS
42	Q	60	LYS
45	V	349	ASN
5	E	155	ALA
6	F	82	THR
6	F	232	SER
6	F	311	HIS
7	G	251	PRO
7	G	253	PHE
12	L	220	GLN
13	M	108	GLU
23	h	11	ILE
27	l	126	LEU
30	o	29	TYR
36	u	39	PRO
36	u	75	TYR
4	D	125	ALA
6	F	189	ALA
7	G	125	VAL
16	a	81	TYR
16	a	184	LYS
20	e	129	GLY
22	g	125	ALA
29	n	15	VAL

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Mol	Chain	Res	Type
29	n	47	LYS
32	q	7	VAL
24	i	3	GLY
29	n	56	VAL
45	V	327	GLY
5	E	317	ILE
35	t	77	GLY
37	v	21	THR
6	F	317	PRO
15	O	6	ILE
25	j	80	ARG
30	o	21	ILE
9	I	191	VAL
5	E	90	VAL
8	H	6	ALA

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	D	193/196 (98%)	183 (95%)	10 (5%)	21	44
5	E	318/323 (98%)	302 (95%)	16 (5%)	22	44
6	F	288/289 (100%)	274 (95%)	14 (5%)	22	45
7	G	244/245 (100%)	225 (92%)	19 (8%)	11	33
8	H	134/153 (88%)	129 (96%)	5 (4%)	30	51
9	I	186/205 (91%)	173 (93%)	13 (7%)	14	37
10	J	187/208 (90%)	174 (93%)	13 (7%)	14	37
11	K	171/171 (100%)	160 (94%)	11 (6%)	16	38
12	L	177/187 (95%)	164 (93%)	13 (7%)	13	35
13	M	147/150 (98%)	139 (95%)	8 (5%)	20	43
14	N	154/159 (97%)	142 (92%)	12 (8%)	11	33
15	O	107/109 (98%)	101 (94%)	6 (6%)	19	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	a	175/176 (99%)	166 (95%)	9 (5%)	21	44
17	b	160/162 (99%)	155 (97%)	5 (3%)	35	56
18	c	140/146 (96%)	132 (94%)	8 (6%)	18	42
19	d	150/151 (99%)	145 (97%)	5 (3%)	33	55
20	e	153/154 (99%)	146 (95%)	7 (5%)	24	46
21	f	156/156 (100%)	150 (96%)	6 (4%)	29	51
22	g	136/137 (99%)	125 (92%)	11 (8%)	11	32
23	h	87/107 (81%)	86 (99%)	1 (1%)	65	73
24	i	104/105 (99%)	101 (97%)	3 (3%)	37	58
25	j	57/129 (44%)	57 (100%)	0	100	100
26	k	104/118 (88%)	96 (92%)	8 (8%)	12	33
27	l	109/110 (99%)	103 (94%)	6 (6%)	19	43
28	m	115/116 (99%)	109 (95%)	6 (5%)	21	44
29	n	118/119 (99%)	113 (96%)	5 (4%)	26	49
30	o	46/47 (98%)	43 (94%)	3 (6%)	15	38
31	p	81/88 (92%)	80 (99%)	1 (1%)	63	73
32	q	92/97 (95%)	87 (95%)	5 (5%)	20	43
33	r	109/111 (98%)	101 (93%)	8 (7%)	13	35
34	s	43/91 (47%)	42 (98%)	1 (2%)	44	64
35	t	95/103 (92%)	93 (98%)	2 (2%)	47	65
36	u	104/105 (99%)	99 (95%)	5 (5%)	23	45
37	v	81/82 (99%)	73 (90%)	8 (10%)	7	25
38	w	70/71 (99%)	67 (96%)	3 (4%)	26	48
39	x	68/69 (99%)	67 (98%)	1 (2%)	57	70
40	y	45/46 (98%)	43 (96%)	2 (4%)	25	48
41	z	47/116 (40%)	45 (96%)	2 (4%)	26	48
42	Q	90/91 (99%)	83 (92%)	7 (8%)	11	33
43	R	71/72 (99%)	69 (97%)	2 (3%)	38	59
45	V	224/791 (28%)	198 (88%)	26 (12%)	5	20
All	All	5336/6261 (85%)	5040 (94%)	296 (6%)	21	43

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	17	THR
4	D	23	ARG
4	D	74	GLU
4	D	96	LEU
4	D	116	VAL
4	D	122	ASP
4	D	134	VAL
4	D	207	VAL
4	D	227	ARG
4	D	230	VAL
5	E	10	ARG
5	E	19	ARG
5	E	25	ILE
5	E	85	VAL
5	E	115	LYS
5	E	169	THR
5	E	188	ILE
5	E	232	ARG
5	E	238	LEU
5	E	252	ILE
5	E	296	THR
5	E	305	ILE
5	E	324	VAL
5	E	339	ARG
5	E	351	LEU
5	E	364	LYS
6	F	52	VAL
6	F	67	THR
6	F	69	ARG
6	F	73	ARG
6	F	74	ILE
6	F	99	MET
6	F	112	LYS
6	F	150	LEU
6	F	154	THR
6	F	179	LEU
6	F	182	LEU
6	F	246	ARG
6	F	307	GLN
6	F	361	HIS
7	G	13	SER
7	G	15	ARG
7	G	18	THR

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Mol	Chain	Res	Type
7	G	22	ARG
7	G	23	ARG
7	G	24	ARG
7	G	41	LYS
7	G	75	LEU
7	G	92	LEU
7	G	105	ILE
7	G	115	LEU
7	G	131	LEU
7	G	151	GLN
7	G	193	GLU
7	G	204	VAL
7	G	211	LEU
7	G	259	LYS
7	G	273	ARG
7	G	279	LYS
8	H	34	LEU
8	H	64	LEU
8	H	65	ILE
8	H	84	VAL
8	H	155	LEU
9	I	24	GLU
9	I	82	LYS
9	I	83	LEU
9	I	84	VAL
9	I	88	ARG
9	I	92	ILE
9	I	124	LEU
9	I	125	GLU
9	I	129	LEU
9	I	145	ARG
9	I	179	LEU
9	I	218	ARG
9	I	239	LEU
10	J	41	GLN
10	J	57	ARG
10	J	63	LYS
10	J	65	LEU
10	J	92	LYS
10	J	136	LEU
10	J	150	LEU
10	J	163	VAL

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Mol	Chain	Res	Type
10	J	169	LEU
10	J	201	THR
10	J	232	HIS
10	J	240	ASN
10	J	248	LYS
11	K	5	GLN
11	K	23	ARG
11	K	41	ILE
11	K	48	VAL
11	K	49	ASN
11	K	52	LEU
11	K	118	LEU
11	K	139	ASN
11	K	164	ILE
11	K	166	ARG
11	K	177	ASP
12	L	7	ARG
12	L	30	LYS
12	L	33	ILE
12	L	40	LYS
12	L	48	LEU
12	L	52	LEU
12	L	90	ARG
12	L	115	MET
12	L	163	GLN
12	L	165	ILE
12	L	169	LYS
12	L	203	LYS
12	L	208	ASN
13	M	12	LEU
13	M	13	LYS
13	M	40	LEU
13	M	80	LEU
13	M	81	GLU
13	M	107	ASP
13	M	130	VAL
13	M	142	LYS
14	N	23	LYS
14	N	24	VAL
14	N	36	ARG
14	N	49	ARG
14	N	58	VAL

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Mol	Chain	Res	Type
14	N	67	ARG
14	N	101	ARG
14	N	104	ARG
14	N	124	ILE
14	N	131	LYS
14	N	136	GLU
14	N	190	LYS
15	O	7	VAL
15	O	12	TRP
15	O	20	VAL
15	O	28	SER
15	O	53	VAL
15	O	72	LEU
16	a	22	LEU
16	a	27	VAL
16	a	50	ARG
16	a	133	ILE
16	a	138	GLN
16	a	174	ILE
16	a	180	PHE
16	a	183	THR
16	a	201	ARG
17	b	34	VAL
17	b	43	ILE
17	b	124	LEU
17	b	125	ARG
17	b	155	LYS
18	c	24	VAL
18	c	52	LEU
18	c	112	LEU
18	c	120	ASN
18	c	125	GLN
18	c	127	ARG
18	c	168	LEU
18	c	180	LYS
19	d	26	LEU
19	d	39	ARG
19	d	49	LEU
19	d	135	GLN
19	d	138	LEU
20	e	17	VAL
20	e	25	ASP

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Mol	Chain	Res	Type
20	e	44	LEU
20	e	74	ARG
20	e	99	LEU
20	e	103	ARG
20	e	138	LEU
21	f	12	ARG
21	f	45	LEU
21	f	50	LYS
21	f	61	ILE
21	f	71	LYS
21	f	137	ARG
22	g	12	ARG
22	g	32	LYS
22	g	75	ILE
22	g	79	MET
22	g	80	VAL
22	g	83	ARG
22	g	96	ILE
22	g	102	ARG
22	g	126	VAL
22	g	127	GLN
22	g	128	LEU
23	h	10	LYS
24	i	34	LEU
24	i	83	LYS
24	i	132	ASN
26	k	34	LEU
26	k	63	ILE
26	k	70	GLU
26	k	115	ARG
26	k	125	ARG
26	k	133	LEU
26	k	135	ILE
26	k	142	ILE
27	l	13	ARG
27	l	37	LYS
27	l	50	ILE
27	l	56	VAL
27	l	76	LEU
27	l	126	LEU
28	m	14	VAL
28	m	24	VAL

