Full wwPDB EM Validation Report

Jul 17, 2024 – 11:00 AM EDT

PDB ID	:	8W2O
EMDB ID	:	EMD-43753
Title	:	Yeast U1 snRNP with humanized U1C Zinc-Finger domain
Authors	:	Shi, S.S.; Kuang, Z.L.; Zhao, R.
Deposited on	:	2024-02-20
Resolution	:	3.49 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:

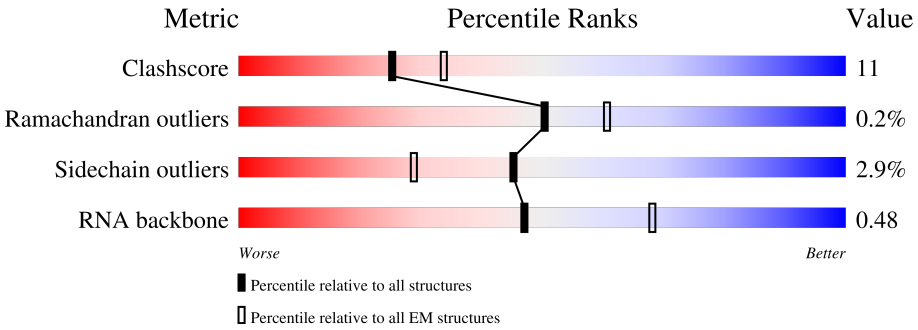
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	47% 8% · 44%
2	B	231	53% 23% · 23%
3	C	350	29% 7% · 62%
4	D	544	77% 22% ·
5	E	629	77% 14% 8%
6	F	523	29% 6% 65%
7	G	492	37% 11% 53%

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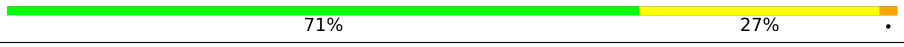
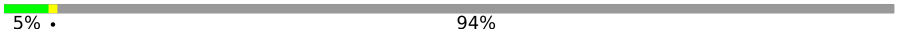
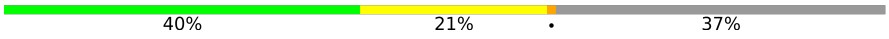
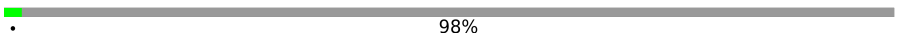
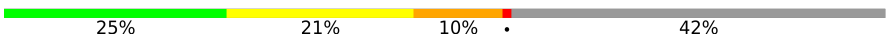
Mol	Chain	Length	Quality of chain
8	H	52	
9	I	261	
10	K	196	
11	L	146	
12	M	110	
13	N	101	
14	O	94	
15	P	86	
16	Q	77	
17	r	187	
18	R	568	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 28117 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 U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	169	1092	675	207	209	1	0	0

- Molecule 2 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	178	1462	907	280	268	7	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	PRO	THR	engineered mutation	UNP Q05900
B	3	LYS	ARG	engineered mutation	UNP Q05900
B	4	PHE	TYR	engineered mutation	UNP Q05900
B	7	ASP	GLU	engineered mutation	UNP Q05900
B	10	ASP	HIS	engineered mutation	UNP Q05900
B	11	THR	SER	engineered mutation	UNP Q05900
B	17	SER	THR	engineered mutation	UNP Q05900
B	18	PRO	LEU	engineered mutation	UNP Q05900
B	23	THR	SER	engineered mutation	UNP Q05900
B	25	CYS	LEU	engineered mutation	UNP Q05900
B	26	SER	VAL	engineered mutation	UNP Q05900
B	28	ARG	LYS	engineered mutation	UNP Q05900
B	29	LYS	ASN	engineered mutation	UNP Q05900
B	31	LYS	LEU	engineered mutation	UNP Q05900
B	32	GLU	ARG	engineered mutation	UNP Q05900
B	33	ASN	ILE	engineered mutation	UNP Q05900
B	34	VAL	THR	engineered mutation	UNP Q05900
B	35	LYS	ALA	engineered mutation	UNP Q05900

