



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:56 AM UTC

PDB ID : 8CBJ / pdb_00008cbj
EMDB ID : EMD-16541
Title : Cryo-EM structure of Otu2-bound cytoplasmic pre-40S ribosome biogenesis complex
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2023-01-25
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

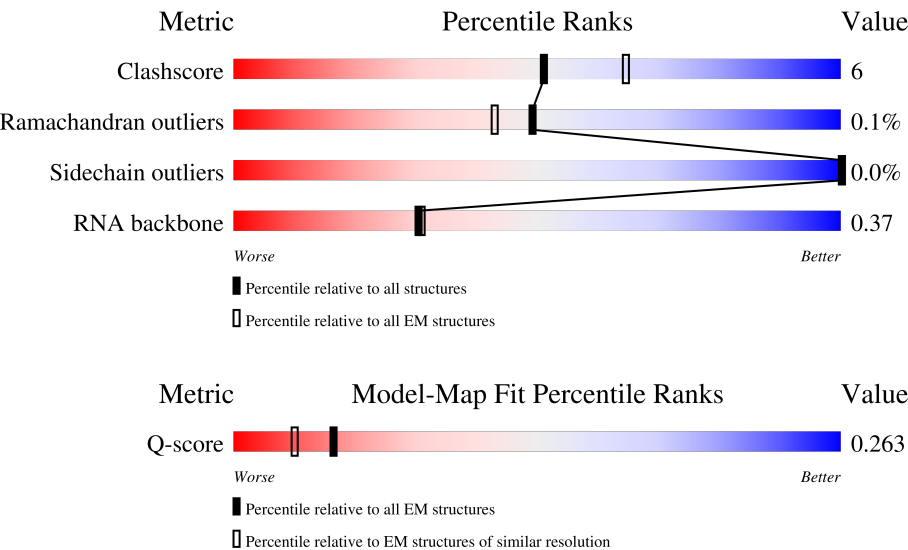
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	b	82	83%12%. 6% 82%12%6% 5%62%34%
2	c	67	
3	d	56	

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Mol	Chain	Length	Quality of chain
4	e	63	
5	g	319	
6	h	274	
7	i	483	
8	j	463	
9	k	788	
10	l	425	
11	A	252	
12	B	255	
13	C	254	
14	D	240	
15	E	261	
16	F	225	
17	G	236	
18	H	190	
19	I	200	
20	J	197	
21	L	156	
22	M	143	
23	N	151	
24	O	137	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	

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Mol	Chain	Length	Quality of chain
29	T	144	
30	U	121	
31	V	87	
32	W	130	
33	X	145	
34	Y	135	
35	Z	108	
36	a	459	
37	y	318	
38	2	2012	
39	K	307	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 87884 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 2 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 3 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	37	Total	C	N	O	S	0	0
			302	186	62	50	4		

- Molecule 4 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	48	Total	C	N	O	S	0	0
			384	242	81	59	2		

- Molecule 5 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	317	Total	C	N	O	S	0	0
			2431	1538	417	468	8		

- Molecule 6 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 7 is a protein called ENP1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	262	Total	C	N	O	S	0	0
			2133	1388	364	378	3		

- Molecule 8 is a protein called LTV1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	46	Total	C	N	O	S	0	0
			396	242	57	95	2		

- Molecule 9 is a protein called TSR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	670	Total	C	N	O	S	0	0
			5402	3449	937	1002	14		

- Molecule 10 is a protein called non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	286	Total	C	N	O	S	0	0
			2322	1464	410	430	18		

- Molecule 11 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	206	Total	C	N	O	S	0	0
			1611	1036	285	288	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP B3LI22

- Molecule 12 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 13 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 14 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	202	Total	C	N	O	S	0	0
			1576	998	290	282	6		

- Molecule 15 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 16 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 17 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	232	Total	C	N	O	S	0	0
			1873	1172	366	332	3		

- Molecule 18 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	H	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 19 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 20 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 21 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 22 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	125	Total	C	N	O	S	0	0
			941	591	166	182	2		

- Molecule 23 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 24 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	127	Total	C	N	O	S	0	0
			926	569	185	169	3		

- Molecule 25 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	127	Total	C	N	O	S	0	0
			1001	637	186	171	7		

- Molecule 26 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Q	127	Total	C	N	O	0	0
			993	640	177	176		

- Molecule 27 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 28 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	135	Total	C	N	O	S	0	0
			1110	696	215	197	2		

- Molecule 29 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 30 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	103	Total	C	N	O	S	0	0
			819	519	148	151	1		

- Molecule 31 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 32 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 33 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 34 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Y	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 35 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Z	63	Total	C	N	O	0	0
			512	328	94	90		

- Molecule 36 is a protein called 20S-pre-rRNA D-site endonuclease NOB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	a	272	Total	C	N	O	0	0
			1343	799	272	272		

- Molecule 37 is a protein called rRNA adenine N(6)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	154	Total	C	N	O	S	0	0
			1245	788	223	225	9		

- Molecule 38 is a RNA chain called 20S pre-ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	1767	Total	C	N	O	P	0	0
			37662	16836	6672	12387	1767		

- Molecule 39 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	K	99	Total	C	N	O	0	0
			494	296	99	99		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	178	SER	CYS	engineered mutation	UNP P38747

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	b	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

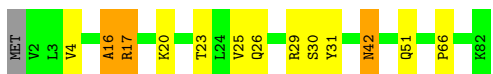
Mol	Chain	Residues	Atoms		AltConf
41	2	46	Total 46	Mg 46	0

3 Residue-property plots [i](#)

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: 40S ribosomal protein S27-A

Chain b: 



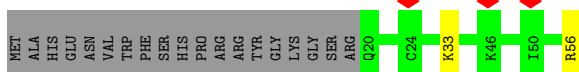
- Molecule 2: 40S ribosomal protein S28-A

Chain c: 



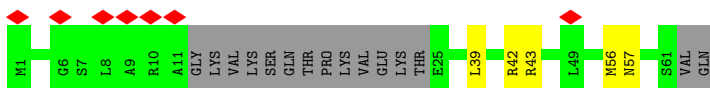
- Molecule 3: RPS29A isoform 1

Chain d: 



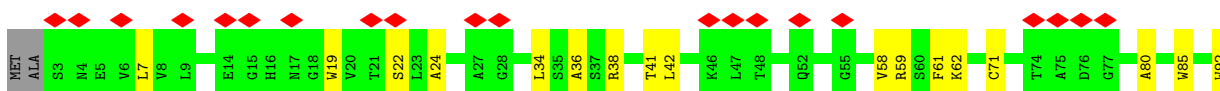
- Molecule 4: 40S ribosomal protein S30-A

Chain e: 



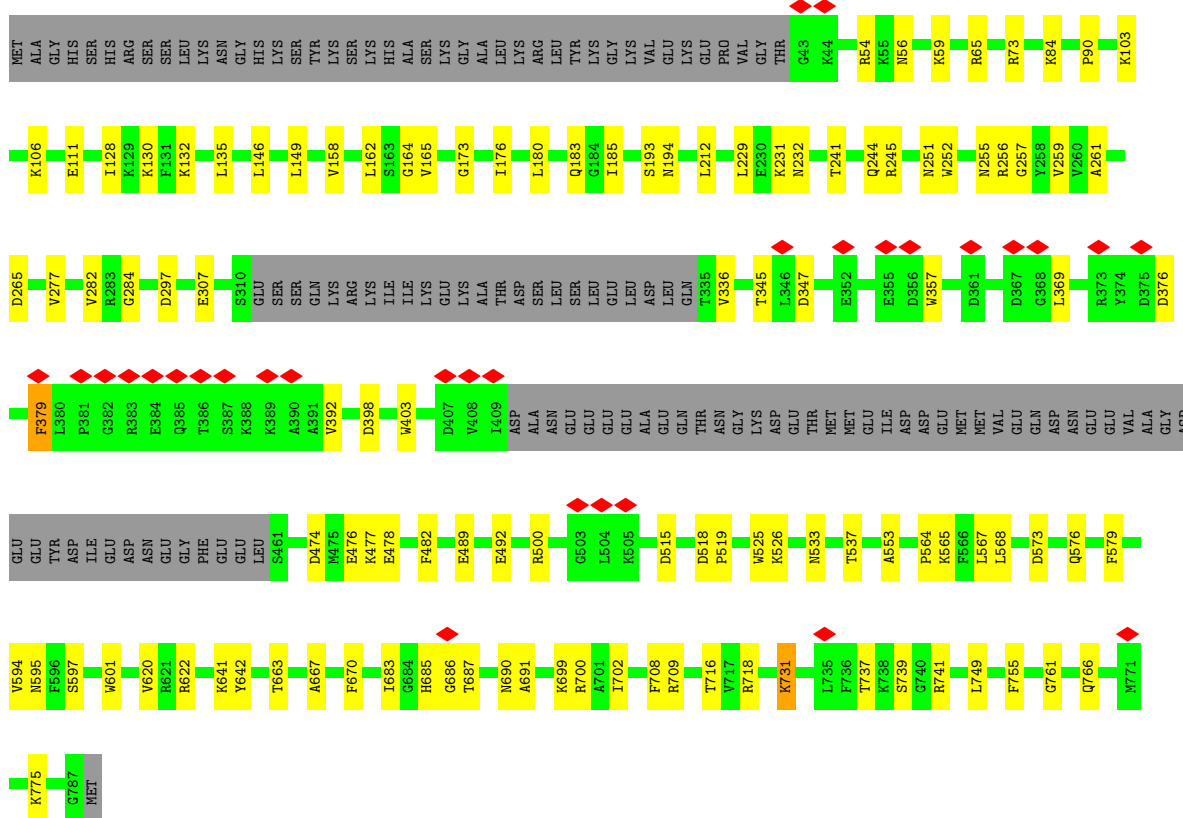
- Molecule 5: Guanine nucleotide-binding protein subunit beta-like protein

Chain g: 



- Molecule 9: TSR1 isoform 1

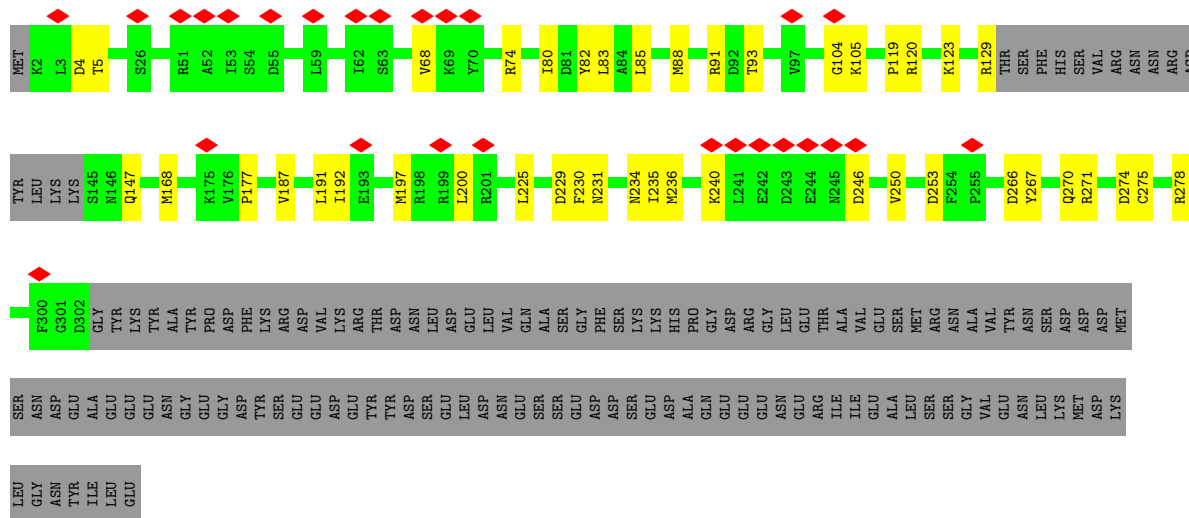
Chain k:



- Molecule 10: non-specific serine/threonine protein kinase

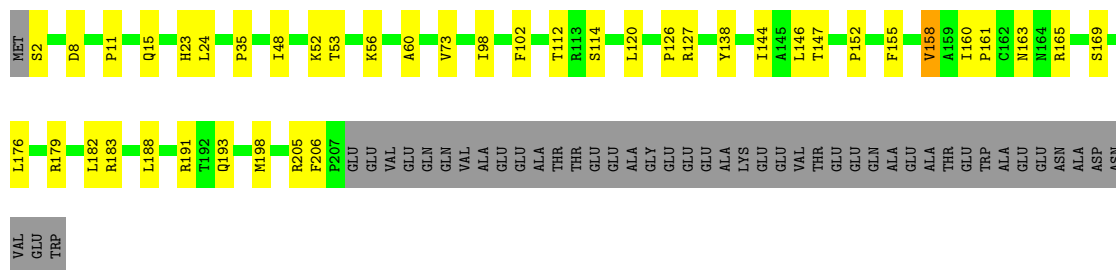
Chain 1:





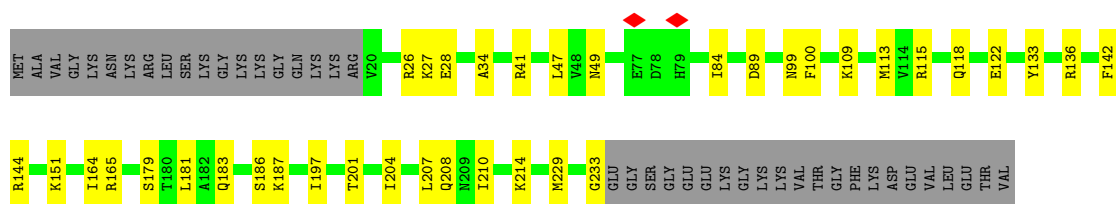
• Molecule 11: 40S ribosomal protein S0-A

Chain A: 65% 16% 18%



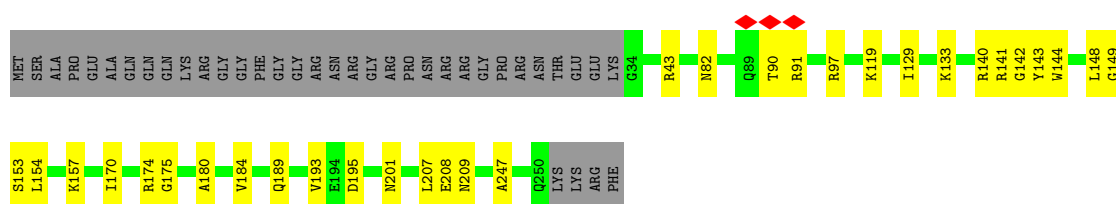
• Molecule 12: 40S ribosomal protein S1-A

Chain B: 69% 15% 16%

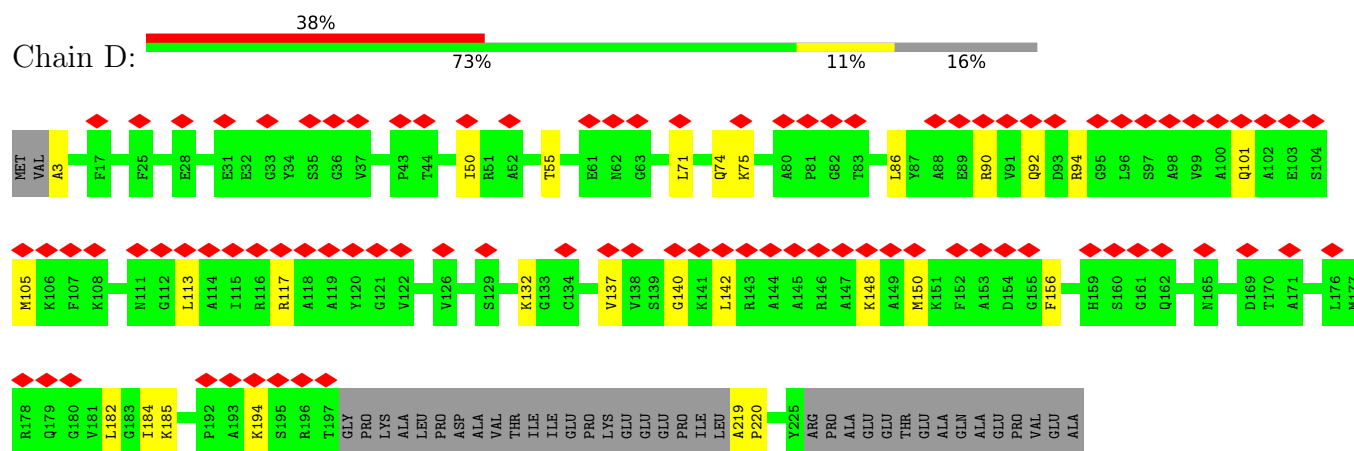


• Molecule 13: 40S ribosomal protein S2

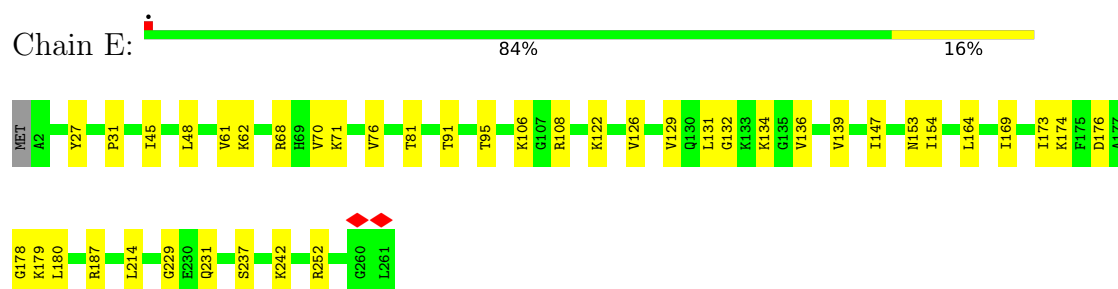
Chain C: 73% 12% 15%



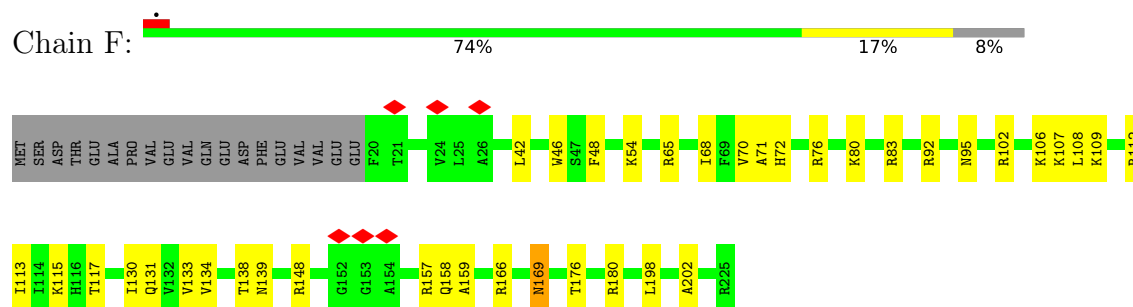
- Molecule 14: 40S ribosomal protein S3



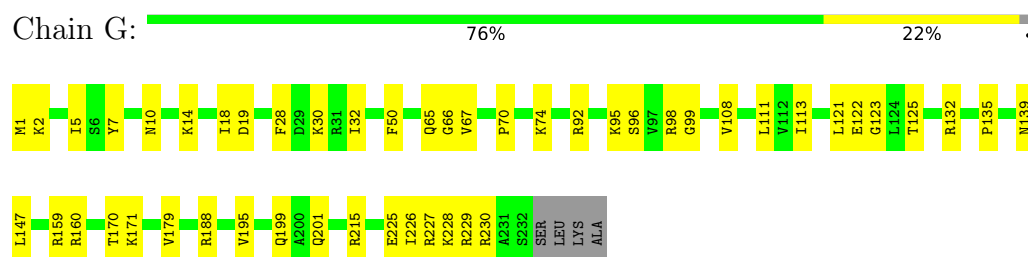
- Molecule 15: 40S ribosomal protein S4-B



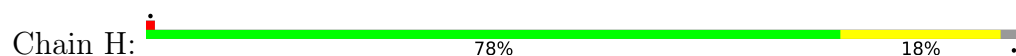
- Molecule 16: 40S ribosomal protein S5

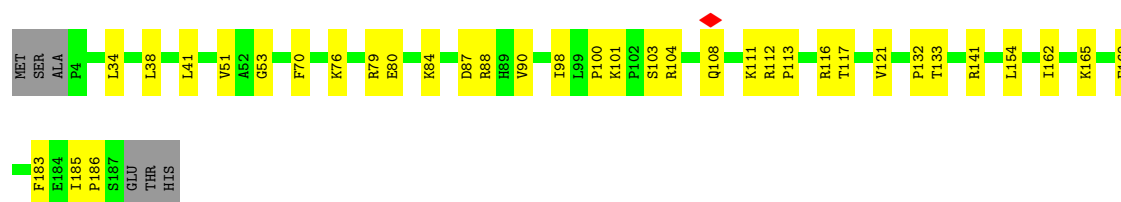


- Molecule 17: 40S ribosomal protein S6-B



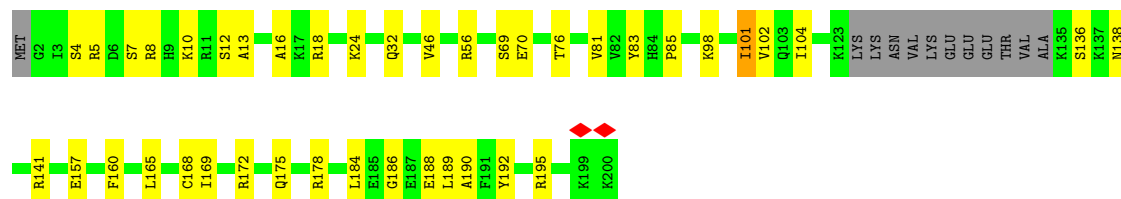
- Molecule 18: 40S ribosomal protein S7-A





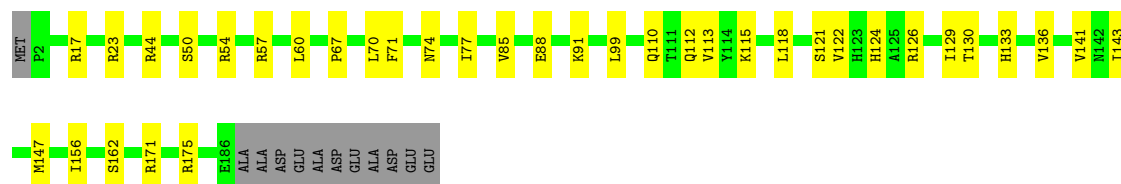
- Molecule 19: 40S ribosomal protein S8-A

Chain I: 74% 20% 6%



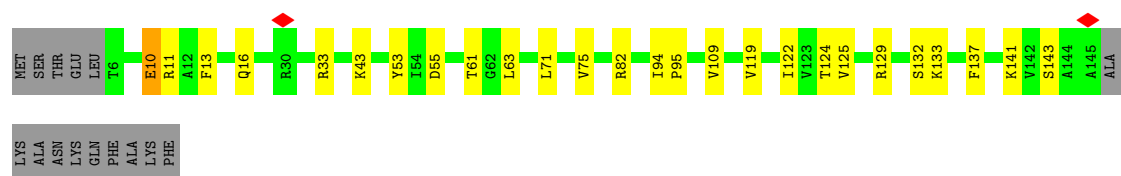
- Molecule 20: 40S ribosomal protein S9-A

Chain J: 76% 18% 6%



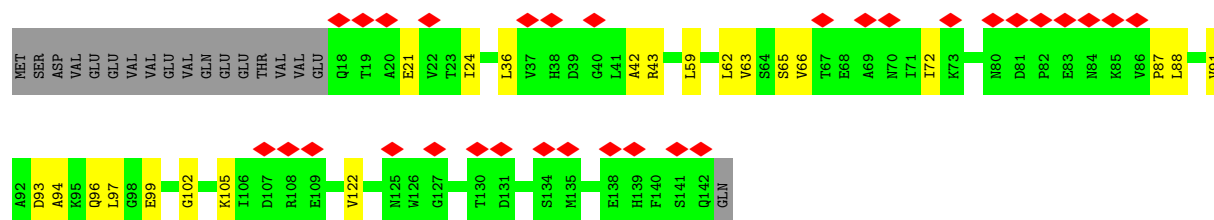
- Molecule 21: 40S ribosomal protein S11-A

Chain L: 73% 16% 10%



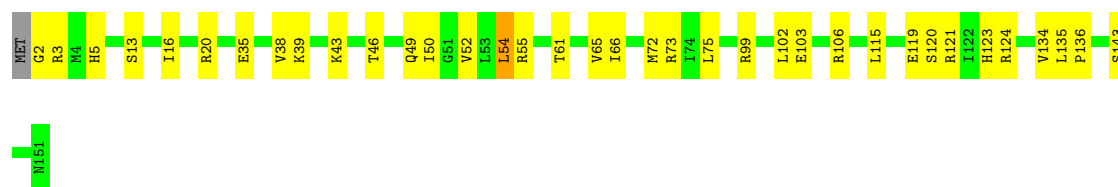
- Molecule 22: 40S ribosomal protein S12

Chain M: 22% 72% 15% 13%



- Molecule 23: 40S ribosomal protein S13

Chain N:  75% 23% ..