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Mol	Chain	Res	Type
28	m	34	LYS
28	m	120	GLU
28	m	121	ARG
28	m	126	LYS
29	n	34	MET
29	n	56	VAL
29	n	120	ASN
29	n	130	VAL
29	n	133	LEU
30	o	22	LYS
30	o	25	LYS
30	o	59	LYS
31	p	87	VAL
32	q	16	LEU
32	q	55	LEU
32	q	79	ARG
32	q	82	GLU
32	q	86	LYS
33	r	19	ARG
33	r	27	ARG
33	r	33	ARG
33	r	44	ARG
33	r	47	ARG
33	r	75	LEU
33	r	125	ARG
33	r	128	LEU
34	s	37	THR
35	t	29	ILE
35	t	58	ARG
36	u	20	GLN
36	u	21	LEU
36	u	71	LYS
36	u	115	LYS
36	u	119	LYS
37	v	7	ILE
37	v	20	MET
37	v	26	ILE
37	v	45	ARG
37	v	57	LEU
37	v	58	ILE
37	v	75	LYS
37	v	76	ARG

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Mol	Chain	Res	Type
38	w	17	THR
38	w	24	ARG
38	w	25	ARG
39	x	67	GLN
40	y	21	ARG
40	y	23	LEU
41	z	85	LEU
41	z	127	LEU
42	Q	35	LEU
42	Q	61	LYS
42	Q	71	ARG
42	Q	78	LYS
42	Q	83	LEU
42	Q	99	GLN
42	Q	100	LYS
43	R	31	ILE
43	R	45	LYS
45	V	162	ARG
45	V	164	LYS
45	V	171	PHE
45	V	177	LEU
45	V	179	LEU
45	V	185	VAL
45	V	209	LYS
45	V	221	LYS
45	V	228	LEU
45	V	265	LYS
45	V	278	LYS
45	V	286	MET
45	V	291	LEU
45	V	299	SER
45	V	307	ASN
45	V	350	ASP
45	V	362	ILE
45	V	364	HIS
45	V	370	MET
45	V	376	ASN
45	V	387	LEU
45	V	390	ASP
45	V	391	TYR
45	V	397	LEU
45	V	400	LYS

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Mol	Chain	Res	Type
45	V	401	LEU

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

Mol	Chain	Res	Type
4	D	8	GLN
4	D	115	ASN
5	E	11	HIS
6	F	48	GLN
6	F	114	ASN
6	F	175	HIS
6	F	213	ASN
6	F	311	HIS
7	G	32	GLN
7	G	90	HIS
7	G	206	GLN
7	G	264	GLN
8	H	4	GLN
8	H	167	ASN
9	I	52	GLN
9	I	81	HIS
9	I	93	ASN
9	I	197	GLN
9	I	231	ASN
10	J	79	GLN
10	J	145	ASN
10	J	192	GLN
10	J	240	ASN
11	K	5	GLN
11	K	49	ASN
11	K	59	ASN
11	K	96	HIS
11	K	139	ASN
12	L	14	ASN
12	L	123	HIS
12	L	163	GLN
13	M	20	ASN
13	M	43	GLN
14	N	19	GLN
14	N	25	HIS
14	N	103	ASN
16	a	15	GLN

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Mol	Chain	Res	Type
16	a	87	GLN
17	b	42	ASN
17	b	72	HIS
17	b	182	ASN
17	b	193	GLN
18	c	55	GLN
18	c	97	ASN
18	c	133	HIS
18	c	172	GLN
19	d	15	HIS
19	d	73	GLN
19	d	135	GLN
20	e	34	GLN
20	e	36	ASN
20	e	39	ASN
20	e	68	GLN
20	e	166	ASN
21	f	63	GLN
21	f	65	ASN
22	g	26	HIS
22	g	54	HIS
22	g	103	GLN
23	h	52	ASN
23	h	101	ASN
24	i	132	ASN
26	k	85	GLN
27	l	42	GLN
28	m	106	GLN
28	m	127	ASN
29	n	62	HIS
29	n	64	GLN
30	o	17	HIS
32	q	43	HIS
33	r	13	HIS
33	r	20	HIS
33	r	88	HIS
33	r	98	HIS
33	r	104	ASN
34	s	24	ASN
35	t	69	HIS
36	u	16	GLN
40	y	4	GLN

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Mol	Chain	Res	Type
40	y	20	ASN
41	z	90	ASN
42	Q	47	GLN
42	Q	82	GLN
45	V	160	GLN
45	V	163	GLN
45	V	231	GLN
45	V	272	GLN
45	V	332	ASN
45	V	349	ASN
45	V	351	GLN
45	V	378	ASN
45	V	388	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3201/3396 (94%)	779 (24%)	77 (2%)
2	B	120/121 (99%)	22 (18%)	2 (1%)
3	C	157/158 (99%)	38 (24%)	3 (1%)
All	All	3478/3675 (94%)	839 (24%)	82 (2%)

All (839) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	A
1	A	22	G
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
1	A	75	G
1	A	89	A
1	A	92	G
1	A	105	C
1	A	109	A

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Mol	Chain	Res	Type
1	A	110	G
1	A	111	C
1	A	116	A
1	A	118	U
1	A	122	A
1	A	123	A
1	A	136	G
1	A	137	G
1	A	143	G
1	A	150	A
1	A	156	G
1	A	157	A
1	A	161	G
1	A	166	C
1	A	167	U
1	A	168	U
1	A	170	G
1	A	173	G
1	A	177	U
1	A	182	U
1	A	184	U
1	A	187	A
1	A	190	U
1	A	191	U
1	A	192	C
1	A	198	A
1	A	200	C
1	A	210	U
1	A	211	A
1	A	218	G
1	A	219	A
1	A	240	U
1	A	241	G
1	A	243	G
1	A	245	U
1	A	246	U
1	A	247	C
1	A	249	U
1	A	250	U
1	A	252	U
1	A	266	A
1	A	269	G

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Mol	Chain	Res	Type
1	A	286	U
1	A	295	A
1	A	305	U
1	A	315	C
1	A	317	A
1	A	323	A
1	A	329	U
1	A	338	A
1	A	339	C
1	A	376	G
1	A	381	U
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	417	A
1	A	420	G
1	A	421	G
1	A	422	A
1	A	429	U
1	A	436	A
1	A	439	C
1	A	440	A
1	A	495	G
1	A	507	U
1	A	510	G
1	A	518	G
1	A	519	A
1	A	520	U
1	A	521	A
1	A	523	A
1	A	526	C
1	A	531	G
1	A	536	U
1	A	539	C
1	A	541	U
1	A	543	C
1	A	546	C
1	A	547	G

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Mol	Chain	Res	Type
1	A	548	G
1	A	549	U
1	A	551	A
1	A	553	U
1	A	555	U
1	A	556	U
1	A	557	A
1	A	559	A
1	A	560	G
1	A	569	A
1	A	570	A
1	A	579	G
1	A	588	G
1	A	589	A
1	A	592	A
1	A	598	A
1	A	600	G
1	A	604	G
1	A	611	A
1	A	619	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	634	C
1	A	636	C
1	A	649	A
1	A	660	A
1	A	662	U
1	A	676	G
1	A	677	A
1	A	681	U
1	A	683	U
1	A	684	G
1	A	687	U
1	A	689	U
1	A	690	A
1	A	691	A
1	A	696	C
1	A	705	A
1	A	710	A
1	A	712	G
1	A	715	A

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Mol	Chain	Res	Type
1	A	716	A
1	A	720	A
1	A	725	G
1	A	735	A
1	A	739	G
1	A	748	U
1	A	764	U
1	A	766	U
1	A	767	U
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G
1	A	785	G
1	A	786	A
1	A	792	G
1	A	799	G
1	A	801	A
1	A	806	A
1	A	808	A
1	A	814	U
1	A	817	A
1	A	830	A
1	A	849	C
1	A	857	G
1	A	861	C
1	A	868	C
1	A	874	U
1	A	879	U
1	A	890	C
1	A	894	G
1	A	895	A
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	911	C
1	A	914	A
1	A	916	G
1	A	917	A
1	A	921	A

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Mol	Chain	Res	Type
1	A	923	C
1	A	925	A
1	A	937	G
1	A	941	G
1	A	944	C
1	A	958	C
1	A	959	C
1	A	960	U
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	1001	G
1	A	1002	A
1	A	1009	A
1	A	1010	G
1	A	1013	G
1	A	1015	U
1	A	1017	C
1	A	1018	G
1	A	1019	G
1	A	1021	G
1	A	1024	G
1	A	1025	A
1	A	1026	A
1	A	1029	G
1	A	1030	A
1	A	1031	C
1	A	1034	U
1	A	1036	A
1	A	1037	C
1	A	1040	A
1	A	1041	U
1	A	1047	A
1	A	1049	C
1	A	1057	A
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1073	U