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	132	Total	C	N	O	S	0	0
			1042	663	188	187	4		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLY	-	expression tag	UNP P32605
C	300	ARG	-	expression tag	UNP P32605
C	301	ARG	-	expression tag	UNP P32605
C	302	ILE	-	expression tag	UNP P32605
C	303	PRO	-	expression tag	UNP P32605
C	304	GLY	-	expression tag	UNP P32605
C	305	LEU	-	expression tag	UNP P32605
C	306	ILE	-	expression tag	UNP P32605
C	307	ASN	-	expression tag	UNP P32605
C	308	PRO	-	expression tag	UNP P32605
C	309	TRP	-	expression tag	UNP P32605
C	310	LYS	-	expression tag	UNP P32605
C	311	ARG	-	expression tag	UNP P32605
C	312	ARG	-	expression tag	UNP P32605
C	313	TRP	-	expression tag	UNP P32605
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
C	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
C	320	VAL	-	expression tag	UNP P32605
C	321	SER	-	expression tag	UNP P32605
C	322	ALA	-	expression tag	UNP P32605
C	323	ALA	-	expression tag	UNP P32605
C	324	ASN	-	expression tag	UNP P32605
C	325	ARG	-	expression tag	UNP P32605
C	326	PHE	-	expression tag	UNP P32605
C	327	LYS	-	expression tag	UNP P32605
C	328	LYS	-	expression tag	UNP P32605
C	329	ILE	-	expression tag	UNP P32605
C	330	SER	-	expression tag	UNP P32605
C	331	SER	-	expression tag	UNP P32605
C	332	SER	-	expression tag	UNP P32605
C	333	GLY	-	expression tag	UNP P32605
C	334	ALA	-	expression tag	UNP P32605
C	335	LEU	-	expression tag	UNP P32605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	336	ASP	-	expression tag	UNP P32605
C	337	TYR	-	expression tag	UNP P32605
C	338	ASP	-	expression tag	UNP P32605
C	339	ILE	-	expression tag	UNP P32605
C	340	PRO	-	expression tag	UNP P32605
C	341	THR	-	expression tag	UNP P32605
C	342	THR	-	expression tag	UNP P32605
C	343	ALA	-	expression tag	UNP P32605
C	344	SER	-	expression tag	UNP P32605
C	345	GLU	-	expression tag	UNP P32605
C	346	ASN	-	expression tag	UNP P32605
C	347	LEU	-	expression tag	UNP P32605
C	348	TYR	-	expression tag	UNP P32605
C	349	PHE	-	expression tag	UNP P32605
C	350	GLN	-	expression tag	UNP P32605

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	541	Total	C	N	O	S	0	0
			4523	2968	719	816	20		

- Molecule 5 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	576	Total	C	N	O	S	0	0
			3985	2530	694	752	9		

- Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	183	Total	C	N	O	S	0	0
			1401	880	240	270	11		

- Molecule 7 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	232	Total	C	N	O	S	0	0
			1897	1232	310	343	12		

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	52	Total	C	N	O	S	0	0
			420	266	74	79	1		

- Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	16	Total	C	N	O	S	0	0
			125	77	22	24	2		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	123	Total	C	N	O	S	0	0
			1003	632	190	178	3		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	119	Total	C	N	O	S	0	0
			921	578	164	176	3		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	107	Total	C	N	O	S	0	0
			862	547	159	152	4		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	91	Total	C	N	O	S	0	0
			695	443	119	130	3		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	75	Total	C	N	O	S	0	0
			573	381	92	97	3		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	74	Total	C	N	O	S	0	0
			580	375	103	101	1		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	71	Total	C	N	O	S	0	0
			537	342	95	99	1		

- Molecule 17 is a RNA chain called ACT1 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	3	Total	C	N	O	P	0	0
			62	28	9	22	3		

- Molecule 18 is a RNA chain called U1 snRNA.