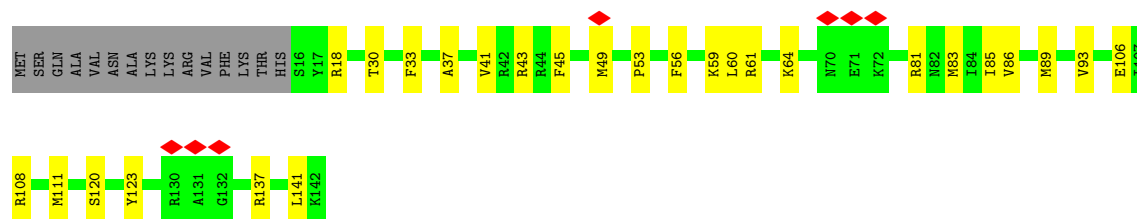
- Molecule 24: 40S ribosomal protein S14-A

Chain O:  72% 20% 7%



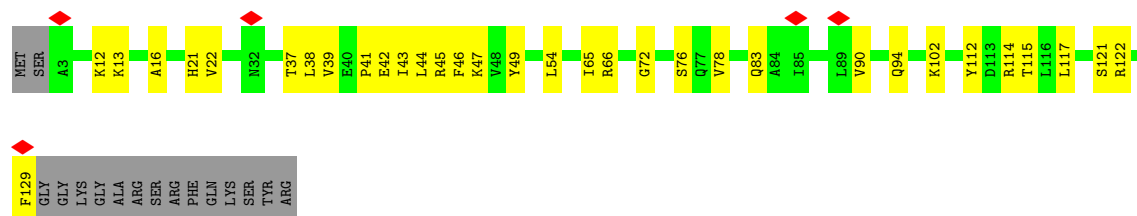
- Molecule 25: RPS15 isoform 1

Chain P:  5% 70% 19% 11%



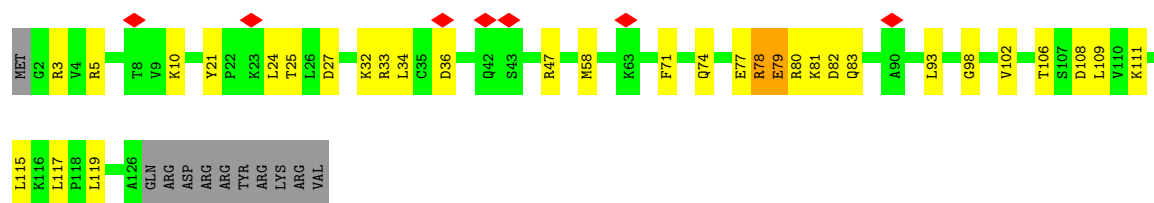
- Molecule 26: 40S ribosomal protein S16-A

Chain Q:  66% 23% 11%



- Molecule 27: 40S ribosomal protein S17-A

Chain R:  5% 68% 22% 8%



- Molecule 28: 40S ribosomal protein S18-A

Chain S:  79% 14% 8%



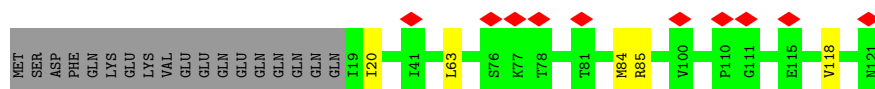
- Molecule 29: 40S ribosomal protein S19-A

Chain T:  8% 88% 12%



- Molecule 30: 40S ribosomal protein S20

Chain U:  8% 81% 15%



- Molecule 31: 40S ribosomal protein S21-A

Chain V:  87% 13%



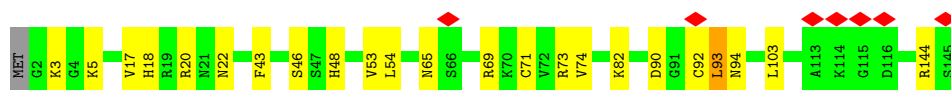
- Molecule 32: 40S ribosomal protein S22-A

Chain W:  74% 24% 2%



- Molecule 33: 40S ribosomal protein S23-A

Chain X:  5% 83% 15%

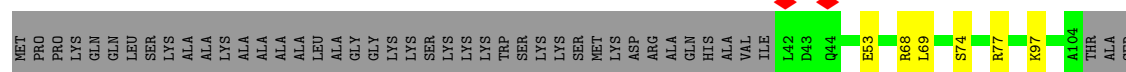


- Molecule 34: 40S ribosomal protein S24-A

Chain Y:  82% 17%

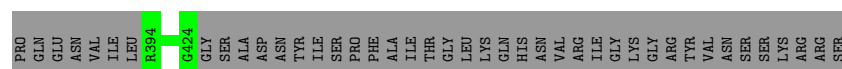
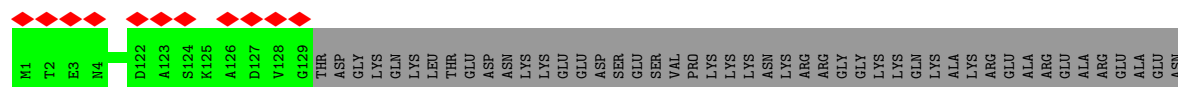


- Molecule 35: 40S ribosomal protein S25-A

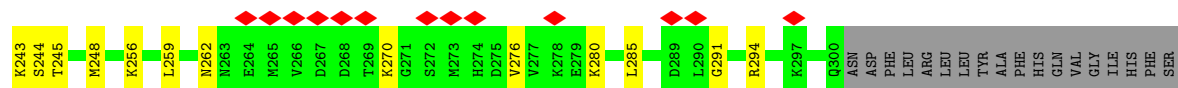
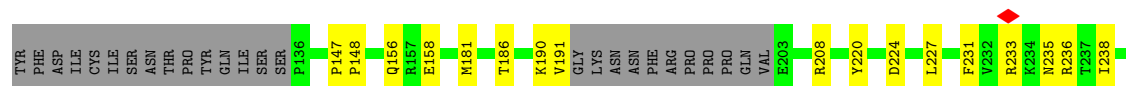
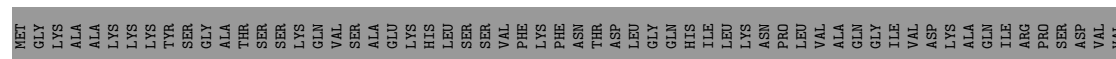


GLU

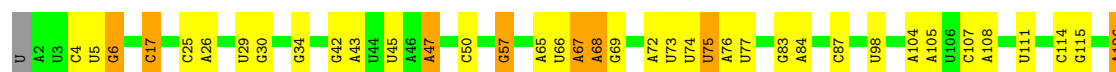
Chain a: 5% 59% 41%

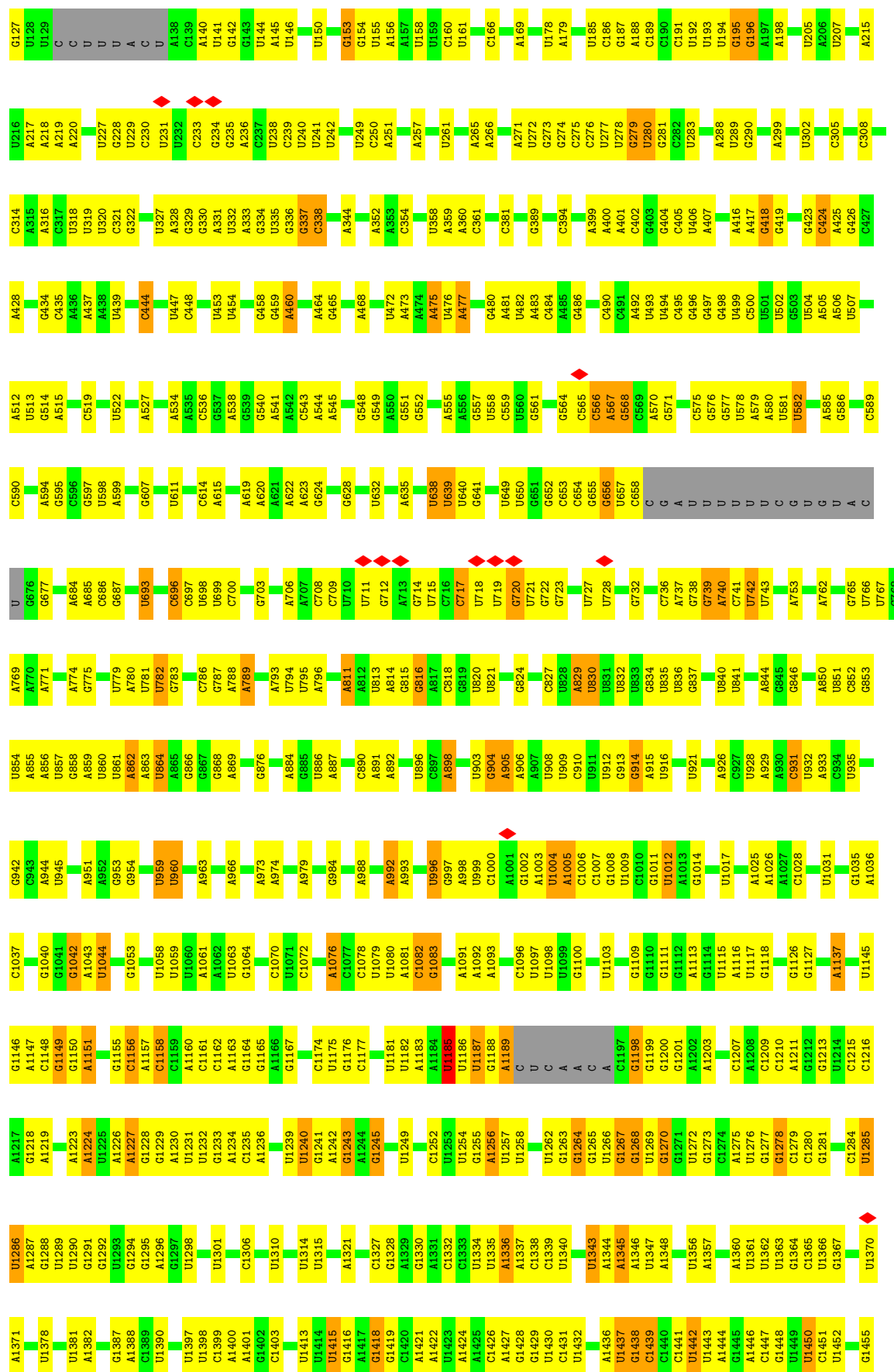


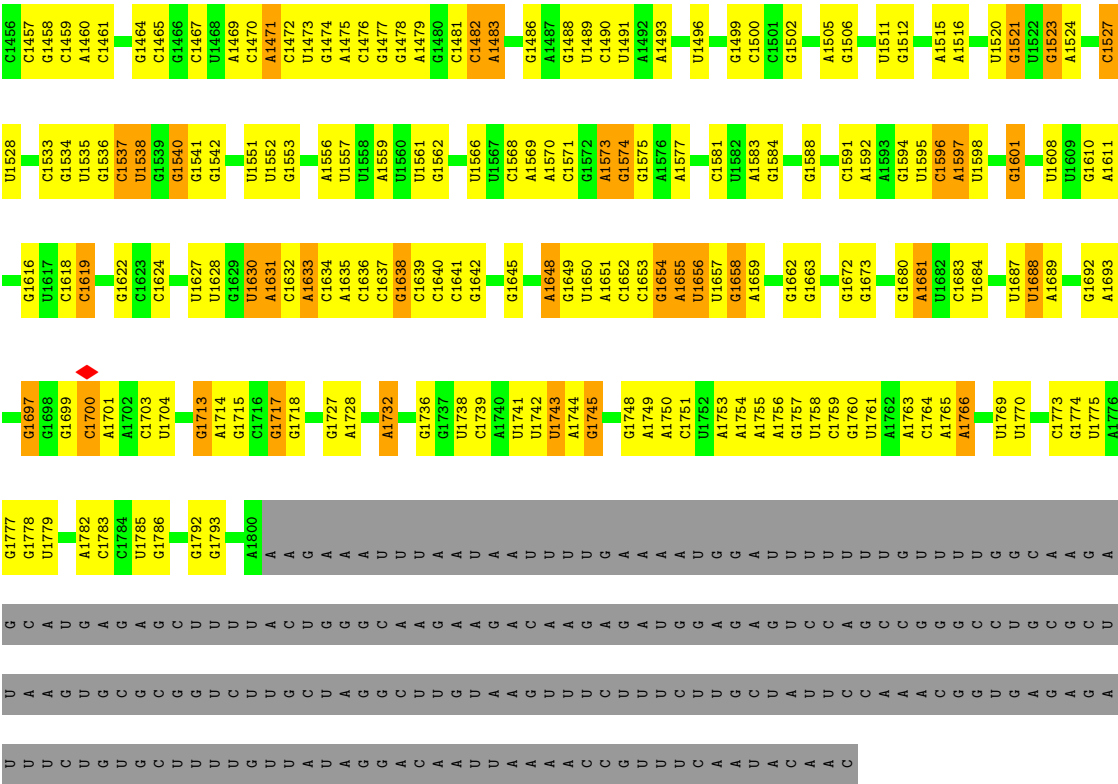
Chain γ :



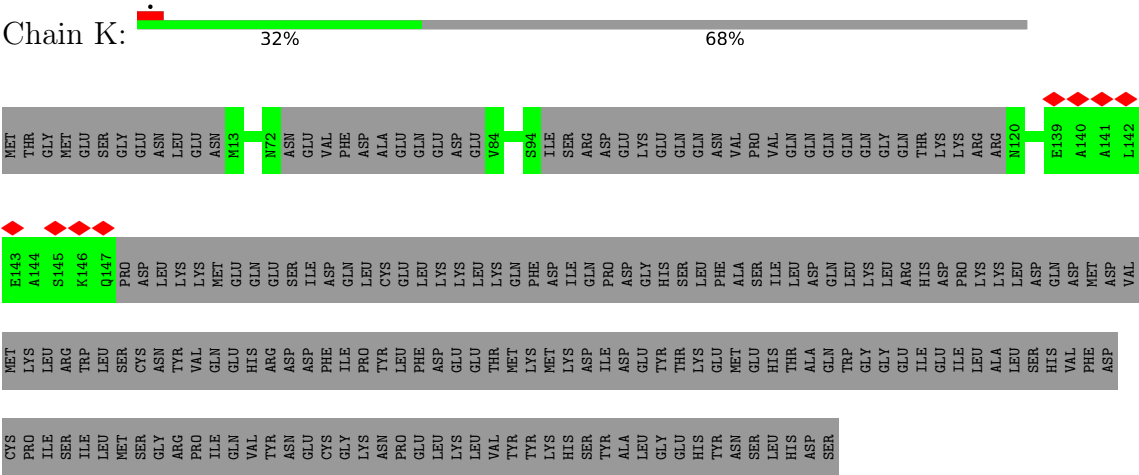
Chain 2:







● Molecule 39: OTU domain-containing protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.970	Depositor
Minimum map value	-1.474	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	b	0.34	0/620	0.77	3/838 (0.4%)
2	c	0.25	0/499	0.66	0/670
3	d	0.24	0/306	0.66	0/404
4	e	0.35	0/390	0.73	0/517
5	g	0.19	0/2484	0.48	2/3382 (0.1%)
6	h	0.37	0/1462	0.85	1/1969 (0.1%)
7	i	0.27	0/2188	0.63	3/2970 (0.1%)
8	j	0.16	0/403	0.39	0/543
9	k	0.25	0/5528	0.63	5/7477 (0.1%)
10	l	0.27	0/2368	0.71	2/3181 (0.1%)
11	A	0.35	0/1653	0.75	2/2261 (0.1%)
12	B	0.28	0/1735	0.74	1/2335 (0.0%)
13	C	0.34	0/1665	0.74	2/2263 (0.1%)
14	D	0.24	0/1596	0.56	1/2142 (0.0%)
15	E	0.39	0/2109	0.79	7/2839 (0.2%)
16	F	0.32	0/1629	0.71	2/2202 (0.1%)
17	G	0.27	0/1897	0.59	0/2532
18	H	0.32	0/1506	0.80	0/2028
19	I	0.42	1/1514 (0.1%)	0.73	1/2021 (0.0%)
20	J	0.41	1/1519 (0.1%)	0.83	2/2035 (0.1%)
21	L	0.38	0/1155	0.67	0/1557
22	M	0.22	0/949	0.52	0/1284
23	N	0.33	0/1215	0.77	2/1638 (0.1%)
24	O	0.28	0/937	0.65	0/1261
25	P	0.25	0/1022	0.64	1/1373 (0.1%)
26	Q	0.26	0/1011	0.61	0/1362
27	R	0.31	0/1010	0.86	5/1355 (0.4%)
28	S	0.25	0/1128	0.68	0/1518
29	T	0.28	0/1130	0.66	2/1517 (0.1%)
30	U	0.19	0/829	0.47	0/1121
31	V	0.39	0/693	0.78	0/935
32	W	0.46	0/1038	0.87	2/1395 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	X	0.36	0/1139	0.65	1/1518 (0.1%)
34	Y	0.34	0/1087	0.69	0/1449
35	Z	0.28	0/519	0.67	1/696 (0.1%)
36	a	0.11	0/1340	0.31	0/1861
37	y	0.27	0/1265	0.74	1/1702 (0.1%)
38	2	0.30	0/42123	0.48	8/65631 (0.0%)
39	K	0.13	0/491	0.31	0/682
All	All	0.30	2/93152 (0.0%)	0.59	57/134464 (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
9	k	0	1
12	B	0	1
20	J	0	1
21	L	0	1
27	R	0	1
37	y	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	I	101	ILE	CG1-CD1	-6.09	1.28	1.51
20	J	143	ILE	CG1-CD1	-5.27	1.31	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	1185	U	OP2-P-O3'	-9.97	78.07	108.00
15	E	237	SER	CA-C-N	7.52	132.12	120.68
15	E	237	SER	C-N-CA	7.52	132.12	120.68
9	k	379	PHE	CA-C-N	6.91	140.60	120.97
9	k	379	PHE	C-N-CA	6.91	140.60	120.97
1	b	17	ARG	CA-CB-CG	6.82	127.75	114.10
10	l	91	ARG	CA-C-N	6.81	132.06	122.46
10	l	91	ARG	C-N-CA	6.81	132.06	122.46
23	N	134	VAL	N-CA-C	-6.56	106.34	112.83
32	W	82	LYS	CA-CB-CG	6.42	126.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	95	THR	CA-C-N	6.32	133.61	121.54
15	E	95	THR	C-N-CA	6.32	133.61	121.54
7	i	373	LYS	CA-CB-CG	6.14	126.39	114.10
25	P	86	VAL	CB-CA-C	5.95	117.12	110.52
27	R	77	GLU	N-CA-CB	5.80	119.31	110.44
20	J	115	LYS	CB-CG-CD	5.79	124.61	111.30
27	R	79	GLU	N-CA-CB	5.77	119.03	110.49
29	T	109	GLU	N-CA-CB	5.75	119.20	110.28
38	2	1700	C	P-O3'-C3'	5.74	128.81	120.20
13	C	189	GLN	N-CA-CB	5.73	119.46	110.46
38	2	1156	C	P-O3'-C3'	5.67	128.70	120.20
6	h	217	GLU	N-CA-CB	5.65	118.62	110.20
29	T	109	GLU	CA-CB-CG	5.64	125.39	114.10
38	2	782	U	P-O3'-C3'	5.64	128.66	120.20
32	W	119	LYS	CB-CG-CD	5.61	124.20	111.30
27	R	78	ARG	CA-C-N	-5.60	113.30	122.54
27	R	78	ARG	C-N-CA	-5.60	113.30	122.54
13	C	189	GLN	CA-CB-CG	5.52	125.14	114.10
38	2	1343	U	P-O3'-C3'	5.50	128.44	120.20
9	k	476	GLU	N-CA-CB	5.42	119.23	110.40
38	2	1185	U	OP1-P-O3'	-5.41	91.76	108.00
33	X	93	LEU	CA-CB-CG	5.41	135.22	116.30
35	Z	69	LEU	CA-CB-CG	5.41	135.22	116.30
5	g	164	ASP	CA-C-N	5.39	131.83	121.54
5	g	164	ASP	C-N-CA	5.39	131.83	121.54
16	F	169	ASN	CA-C-N	-5.33	112.74	122.38
16	F	169	ASN	C-N-CA	-5.33	112.74	122.38
20	J	147	MET	CB-CG-SD	5.32	128.67	112.70
9	k	731	LYS	CA-CB-CG	5.30	124.69	114.10
7	i	373	LYS	CB-CA-C	-5.26	102.39	110.81
37	y	181	MET	CA-CB-CG	5.22	124.54	114.10
27	R	77	GLU	CA-CB-CG	5.18	124.46	114.10
14	D	150	MET	CB-CG-SD	5.16	128.19	112.70
23	N	54	LEU	CA-CB-CG	5.14	134.28	116.30
15	E	214	LEU	CA-C-N	5.13	131.35	121.54
15	E	214	LEU	C-N-CA	5.13	131.35	121.54
15	E	62	LYS	CA-CB-CG	5.11	124.33	114.10
38	2	418	G	C2'-C3'-O3'	5.11	121.36	113.70
19	I	188	GLU	CA-CB-CG	5.10	124.31	114.10
38	2	1004	U	C2-N1-C1'	5.10	133.00	117.70
11	A	188	LEU	CA-C-N	5.06	127.12	120.60
11	A	188	LEU	C-N-CA	5.06	127.12	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	90	PRO	CA-N-CD	-5.05	104.92	112.00
1	b	16	ALA	CA-C-N	5.05	127.98	120.31
1	b	16	ALA	C-N-CA	5.05	127.98	120.31
12	B	142	PHE	N-CA-C	5.02	114.92	108.34
7	i	426	GLN	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	B	144	ARG	Peptide
20	J	112	GLN	Peptide
21	L	10	GLU	Peptide
27	R	21	TYR	Peptide
9	k	392	VAL	Peptide
37	y	270	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	b	610	0	629	10	0
2	c	497	0	535	6	0
3	d	302	0	297	4	0
4	e	384	0	423	5	0
5	g	2431	0	2381	25	0
6	h	1436	0	1515	16	0
7	i	2133	0	2172	30	0
8	j	396	0	322	6	0
9	k	5402	0	5276	66	0
10	l	2322	0	2305	27	0
11	A	1611	0	1616	28	0
12	B	1709	0	1784	23	0
13	C	1635	0	1723	20	0
14	D	1576	0	1650	15	0
15	E	2068	0	2154	24	0
16	F	1609	0	1675	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1873	0	1980	36	0
18	H	1481	0	1572	23	0
19	I	1489	0	1525	35	0
20	J	1494	0	1573	23	0
21	L	1129	0	1196	17	0
22	M	941	0	982	12	0
23	N	1192	0	1255	25	0
24	O	926	0	950	25	0
25	P	1001	0	1042	19	0
26	Q	993	0	1051	23	0
27	R	1000	0	1063	22	0
28	S	1110	0	1134	12	0
29	T	1112	0	1124	13	0
30	U	819	0	885	3	0
31	V	684	0	672	8	0
32	W	1021	0	1060	19	0
33	X	1121	0	1196	15	0
34	Y	1073	0	1132	16	0
35	Z	512	0	551	5	0
36	a	1343	0	618	2	0
37	y	1245	0	1284	18	0
38	2	37662	0	18947	304	0
39	K	494	0	225	0	0
40	b	1	0	0	0	0
40	d	1	0	0	0	0
41	2	46	0	0	0	0
All	All	87884	0	69474	840	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 6.