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Mol	Chain	Res	Type
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	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	1129	A
1	A	1131	G
1	A	1140	G
1	A	1153	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1188	U
1	A	1191	U
1	A	1192	C
1	A	1200	A
1	A	1201	C
1	A	1208	U
1	A	1212	A
1	A	1213	G
1	A	1217	A
1	A	1219	C
1	A	1222	G
1	A	1223	A
1	A	1230	G
1	A	1232	C
1	A	1236	G
1	A	1237	G
1	A	1240	A
1	A	1241	U
1	A	1242	G
1	A	1243	G
1	A	1244	A
1	A	1245	A
1	A	1246	G
1	A	1247	U
1	A	1248	C

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Mol	Chain	Res	Type
1	A	1249	G
1	A	1253	U
1	A	1257	C
1	A	1258	U
1	A	1260	A
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1266	G
1	A	1267	U
1	A	1270	A
1	A	1271	A
1	A	1272	C
1	A	1274	A
1	A	1276	U
1	A	1278	A
1	A	1279	C
1	A	1285	G
1	A	1287	A
1	A	1289	G
1	A	1305	U
1	A	1307	G
1	A	1308	A
1	A	1309	U
1	A	1313	G
1	A	1316	C
1	A	1325	U
1	A	1329	U
1	A	1330	A
1	A	1331	U
1	A	1340	G
1	A	1348	U
1	A	1349	G
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1356	U
1	A	1357	G
1	A	1364	C
1	A	1383	G
1	A	1385	C
1	A	1386	A

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Mol	Chain	Res	Type
1	A	1392	G
1	A	1393	A
1	A	1399	A
1	A	1400	G
1	A	1414	G
1	A	1416	C
1	A	1419	A
1	A	1434	G
1	A	1437	C
1	A	1446	A
1	A	1450	G
1	A	1455	U
1	A	1460	A
1	A	1481	A
1	A	1482	A
1	A	1498	A
1	A	1500	G
1	A	1508	C
1	A	1512	U
1	A	1527	C
1	A	1531	C
1	A	1533	U
1	A	1536	G
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	1565	G
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	1574	C
1	A	1576	G
1	A	1577	G
1	A	1578	C
1	A	1579	C

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Mol	Chain	Res	Type
1	A	1582	C
1	A	1583	A
1	A	1587	A
1	A	1589	A
1	A	1593	A
1	A	1611	G
1	A	1618	G
1	A	1620	U
1	A	1622	U
1	A	1628	C
1	A	1629	U
1	A	1630	U
1	A	1642	A
1	A	1643	A
1	A	1645	U
1	A	1657	C
1	A	1664	G
1	A	1666	G
1	A	1678	G
1	A	1683	A
1	A	1703	U
1	A	1716	U
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1741	A
1	A	1742	U
1	A	1749	A
1	A	1750	A
1	A	1751	G
1	A	1760	A
1	A	1761	C
1	A	1762	C
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1775	G
1	A	1779	C
1	A	1780	G
1	A	1797	A
1	A	1798	A
1	A	1808	G

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Mol	Chain	Res	Type
1	A	1812	G
1	A	1813	A
1	A	1814	A
1	A	1815	U
1	A	1816	A
1	A	1817	G
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1840	U
1	A	1841	A
1	A	1842	A
1	A	1846	C
1	A	1847	A
1	A	1849	C
1	A	1850	A
1	A	1855	U
1	A	1858	A
1	A	1859	A
1	A	1866	C
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1908	A
1	A	1910	A
1	A	1936	A
1	A	1951	C
1	A	1952	G
1	A	1953	G
1	A	1954	G
1	A	2095	G
1	A	2099	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2112	U
1	A	2113	A
1	A	2114	C
1	A	2115	G
1	A	2120	A
1	A	2121	G

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Mol	Chain	Res	Type
1	A	2122	G
1	A	2131	A
1	A	2134	G
1	A	2140	U
1	A	2158	A
1	A	2169	G
1	A	2180	G
1	A	2185	G
1	A	2192	C
1	A	2193	U
1	A	2198	A
1	A	2204	C
1	A	2205	U
1	A	2210	G
1	A	2211	U
1	A	2228	A
1	A	2239	G
1	A	2244	A
1	A	2245	C
1	A	2246	G
1	A	2250	G
1	A	2252	A
1	A	2253	G
1	A	2255	A
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2270	A
1	A	2273	G
1	A	2274	U
1	A	2276	G
1	A	2279	A
1	A	2281	A
1	A	2282	U
1	A	2285	C
1	A	2288	G
1	A	2298	U
1	A	2307	G
1	A	2308	C
1	A	2310	U
1	A	2313	A
1	A	2314	U

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Mol	Chain	Res	Type
1	A	2315	G
1	A	2327	U
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2337	C
1	A	2357	A
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	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	2418	G
1	A	2419	A
1	A	2421	U
1	A	2422	C
1	A	2425	G
1	A	2434	U
1	A	2435	G
1	A	2437	G
1	A	2438	A
1	A	2440	G
1	A	2442	G
1	A	2443	A
1	A	2444	C
1	A	2445	A
1	A	2446	U
1	A	2448	G
1	A	2449	A
1	A	2450	G
1	A	2451	G
1	A	2452	G
1	A	2453	U
1	A	2454	G
1	A	2455	U

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Mol	Chain	Res	Type
1	A	2456	A
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
1	A	2472	U
1	A	2473	C
1	A	2474	G
1	A	2475	G
1	A	2477	G
1	A	2481	G
1	A	2484	A
1	A	2487	U
1	A	2488	A
1	A	2491	A
1	A	2492	C
1	A	2494	A
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	2505	U
1	A	2506	U
1	A	2507	C
1	A	2508	U
1	A	2513	U
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2530	G
1	A	2531	C
1	A	2532	U
1	A	2533	G
1	A	2537	U
1	A	2538	U

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Mol	Chain	Res	Type
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2544	U
1	A	2547	A
1	A	2548	C
1	A	2549	G
1	A	2550	U
1	A	2552	C
1	A	2554	A
1	A	2555	G
1	A	2558	U
1	A	2561	A
1	A	2562	A
1	A	2565	U
1	A	2566	C
1	A	2568	C
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2575	G
1	A	2576	G
1	A	2582	C
1	A	2585	G
1	A	2586	G
1	A	2593	A
1	A	2594	C
1	A	2602	G
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2621	G
1	A	2626	A
1	A	2652	U
1	A	2655	U
1	A	2656	A
1	A	2657	A
1	A	2665	U

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Mol	Chain	Res	Type
1	A	2674	A
1	A	2677	G
1	A	2681	U
1	A	2689	A
1	A	2691	A
1	A	2692	A
1	A	2694	A
1	A	2696	A
1	A	2703	A
1	A	2704	A
1	A	2713	U
1	A	2719	U
1	A	2726	C
1	A	2728	G
1	A	2729	U
1	A	2737	C
1	A	2752	U
1	A	2753	G
1	A	2754	G
1	A	2762	A
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2816	G
1	A	2817	A
1	A	2821	C
1	A	2841	G
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2847	A
1	A	2849	C
1	A	2850	G
1	A	2861	U
1	A	2867	C
1	A	2871	G

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Mol	Chain	Res	Type
1	A	2872	A
1	A	2887	A
1	A	2898	G
1	A	2899	C
1	A	2904	U
1	A	2907	G
1	A	2914	G
1	A	2921	U
1	A	2923	U
1	A	2935	U
1	A	2936	A
1	A	2938	G
1	A	2941	A
1	A	2942	C
1	A	2947	G
1	A	2971	A
1	A	2975	U
1	A	2983	C
1	A	2996	U
1	A	2997	G
1	A	3004	C
1	A	3011	A
1	A	3012	A
1	A	3014	U
1	A	3028	G
1	A	3048	A
1	A	3049	A
1	A	3056	U
1	A	3057	U
1	A	3058	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3092	C
1	A	3102	G
1	A	3109	G
1	A	3110	C
1	A	3114	A
1	A	3115	C
1	A	3117	C
1	A	3122	A

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Mol	Chain	Res	Type
1	A	3124	G
1	A	3128	G
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	3155	U
1	A	3156	U
1	A	3157	U
1	A	3163	A
1	A	3164	C
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	3187	A
1	A	3196	U
1	A	3197	G
1	A	3200	G
1	A	3202	G
1	A	3207	U
1	A	3208	G
1	A	3212	C
1	A	3213	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3228	C
1	A	3229	G
1	A	3232	G
1	A	3234	A
1	A	3243	A
1	A	3244	A
1	A	3245	A
1	A	3246	G
1	A	3247	G

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Mol	Chain	Res	Type
1	A	3249	C
1	A	3259	U
1	A	3260	G
1	A	3261	C
1	A	3263	G
1	A	3270	U
1	A	3271	G
1	A	3275	U
1	A	3276	G
1	A	3279	A
1	A	3280	U
1	A	3283	U
1	A	3284	G
1	A	3286	G
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3308	C
1	A	3313	U
1	A	3316	A
1	A	3317	U
1	A	3318	G
1	A	3319	U
1	A	3320	A
1	A	3324	C
1	A	3325	G
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	3357	U
1	A	3363	U
1	A	3366	G
1	A	3368	U
1	A	3369	G