All (840) 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)
38:2:1175:U:H3	38:2:1464:G:H1	1.01	1.00
38:2:1213:G:H1	38:2:1450:U:H3	1.13	0.96
38:2:641:G:H1	38:2:693:U:H3	0.97	0.94
38:2:273:G:H1	38:2:283:U:H3	1.14	0.94
38:2:898:A:H62	38:2:914:G:N2	1.66	0.94
38:2:1688:U:H3	38:2:1713:G:H1	0.97	0.92
38:2:1658:G:H1	38:2:1743:U:H3	0.95	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:706:A:H2	38:2:732:G:H1	1.14	0.90
38:2:699:U:H3	38:2:739:G:H1	1.19	0.89
38:2:898:A:H62	38:2:914:G:H21	1.20	0.87
12:B:109:LYS:O	12:B:113:MET:HB2	1.81	0.81
38:2:898:A:N6	38:2:914:G:H21	1.79	0.81
38:2:1335:U:H3	38:2:1416:G:H1	1.28	0.79
38:2:717:C:H42	38:2:720:G:N2	1.80	0.78
38:2:717:C:N4	38:2:720:G:H22	1.83	0.77
38:2:1145:U:H3	38:2:1633:A:H62	1.33	0.75
38:2:1697:G:H1	38:2:1704:U:H3	1.35	0.75
38:2:717:C:H42	38:2:720:G:H22	1.36	0.74
38:2:1267:G:H1	38:2:1442:U:HO2'	1.33	0.73
15:E:252:ARG:HH22	20:J:71:PHE:HA	1.55	0.71
38:2:1471:A:H62	38:2:1538:U:H3	1.37	0.70
35:Z:77:ARG:NH2	38:2:1534:G:N7	2.42	0.68
38:2:1273:G:O6	38:2:1437:U:C4	2.47	0.68
19:I:172:ARG:NH2	38:2:331:A:N7	2.45	0.65
9:k:708:PHE:HB2	9:k:718:ARG:HB2	1.78	0.64
38:2:1272:U:H3	38:2:1438:G:H1	1.44	0.64
38:2:996:U:H3	38:2:1008:G:H1	1.45	0.64
14:D:137:VAL:HB	14:D:185:LYS:HB2	1.80	0.64
10:l:5:THR:HB	25:P:141:LEU:HD11	1.81	0.63
1:b:4:VAL:HG11	31:V:71:ARG:HD3	1.80	0.63
16:F:108:LEU:HD22	38:2:1528:U:H5''	1.80	0.63
38:2:706:A:H2	38:2:732:G:N1	1.93	0.63
5:g:80:ALA:HB3	5:g:92:TRP:HB2	1.81	0.62
38:2:1149:G:H1	38:2:1628:U:H3	1.48	0.61
9:k:261:ALA:HB3	9:k:579:PHE:HB3	1.81	0.61
5:g:127:ARG:HD2	27:R:33:ARG:HD3	1.82	0.61
18:H:34:LEU:O	18:H:38:LEU:HB2	1.99	0.61
4:e:42:ARG:HH12	38:2:589:C:H5''	1.65	0.61
38:2:868:G:H1	38:2:960:U:H3	1.45	0.61
7:i:262:ALA:O	7:i:266:PHE:HB2	2.00	0.61
16:F:107:LYS:HE3	38:2:1610:G:H5''	1.81	0.61
23:N:5:HIS:HD2	23:N:121:ARG:HE	1.48	0.61
9:k:241:THR:HG22	9:k:245:ARG:HH21	1.66	0.60
15:E:45:ILE:HG13	15:E:61:VAL:HG11	1.83	0.60
5:g:107:LYS:HE3	5:g:128:ASP:HB2	1.84	0.60
14:D:140:GLY:HA3	14:D:182:LEU:HG	1.84	0.60
19:I:16:ALA:HB2	38:2:354:C:H5''	1.84	0.60
23:N:61:THR:HG23	38:2:959:U:H1'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:1174:C:H42	38:2:1465:C:H42	1.49	0.60
38:2:1472:C:O2'	38:2:1534:G:N2	2.34	0.60
12:B:207:LEU:HB3	12:B:210:ILE:HD11	1.83	0.60
38:2:1684:U:H3	38:2:1717:G:H1	1.49	0.60
7:i:307:VAL:HG12	7:i:341:VAL:HG11	1.83	0.60
19:I:98:LYS:HB3	38:2:329:G:H5''	1.82	0.60
19:I:5:ARG:NH2	38:2:332:U:O2'	2.35	0.60
7:i:396:ARG:NH1	7:i:408:ASP:OD2	2.35	0.60
16:F:70:VAL:HG21	26:Q:47:LYS:HG2	1.83	0.60
7:i:279:ILE:HG13	7:i:283:LEU:HB2	1.83	0.60
38:2:1638:G:H1	38:2:1766:A:H62	1.49	0.60
9:k:749:LEU:H	9:k:755:PHE:HA	1.67	0.59
10:l:231:ASN:ND2	38:2:1575:G:N3	2.50	0.59
7:i:214:TYR:HA	7:i:217:VAL:HG12	1.84	0.59
5:g:178:VAL:HB	5:g:192:PHE:HB2	1.85	0.59
1:b:26:GLN:NE2	38:2:864:U:O2	2.35	0.59
5:g:19:TRP:HB2	5:g:38:ARG:HD2	1.84	0.59
25:P:60:LEU:HD21	25:P:89:MET:HB3	1.84	0.59
33:X:69:ARG:NH2	33:X:71:CYS:SG	2.76	0.59
10:l:197:MET:HA	10:l:200:LEU:HB2	1.85	0.59
10:l:236:MET:HB3	10:l:250:VAL:HB	1.85	0.58
9:k:180:LEU:HB3	9:k:185:ILE:HD11	1.85	0.58
33:X:82:LYS:NZ	38:2:1650:U:OP1	2.36	0.58
38:2:1310:U:O2'	38:2:1401:A:N1	2.37	0.58
27:R:93:LEU:HB3	27:R:98:GLY:HA2	1.85	0.58
38:2:279:G:H8	38:2:280:U:H4'	1.69	0.58
38:2:984:G:H1	38:2:1017:U:H3	1.49	0.58
9:k:737:THR:HG22	9:k:739:SER:H	1.68	0.58
11:A:11:PRO:HG3	27:R:115:LEU:HD22	1.84	0.57
38:2:1213:G:N2	38:2:1450:U:O2	2.33	0.57
26:Q:21:HIS:HB2	26:Q:66:ARG:HB2	1.86	0.57
18:H:51:VAL:HG23	18:H:53:GLY:H	1.69	0.57
7:i:444:VAL:HG11	7:i:457:ARG:HB3	1.86	0.57
6:h:109:LEU:O	6:h:113:TRP:HB2	2.05	0.57
9:k:164:GLY:H	9:k:194:ASN:HB2	1.69	0.57
17:G:74:LYS:HA	17:G:96:SER:HA	1.87	0.57
19:I:178:ARG:NH2	38:2:207:U:O2	2.37	0.57
38:2:706:A:C2	38:2:732:G:N1	2.53	0.57
7:i:446:GLN:HG3	7:i:447:ARG:HG3	1.87	0.57
11:A:15:GLN:HB2	27:R:117:LEU:HD11	1.85	0.57
17:G:66:GLY:HA2	38:2:1681:A:H1'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:16:VAL:O	24:O:18:ARG:NH1	2.38	0.57
38:2:1285:U:H5'	38:2:1286:U:H4'	1.87	0.57
11:A:183:ARG:NH2	11:A:191:ARG:O	2.37	0.56
18:H:98:ILE:HG12	18:H:121:VAL:HG21	1.87	0.56
25:P:83:MET:HE1	25:P:89:MET:HE1	1.86	0.56
38:2:886:U:H2'	38:2:887:A:H8	1.70	0.56
18:H:41:LEU:HB3	18:H:70:PHE:HE1	1.69	0.56
20:J:88:GLU:O	20:J:91:LYS:NZ	2.36	0.56
38:2:1240:U:N3	38:2:1245:G:N7	2.54	0.56
15:E:48:LEU:HD11	15:E:70:VAL:HG21	1.88	0.56
24:O:121:VAL:O	38:2:886:U:O2'	2.24	0.56
9:k:766:GLN:NE2	38:2:1439:C:O2	2.39	0.56
26:Q:39:VAL:HG12	26:Q:41:PRO:HD2	1.88	0.56
38:2:1594:G:OP2	38:2:1596:C:N4	2.38	0.56
10:l:197:MET:HE1	10:l:235:ILE:HB	1.87	0.56
25:P:108:ARG:H	25:P:111:MET:HE3	1.71	0.56
38:2:706:A:N1	38:2:732:G:O6	2.38	0.56
38:2:1291:G:H2'	38:2:1292:G:H8	1.71	0.56
15:E:71:LYS:HB2	15:E:91:THR:HB	1.88	0.56
37:y:186:THR:HG22	37:y:208:ARG:HH21	1.71	0.56
32:W:90:THR:HA	32:W:94:LEU:HD13	1.86	0.55
30:U:20:ILE:HD11	30:U:118:VAL:HG13	1.88	0.55
38:2:1631:A:H5'	38:2:1633:A:H5''	1.88	0.55
16:F:166:ARG:HH21	38:2:1163:A:H4'	1.72	0.55
18:H:132:PRO:HD2	18:H:162:ILE:HD11	1.87	0.55
38:2:1082:C:H42	38:2:1091:A:H62	1.52	0.55
9:k:103:LYS:NZ	9:k:193:SER:O	2.40	0.55
19:I:168:CYS:SG	19:I:169:ILE:N	2.78	0.55
7:i:240:ARG:NH2	8:j:387:ASP:O	2.40	0.55
10:l:104:GLY:O	10:l:129:ARG:NH2	2.40	0.55
16:F:80:LYS:HB3	16:F:83:ARG:HB2	1.88	0.55
17:G:201:GLN:NE2	38:2:126:A:OP2	2.40	0.55
5:g:108:SER:HB3	5:g:128:ASP:HB3	1.87	0.55
6:h:241:ARG:NH2	38:2:905:A:OP1	2.39	0.55
17:G:215:ARG:O	17:G:215:ARG:NH1	2.39	0.55
34:Y:104:SER:OG	34:Y:105:ARG:N	2.38	0.55
17:G:67:VAL:HG13	17:G:99:GLY:HA2	1.88	0.55
2:c:58:GLU:HB2	2:c:61:ARG:HE	1.72	0.55
15:E:187:ARG:NH2	38:2:753:A:N7	2.55	0.55
19:I:8:ARG:HG3	19:I:18:ARG:HD2	1.89	0.55
17:G:135:PRO:HG2	17:G:141:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:43:LYS:NZ	38:2:740:A:OP2	2.41	0.54
25:P:53:PRO:HA	25:P:56:PHE:HB2	1.89	0.54
23:N:102:LEU:HD21	23:N:115:LEU:HD22	1.90	0.54
38:2:394:C:H42	38:2:401:A:H62	1.54	0.54
38:2:1356:U:H2'	38:2:1357:A:H8	1.72	0.54
13:C:82:ASN:HD21	13:C:207:LEU:HD12	1.73	0.54
5:g:292:LEU:HD12	5:g:301:LEU:HD11	1.90	0.54
11:A:112:THR:HG22	11:A:114:SER:H	1.73	0.54
13:C:180:ALA:HB1	13:C:184:VAL:HG13	1.89	0.54
17:G:50:PHE:HB3	17:G:111:LEU:HD22	1.89	0.54
7:i:357:SER:HA	7:i:360:LEU:HD12	1.89	0.54
14:D:55:THR:HB	14:D:92:GLN:H	1.73	0.54
15:E:126:VAL:HG21	15:E:154:ILE:HD11	1.90	0.54
15:E:178:GLY:O	15:E:231:GLN:NE2	2.41	0.54
38:2:1469:A:H4'	38:2:1541:G:H4'	1.88	0.54
20:J:17:ARG:O	20:J:23:ARG:NH2	2.40	0.54
20:J:113:VAL:HG21	20:J:129:ILE:HD11	1.88	0.54
24:O:15:GLY:H	24:O:79:VAL:HA	1.72	0.54
26:Q:94:GLN:HB2	26:Q:102:LYS:HE2	1.89	0.54
32:W:16:ASN:ND2	38:2:1037:C:O2	2.40	0.54
16:F:102:ARG:NH2	38:2:1470:C:OP2	2.41	0.54
7:i:379:LYS:HZ3	7:i:427:ARG:HB2	1.73	0.54
13:C:90:THR:HG22	13:C:91:ARG:HG3	1.90	0.54
16:F:76:ARG:HD3	26:Q:122:ARG:HG3	1.90	0.54
18:H:116:ARG:NH2	38:2:858:G:OP1	2.41	0.54
31:V:25:LYS:NZ	31:V:27:ASP:OD2	2.40	0.54
19:I:10:LYS:NZ	38:2:337:G:O2'	2.41	0.53
19:I:175:GLN:NE2	38:2:331:A:OP2	2.39	0.53
38:2:1227:A:O4'	38:2:1255:G:N2	2.41	0.53
18:H:103:SER:OG	18:H:104:ARG:N	2.41	0.53
38:2:1537:C:O2'	38:2:1540:G:O6	2.27	0.53
12:B:214:LYS:NZ	38:2:886:U:OP1	2.35	0.53
22:M:42:ALA:HB3	22:M:122:VAL:HB	1.88	0.53
26:Q:114:ARG:HH21	26:Q:115:THR:HG22	1.74	0.53
27:R:25:THR:HG23	27:R:27:ASP:H	1.72	0.53
10:l:120:ARG:HA	10:l:191:LEU:H	1.73	0.53
24:O:136:ARG:NH1	38:2:903:U:OP1	2.41	0.53
37:y:245:THR:HA	37:y:248:MET:HE2	1.91	0.53
7:i:409:ALA:O	7:i:447:ARG:NH1	2.41	0.53
15:E:108:ARG:NH2	38:2:788:A:OP2	2.37	0.53
17:G:70:PRO:HA	17:G:98:ARG:HH12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:192:TYR:HE1	21:L:13:PHE:HB2	1.73	0.53
20:J:171:ARG:NH2	38:2:538:A:OP2	2.41	0.53
37:y:227:LEU:O	37:y:231:PHE:HB3	2.09	0.53
15:E:176:ASP:HB2	15:E:179:LYS:HE3	1.89	0.53
16:F:133:VAL:HG22	16:F:198:LEU:HD21	1.90	0.53
17:G:188:ARG:HD3	38:2:283:U:H5''	1.90	0.53
25:P:137:ARG:NH2	38:2:1181:U:OP2	2.42	0.53
38:2:829:A:H4'	38:2:830:U:H5'	1.91	0.53
13:C:91:ARG:NH1	38:2:1289:U:OP2	2.42	0.53
23:N:46:THR:OG1	23:N:49:GLN:OE1	2.26	0.53
25:P:45:PHE:HA	25:P:49:MET:HE1	1.90	0.53
38:2:1588:G:H1	38:2:1608:U:H3	1.57	0.53
19:I:172:ARG:NH1	38:2:330:G:OP2	2.41	0.53
29:T:102:ARG:NH2	38:2:1500:C:OP2	2.38	0.52
38:2:47:A:N7	38:2:98:U:O2'	2.42	0.52
38:2:1656:U:H3	38:2:1745:G:H22	1.56	0.52
16:F:112:ARG:HH22	35:Z:97:LYS:HB3	1.74	0.52
32:W:115:GLU:O	32:W:119:LYS:HB2	2.09	0.52
1:b:30:SER:OG	1:b:31:TYR:N	2.41	0.52
11:A:23:HIS:HA	11:A:48:ILE:HG12	1.92	0.52
14:D:94:ARG:O	14:D:101:GLN:NE2	2.42	0.52
22:M:99:GLU:OE1	22:M:105:LYS:NZ	2.40	0.52
24:O:41:ARG:NH1	38:2:896:U:O2	2.42	0.52
32:W:2:THR:OG1	32:W:3:ARG:N	2.41	0.52
34:Y:38:ASP:OD1	34:Y:41:ARG:NH2	2.43	0.52
11:A:183:ARG:NH1	11:A:193:GLN:O	2.42	0.52
12:B:27:LYS:HD3	12:B:47:LEU:HD21	1.90	0.52
13:C:129:ILE:O	13:C:133:LYS:HB2	2.09	0.52
16:F:176:THR:HB	16:F:180:ARG:HH22	1.75	0.52
17:G:160:ARG:NH2	38:2:68:A:OP1	2.43	0.52
25:P:43:ARG:NH2	38:2:1552:U:OP2	2.42	0.52
1:b:17:ARG:NH1	38:2:1070:C:O3'	2.42	0.52
32:W:30:SER:OG	32:W:31:SER:N	2.42	0.52
38:2:1263:G:N2	38:2:1264:G:O6	2.43	0.52
34:Y:112:LYS:NZ	38:2:57:G:OP1	2.37	0.52
13:C:153:SER:OG	13:C:154:LEU:N	2.42	0.52
19:I:83:TYR:OH	21:L:11:ARG:NH1	2.43	0.52
38:2:862:A:O2'	38:2:963:A:N6	2.41	0.52
18:H:111:LYS:O	38:2:811:A:N6	2.40	0.52
20:J:136:VAL:HG12	20:J:156:ILE:HG12	1.92	0.52
21:L:55:ASP:OD1	21:L:82:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:29:HIS:HD2	24:O:41:ARG:HG3	1.75	0.52
38:2:1335:U:O2	38:2:1416:G:N2	2.40	0.52
12:B:204:ILE:O	38:2:1064:G:O2'	2.27	0.52
38:2:1243:G:H21	38:2:1451:C:H1'	1.74	0.52
5:g:41:THR:HG22	5:g:62:LYS:HB2	1.92	0.51
9:k:162:LEU:HD13	9:k:212:LEU:HD12	1.92	0.51
11:A:2:SER:N	31:V:77:GLY:O	2.43	0.51
7:i:360:LEU:HB3	7:i:393:TYR:HB2	1.92	0.51
9:k:594:VAL:HA	9:k:691:ALA:HA	1.92	0.51
13:C:43:ARG:NH1	13:C:247:ALA:O	2.43	0.51
9:k:709:ARG:NH1	38:2:1209:C:OP2	2.43	0.51
38:2:996:U:O2	38:2:1008:G:N2	2.40	0.51
18:H:141:ARG:NH1	32:W:49:GLU:OE1	2.44	0.51
19:I:7:SER:OG	38:2:336:G:N2	2.41	0.51
38:2:29:U:H2'	38:2:30:G:H8	1.76	0.51
18:H:101:LYS:H	38:2:639:U:H5	1.59	0.51
20:J:110:GLN:HE21	20:J:122:VAL:HG12	1.75	0.51
22:M:59:LEU:HA	22:M:87:PRO:HG2	1.91	0.51
23:N:121:ARG:NH1	38:2:868:G:OP1	2.38	0.51
31:V:34:ILE:HB	31:V:53:TYR:HB2	1.92	0.51
19:I:186:GLY:O	19:I:190:ALA:HB2	2.11	0.51
38:2:273:G:N2	38:2:283:U:O2	2.39	0.51
6:h:155:GLY:HA2	6:h:158:PHE:HD2	1.76	0.51
9:k:403:TRP:NE1	25:P:123:TYR:O	2.42	0.51
17:G:132:ARG:NH1	38:2:150:U:O4'	2.44	0.51
34:Y:78:SER:OG	34:Y:81:GLU:OE1	2.29	0.51
17:G:171:LYS:NZ	38:2:67:A:OP1	2.44	0.51
19:I:141:ARG:NH2	38:2:195:G:O6	2.44	0.51
25:P:81:ARG:NH1	25:P:120:SER:O	2.43	0.51
34:Y:25:VAL:HG11	34:Y:40:LEU:HD21	1.93	0.51
38:2:1688:U:O2	38:2:1713:G:N2	2.37	0.51
9:k:128:ILE:HG12	9:k:130:LYS:H	1.75	0.51
16:F:70:VAL:HG13	26:Q:43:ILE:HG22	1.92	0.51
18:H:87:ASP:O	18:H:88:ARG:NH1	2.38	0.51
26:Q:37:THR:O	26:Q:45:ARG:NH1	2.44	0.51
38:2:65:A:H2	38:2:84:A:H62	1.59	0.51
38:2:1658:G:O6	38:2:1743:U:O4	2.28	0.51
9:k:357:TRP:NE1	9:k:515:ASP:OD1	2.44	0.50
24:O:46:MET:HG3	24:O:47:LYS:HE3	1.92	0.50
34:Y:131:ARG:NH2	38:2:154:G:OP2	2.40	0.50
5:g:7:LEU:HD22	5:g:313:TRP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:97:ARG:NH2	38:2:1291:G:OP1	2.45	0.50
23:N:35:GLU:OE1	23:N:39:LYS:NZ	2.41	0.50
27:R:24:LEU:HD23	27:R:34:LEU:HD13	1.93	0.50
12:B:136:ARG:NH2	38:2:884:A:OP1	2.45	0.50
17:G:14:LYS:NZ	17:G:122:GLU:OE1	2.44	0.50
37:y:238:ILE:HB	37:y:291:GLY:HA2	1.93	0.50
9:k:252:TRP:HH2	9:k:620:VAL:HG13	1.76	0.50
23:N:35:GLU:HA	23:N:38:VAL:HG12	1.92	0.50
37:y:243:LYS:HA	37:y:248:MET:HB3	1.92	0.50
5:g:222:LEU:HB3	5:g:231:MET:HE3	1.94	0.50
12:B:109:LYS:O	12:B:113:MET:CB	2.57	0.50
13:C:142:GLY:N	13:C:153:SER:O	2.40	0.50
17:G:2:LYS:NZ	38:2:154:G:OP1	2.44	0.50
23:N:2:GLY:N	38:2:1035:G:OP1	2.44	0.50
27:R:79:GLU:O	27:R:83:GLN:HB3	2.12	0.50
38:2:1255:G:H21	38:2:1256:A:H62	1.59	0.50
11:A:98:ILE:HG21	11:A:102:PHE:HD1	1.77	0.50
38:2:898:A:N6	38:2:914:G:N2	2.43	0.50
33:X:90:ASP:HB3	33:X:93:LEU:H	1.77	0.50
5:g:22:SER:HB3	5:g:36:ALA:HB3	1.93	0.50
11:A:73:VAL:HG12	11:A:120:LEU:HB3	1.94	0.50
38:2:1697:G:O6	38:2:1704:U:O4	2.30	0.50
6:h:98:LYS:NZ	6:h:138:GLU:OE1	2.41	0.49
38:2:67:A:N6	38:2:83:G:O2'	2.45	0.49
38:2:144:U:H2'	38:2:145:A:H8	1.77	0.49
2:c:64:ARG:HG2	2:c:65:ARG:HD2	1.92	0.49
5:g:248:ASN:ND2	5:g:297:ASP:O	2.45	0.49
16:F:106:LYS:HE3	38:2:1527:C:H4'	1.93	0.49
19:I:138:ASN:OD1	19:I:141:ARG:NH1	2.45	0.49
32:W:82:LYS:HG3	32:W:84:GLY:H	1.76	0.49
5:g:309:VAL:O	5:g:311:ARG:NH1	2.46	0.49
7:i:361:ARG:HD3	8:j:369:GLU:HG2	1.94	0.49
16:F:46:TRP:HB3	16:F:130:ILE:HD11	1.93	0.49
19:I:141:ARG:NH2	38:2:196:G:O6	2.44	0.49
23:N:103:GLU:O	23:N:106:ARG:NH1	2.44	0.49
35:Z:74:SER:OG	38:2:1534:G:OP2	2.30	0.49
38:2:50:C:H2'	38:2:424:C:H41	1.77	0.49
38:2:929:A:OP2	38:2:931:C:N4	2.44	0.49
38:2:1561:U:H2'	38:2:1562:G:H8	1.77	0.49
7:i:408:ASP:HA	7:i:411:ARG:HD2	1.94	0.49
19:I:10:LYS:HD2	38:2:338:C:H5''	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:X:3:LYS:NZ	38:2:614:C:OP1	2.36	0.49
7:i:411:ARG:O	7:i:447:ARG:NH2	2.43	0.49
9:k:670:PHE:HA	9:k:683:ILE:HG12	1.95	0.49
11:A:52:LYS:O	11:A:56:LYS:HB2	2.12	0.49
29:T:122:ARG:NH1	38:2:1499:G:OP1	2.45	0.49
6:h:178:ASP:O	24:O:103:ARG:NH1	2.45	0.49
7:i:362:LEU:O	7:i:396:ARG:NH2	2.46	0.49
10:l:4:ASP:O	10:l:82:TYR:OH	2.30	0.49
10:l:229:ASP:O	10:l:234:ASN:ND2	2.40	0.49
38:2:953:G:H2'	38:2:954:G:H8	1.77	0.49
16:F:133:VAL:HA	16:F:198:LEU:HD11	1.94	0.49
27:R:5:ARG:O	27:R:10:LYS:NZ	2.45	0.49
29:T:16:ASN:OD1	29:T:56:LYS:NZ	2.40	0.49
34:Y:7:ILE:HD13	34:Y:43:LYS:HG2	1.93	0.49
38:2:1082:C:O2'	38:2:1083:G:O4'	2.30	0.49
1:b:42:ASN:C	1:b:42:ASN:HD22	2.20	0.49
18:H:133:THR:HG21	18:H:154:LEU:HD23	1.95	0.49
19:I:46:VAL:HG21	19:I:56:ARG:HE	1.76	0.49
19:I:195:ARG:HH12	21:L:11:ARG:HA	1.78	0.49
38:2:1673:G:O6	38:2:1728:A:N1	2.46	0.49
10:l:80:ILE:HA	10:l:83:LEU:HG	1.95	0.49
19:I:69:SER:OG	19:I:70:GLU:OE1	2.31	0.49
20:J:74:ASN:HA	20:J:77:ILE:HG22	1.95	0.49
38:2:1482:C:OP2	38:2:1521:G:N2	2.40	0.49
7:i:276:GLN:HA	7:i:279:ILE:HG22	1.95	0.49
9:k:231:LYS:NZ	9:k:232:ASN:OD1	2.43	0.49
27:R:71:PHE:O	27:R:74:GLN:N	2.46	0.49
31:V:33:GLN:NE2	31:V:53:TYR:O	2.46	0.49
38:2:1243:G:N2	38:2:1451:C:O2	2.46	0.49
38:2:1556:A:H61	38:2:1597:A:H2	1.61	0.49
15:E:134:LYS:NZ	38:2:205:U:OP1	2.45	0.48
37:y:235:ASN:O	37:y:294:ARG:NH1	2.45	0.48
38:2:1470:C:OP1	38:2:1540:G:O2'	2.31	0.48
3:d:33:LYS:HE2	38:2:1594:G:H4'	1.96	0.48
9:k:500:ARG:HH12	9:k:519:PRO:HG2	1.77	0.48
13:C:209:ASN:ND2	38:2:1298:U:O2	2.46	0.48
23:N:72:MET:HA	23:N:75:LEU:HB3	1.95	0.48
35:Z:77:ARG:NH1	38:2:1533:C:OP2	2.45	0.48
1:b:16:ALA:O	1:b:29:ARG:NH1	2.46	0.48
9:k:103:LYS:HB3	9:k:229:LEU:HB3	1.94	0.48
9:k:307:GLU:HG3	9:k:336:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:267:TYR:O	10:l:271:ARG:HB2	2.13	0.48
11:A:176:LEU:HA	11:A:179:ARG:HG2	1.95	0.48
16:F:42:LEU:HD12	16:F:48:PHE:HB2	1.95	0.48
23:N:73:ARG:NH2	38:2:859:A:O2'	2.45	0.48
24:O:41:ARG:NH2	38:2:916:U:O4	2.46	0.48
38:2:1213:G:H1'	38:2:1243:G:H1	1.77	0.48
11:A:35:PRO:O	11:A:52:LYS:NZ	2.40	0.48
5:g:237:GLN:OE1	5:g:261:LYS:NZ	2.46	0.48
38:2:1381:U:H2'	38:2:1382:A:H8	1.77	0.48
14:D:132:LYS:NZ	14:D:156:PHE:O	2.46	0.48
19:I:136:SER:OG	38:2:188:A:OP1	2.31	0.48
20:J:85:VAL:HG12	20:J:99:LEU:HD11	1.94	0.48
34:Y:37:LYS:HG3	38:2:522:U:H5''	1.94	0.48
34:Y:105:ARG:NH2	38:2:458:G:OP2	2.47	0.48
38:2:1115:U:H2'	38:2:1116:A:H8	1.78	0.48
5:g:24:ALA:HB3	5:g:34:LEU:HB3	1.96	0.48
25:P:93:VAL:HA	25:P:106:GLU:HA	1.95	0.48
37:y:233:ARG:NH1	38:2:1012:U:O2	2.41	0.48
7:i:317:PHE:O	7:i:321:PHE:HB3	2.13	0.48
10:l:74:ARG:HH21	10:l:147:GLN:H	1.61	0.48
16:F:68:ILE:HG13	16:F:71:ALA:H	1.78	0.48
20:J:44:ARG:NH1	38:2:473:A:OP1	2.41	0.48
21:L:33:ARG:NH2	21:L:53:TYR:O	2.41	0.48
26:Q:72:GLY:O	38:2:1482:C:O2'	2.31	0.48
38:2:1345:A:O2'	38:2:1348:A:N6	2.43	0.48
9:k:699:LYS:HZ3	9:k:775:LYS:HG3	1.79	0.48
10:l:105:LYS:NZ	38:2:1577:A:O3'	2.46	0.48
10:l:177:PRO:HB3	10:l:192:ILE:HD11	1.96	0.48
18:H:108:GLN:NE2	38:2:742:U:OP1	2.46	0.48
28:S:27:LYS:NZ	28:S:55:HIS:O	2.46	0.48
6:h:252:LEU:HD21	24:O:134:GLY:HA3	1.96	0.48
32:W:122:SER:OG	32:W:123:GLY:N	2.47	0.48
33:X:65:ASN:ND2	38:2:570:A:OP2	2.47	0.48
38:2:795:U:H2'	38:2:796:A:H8	1.79	0.48
38:2:1005:A:O2'	38:2:1006:C:O4'	2.29	0.48
12:B:186:SER:OG	12:B:187:LYS:NZ	2.45	0.47
19:I:186:GLY:O	19:I:190:ALA:CB	2.62	0.47
20:J:133:HIS:NE2	38:2:512:A:O2'	2.43	0.47
34:Y:19:ALA:HB3	34:Y:81:GLU:HG2	1.95	0.47
38:2:1397:U:O2'	38:2:1400:A:N6	2.47	0.47
10:l:123:LYS:HB3	10:l:187:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:H:112:ARG:NH2	18:H:117:THR:OG1	2.48	0.47
25:P:43:ARG:HH21	38:2:1551:U:H3'	1.80	0.47
38:2:598:U:H2'	38:2:599:A:H8	1.78	0.47
38:2:1511:U:H2'	38:2:1512:G:H8	1.79	0.47
9:k:84:LYS:HB2	9:k:135:LEU:HD13	1.96	0.47
9:k:687:THR:OG1	33:X:144:ARG:NH1	2.46	0.47
10:l:234:ASN:HD21	10:l:253:ASP:HB2	1.79	0.47
14:D:3:ALA:N	38:2:1491:U:OP2	2.47	0.47
38:2:1552:U:O2'	38:2:1597:A:O2'	2.29	0.47
34:Y:41:ARG:HG3	34:Y:55:VAL:HG23	1.96	0.47
3:d:56:ARG:NH2	38:2:1334:U:O2	2.39	0.47
7:i:326:VAL:HA	7:i:330:CYS:HB2	1.95	0.47
11:A:198:MET:SD	11:A:198:MET:N	2.88	0.47
18:H:162:ILE:HG23	18:H:169:PHE:HE2	1.79	0.47
19:I:5:ARG:NH1	38:2:336:G:O6	2.47	0.47
19:I:18:ARG:NH1	38:2:105:A:OP1	2.46	0.47
33:X:48:HIS:HB3	33:X:103:LEU:HD11	1.97	0.47
36:a:337:VAL:HA	36:a:348:PRO:HA	1.96	0.47
2:c:8:THR:OG1	2:c:56:LEU:O	2.31	0.47
2:c:18:ARG:HG3	38:2:1616:G:H4'	1.97	0.47
9:k:398:ASP:OD1	9:k:398:ASP:N	2.48	0.47
19:I:184:LEU:HB3	19:I:189:LEU:HB2	1.97	0.47
20:J:113:VAL:HG13	20:J:118:LEU:HB2	1.97	0.47
23:N:119:GLU:OE1	23:N:123:HIS:NE2	2.47	0.47
38:2:1182:U:H3	38:2:1185:U:H5''	1.79	0.47
7:i:270:LEU:HD13	7:i:274:GLU:HG2	1.97	0.47
9:k:65:ARG:HH12	38:2:434:G:P	2.37	0.47
15:E:180:LEU:N	15:E:229:GLY:O	2.44	0.47
16:F:72:HIS:HD1	16:F:107:LYS:HD2	1.80	0.47
20:J:130:THR:OG1	38:2:475:A:OP1	2.29	0.47
26:Q:46:PHE:HA	26:Q:49:TYR:HB2	1.96	0.47
28:S:104:ASN:OD1	28:S:107:SER:OG	2.32	0.47
29:T:89:ARG:NH1	38:2:1601:G:O4'	2.47	0.47
38:2:979:A:N3	38:2:1775:U:O2'	2.45	0.47
38:2:1662:G:H2'	38:2:1663:G:H8	1.80	0.47
9:k:180:LEU:HA	9:k:183:GLN:HG2	1.96	0.47
11:A:24:LEU:HD13	36:a:306:ALA:HB1	1.97	0.47
22:M:91:VAL:HG21	22:M:97:LEU:HD13	1.96	0.47
26:Q:44:LEU:HB3	26:Q:78:VAL:HG11	1.96	0.47
27:R:106:THR:HA	27:R:109:LEU:HG	1.96	0.47
37:y:285:LEU:HD13	37:y:291:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:632:U:O2'	38:2:1103:U:OP1	2.32	0.47
12:B:151:LYS:NZ	38:2:1044:U:OP2	2.46	0.47
17:G:28:PHE:O	17:G:30:LYS:NZ	2.44	0.47
37:y:244:SER:OG	38:2:1012:U:O3'	2.32	0.47
38:2:706:A:N1	38:2:732:G:C6	2.83	0.47
38:2:973:A:H2'	38:2:974:A:H8	1.79	0.47
3:d:56:ARG:HH12	38:2:1418:G:H1'	1.80	0.47
12:B:49:ASN:ND2	38:2:896:U:OP1	2.47	0.47
17:G:179:VAL:HG11	38:2:140:A:H1'	1.97	0.47
18:H:90:VAL:O	18:H:165:LYS:NZ	2.46	0.47
26:Q:66:ARG:HH12	38:2:1365:C:H5''	1.79	0.47
9:k:146:LEU:HD23	9:k:149:LEU:HD12	1.95	0.46
9:k:595:ASN:N	9:k:690:ASN:O	2.46	0.46
18:H:117:THR:OG1	38:2:638:U:O3'	2.33	0.46
7:i:256:PRO:HB2	7:i:302:HIS:HB2	1.98	0.46
26:Q:42:GLU:OE1	38:2:1528:U:O2'	2.33	0.46
29:T:138:GLN:HA	29:T:141:GLU:HB2	1.96	0.46
38:2:1785:U:H2'	38:2:1786:G:H8	1.79	0.46
10:l:240:LYS:HB2	10:l:246:ASP:HB2	1.97	0.46
35:Z:53:GLU:HG2	35:Z:68:ARG:HH21	1.80	0.46
38:2:1175:U:H2'	38:2:1176:G:H8	1.81	0.46
5:g:42:LEU:HB2	5:g:61:PHE:HB2	1.97	0.46
7:i:270:LEU:O	7:i:313:LYS:NZ	2.46	0.46
9:k:73:ARG:NH2	9:k:244:GLN:O	2.48	0.46
9:k:376:ASP:OD1	9:k:376:ASP:N	2.48	0.46
9:k:573:ASP:HB3	9:k:576:GLN:HB2	1.97	0.46
9:k:667:ALA:O	9:k:686:GLY:N	2.48	0.46
10:l:230:PHE:HE2	10:l:235:ILE:HD11	1.81	0.46
12:B:26:ARG:NH2	12:B:28:GLU:OE2	2.44	0.46
26:Q:13:LYS:O	26:Q:76:SER:OG	2.33	0.46
38:2:711:U:H3	38:2:727:U:H3	1.63	0.46
16:F:106:LYS:HG3	16:F:109:LYS:HB2	1.97	0.46
23:N:52:VAL:HG22	23:N:55:ARG:HH21	1.81	0.46
27:R:108:ASP:HA	27:R:111:LYS:HG2	1.98	0.46
38:2:992:A:H2	38:2:1012:U:H3	1.62	0.46
38:2:1688:U:O4	38:2:1713:G:O6	2.33	0.46
5:g:217:ASP:OD1	5:g:217:ASP:N	2.49	0.46
10:l:85:LEU:HD21	25:P:141:LEU:HB3	1.98	0.46
15:E:68:ARG:HE	15:E:76:VAL:HG11	1.80	0.46
16:F:76:ARG:NH1	26:Q:121:SER:OG	2.49	0.46
19:I:4:SER:HB2	19:I:24:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:12:SER:OG	19:I:13:ALA:N	2.49	0.46
19:I:157:GLU:HA	19:I:160:PHE:HB2	1.97	0.46
21:L:16:GLN:NE2	21:L:61:THR:O	2.48	0.46
38:2:699:U:O2	38:2:739:G:N2	2.43	0.46
9:k:641:LYS:NZ	9:k:642:TYR:O	2.41	0.46
11:A:127:ARG:HD2	11:A:152:PRO:HG3	1.98	0.46
24:O:136:ARG:NH2	38:2:904:G:OP2	2.49	0.46