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Mol	Chain	Res	Type
1	A	3375	A
1	A	3378	C
1	A	3382	U
1	A	3383	G
1	A	3386	G
1	A	3390	G
1	A	3396	U
2	B	10	C
2	B	19	C
2	B	22	A
2	B	42	A
2	B	49	G
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	56	A
2	B	60	G
2	B	65	G
2	B	71	G
2	B	73	C
2	B	91	G
2	B	99	G
2	B	101	G
2	B	102	A
2	B	112	G
2	B	114	U
2	B	120	C
2	B	121	U
3	C	2	A
3	C	23	U
3	C	24	G
3	C	34	U
3	C	35	C
3	C	50	C
3	C	52	A
3	C	53	A
3	C	57	C
3	C	59	A
3	C	62	C
3	C	63	G
3	C	80	A

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Mol	Chain	Res	Type
3	C	81	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	91	C
3	C	95	G
3	C	104	A
3	C	106	C
3	C	108	C
3	C	111	A
3	C	113	U
3	C	125	U
3	C	126	A
3	C	129	C
3	C	136	G
3	C	138	A
3	C	146	U
3	C	148	G
3	C	151	C
3	C	152	G
3	C	155	A
3	C	158	U

All (82) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	65	A
1	A	169	U
1	A	239	G
1	A	518	G
1	A	547	G
1	A	558	U
1	A	588	G
1	A	594	U
1	A	599	C
1	A	619	A
1	A	770	G
1	A	873	C
1	A	896	A

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Mol	Chain	Res	Type
1	A	916	G
1	A	959	C
1	A	960	U
1	A	979	U
1	A	993	G
1	A	1064	A
1	A	1097	G
1	A	1103	A
1	A	1263	A
1	A	1307	G
1	A	1329	U
1	A	1352	A
1	A	1355	A
1	A	1482	A
1	A	1554	U
1	A	1556	C
1	A	1562	C
1	A	1576	G
1	A	1716	U
1	A	1778	G
1	A	1814	A
1	A	1815	U
1	A	1816	A
1	A	1820	U
1	A	1841	A
1	A	1846	C
1	A	1858	A
1	A	2101	C
1	A	2112	U
1	A	2144	A
1	A	2209	U
1	A	2249	G
1	A	2269	U
1	A	2281	A
1	A	2418	G
1	A	2434	U
1	A	2453	U
1	A	2495	C
1	A	2496	C
1	A	2501	U
1	A	2506	U
1	A	2513	U

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Mol	Chain	Res	Type
1	A	2537	U
1	A	2541	U
1	A	2585	G
1	A	2593	A
1	A	2754	G
1	A	2801	A
1	A	2983	C
1	A	3003	G
1	A	3048	A
1	A	3055	U
1	A	3056	U
1	A	3057	U
1	A	3078	U
1	A	3195	U
1	A	3218	A
1	A	3228	C
1	A	3242	G
1	A	3269	U
1	A	3317	U
1	A	3350	C
1	A	3351	U
1	A	3353	G
2	B	52	G
2	B	111	U
3	C	80	A
3	C	82	U
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](#)

Of 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

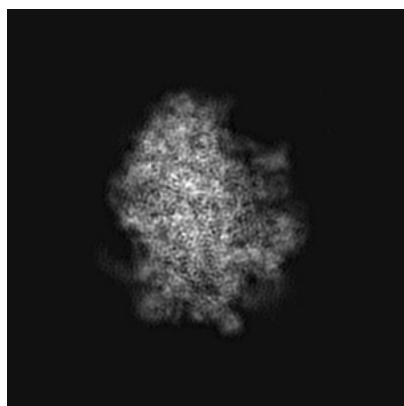
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8368. These allow visual inspection of the internal detail of the map and identification of artifacts.

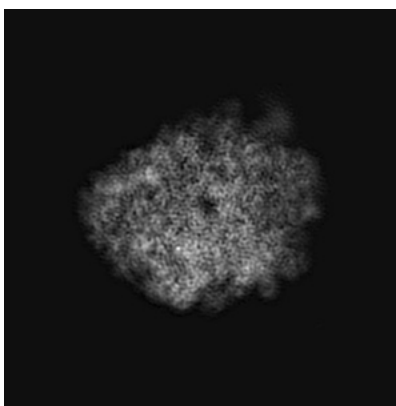
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

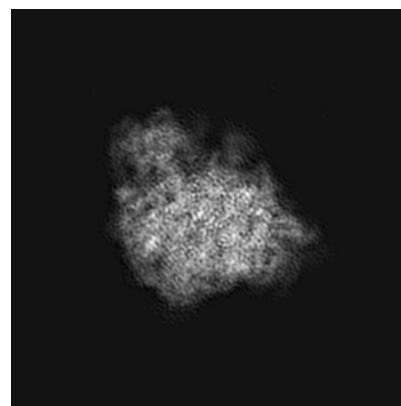
6.1.1 Primary map



X

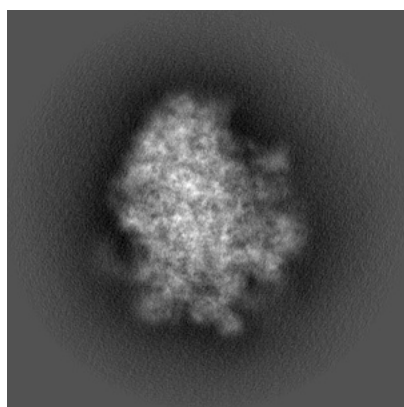


Y

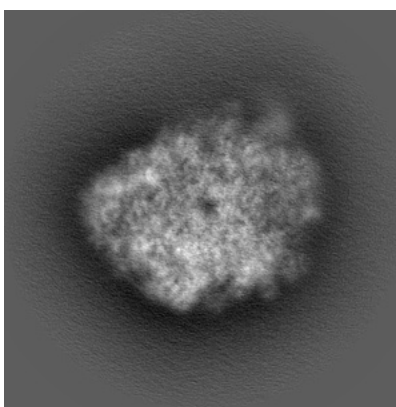


Z

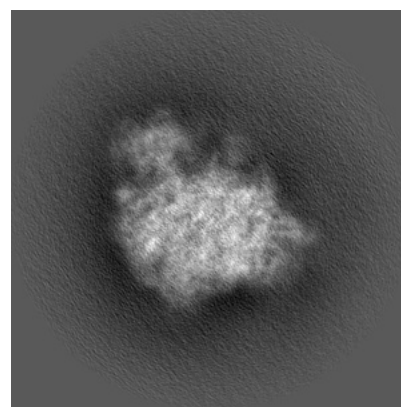
6.1.2 Raw map



X



Y

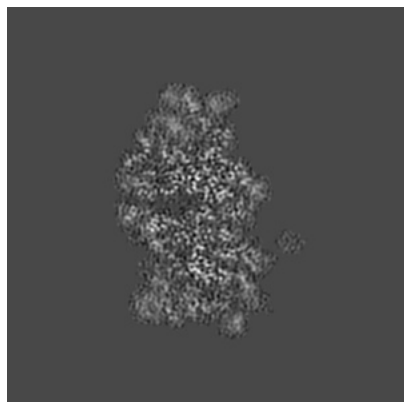


Z

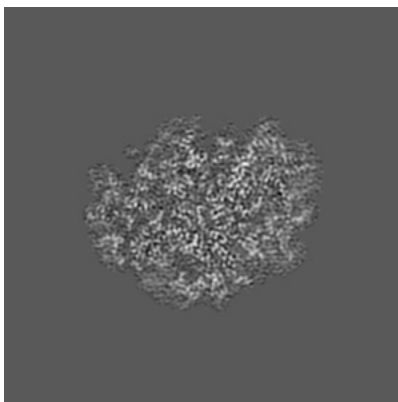
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

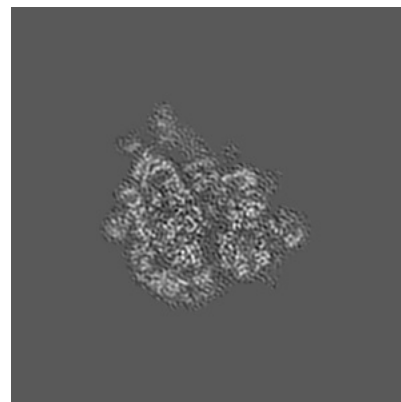
6.2.1 Primary map



X Index: 160

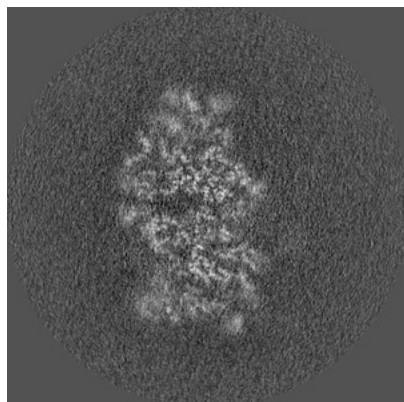


Y Index: 160

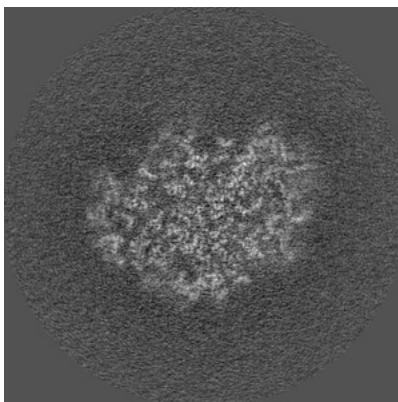


Z Index: 160

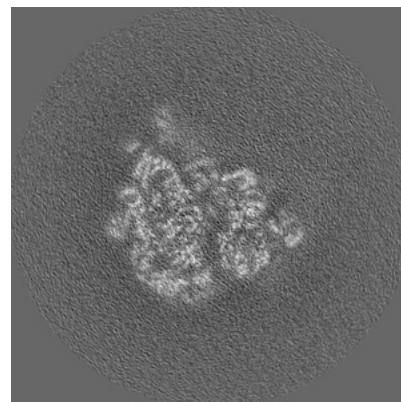
6.2.2 Raw map



X Index: 160



Y Index: 160

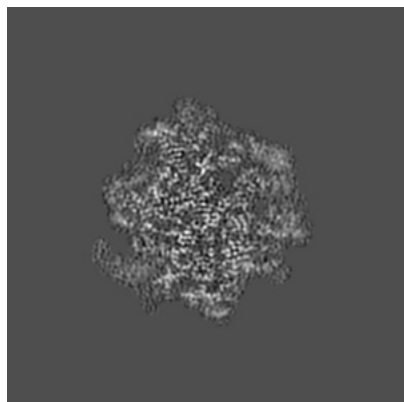


Z Index: 160

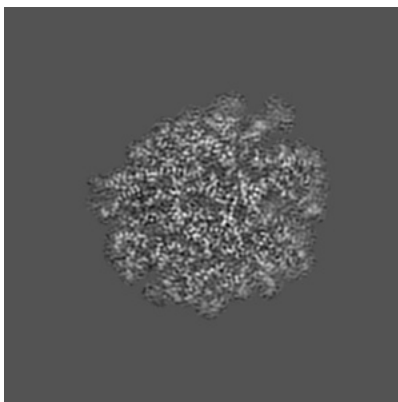
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

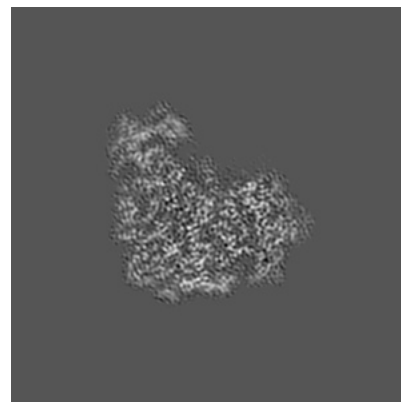
6.3.1 Primary map



X Index: 129

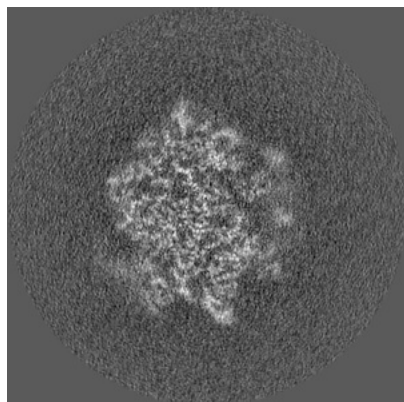


Y Index: 142

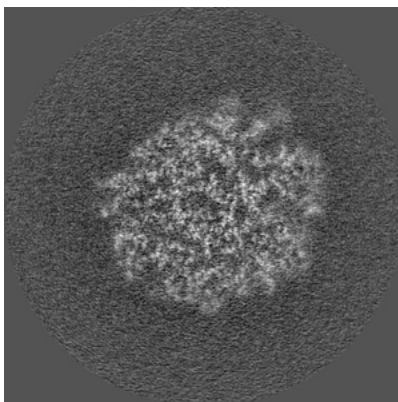


Z Index: 151

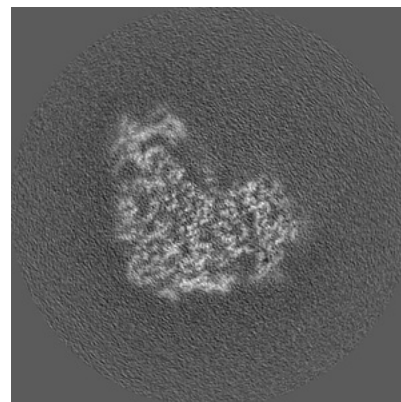
6.3.2 Raw map



X Index: 135



Y Index: 142

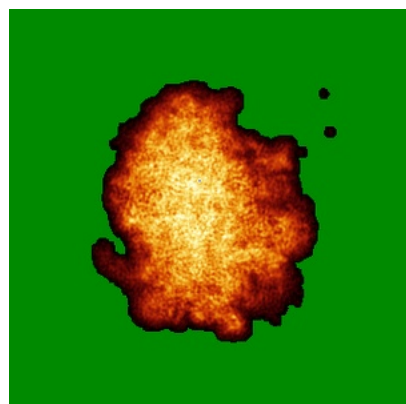


Z Index: 151

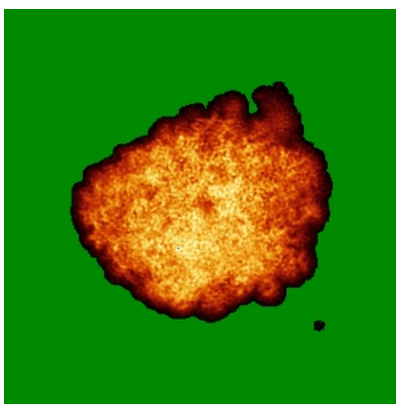
The images above show the largest variance slices of the map in three orthogonal directions.