37:y:190:LYS:NZ	37:y:191:VAL:O	2.48	0.46
9:k:256:ARG:NH1	9:k:663:THR:OG1	2.48	0.46
9:k:565:LYS:HD2	9:k:568:LEU:HD12	1.98	0.46
12:B:122:GLU:O	12:B:165:ARG:NH1	2.46	0.46
21:L:122:ILE:HG13	21:L:143:SER:HB2	1.97	0.46
23:N:65:VAL:HG13	23:N:66:ILE:HG23	1.98	0.46
26:Q:16:ALA:HB2	26:Q:72:GLY:HA3	1.97	0.46
28:S:97:ASP:OD1	28:S:97:ASP:N	2.48	0.46
29:T:77:ASN:HB3	29:T:95:ASP:HB3	1.98	0.46
9:k:265:ASP:HB2	9:k:277:VAL:HB	1.97	0.46
9:k:533:ASN:O	9:k:537:THR:OG1	2.30	0.46
9:k:700:ARG:HD3	9:k:702:ILE:HD11	1.98	0.46
22:M:43:ARG:NH2	38:2:1255:G:O2'	2.49	0.46
23:N:20:ARG:NH2	38:2:861:U:O3'	2.48	0.46
23:N:39:LYS:O	23:N:43:LYS:NZ	2.47	0.46
23:N:50:ILE:O	23:N:54:LEU:HB2	2.16	0.46
28:S:115:ARG:HA	28:S:118:LYS:HE3	1.97	0.46
37:y:220:TYR:O	37:y:224:ASP:HB2	2.15	0.46
38:2:476:U:OP1	38:2:477:A:O2'	2.29	0.46
38:2:890:C:H2'	38:2:891:A:H8	1.81	0.46
21:L:75:VAL:HG13	21:L:119:VAL:HA	1.97	0.46
22:M:62:LEU:HD11	22:M:88:LEU:HD22	1.98	0.46
27:R:78:ARG:O	27:R:81:LYS:NZ	2.38	0.46
27:R:117:LEU:HD23	27:R:119:LEU:HD21	1.98	0.46
38:2:814:A:O2'	38:2:816:G:OP2	2.33	0.46
38:2:1187:U:O2	38:2:1198:G:O6	2.33	0.46
38:2:1483:A:OP2	38:2:1521:G:N2	2.43	0.46
1:b:20:LYS:NZ	23:N:13:SER:O	2.39	0.45
9:k:282:VAL:HG13	9:k:553:ALA:HA	1.96	0.45
16:F:139:ASN:ND2	16:F:202:ALA:O	2.48	0.45
17:G:121:LEU:O	17:G:125:THR:OG1	2.31	0.45
17:G:142:ARG:HG3	17:G:147:LEU:HB2	1.98	0.45
38:2:568:G:N2	38:2:582:U:O2'	2.48	0.45
6:h:223:ARG:HB2	6:h:234:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:267:TYR:HA	10:l:270:GLN:HG3	1.99	0.45
13:C:175:GLY:N	13:C:195:ASP:OD1	2.42	0.45
16:F:92:ARG:NH2	16:F:169:ASN:OD1	2.47	0.45
20:J:67:PRO:HA	20:J:70:LEU:HG	1.98	0.45
30:U:85:ARG:NH2	38:2:1336:A:OP1	2.49	0.45
32:W:14:ILE:HD13	32:W:25:VAL:HG11	1.98	0.45
32:W:41:MET:HG2	32:W:129:VAL:HG11	1.99	0.45
33:X:54:LEU:HD12	33:X:73:ARG:HG3	1.97	0.45
2:c:18:ARG:HD3	2:c:26:THR:HB	1.99	0.45
7:i:408:ASP:OD1	7:i:411:ARG:NH1	2.45	0.45
8:j:396:GLU:HA	8:j:399:LEU:HD12	1.97	0.45
20:J:50:SER:OG	20:J:54:ARG:NH1	2.49	0.45
20:J:121:SER:OG	20:J:122:VAL:N	2.49	0.45
21:L:109:VAL:HG11	21:L:125:VAL:HG11	1.98	0.45
22:M:36:LEU:HD22	22:M:102:GLY:HA3	1.98	0.45
23:N:99:ARG:NH2	23:N:143:SER:O	2.49	0.45
24:O:74:VAL:HG23	24:O:76:ILE:HG12	1.99	0.45
29:T:7:ARG:NH1	38:2:1366:U:O2'	2.49	0.45
38:2:1553:G:N1	38:2:1556:A:OP2	2.50	0.45
6:h:153:GLN:HG2	24:O:103:ARG:HA	1.97	0.45
11:A:146:LEU:HD23	11:A:160:ILE:HB	1.98	0.45
17:G:2:LYS:HB3	17:G:108:VAL:HG22	1.98	0.45
17:G:7:TYR:HD2	17:G:10:ASN:H	1.64	0.45
38:2:656:G:O2'	38:2:657:U:O4'	2.34	0.45
38:2:1151:A:H62	38:2:1627:U:H3	1.65	0.45
38:2:1777:G:H2'	38:2:1778:G:C8	2.51	0.45
26:Q:12:LYS:O	26:Q:83:GLN:NE2	2.44	0.45
29:T:75:LYS:O	29:T:79:LEU:HB2	2.17	0.45
37:y:276:VAL:HA	37:y:280:LYS:HB2	1.97	0.45
38:2:1573:A:OP1	38:2:1574:G:N2	2.49	0.45
10:l:266:ASP:N	10:l:266:ASP:OD1	2.46	0.45
13:C:119:LYS:NZ	38:2:1291:G:OP1	2.50	0.45
16:F:65:ARG:HA	16:F:65:ARG:HD3	1.83	0.45
17:G:140:ASN:HA	17:G:143:LYS:HG2	1.99	0.45
21:L:63:LEU:O	21:L:129:ARG:NH1	2.50	0.45
9:k:741:ARG:HD3	9:k:761:GLY:H	1.82	0.45
13:C:201:ASN:OD1	38:2:607:G:O2'	2.33	0.45
28:S:49:LYS:HE3	28:S:79:TYR:HB3	1.98	0.45
32:W:28:ARG:HG3	32:W:60:LYS:HG2	1.98	0.45
32:W:69:LEU:HD11	32:W:72:CYS:HB3	1.98	0.45
38:2:1638:G:H1	38:2:1766:A:N6	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:187:VAL:HG13	6:h:251:ILE:HD11	1.99	0.45
11:A:8:ASP:OD1	11:A:8:ASP:N	2.50	0.45
11:A:205:ARG:NH1	11:A:206:PHE:O	2.49	0.45
15:E:242:LYS:HD3	15:E:242:LYS:HA	1.77	0.45
19:I:81:VAL:HG22	19:I:102:VAL:HG12	1.99	0.45
38:2:551:G:H2'	38:2:552:G:H8	1.82	0.45
17:G:227:ARG:HH21	17:G:230:ARG:HD2	1.82	0.45
24:O:90:ARG:HG2	24:O:91:THR:H	1.82	0.45
29:T:39:THR:OG1	38:2:1478:G:OP1	2.34	0.45
38:2:273:G:O6	38:2:283:U:O4	2.34	0.45
38:2:641:G:O6	38:2:693:U:O4	2.35	0.45
9:k:54:ARG:NH1	38:2:358:U:OP1	2.43	0.45
9:k:478:GLU:O	9:k:482:PHE:N	2.50	0.45
9:k:564:PRO:HG2	9:k:567:LEU:HD12	1.99	0.45
21:L:132:SER:OG	21:L:133:LYS:N	2.50	0.45
27:R:3:ARG:NH1	38:2:1415:U:OP1	2.49	0.45
34:Y:29:HIS:HB2	34:Y:32:ARG:HB2	1.99	0.45
38:2:992:A:O2'	38:2:1785:U:O2	2.33	0.45
9:k:601:TRP:HE1	9:k:685:HIS:HB3	1.82	0.44
11:A:155:PHE:HD1	31:V:60:ARG:HG2	1.82	0.44
12:B:118:GLN:OE1	12:B:208:GLN:NE2	2.49	0.44
28:S:2:SER:OG	28:S:3:LEU:N	2.49	0.44
38:2:566:C:OP2	38:2:567:A:N6	2.50	0.44
6:h:94:PHE:O	24:O:111:ARG:NH1	2.41	0.44
15:E:106:LYS:NZ	38:2:789:A:O2'	2.49	0.44
15:E:122:LYS:HB3	15:E:164:LEU:HD11	1.99	0.44
16:F:112:ARG:HA	16:F:115:LYS:HG2	1.99	0.44
18:H:154:LEU:HD11	18:H:183:PHE:HD2	1.81	0.44
22:M:93:ASP:HB2	22:M:96:GLN:HB2	1.99	0.44
14:D:75:LYS:HA	14:D:75:LYS:HD3	1.86	0.44
38:2:289:U:H2'	38:2:290:G:H8	1.82	0.44
38:2:1775:U:H3	38:2:1786:G:H1	1.65	0.44
12:B:164:ILE:HG23	12:B:201:THR:HG21	1.99	0.44
15:E:27:TYR:OH	38:2:460:A:O2'	2.35	0.44
20:J:133:HIS:ND1	20:J:162:SER:OG	2.36	0.44
27:R:24:LEU:HB2	27:R:58:MET:HE3	1.98	0.44
32:W:6:VAL:HG12	32:W:34:ILE:HD11	2.00	0.44
9:k:106:LYS:NZ	9:k:111:GLU:OE1	2.50	0.44
14:D:142:LEU:HD12	14:D:148:LYS:HD2	1.99	0.44
15:E:147:ILE:HG21	15:E:169:ILE:HG13	1.98	0.44
20:J:175:ARG:NH1	38:2:538:A:OP1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:99:ARG:HA	23:N:102:LEU:HG	1.99	0.44
38:2:1630:U:H2'	38:2:1631:A:H4'	1.99	0.44
9:k:251:ASN:O	9:k:255:ASN:ND2	2.51	0.44
9:k:474:ASP:HA	9:k:477:LYS:HG2	1.99	0.44
19:I:83:TYR:HD2	19:I:101:ILE:HD12	1.80	0.44
26:Q:22:VAL:HG13	26:Q:65:ILE:HG13	1.99	0.44
10:l:119:PRO:HB2	10:l:191:LEU:HD22	1.99	0.44
11:A:179:ARG:HA	11:A:182:LEU:HG	1.99	0.44
18:H:112:ARG:HA	18:H:113:PRO:HD3	1.91	0.44
38:2:1476:C:H2'	38:2:1477:G:H8	1.83	0.44
7:i:266:PHE:HD2	7:i:270:LEU:HD11	1.83	0.44
7:i:434:GLN:HG2	7:i:465:SER:HB2	2.00	0.44
9:k:297:ASP:OD1	9:k:622:ARG:NH2	2.49	0.44
11:A:138:TYR:OH	38:2:1296:A:OP1	2.34	0.44
16:F:131:GLN:HA	16:F:134:VAL:HG12	1.99	0.44
20:J:141:VAL:HG12	38:2:767:U:H6	1.81	0.44
23:N:135:LEU:HD12	23:N:136:PRO:HD2	2.00	0.44
25:P:30:THR:HA	25:P:33:PHE:HD2	1.82	0.44
38:2:472:U:O2'	38:2:769:A:N3	2.39	0.44
38:2:1521:G:O2'	38:2:1523:G:OP2	2.29	0.44
17:G:159:ARG:HH21	17:G:170:THR:HG23	1.83	0.44
23:N:5:HIS:NE2	23:N:120:SER:OG	2.51	0.44
27:R:82:ASP:OD1	27:R:82:ASP:N	2.48	0.44
32:W:56:HIS:O	38:2:861:U:O2'	2.31	0.44
38:2:1645:G:H22	38:2:1756:A:H2	1.66	0.44
4:e:56:MET:SD	4:e:56:MET:N	2.91	0.43
10:l:275:CYS:HA	10:l:278:ARG:HG2	2.00	0.43
13:C:140:ARG:NH2	31:V:1:MET:SD	2.86	0.43
38:2:1658:G:N2	38:2:1743:U:O2	2.41	0.43
6:h:129:ARG:HA	6:h:129:ARG:HD3	1.83	0.43
12:B:133:TYR:HE1	12:B:181:LEU:HD13	1.83	0.43
16:F:113:ILE:O	16:F:117:THR:OG1	2.31	0.43
23:N:16:ILE:O	32:W:57:ARG:NH2	2.50	0.43
29:T:89:ARG:HH22	38:2:1467:C:H1'	1.82	0.43
37:y:156:GLN:HE22	37:y:158:GLU:HB2	1.82	0.43
38:2:1278:G:H22	38:2:1430:U:H3	1.66	0.43
38:2:1290:U:H2'	38:2:1291:G:C8	2.53	0.43
2:c:64:ARG:HE	2:c:65:ARG:HH11	1.66	0.43
12:B:197:ILE:HG21	12:B:210:ILE:HG21	1.99	0.43
16:F:148:ARG:HH12	16:F:157:ARG:HE	1.65	0.43
20:J:54:ARG:HG3	20:J:57:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:10:GLU:HG2	21:L:11:ARG:H	1.82	0.43
25:P:37:ALA:HB1	25:P:41:VAL:HB	2.00	0.43
9:k:158:VAL:HG21	9:k:185:ILE:HD12	2.00	0.43
24:O:18:ARG:HH12	24:O:31:THR:HG22	1.83	0.43
32:W:51:GLU:N	32:W:62:VAL:O	2.43	0.43
24:O:31:THR:HB	24:O:38:THR:HA	2.01	0.43
24:O:49:LYS:HA	24:O:49:LYS:HD3	1.87	0.43
25:P:56:PHE:HA	25:P:59:LYS:HE3	2.01	0.43
32:W:87:GLU:OE2	32:W:117:ARG:NH2	2.48	0.43
38:2:17:C:O2'	38:2:1137:A:N1	2.50	0.43
38:2:1035:G:H2'	38:2:1036:A:H8	1.84	0.43
38:2:1591:C:H2'	38:2:1592:A:H8	1.82	0.43
5:g:59:ARG:NH2	5:g:96:THR:O	2.51	0.43
24:O:48:VAL:HG12	24:O:50:ALA:H	1.83	0.43
25:P:61:ARG:HA	25:P:64:LYS:HB2	2.00	0.43
37:y:256:LYS:HA	37:y:259:LEU:HG	1.99	0.43
38:2:513:U:H2'	38:2:514:G:C8	2.54	0.43
38:2:1488:G:H3'	38:2:1515:A:H61	1.84	0.43
9:k:708:PHE:N	9:k:716:THR:O	2.51	0.43
13:C:208:GLU:OE2	13:C:208:GLU:N	2.50	0.43
15:E:173:ILE:HD13	15:E:229:GLY:HA2	2.00	0.43
38:2:67:A:O2'	38:2:69:G:OP1	2.36	0.43
13:C:144:TRP:HZ3	20:J:60:LEU:HD23	1.84	0.43
16:F:158:GLN:NE2	16:F:159:ALA:O	2.50	0.43
22:M:66:VAL:HB	22:M:72:ILE:HD11	2.01	0.43
38:2:1223:A:H2'	38:2:1224:A:C8	2.54	0.43
38:2:1273:G:O6	38:2:1437:U:O4	2.37	0.43
9:k:379:PHE:CE2	9:k:731:LYS:HG3	2.54	0.43
17:G:140:ASN:OD1	17:G:143:LYS:NZ	2.47	0.43
20:J:110:GLN:HE22	20:J:126:ARG:HB2	1.83	0.43
20:J:121:SER:H	20:J:124:HIS:HB3	1.84	0.43
26:Q:66:ARG:NH2	38:2:1366:U:OP2	2.52	0.43
27:R:33:ARG:HA	27:R:36:ASP:HB2	1.99	0.43
33:X:94:ASN:OD1	33:X:94:ASN:N	2.50	0.43
38:2:1177:C:H5''	38:2:1189:A:H61	1.83	0.43
38:2:1286:U:H6	38:2:1286:U:H2'	1.70	0.43
5:g:135:THR:HG22	5:g:139:GLN:H	1.84	0.43
38:2:5:U:H2'	38:2:6:G:H8	1.84	0.43
15:E:31:PRO:HA	15:E:81:THR:HB	1.99	0.42
34:Y:55:VAL:HG12	34:Y:75:VAL:HA	2.01	0.42
38:2:5:U:H2'	38:2:6:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:87:C:O2'	38:2:169:A:N1	2.41	0.42
38:2:1265:G:OP2	38:2:1265:G:N2	2.43	0.42
11:A:205:ARG:HD2	27:R:80:ARG:HH12	1.84	0.42
17:G:5:ILE:HD11	17:G:113:ILE:HG12	2.01	0.42
25:P:18:ARG:NH1	28:S:90:ASN:O	2.52	0.42
26:Q:54:LEU:HD21	26:Q:112:TYR:HB3	2.01	0.42
38:2:953:G:H2'	38:2:954:G:C8	2.54	0.42
6:h:268:SER:O	6:h:272:GLU:HB2	2.20	0.42
17:G:229:ARG:HH12	38:2:703:G:H5'	1.83	0.42
23:N:3:ARG:H	38:2:866:G:H5''	1.83	0.42
24:O:82:LYS:HG3	24:O:84:ARG:HH21	1.84	0.42
38:2:717:C:N4	38:2:720:G:N2	2.49	0.42
4:e:57:ASN:HB3	38:2:557:G:H5''	2.02	0.42
9:k:132:LYS:HA	9:k:132:LYS:HD3	1.82	0.42
11:A:163:ASN:O	11:A:169:SER:OG	2.33	0.42
13:C:157:LYS:HE2	13:C:170:ILE:HG23	2.00	0.42
33:X:92:CYS:SG	38:2:566:C:N4	2.93	0.42
11:A:60:ALA:HB1	11:A:144:ILE:HD12	2.01	0.42
24:O:18:ARG:HA	24:O:84:ARG:HH22	1.84	0.42
24:O:31:THR:OG1	24:O:32:ASP:N	2.52	0.42
38:2:1648:A:H2'	38:2:1649:G:H8	1.83	0.42
3:d:56:ARG:HH11	26:Q:129:PHE:HZ	1.68	0.42
6:h:113:TRP:HH2	6:h:128:VAL:HG11	1.85	0.42
9:k:56:ASN:HA	9:k:59:LYS:HG2	2.02	0.42
9:k:597:SER:OG	9:k:687:THR:N	2.50	0.42
24:O:22:SER:OG	24:O:23:PHE:N	2.52	0.42
26:Q:37:THR:HG23	26:Q:38:LEU:HG	2.01	0.42
27:R:32:LYS:HE3	27:R:47:ARG:HH12	1.85	0.42
28:S:39:GLY:H	38:2:1566:U:H5''	1.85	0.42
5:g:58:VAL:HG12	5:g:59:ARG:HG2	2.00	0.42
16:F:54:LYS:HB2	16:F:138:THR:HG21	2.01	0.42
21:L:71:LEU:HD22	21:L:137:PHE:HE1	1.84	0.42
34:Y:15:ASN:HB3	34:Y:20:ARG:HG3	2.00	0.42
38:2:75:U:N3	38:2:76:A:N3	2.67	0.42
1:b:51:GLN:HA	1:b:66:PRO:HB3	2.02	0.42
16:F:95:ASN:O	38:2:1611:A:O2'	2.37	0.42
17:G:1:MET:N	17:G:18:ILE:O	2.41	0.42
17:G:92:ARG:O	38:2:405:C:O2'	2.31	0.42
18:H:100:PRO:HB2	38:2:696:C:H41	1.84	0.42
26:Q:90:VAL:HG21	26:Q:117:LEU:HD11	2.01	0.42
29:T:76:LEU:HD23	29:T:79:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:525:TRP:HE3	9:k:526:LYS:HD3	1.85	0.42
10:l:168:MET:HE1	10:l:225:LEU:HD11	2.02	0.42
15:E:27:TYR:O	38:2:447:U:O2'	2.31	0.42
17:G:14:LYS:HE3	17:G:123:GLY:HA3	2.02	0.42
17:G:32:ILE:O	17:G:65:GLN:NE2	2.49	0.42
23:N:124:ARG:NH1	38:2:628:G:OP1	2.42	0.42
32:W:80:ASN:ND2	32:W:124:LYS:HG2	2.34	0.42
33:X:43:PHE:O	33:X:46:SER:OG	2.36	0.42
37:y:243:LYS:HE3	37:y:243:LYS:HB2	1.86	0.42
38:2:107:C:H2'	38:2:108:A:H8	1.85	0.42
38:2:585:A:H2'	38:2:586:G:H8	1.85	0.42
38:2:1158:C:O2'	38:2:1581:C:OP2	2.33	0.42
38:2:1210:C:H2'	38:2:1211:A:C8	2.55	0.42
11:A:126:PRO:HG3	11:A:147:THR:HG22	2.01	0.42
14:D:113:LEU:HD22	14:D:117:ARG:HH21	1.85	0.42
15:E:132:GLY:N	15:E:136:VAL:O	2.51	0.42
18:H:76:LYS:HA	18:H:79:ARG:HG2	2.02	0.42
32:W:118:ARG:NH1	38:2:686:C:O3'	2.47	0.42
33:X:17:VAL:HG22	33:X:20:ARG:HH21	1.85	0.42
38:2:836:U:H2'	38:2:837:G:C8	2.55	0.42
6:h:172:ILE:HA	6:h:175:LEU:HD12	2.02	0.41
9:k:500:ARG:HH22	9:k:519:PRO:HD2	1.85	0.41
21:L:124:THR:HB	21:L:141:LYS:HB3	2.02	0.41
28:S:28:ILE:HG12	28:S:61:LEU:HD21	2.01	0.41
38:2:434:G:N2	38:2:437:A:OP2	2.52	0.41
5:g:221:MET:SD	5:g:233:THR:OG1	2.73	0.41
5:g:240:VAL:HG22	5:g:256:THR:HG22	2.02	0.41
12:B:187:LYS:HA	12:B:187:LYS:HD3	1.88	0.41
15:E:153:ASN:O	15:E:174:LYS:NZ	2.52	0.41
19:I:76:THR:HB	19:I:104:ILE:HD11	2.02	0.41
38:2:1654:G:H4'	38:2:1655:A:H8	1.85	0.41
9:k:165:VAL:HG23	9:k:194:ASN:HB3	2.02	0.41
9:k:259:VAL:HG22	9:k:282:VAL:HA	2.03	0.41
12:B:229:MET:O	12:B:233:GLY:N	2.51	0.41
14:D:71:LEU:HA	14:D:74:GLN:HB2	2.03	0.41
17:G:139:ASN:OD1	17:G:142:ARG:NH1	2.53	0.41
22:M:63:VAL:HG12	22:M:65:SER:H	1.85	0.41
27:R:102:VAL:HG13	27:R:106:THR:HB	2.02	0.41
38:2:568:G:N2	38:2:582:U:O2	2.54	0.41
38:2:1268:G:H1'	38:2:1270:G:H5'	2.01	0.41
13:C:143:TYR:OH	13:C:149:GLY:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:219:ALA:HA	14:D:220:PRO:HD3	1.94	0.41
27:R:3:ARG:N	38:2:1403:C:OP1	2.46	0.41
33:X:18:HIS:O	33:X:22:ASN:HB2	2.20	0.41
34:Y:18:LEU:HB2	34:Y:20:ARG:HG2	2.00	0.41
38:2:1042:G:H22	38:2:1076:A:H2	1.68	0.41
38:2:1161:C:H1'	38:2:1619:C:H42	1.86	0.41
38:2:1223:A:H2'	38:2:1224:A:H8	1.84	0.41
38:2:1773:C:H2'	38:2:1774:G:H8	1.83	0.41
10:l:274:ASP:HB3	10:l:278:ARG:HH21	1.85	0.41
17:G:225:GLU:HA	17:G:228:LYS:HG3	2.02	0.41
27:R:71:PHE:HA	27:R:74:GLN:HG3	2.02	0.41
29:T:126:GLU:OE1	38:2:1357:A:O2'	2.33	0.41
37:y:147:PRO:HA	37:y:148:PRO:HD3	1.86	0.41
38:2:107:C:H2'	38:2:108:A:C8	2.55	0.41
38:2:389:G:N2	38:2:1732:A:OP1	2.43	0.41
38:2:406:U:H2'	38:2:407:A:C8	2.54	0.41
5:g:36:ALA:HB2	5:g:71:CYS:HB3	2.03	0.41
11:A:53:THR:HG22	11:A:161:PRO:HG2	2.03	0.41
28:S:16:ARG:NH2	28:S:19:ASN:OD1	2.54	0.41
28:S:110:ARG:HA	28:S:110:ARG:HD3	1.90	0.41
38:2:891:A:H2'	38:2:892:A:H8	1.85	0.41
1:b:20:LYS:HA	1:b:29:ARG:HH21	1.86	0.41
4:e:39:LEU:HD13	4:e:42:ARG:HD2	2.01	0.41
12:B:34:ALA:HB3	12:B:41:ARG:HA	2.01	0.41
12:B:89:ASP:OD2	12:B:99:ASN:ND2	2.52	0.41
13:C:148:LEU:O	13:C:174:ARG:NH2	2.54	0.41
17:G:19:ASP:OD2	17:G:19:ASP:N	2.53	0.41
17:G:195:VAL:HG13	17:G:199:GLN:HE22	1.85	0.41
33:X:53:VAL:HG12	33:X:74:VAL:HG22	2.02	0.41
34:Y:108:ARG:NH1	38:2:444:C:OP2	2.53	0.41
38:2:153:G:H2'	38:2:154:G:H8	1.84	0.41
7:i:240:ARG:HH22	8:j:387:ASP:H	1.68	0.41
12:B:84:ILE:HD11	12:B:100:PHE:HE1	1.84	0.41
38:2:29:U:H2'	38:2:30:G:C8	2.54	0.41
5:g:255:ALA:HB2	5:g:292:LEU:HD22	2.02	0.41
6:h:103:PRO:HB3	12:B:115:ARG:HH22	1.86	0.41
7:i:442:GLU:HA	7:i:445:ARG:HG2	2.01	0.41
9:k:257:GLY:HA2	9:k:284:GLY:HA3	2.03	0.41
9:k:345:THR:OG1	9:k:347:ASP:OD1	2.34	0.41
9:k:369:LEU:HD23	9:k:369:LEU:HA	1.95	0.41
19:I:104:ILE:HG23	19:I:165:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:94:ILE:HA	21:L:95:PRO:HD3	1.94	0.41
22:M:63:VAL:HG11	22:M:94:ALA:HB2	2.02	0.41
24:O:82:LYS:O	24:O:84:ARG:NH2	2.54	0.41
29:T:38:LYS:HE2	29:T:38:LYS:HB2	1.94	0.41
38:2:1145:U:O4	38:2:1633:A:N7	2.53	0.41
38:2:1381:U:H2'	38:2:1382:A:C8	2.55	0.41
38:2:1502:G:N2	38:2:1505:A:OP2	2.50	0.41
1:b:23:THR:OG1	1:b:25:VAL:O	2.36	0.41
6:h:116:ILE:HG12	6:h:168:LEU:HD11	2.03	0.41
14:D:50:ILE:HD11	14:D:86:LEU:HB3	2.01	0.41
25:P:85:ILE:HG13	25:P:89:MET:HE3	2.03	0.41
30:U:63:LEU:HB3	30:U:84:MET:HB2	2.03	0.41
8:j:394:ASP:OD1	8:j:394:ASP:N	2.54	0.40
9:k:173:GLY:HA2	9:k:176:ILE:HD12	2.03	0.40
13:C:141:ARG:HG2	13:C:193:VAL:HG12	2.04	0.40
15:E:129:VAL:HG22	15:E:139:VAL:HG12	2.02	0.40
18:H:185:ILE:HD12	18:H:186:PRO:HD2	2.03	0.40
19:I:32:GLN:OE1	38:2:1727:G:N2	2.50	0.40
33:X:5:LYS:NZ	38:2:614:C:OP2	2.42	0.40
38:2:555:A:N3	38:2:590:C:O2'	2.46	0.40
38:2:1117:U:H2'	38:2:1118:G:C8	2.57	0.40
38:2:1672:G:H2'	38:2:1673:G:C8	2.56	0.40
7:i:414:PRO:HB2	7:i:416:ILE:HG22	2.02	0.40
10:l:231:ASN:HD22	38:2:1575:G:HI'	1.86	0.40
11:A:144:ILE:HG22	11:A:158:VAL:HB	2.02	0.40
14:D:105:MET:HE3	14:D:184:ILE:HD12	2.02	0.40
17:G:95:LYS:NZ	38:2:160:C:O3'	2.51	0.40
17:G:226:ILE:HG12	17:G:229:ARG:HH21	1.85	0.40
24:O:25:ASP:OD2	24:O:25:ASP:N	2.52	0.40
28:S:101:LEU:HD12	28:S:103:ASN:H	1.86	0.40
38:2:187:G:O2'	38:2:198:A:N6	2.54	0.40
38:2:464:A:H2'	38:2:465:G:H8	1.85	0.40
38:2:1126:G:H2'	38:2:1127:G:H8	1.85	0.40
38:2:1226:A:O2'	38:2:1256:A:N6	2.45	0.40
38:2:1489:U:OP2	38:2:1515:A:N6	2.47	0.40
5:g:85:TRP:CD1	5:g:109:ASP:HB2	2.57	0.40
7:i:343:ALA:HB2	7:i:374:ILE:HD12	2.02	0.40
9:k:500:ARG:NH2	9:k:518:ASP:OD1	2.54	0.40
9:k:641:LYS:HE2	9:k:700:ARG:HB3	2.04	0.40
10:l:88:MET:HE3	10:l:93:THR:HB	2.03	0.40
14:D:194:LYS:HA	14:D:194:LYS:HD2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:21:GLU:HB2	22:M:24:ILE:HG13	2.03	0.40
37:y:233:ARG:HB3	37:y:236:ARG:HB2	2.02	0.40
4:e:43:ARG:HH21	38:2:590:C:H5"	1.87	0.40
7:i:232:LEU:HD21	8:j:399:LEU:HA	2.03	0.40
9:k:489:GLU:HB2	9:k:492:GLU:HG2	2.02	0.40
11:A:163:ASN:HD21	11:A:165:ARG:HG2	1.86	0.40
12:B:179:SER:HB2	12:B:183:GLN:HB2	2.03	0.40
18:H:80:GLU:HG3	18:H:84:LYS:NZ	2.36	0.40
19:I:85:PRO:HA	21:L:11:ARG:CZ	2.51	0.40
31:V:13:VAL:HA	31:V:14:PRO:HD3	1.97	0.40
14:D:90:ARG:HB3	14:D:194:LYS:HE3	2.03	0.40
15:E:131:LEU:HD13	38:2:251:A:H2	1.87	0.40
37:y:259:LEU:HA	37:y:262:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
2	c	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
3	d	35/56 (62%)	33 (94%)	2 (6%)	0	100	100
4	e	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	g	315/319 (99%)	296 (94%)	18 (6%)	1 (0%)	36	67
6	h	179/274 (65%)	176 (98%)	3 (2%)	0	100	100
7	i	260/483 (54%)	251 (96%)	9 (4%)	0	100	100
8	j	44/463 (10%)	41 (93%)	3 (7%)	0	100	100
9	k	664/788 (84%)	632 (95%)	32 (5%)	0	100	100
10	l	282/425 (66%)	263 (93%)	18 (6%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A	204/252 (81%)	191 (94%)	12 (6%)	1 (0%)	24	57
12	B	212/255 (83%)	203 (96%)	9 (4%)	0	100	100
13	C	215/254 (85%)	205 (95%)	10 (5%)	0	100	100
14	D	198/240 (82%)	190 (96%)	8 (4%)	0	100	100
15	E	258/261 (99%)	242 (94%)	16 (6%)	0	100	100
16	F	204/225 (91%)	192 (94%)	12 (6%)	0	100	100
17	G	230/236 (98%)	222 (96%)	8 (4%)	0	100	100
18	H	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
19	I	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
20	J	183/197 (93%)	176 (96%)	7 (4%)	0	100	100
21	L	138/156 (88%)	133 (96%)	5 (4%)	0	100	100
22	M	123/143 (86%)	118 (96%)	5 (4%)	0	100	100
23	N	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
24	O	125/137 (91%)	118 (94%)	7 (6%)	0	100	100
25	P	125/142 (88%)	118 (94%)	7 (6%)	0	100	100
26	Q	125/143 (87%)	121 (97%)	4 (3%)	0	100	100
27	R	123/136 (90%)	117 (95%)	6 (5%)	0	100	100
28	S	133/146 (91%)	129 (97%)	4 (3%)	0	100	100
29	T	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
30	U	101/121 (84%)	100 (99%)	1 (1%)	0	100	100
31	V	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
32	W	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
33	X	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
34	Y	132/135 (98%)	130 (98%)	1 (1%)	1 (1%)	16	48
35	Z	61/108 (56%)	59 (97%)	2 (3%)	0	100	100
36	a	266/459 (58%)	266 (100%)	0	0	100	100
37	y	150/318 (47%)	134 (89%)	16 (11%)	0	100	100
39	K	93/307 (30%)	93 (100%)	0	0	100	100
All	All	6371/8438 (76%)	6077 (95%)	290 (5%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	g	237	GLN
34	Y	34	ASN
10	l	68	VAL
11	A	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	70/71 (99%)	69 (99%)	1 (1%)	59	70
2	c	56/60 (93%)	56 (100%)	0	100	100
3	d	33/49 (67%)	33 (100%)	0	100	100
4	e	40/54 (74%)	40 (100%)	0	100	100
5	g	259/262 (99%)	259 (100%)	0	100	100
6	h	158/238 (66%)	158 (100%)	0	100	100
7	i	234/424 (55%)	234 (100%)	0	100	100
8	j	44/419 (10%)	44 (100%)	0	100	100
9	k	580/703 (82%)	580 (100%)	0	100	100
10	l	260/384 (68%)	260 (100%)	0	100	100
11	A	171/210 (81%)	171 (100%)	0	100	100
12	B	191/224 (85%)	191 (100%)	0	100	100
13	C	176/205 (86%)	176 (100%)	0	100	100
14	D	164/195 (84%)	164 (100%)	0	100	100
15	E	221/222 (100%)	221 (100%)	0	100	100
16	F	173/191 (91%)	173 (100%)	0	100	100
17	G	198/201 (98%)	198 (100%)	0	100	100
18	H	165/170 (97%)	165 (100%)	0	100	100
19	I	150/161 (93%)	150 (100%)	0	100	100
20	J	158/166 (95%)	158 (100%)	0	100	100
21	L	125/137 (91%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	M	101/119 (85%)	101 (100%)	0	100	100
23	N	127/128 (99%)	127 (100%)	0	100	100
24	O	91/105 (87%)	91 (100%)	0	100	100
25	P	105/118 (89%)	105 (100%)	0	100	100
26	Q	107/119 (90%)	107 (100%)	0	100	100
27	R	113/124 (91%)	113 (100%)	0	100	100
28	S	120/129 (93%)	120 (100%)	0	100	100
29	T	115/116 (99%)	115 (100%)	0	100	100
30	U	96/114 (84%)	96 (100%)	0	100	100
31	V	74/74 (100%)	74 (100%)	0	100	100
32	W	110/111 (99%)	110 (100%)	0	100	100
33	X	119/120 (99%)	119 (100%)	0	100	100
34	Y	112/113 (99%)	112 (100%)	0	100	100
35	Z	56/89 (63%)	56 (100%)	0	100	100
37	y	141/283 (50%)	141 (100%)	0	100	100
All	All	5213/6608 (79%)	5212 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	b	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
3	d	53	ASN
5	g	159	ASN
5	g	182	ASN
5	g	187	GLN
5	g	224	ASN
5	g	308	ASN
6	h	131	ASN
6	h	232	HIS
6	h	262	ASN
7	i	226	HIS
7	i	250	ASN