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

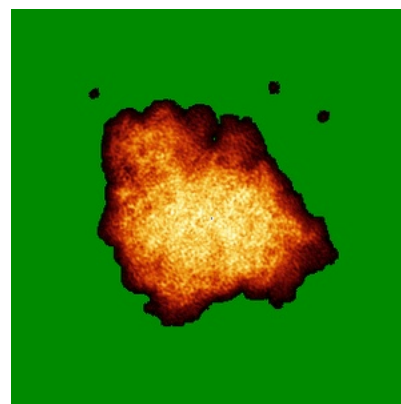
6.4.1 Primary map



X

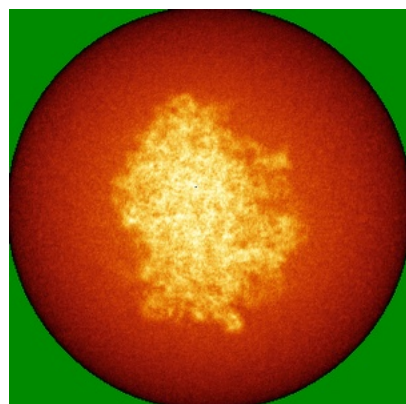


Y

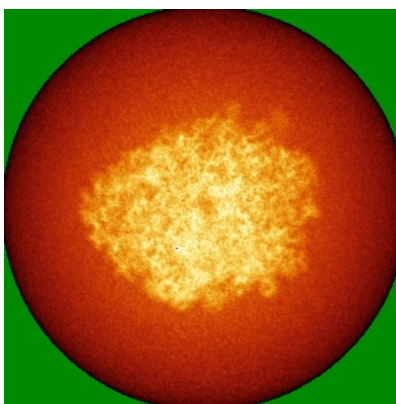


Z

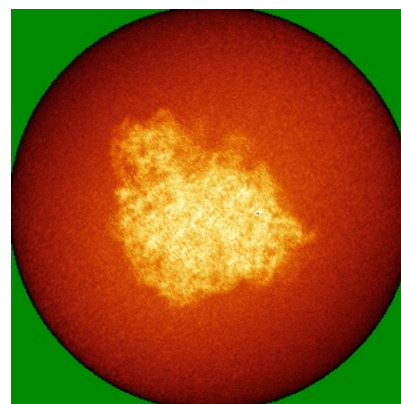
6.4.2 Raw map



X



Y

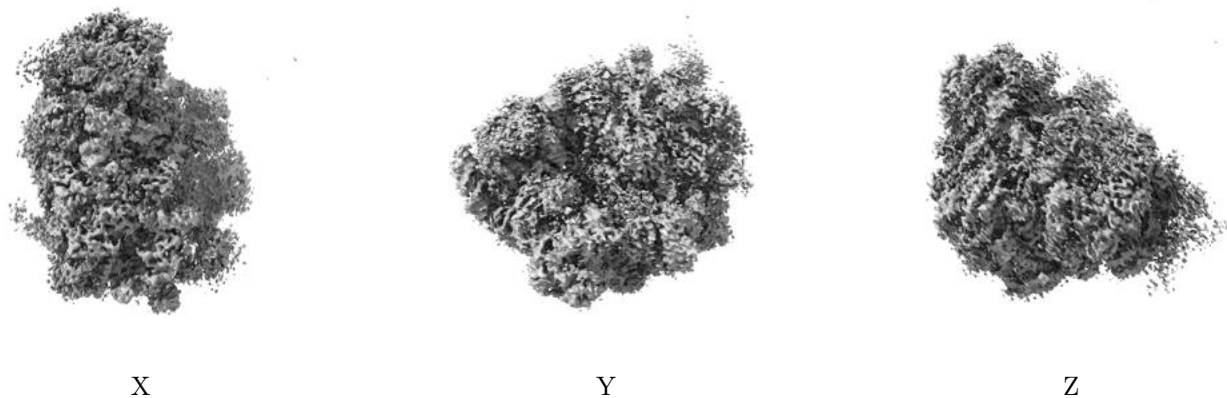


Z

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

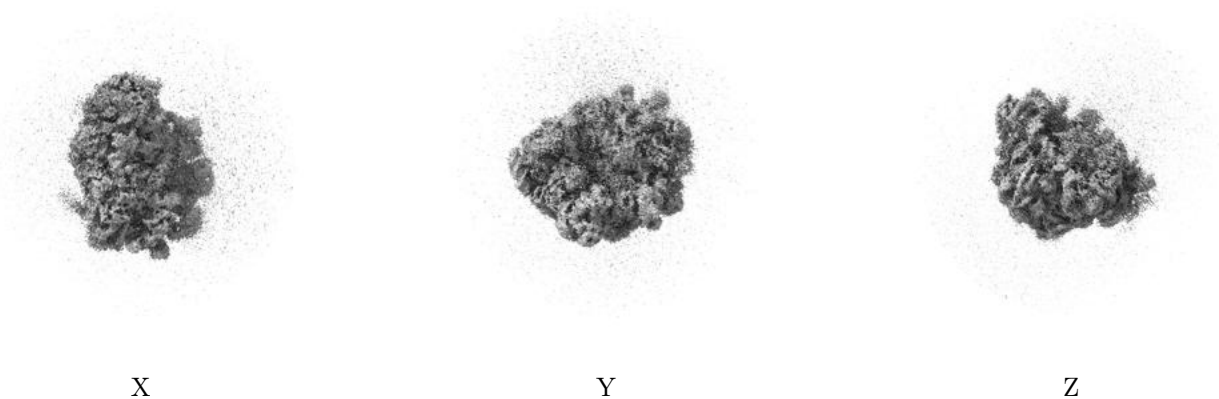
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

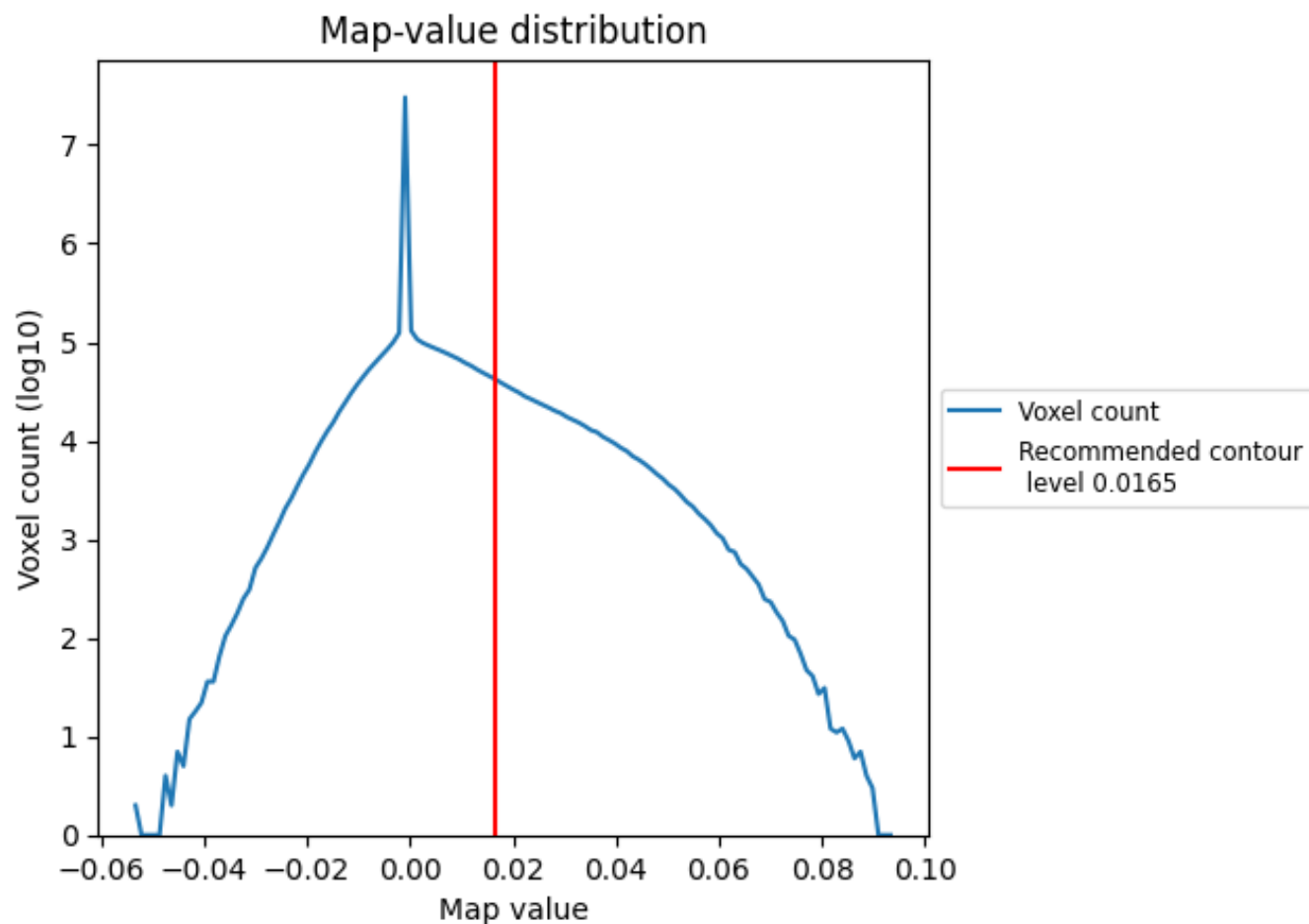
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

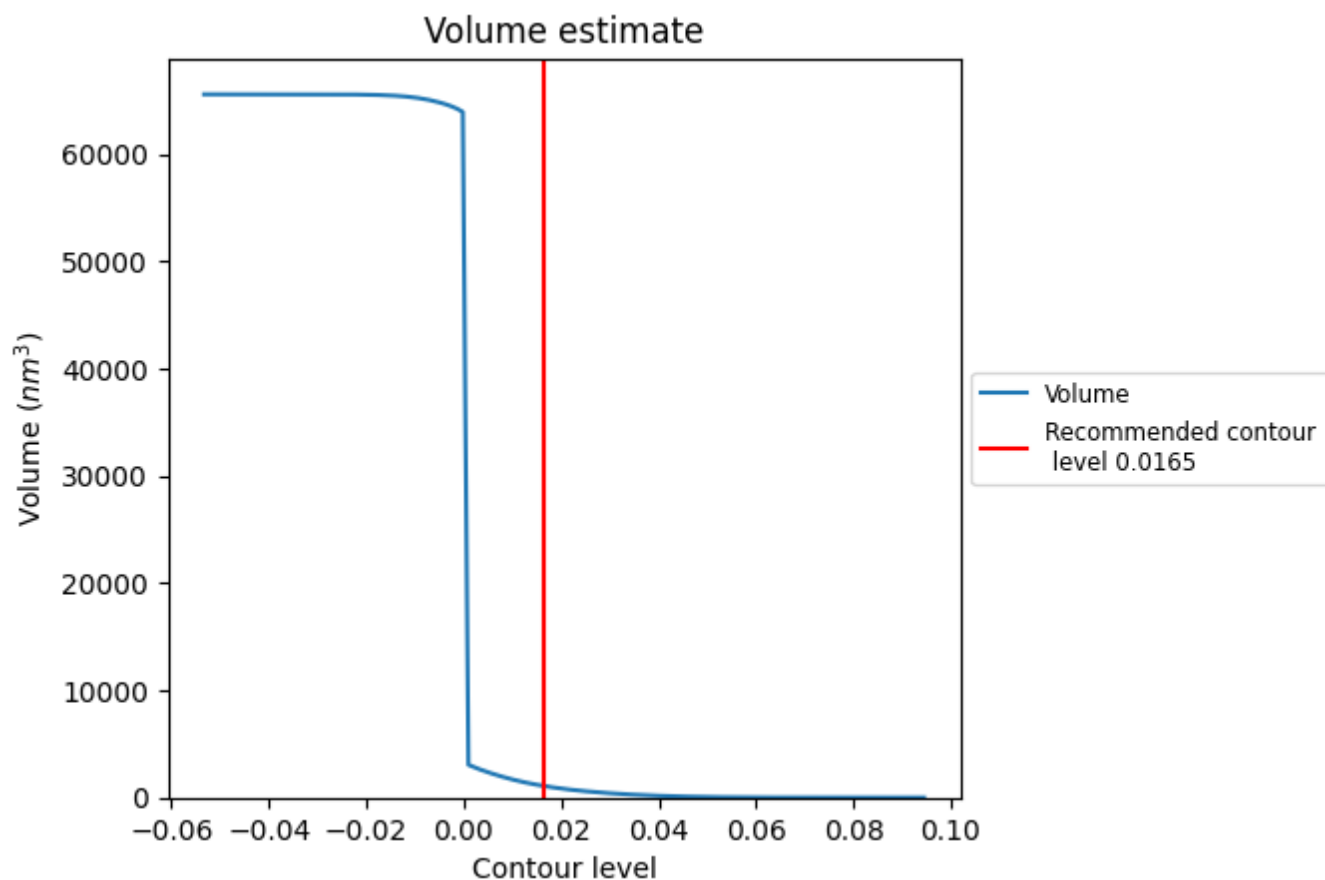
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

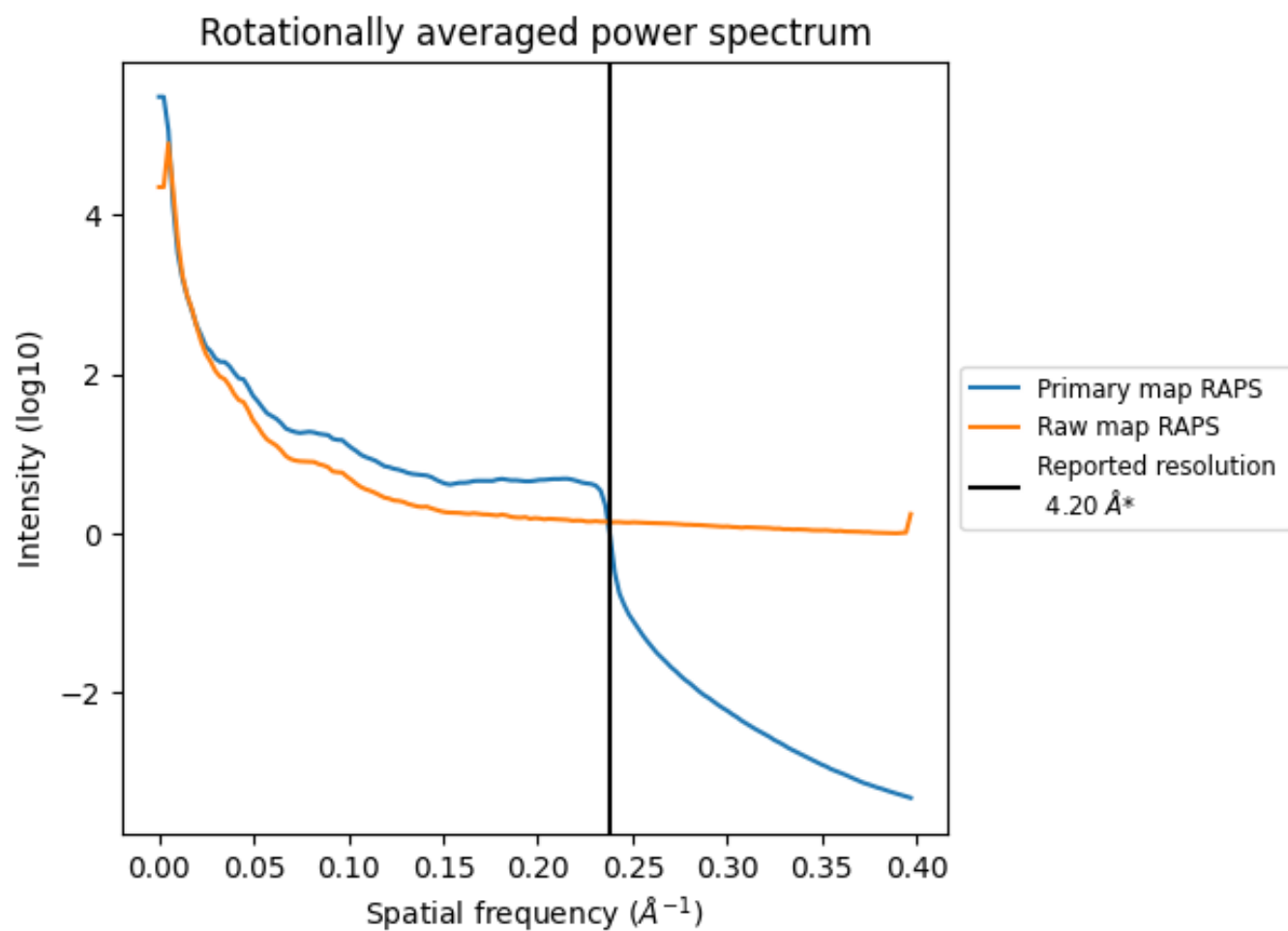
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1077 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 ⓘ

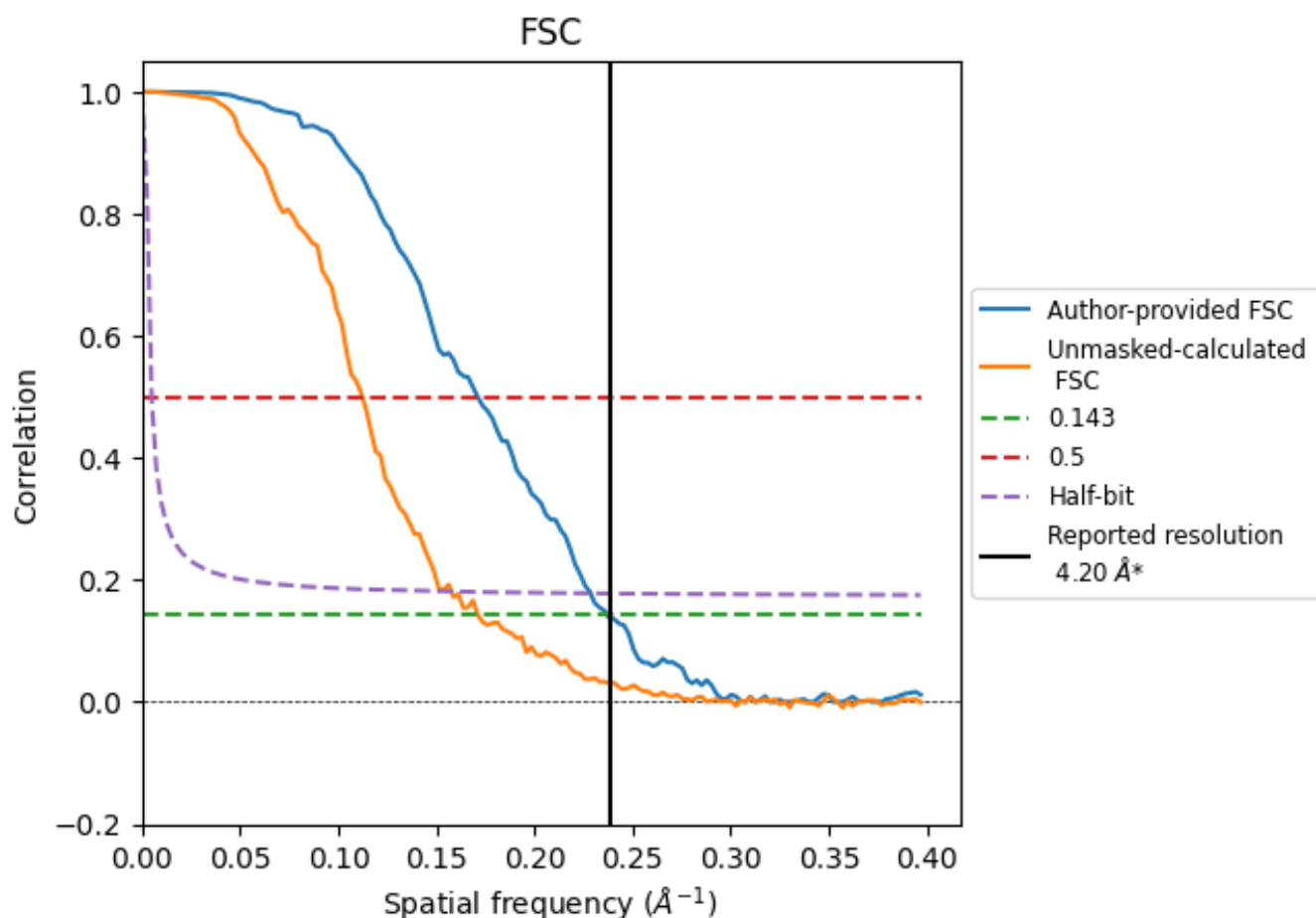


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

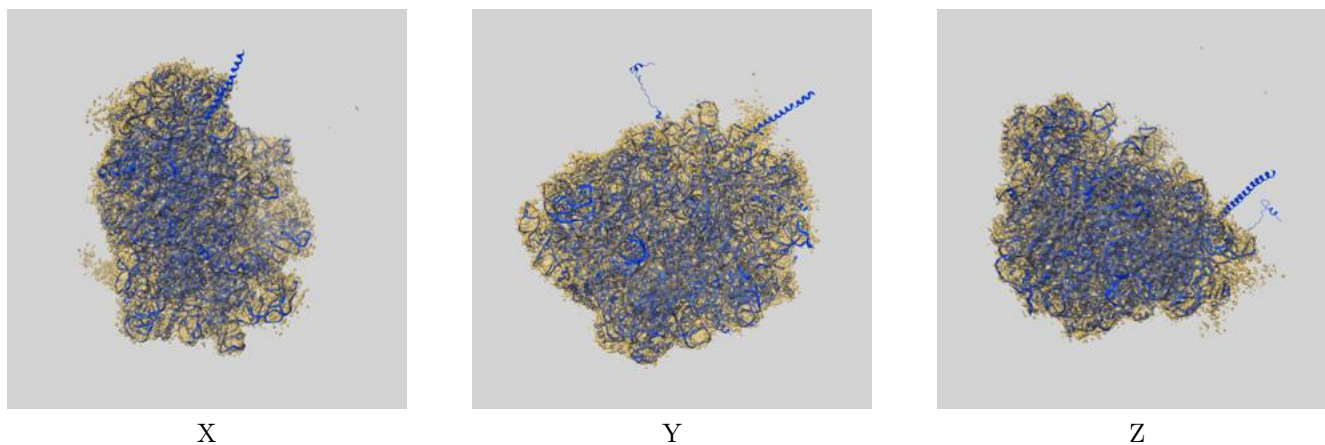
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	5.85	4.38
Unmasked-calculated*	5.85	8.91	6.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.85 differs from the reported value 4.2 by more than 10 %