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Mol	Chain	Res	Type
7	i	436	GLN
8	j	366	ASN
8	j	405	ASN
9	k	509	ASN
9	k	587	HIS
9	k	589	HIS
9	k	617	GLN
9	k	679	ASN
10	l	78	ASN
11	A	15	GLN
11	A	49	ASN
11	A	131	GLN
12	B	40	ASN
12	B	124	ASN
12	B	157	GLN
12	B	209	ASN
12	B	211	HIS
12	B	232	HIS
13	C	147	ASN
13	C	189	GLN
14	D	67	ASN
16	F	139	ASN
16	F	158	GLN
18	H	74	GLN
18	H	108	GLN
18	H	110	GLN
19	I	35	ASN
20	J	176	ASN
21	L	106	ASN
21	L	127	GLN
22	M	111	ASN
23	N	105	ASN
26	Q	100	GLN
28	S	21	ASN
28	S	44	ASN
29	T	101	ASN
30	U	40	ASN
30	U	72	ASN
31	V	21	ASN
32	W	80	ASN
33	X	21	ASN
33	X	28	ASN

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Mol	Chain	Res	Type
34	Y	31	ASN
34	Y	106	GLN
37	y	217	GLN
37	y	274	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	2	1763/2012 (87%)	605 (34%)	18 (1%)