9 Map-model fit ⓘ

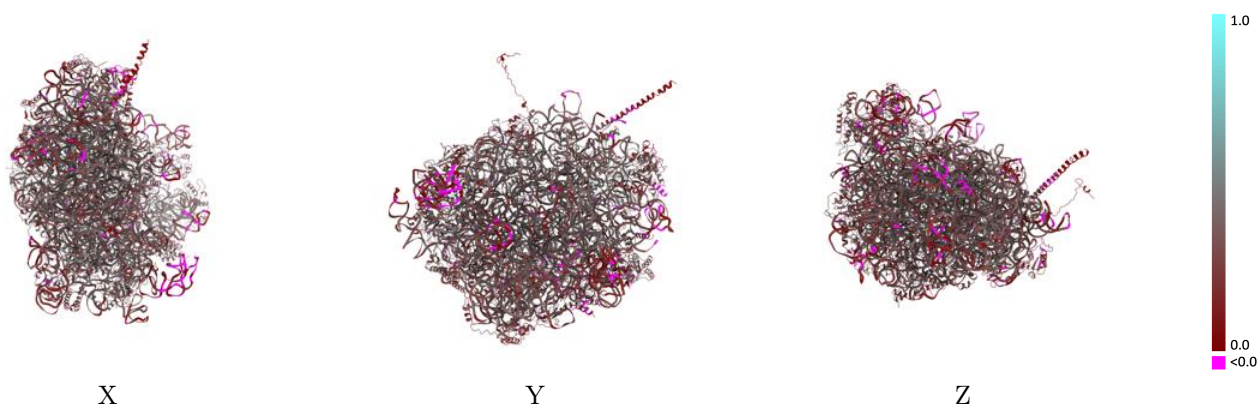
This section contains information regarding the fit between EMDB map EMD-8368 and PDB model 5T6R. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay ⓘ



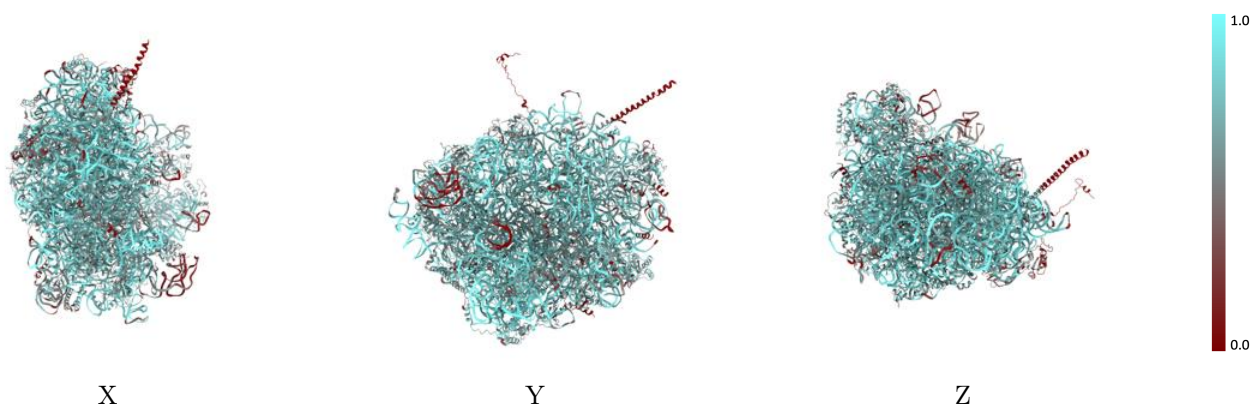
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



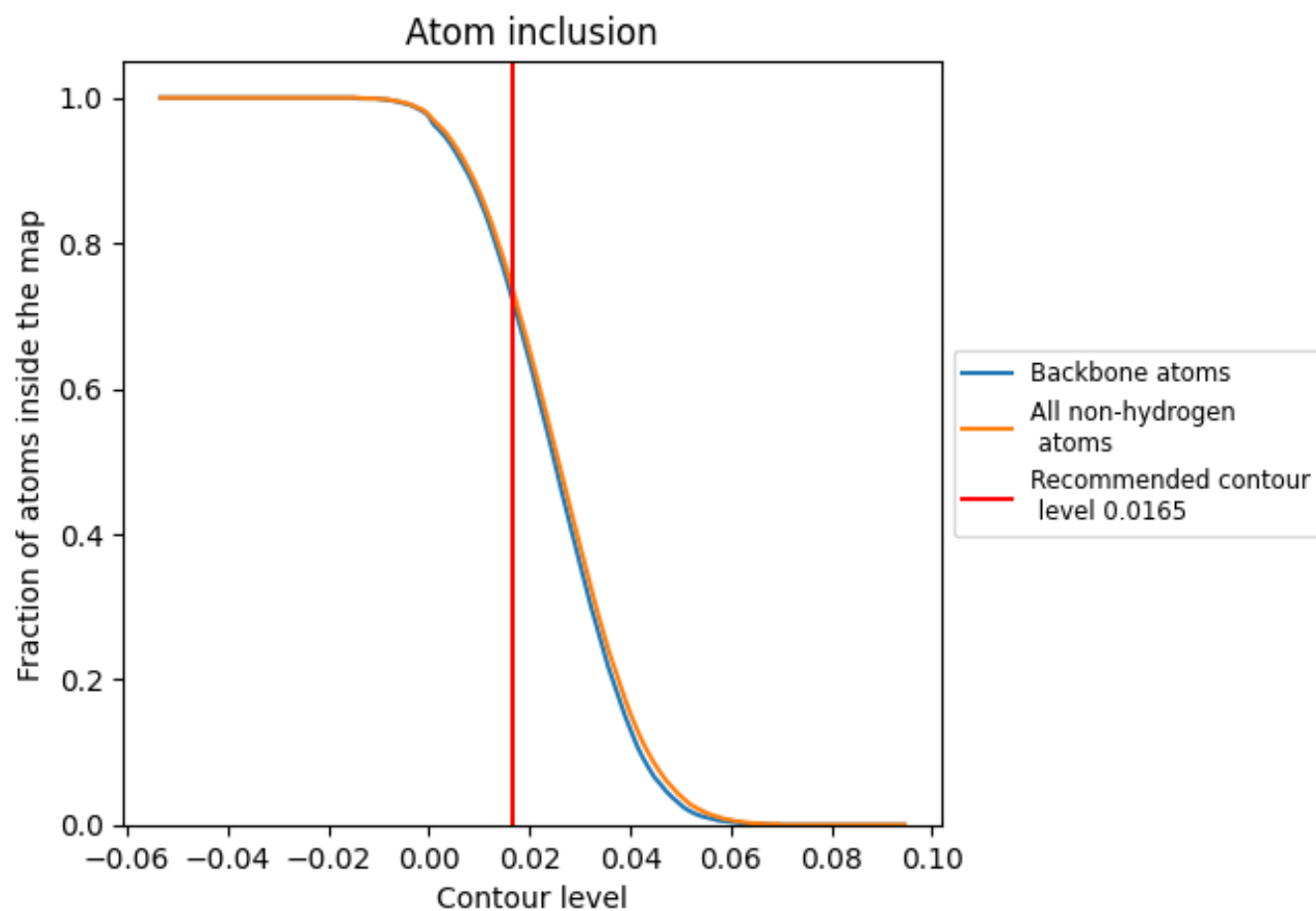
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 74% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7400	 0.3250
A	 0.8230	 0.3290
B	 0.9050	 0.3530
C	 0.8660	 0.3520
D	 0.6730	 0.3640
E	 0.6780	 0.3520
F	 0.6640	 0.3480
G	 0.6510	 0.2870
H	 0.5780	 0.2710
I	 0.6750	 0.3430
J	 0.6260	 0.2860
K	 0.6670	 0.3190
L	 0.5250	 0.2980
M	 0.6180	 0.2730
N	 0.6060	 0.2880
O	 0.6470	 0.3090
Q	 0.5710	 0.2890
R	 0.6430	 0.3190
S	 0.5700	 0.2070
V	 0.5160	 0.2850
a	 0.7030	 0.3720
b	 0.6910	 0.3650
c	 0.6060	 0.3270
d	 0.6530	 0.3480
e	 0.5580	 0.2800
f	 0.6750	 0.3700
g	 0.6570	 0.3530
h	 0.3300	 0.2210
i	 0.5770	 0.2660
j	 0.4440	 0.2280
k	 0.6510	 0.3440
l	 0.6330	 0.3140
m	 0.6400	 0.3020
n	 0.6760	 0.3590
o	 0.5820	 0.3170



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Chain	Atom inclusion	Q-score
p	 0.5840	 0.2710
q	 0.6600	 0.3520
r	 0.6320	 0.3520
s	 0.6780	 0.3860
t	 0.6220	 0.3170
u	 0.6460	 0.3010
v	 0.5450	 0.2580
w	 0.7040	 0.3700
x	 0.5330	 0.2600
y	 0.6340	 0.3470
z	 0.5960	 0.3140