All (605) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
38	2	4	C
38	2	6	G
38	2	17	C
38	2	25	C
38	2	26	A
38	2	34	G
38	2	42	G
38	2	43	A
38	2	45	U
38	2	47	A
38	2	57	G
38	2	66	U
38	2	67	A
38	2	68	A
38	2	72	A
38	2	73	U
38	2	74	U
38	2	75	U
38	2	77	U
38	2	104	A
38	2	111	U
38	2	114	C
38	2	115	G
38	2	126	A
38	2	127	G
38	2	141	U
38	2	142	G
38	2	146	U

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Mol	Chain	Res	Type
38	2	153	G
38	2	155	U
38	2	156	A
38	2	158	U
38	2	161	U
38	2	166	C
38	2	178	U
38	2	179	A
38	2	185	U
38	2	186	C
38	2	189	C
38	2	191	C
38	2	192	U
38	2	193	U
38	2	194	U
38	2	195	G
38	2	196	G
38	2	215	A
38	2	217	A
38	2	218	A
38	2	219	A
38	2	220	A
38	2	227	U
38	2	228	G
38	2	229	U
38	2	230	C
38	2	231	U
38	2	233	C
38	2	234	G
38	2	235	G
38	2	236	A
38	2	238	U
38	2	239	C
38	2	240	U
38	2	241	U
38	2	242	U
38	2	249	U
38	2	250	C
38	2	257	A
38	2	261	U
38	2	265	A
38	2	266	A

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Mol	Chain	Res	Type
38	2	271	A
38	2	272	U
38	2	274	G
38	2	275	C
38	2	276	C
38	2	277	U
38	2	278	U
38	2	279	G
38	2	280	U
38	2	281	G
38	2	288	A
38	2	299	A
38	2	302	U
38	2	305	C
38	2	308	C
38	2	314	C
38	2	316	A
38	2	318	U
38	2	319	U
38	2	320	U
38	2	321	C
38	2	322	G
38	2	327	U
38	2	328	A
38	2	333	A
38	2	334	G
38	2	335	U
38	2	337	G
38	2	338	C
38	2	344	A
38	2	352	A
38	2	359	A
38	2	360	A
38	2	361	C
38	2	381	C
38	2	399	A
38	2	400	A
38	2	402	C
38	2	404	G
38	2	416	A
38	2	417	A
38	2	419	G

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Mol	Chain	Res	Type
38	2	423	G
38	2	424	C
38	2	425	A
38	2	426	G
38	2	428	A
38	2	435	C
38	2	439	U
38	2	444	C
38	2	448	C
38	2	453	U
38	2	454	U
38	2	459	G
38	2	460	A
38	2	468	A
38	2	475	A
38	2	477	A
38	2	480	G
38	2	481	A
38	2	482	U
38	2	483	A
38	2	484	C
38	2	486	G
38	2	490	C
38	2	492	A
38	2	493	U
38	2	494	U
38	2	495	C
38	2	496	G
38	2	497	G
38	2	498	G
38	2	499	U
38	2	500	C
38	2	502	U
38	2	504	U
38	2	505	A
38	2	506	A
38	2	507	U
38	2	515	A
38	2	519	C
38	2	527	A
38	2	534	A
38	2	536	C

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Mol	Chain	Res	Type
38	2	540	G
38	2	541	A
38	2	543	C
38	2	544	A
38	2	545	A
38	2	548	G
38	2	549	G
38	2	558	U
38	2	559	C
38	2	561	G
38	2	564	G
38	2	565	C
38	2	566	C
38	2	567	A
38	2	568	G
38	2	571	G
38	2	575	C
38	2	576	G
38	2	577	G
38	2	578	U
38	2	579	A
38	2	580	A
38	2	581	U
38	2	582	U
38	2	594	A
38	2	595	G
38	2	597	G
38	2	611	U
38	2	615	A
38	2	619	A
38	2	620	A
38	2	622	A
38	2	623	A
38	2	624	G
38	2	635	A
38	2	638	U
38	2	639	U
38	2	640	U
38	2	649	U
38	2	650	U
38	2	652	G
38	2	653	C

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Mol	Chain	Res	Type
38	2	654	C
38	2	655	G
38	2	656	G
38	2	658	C
38	2	677	G
38	2	684	A
38	2	685	A
38	2	687	G
38	2	693	U
38	2	696	C
38	2	697	C
38	2	698	U
38	2	700	C
38	2	708	C
38	2	709	C
38	2	712	G
38	2	714	G
38	2	715	U
38	2	717	C
38	2	718	U
38	2	719	U
38	2	720	G
38	2	721	U
38	2	722	G
38	2	723	G
38	2	728	U
38	2	736	C
38	2	737	A
38	2	738	G
38	2	739	G
38	2	740	A
38	2	741	C
38	2	742	U
38	2	743	U
38	2	762	A
38	2	765	G
38	2	766	U
38	2	771	A
38	2	774	A
38	2	775	G
38	2	779	U
38	2	780	A

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Mol	Chain	Res	Type
38	2	781	U
38	2	782	U
38	2	783	G
38	2	786	C
38	2	787	G
38	2	789	A
38	2	793	A
38	2	794	U
38	2	811	A
38	2	813	U
38	2	815	G
38	2	816	G
38	2	818	C
38	2	820	U
38	2	821	U
38	2	824	G
38	2	827	C
38	2	829	A
38	2	830	U
38	2	832	U
38	2	834	G
38	2	835	U
38	2	840	U
38	2	841	U
38	2	844	A
38	2	846	G
38	2	850	A
38	2	851	U
38	2	852	C
38	2	853	G
38	2	854	U
38	2	855	A
38	2	856	A
38	2	857	U
38	2	860	U
38	2	862	A
38	2	863	A
38	2	864	U
38	2	869	A
38	2	876	G
38	2	898	A
38	2	904	G

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Mol	Chain	Res	Type
38	2	905	A
38	2	906	A
38	2	908	U
38	2	909	U
38	2	910	C
38	2	912	U
38	2	913	G
38	2	914	G
38	2	915	A
38	2	921	U
38	2	926	A
38	2	928	U
38	2	931	C
38	2	932	U
38	2	933	A
38	2	935	U
38	2	942	G
38	2	944	A
38	2	945	U
38	2	951	A
38	2	959	U
38	2	960	U
38	2	966	A
38	2	988	A
38	2	992	A
38	2	993	A
38	2	996	U
38	2	997	G
38	2	998	A
38	2	999	U
38	2	1000	C
38	2	1002	G
38	2	1003	A
38	2	1004	U
38	2	1005	A
38	2	1007	C
38	2	1009	U
38	2	1011	G
38	2	1012	U
38	2	1014	G
38	2	1025	A
38	2	1026	A

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Mol	Chain	Res	Type
38	2	1028	C
38	2	1031	U
38	2	1040	G
38	2	1042	G
38	2	1043	A
38	2	1044	U
38	2	1053	G
38	2	1058	U
38	2	1059	U
38	2	1061	A
38	2	1063	U
38	2	1072	C
38	2	1076	A
38	2	1078	C
38	2	1079	U
38	2	1080	U
38	2	1081	A
38	2	1082	C
38	2	1083	G
38	2	1092	A
38	2	1093	A
38	2	1096	C
38	2	1097	U
38	2	1098	U
38	2	1100	G
38	2	1109	G
38	2	1111	G
38	2	1113	A
38	2	1137	A
38	2	1146	G
38	2	1147	A
38	2	1148	C
38	2	1149	G
38	2	1150	G
38	2	1151	A
38	2	1155	G
38	2	1156	C
38	2	1157	A
38	2	1158	C
38	2	1160	A
38	2	1162	C
38	2	1164	G

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Mol	Chain	Res	Type
38	2	1165	G
38	2	1167	G
38	2	1183	A
38	2	1185	U
38	2	1186	U
38	2	1187	U
38	2	1188	G
38	2	1189	A
38	2	1198	G
38	2	1199	G
38	2	1200	G
38	2	1201	G
38	2	1203	A
38	2	1207	C
38	2	1215	C
38	2	1216	C
38	2	1218	G
38	2	1219	A
38	2	1224	A
38	2	1227	A
38	2	1228	G
38	2	1229	G
38	2	1230	A
38	2	1232	U
38	2	1233	G
38	2	1234	A
38	2	1235	C
38	2	1236	A
38	2	1239	U
38	2	1240	U
38	2	1241	G
38	2	1242	A
38	2	1243	G
38	2	1245	G
38	2	1249	U
38	2	1252	C
38	2	1254	U
38	2	1256	A
38	2	1257	U
38	2	1258	U
38	2	1262	U
38	2	1264	G

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Mol	Chain	Res	Type
38	2	1266	U
38	2	1267	G
38	2	1268	G
38	2	1269	U
38	2	1270	G
38	2	1275	A
38	2	1276	U
38	2	1277	G
38	2	1278	G
38	2	1279	C
38	2	1280	C
38	2	1281	G
38	2	1284	C
38	2	1285	U
38	2	1286	U
38	2	1287	A
38	2	1288	G
38	2	1294	G
38	2	1295	G
38	2	1301	U
38	2	1306	C
38	2	1314	U
38	2	1315	U
38	2	1321	A
38	2	1327	C
38	2	1328	G
38	2	1330	G
38	2	1332	C
38	2	1336	A
38	2	1337	A
38	2	1338	C
38	2	1339	C
38	2	1340	U
38	2	1343	U
38	2	1344	A
38	2	1345	A
38	2	1346	A
38	2	1347	U
38	2	1360	A
38	2	1361	U
38	2	1362	U
38	2	1363	U

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Mol	Chain	Res	Type
38	2	1364	G
38	2	1367	G
38	2	1370	U
38	2	1371	A
38	2	1378	U
38	2	1387	G
38	2	1388	A
38	2	1390	U
38	2	1398	U
38	2	1399	C
38	2	1413	U
38	2	1415	U
38	2	1418	G
38	2	1419	G
38	2	1421	A
38	2	1422	A
38	2	1424	A
38	2	1426	C
38	2	1427	A
38	2	1428	G
38	2	1429	G
38	2	1431	C
38	2	1432	U
38	2	1436	A
38	2	1437	U
38	2	1438	G
38	2	1439	C
38	2	1441	C
38	2	1442	U
38	2	1443	U
38	2	1444	A
38	2	1446	A
38	2	1447	C
38	2	1448	G
38	2	1450	U
38	2	1452	U
38	2	1455	G
38	2	1457	C
38	2	1459	C
38	2	1460	A
38	2	1461	C
38	2	1471	A

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Mol	Chain	Res	Type
38	2	1473	U
38	2	1474	G
38	2	1475	A
38	2	1479	A
38	2	1482	C
38	2	1483	A
38	2	1486	G
38	2	1490	C
38	2	1493	A
38	2	1496	U
38	2	1506	G
38	2	1516	A
38	2	1520	U
38	2	1521	G
38	2	1523	G
38	2	1524	A
38	2	1527	C
38	2	1535	U
38	2	1536	G
38	2	1537	C
38	2	1538	U
38	2	1540	G
38	2	1542	G
38	2	1557	U
38	2	1559	A
38	2	1568	C
38	2	1569	A
38	2	1570	A
38	2	1571	C
38	2	1573	A
38	2	1574	G
38	2	1583	A
38	2	1584	G
38	2	1595	U
38	2	1596	C
38	2	1597	A
38	2	1598	U
38	2	1601	G
38	2	1618	C
38	2	1619	C
38	2	1622	G
38	2	1624	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2	1630	U
38	2	1631	A
38	2	1632	C
38	2	1633	A
38	2	1634	C
38	2	1635	A
38	2	1636	C
38	2	1637	C
38	2	1638	G
38	2	1639	C
38	2	1640	C
38	2	1641	C
38	2	1642	G
38	2	1648	A
38	2	1651	A
38	2	1652	C
38	2	1653	C
38	2	1654	G
38	2	1655	A
38	2	1656	U
38	2	1657	U
38	2	1658	G
38	2	1659	A
38	2	1680	G
38	2	1681	A
38	2	1683	C
38	2	1687	U
38	2	1688	U
38	2	1689	A
38	2	1692	G
38	2	1693	A
38	2	1697	G
38	2	1699	G
38	2	1700	C
38	2	1701	A
38	2	1703	C
38	2	1713	G
38	2	1714	A
38	2	1715	G
38	2	1717	G
38	2	1718	G
38	2	1732	A

Continued on next page...

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Mol	Chain	Res	Type
38	2	1736	G
38	2	1738	U
38	2	1739	C
38	2	1741	U
38	2	1742	U
38	2	1743	U
38	2	1744	A
38	2	1745	G
38	2	1748	G
38	2	1749	A
38	2	1750	A
38	2	1751	C
38	2	1753	A
38	2	1754	A
38	2	1755	A
38	2	1757	G
38	2	1758	U
38	2	1759	C
38	2	1760	G
38	2	1761	U
38	2	1763	A
38	2	1764	C
38	2	1765	A
38	2	1766	A
38	2	1769	U
38	2	1770	U
38	2	1779	U
38	2	1782	A
38	2	1783	C
38	2	1792	G
38	2	1793	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	2	155	U
38	2	278	U
38	2	418	G
38	2	567	A
38	2	782	U
38	2	912	U
38	2	1156	C

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Mol	Chain	Res	Type
38	2	1200	G
38	2	1229	G
38	2	1231	U
38	2	1343	U
38	2	1442	U
38	2	1458	G
38	2	1481	C
38	2	1570	A
38	2	1573	A
38	2	1652	C
38	2	1700	C

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 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1377:U	O3'	1378:U	P	3.49
1	2	902:G	O3'	903:U	P	3.34

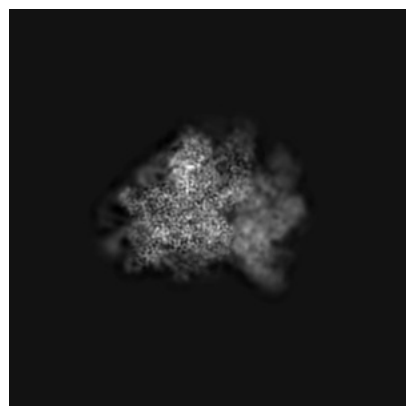
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16541. These allow visual inspection of the internal detail of the map and identification of artifacts.

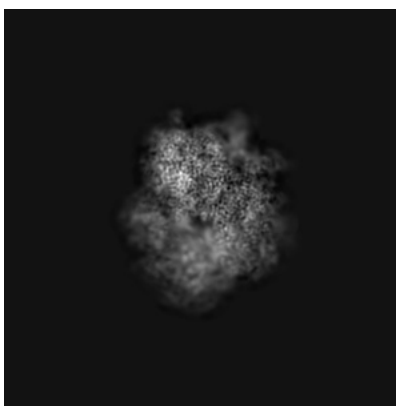
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

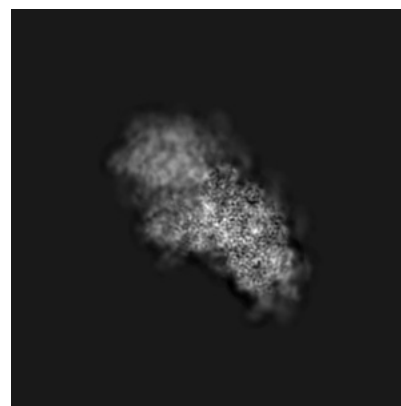
6.1.1 Primary map



X

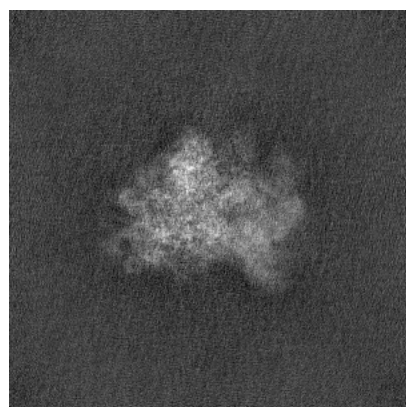


Y

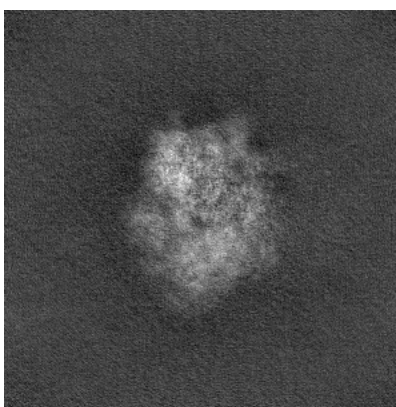


Z

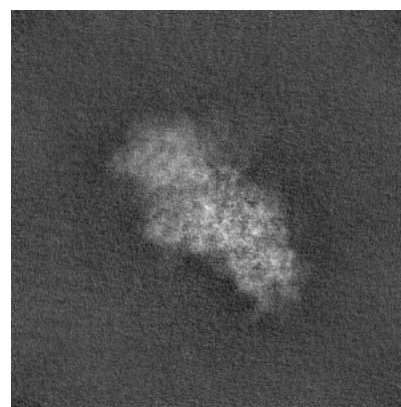
6.1.2 Raw map



X



Y

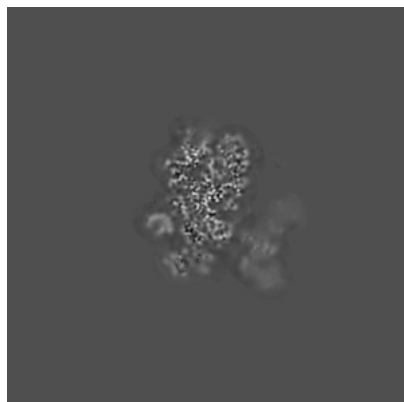


Z

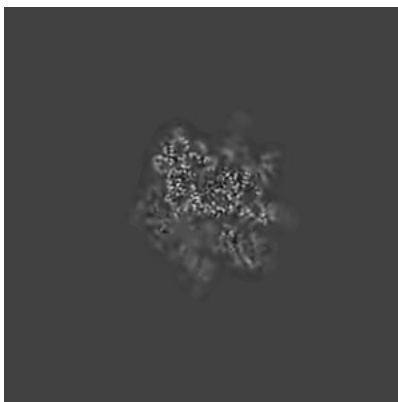
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

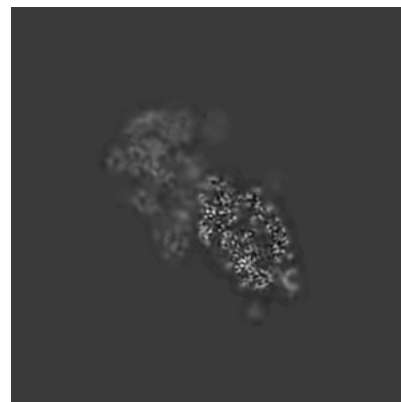
6.2.1 Primary map



X Index: 210

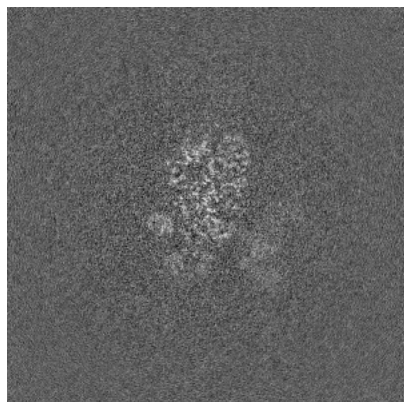


Y Index: 210

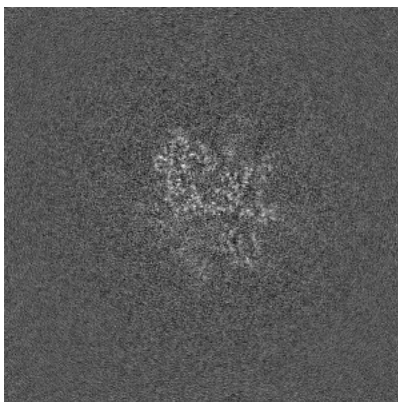


Z Index: 210

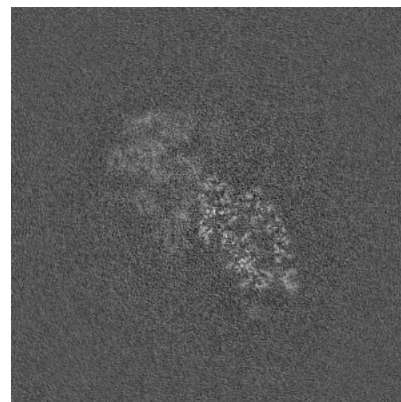
6.2.2 Raw map



X Index: 210



Y Index: 210

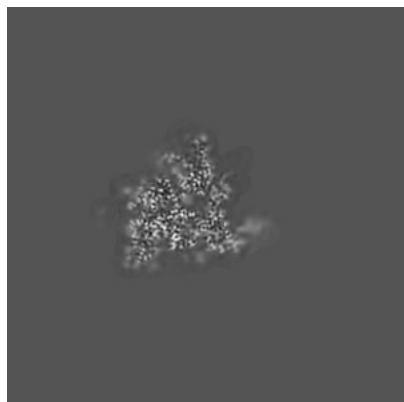


Z Index: 210

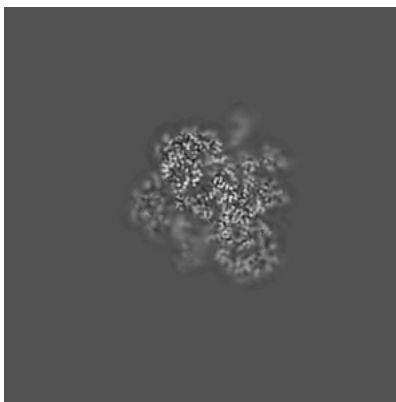
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

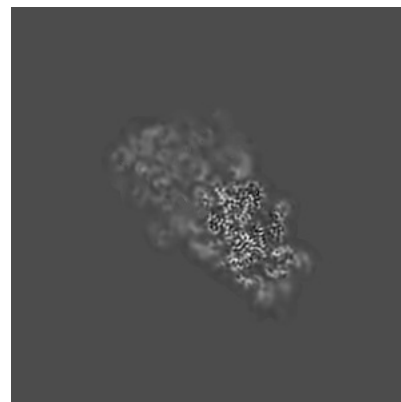
6.3.1 Primary map



X Index: 245

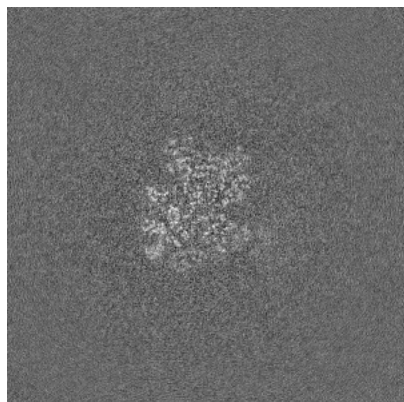


Y Index: 187

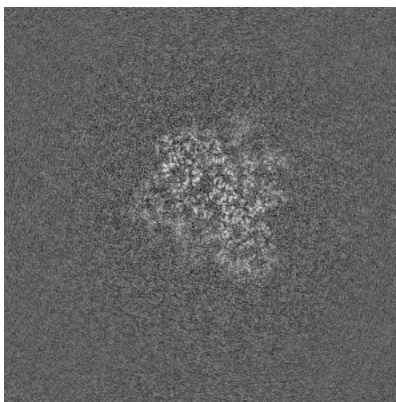


Z Index: 185

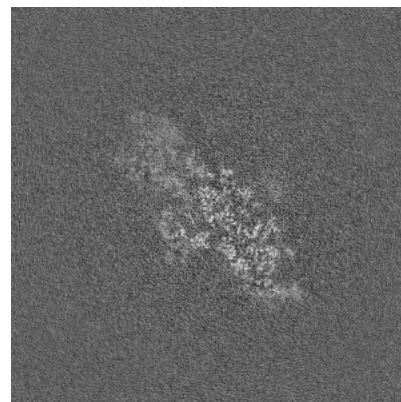
6.3.2 Raw map



X Index: 232



Y Index: 187

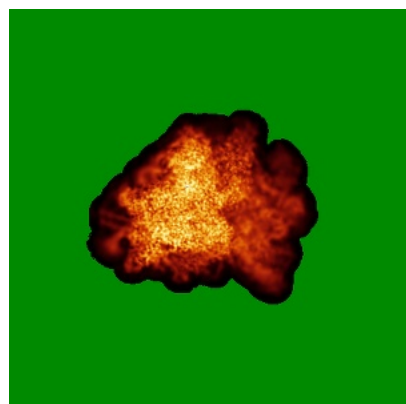


Z Index: 223

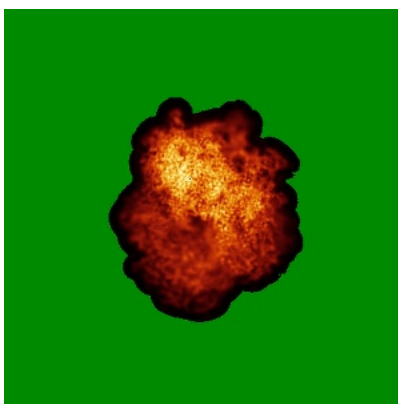
The images above show the largest variance slices of the map in three orthogonal directions.

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

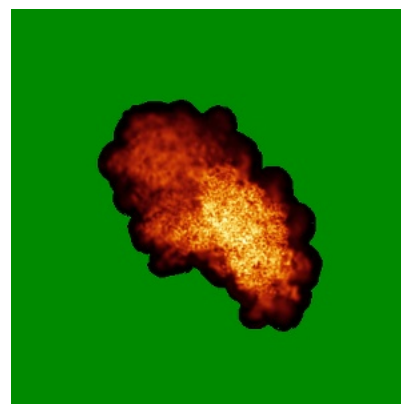
6.4.1 Primary map



X

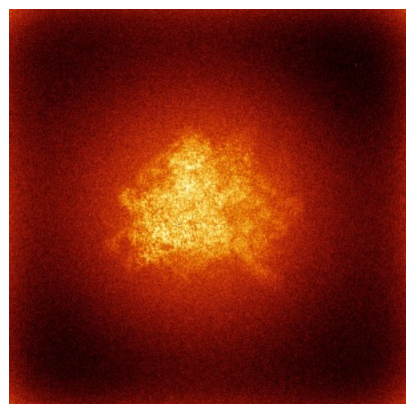


Y

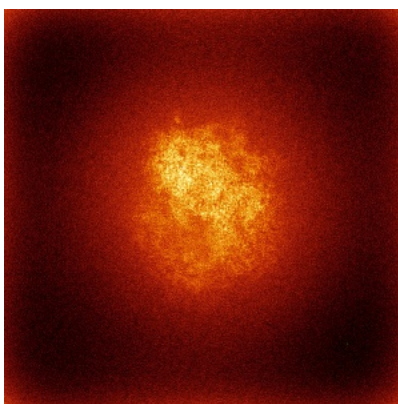


Z

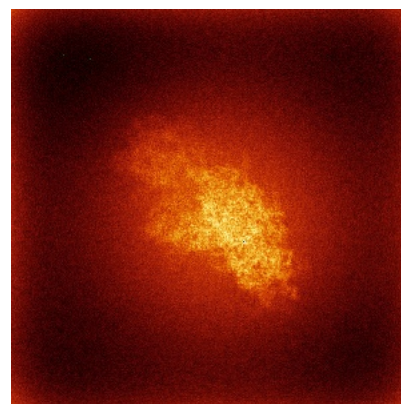
6.4.2 Raw map



X



Y

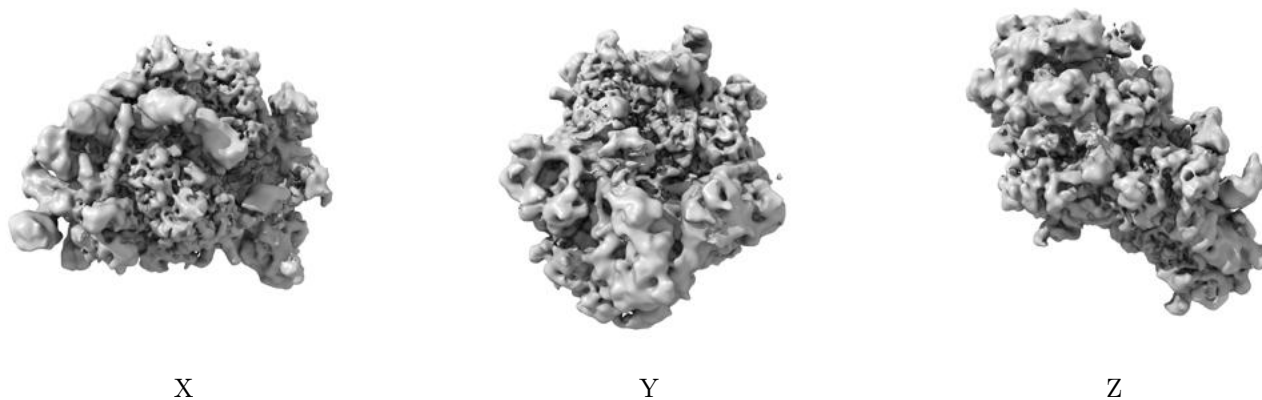


Z

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.

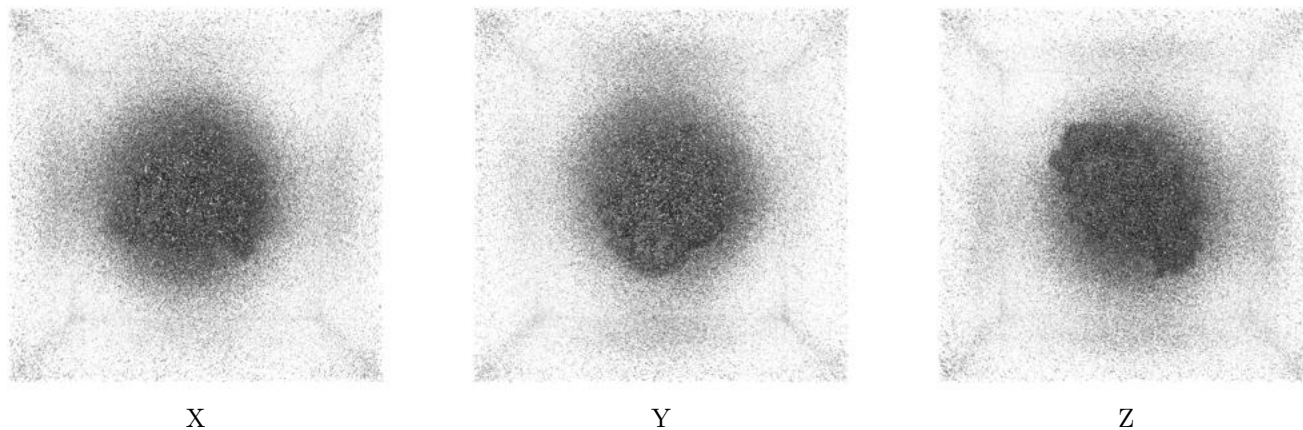
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

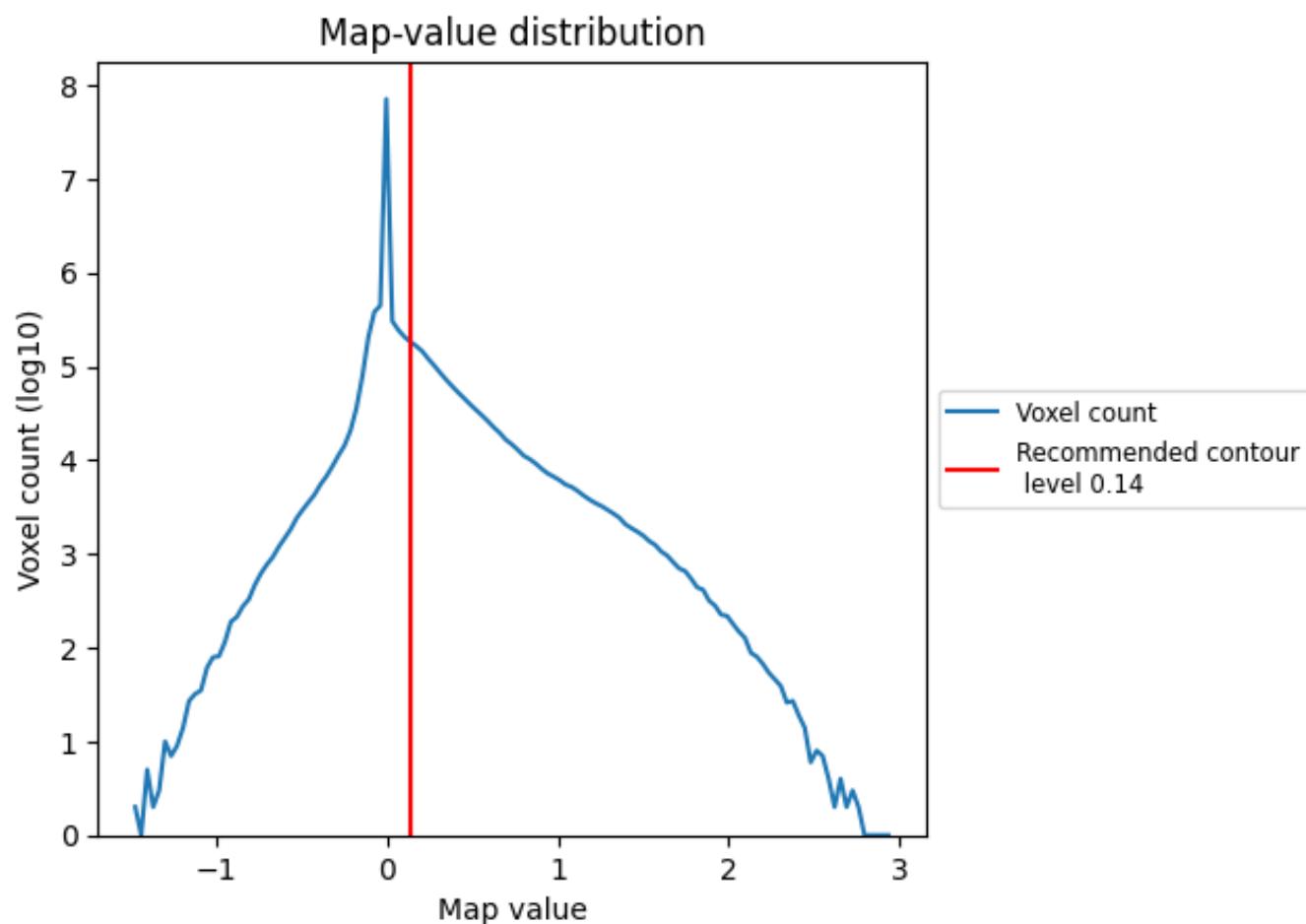
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

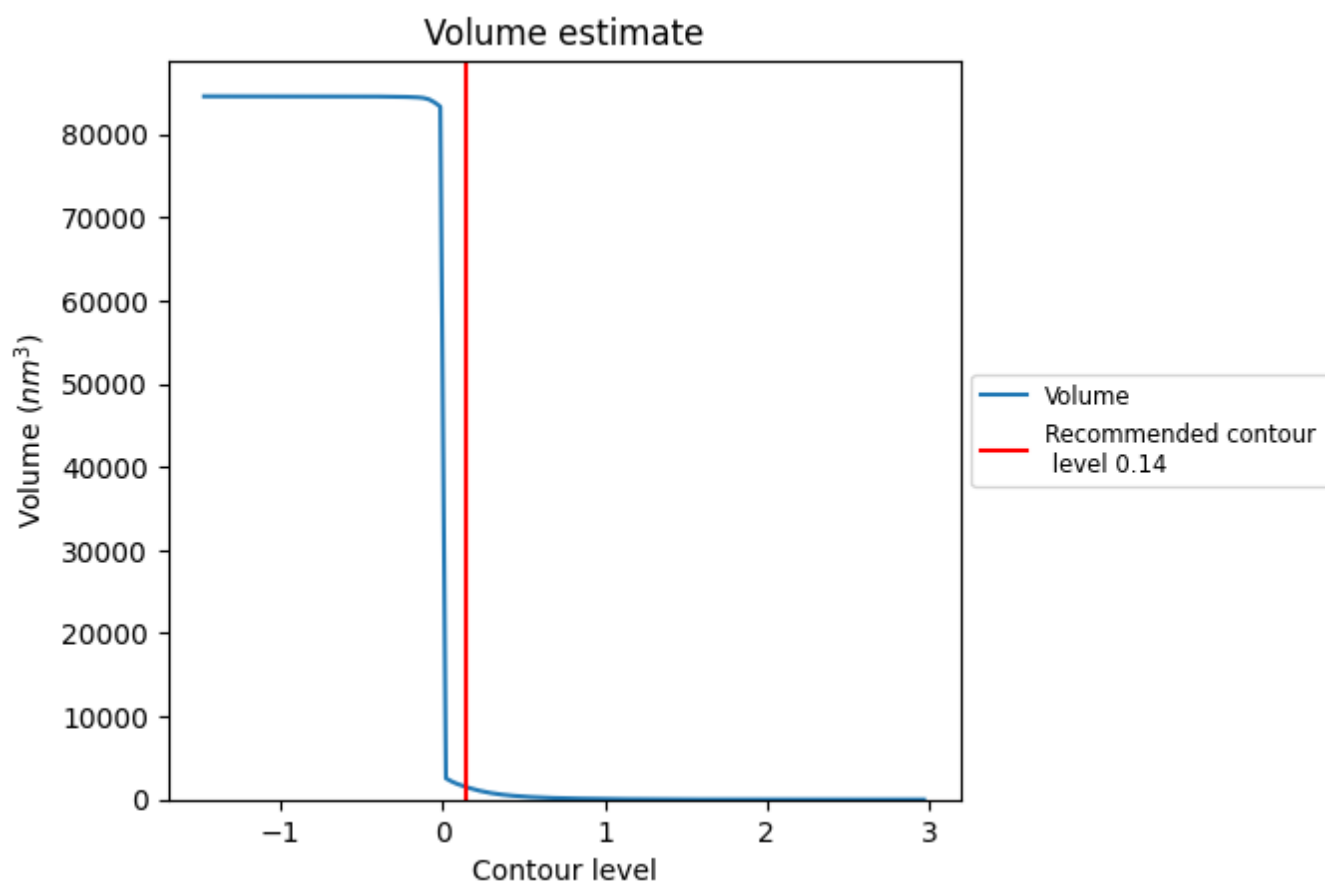
This section contains the results of statistical analysis of the map.

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.

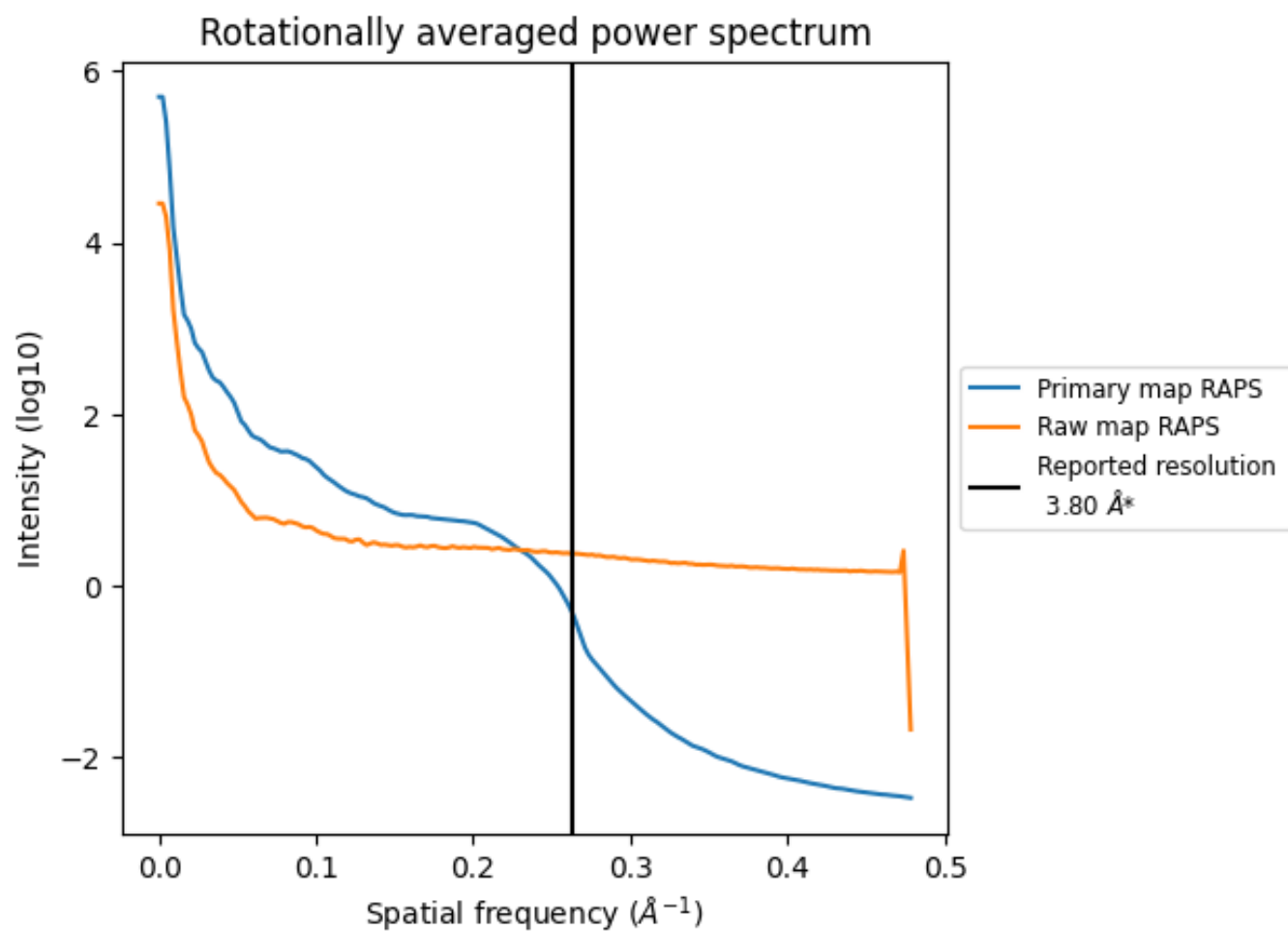
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1532 nm^3 ; this corresponds to an approximate mass of 1384 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 ⓘ

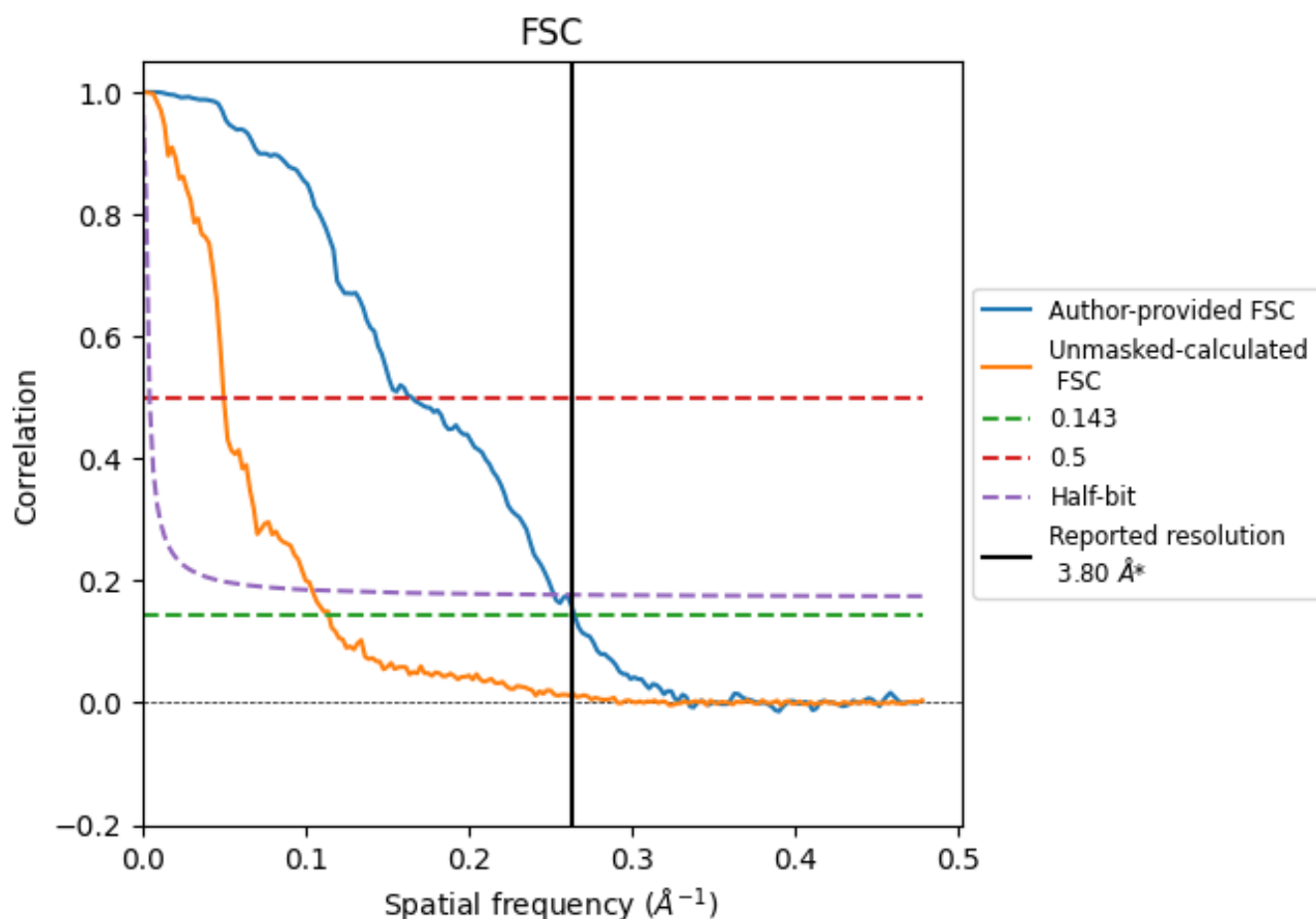


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

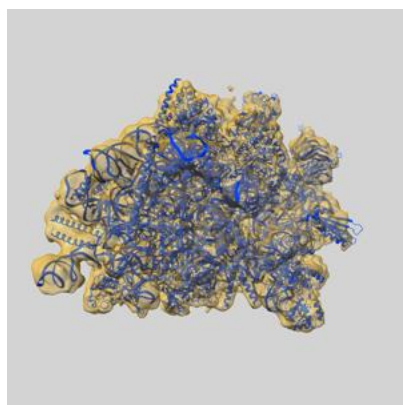
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	6.05	3.96
Unmasked-calculated*	8.73	20.00	9.59

*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 8.73 differs from the reported value 3.8 by more than 10 %

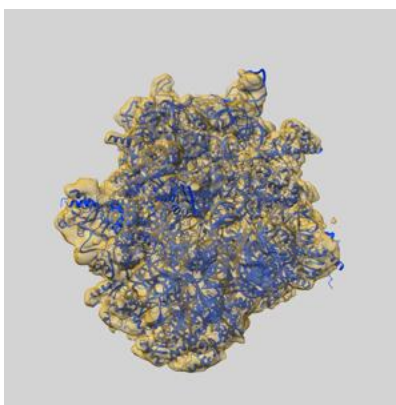
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16541 and PDB model 8CBJ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

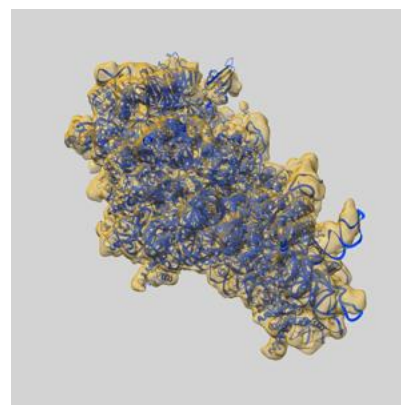
9.1 Map-model overlay [i](#)



X



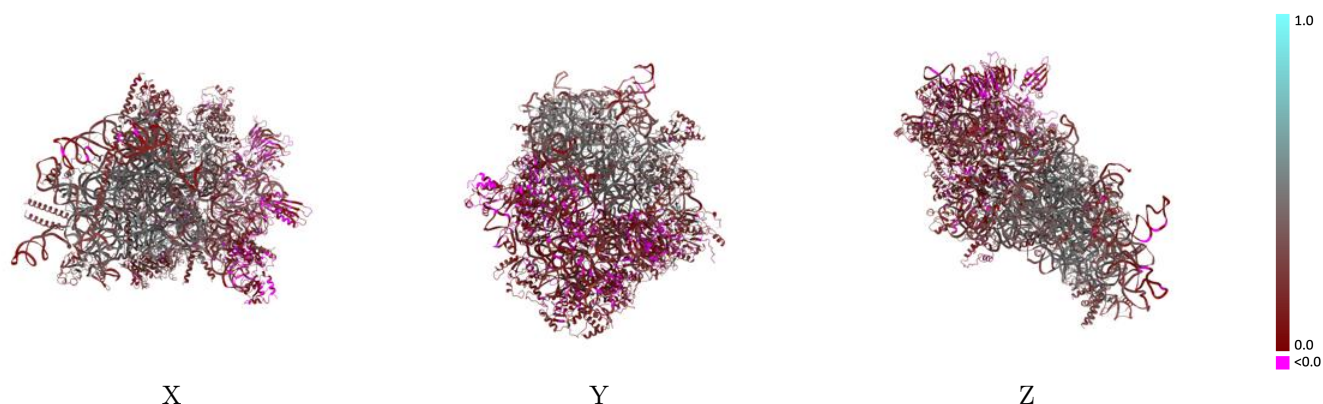
Y



Z

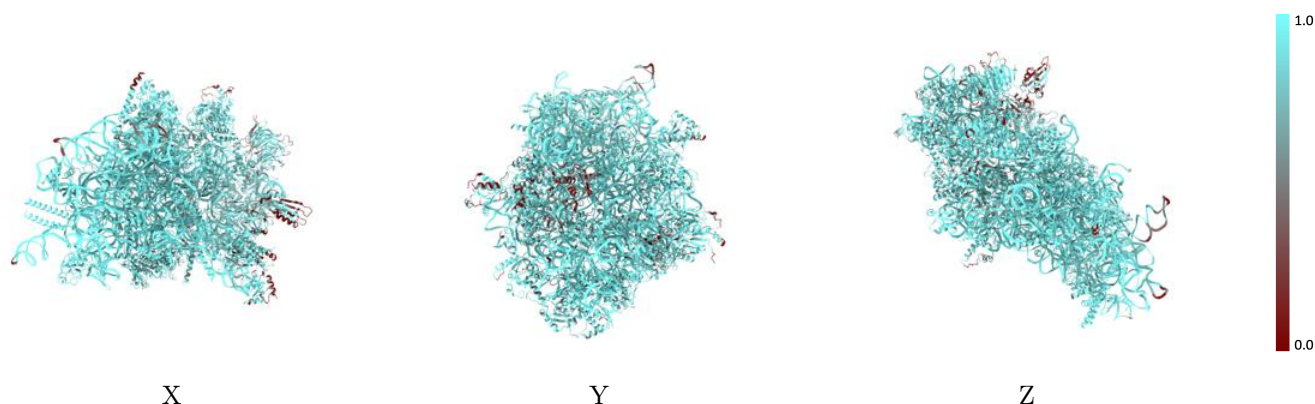
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



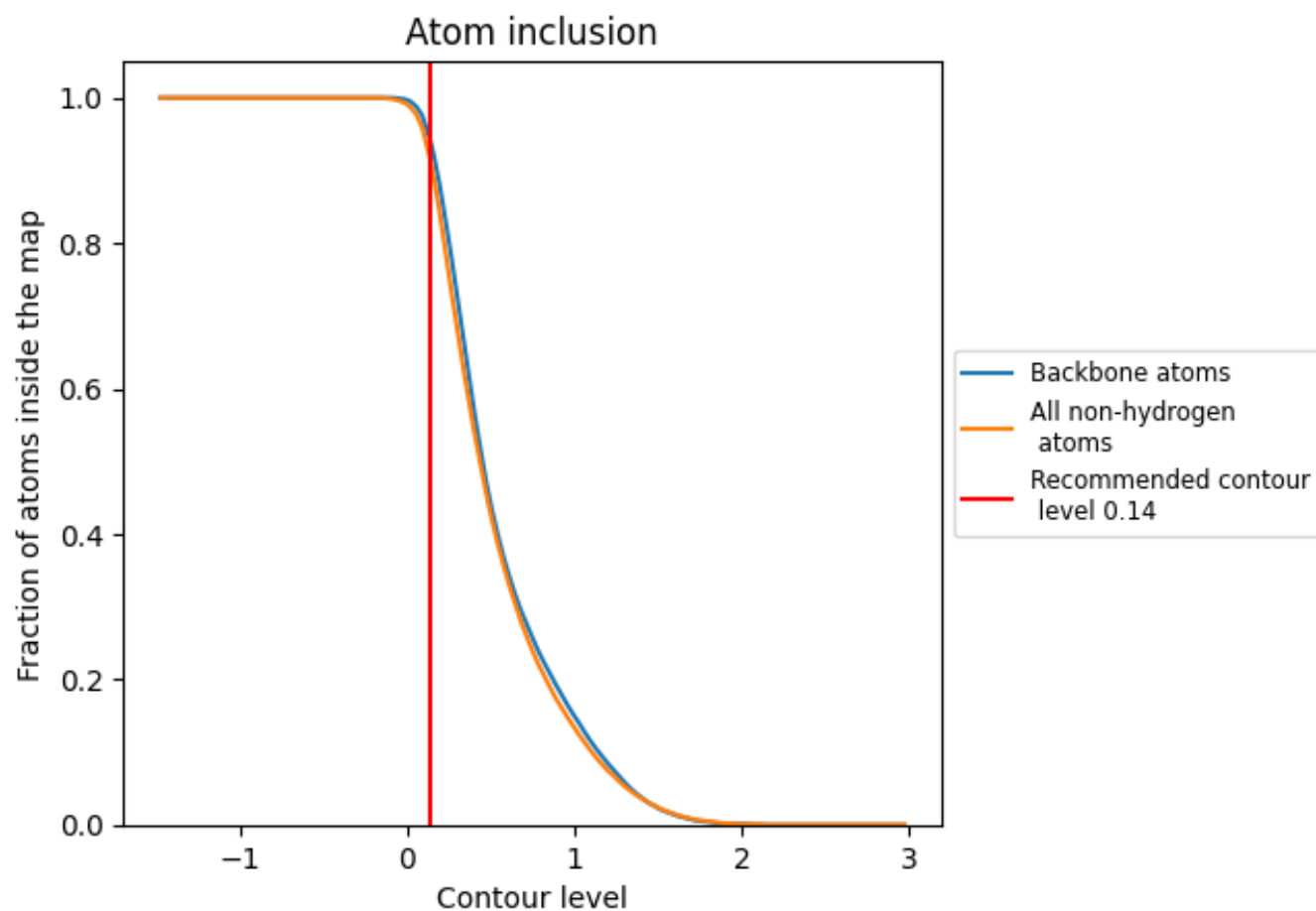
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.2630
2	 0.9730	 0.3030
A	 0.9240	 0.3220
B	 0.8670	 0.2470
C	 0.9470	 0.3950
D	 0.4960	 0.0690
E	 0.9600	 0.4290
F	 0.8850	 0.1280
G	 0.9700	 0.3040
H	 0.9350	 0.2810
I	 0.9680	 0.4050
J	 0.9480	 0.4090
K	 0.9130	 0.2550
L	 0.9600	 0.4520
M	 0.6920	 0.0350
N	 0.9520	 0.3580
O	 0.8890	 0.2580
P	 0.8960	 0.1490
Q	 0.9280	 0.1010
R	 0.8970	 0.1390
S	 0.8720	 0.1350
T	 0.8620	 0.1110
U	 0.8570	 0.0760
V	 0.9650	 0.3930
W	 0.9710	 0.4450
X	 0.9020	 0.3890
Y	 0.9570	 0.3960
Z	 0.8950	 0.1390
a	 0.8880	 0.2310
b	 0.9500	 0.3760
c	 0.9200	 0.1280
d	 0.8940	 0.0880
e	 0.8370	 0.3070
g	 0.7250	 0.0640
h	 0.8500	 0.2060



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Chain	Atom inclusion	Q-score
i	 0.8260	 0.0880
j	 0.5820	 0.0820
k	 0.8260	 0.2090
l	 0.8040	 0.1030
y	 0.7850	 0.1410