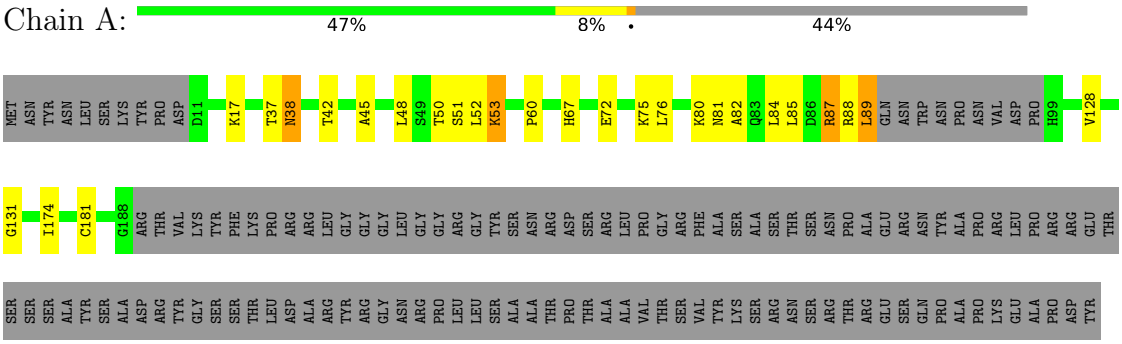
Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	327	Total	C	N	O	P	0	0
			6937	3104	1196	2310	327		

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.

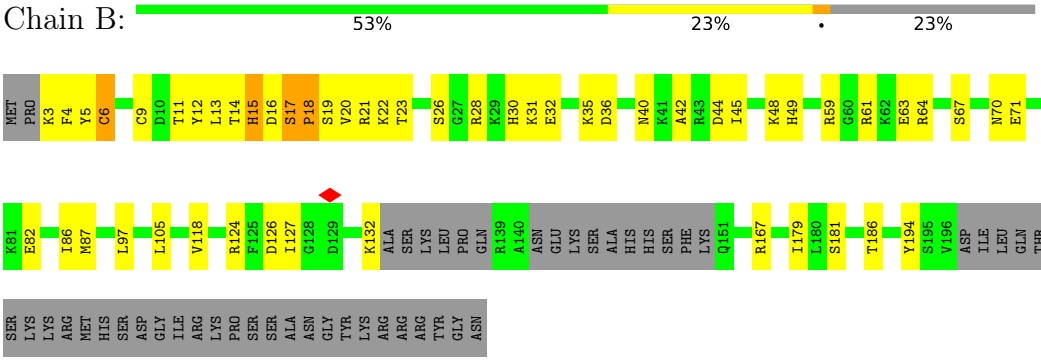
• Molecule 1: U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain A:



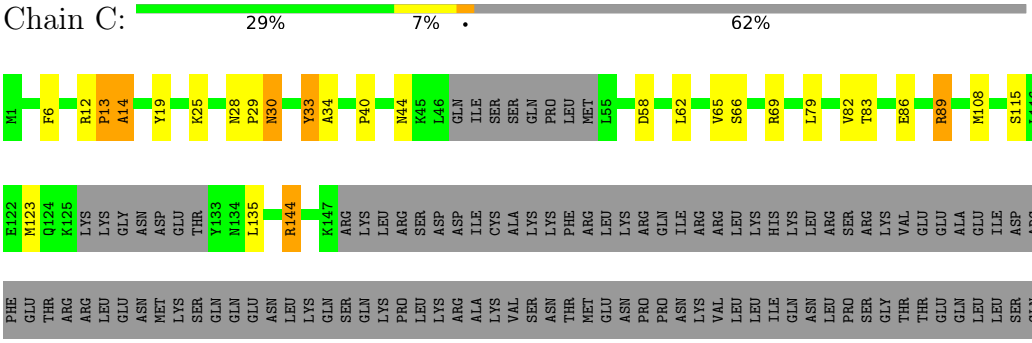
• Molecule 2: U1 small nuclear ribonucleoprotein C

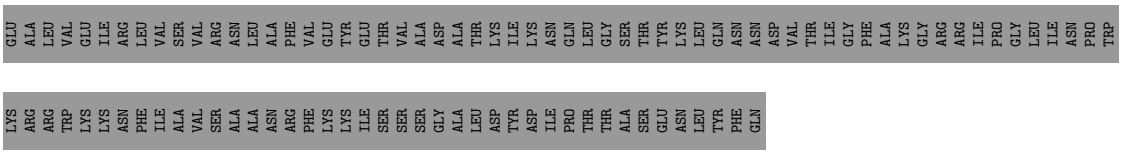
Chain B:



• Molecule 3: U1 small nuclear ribonucleoprotein A

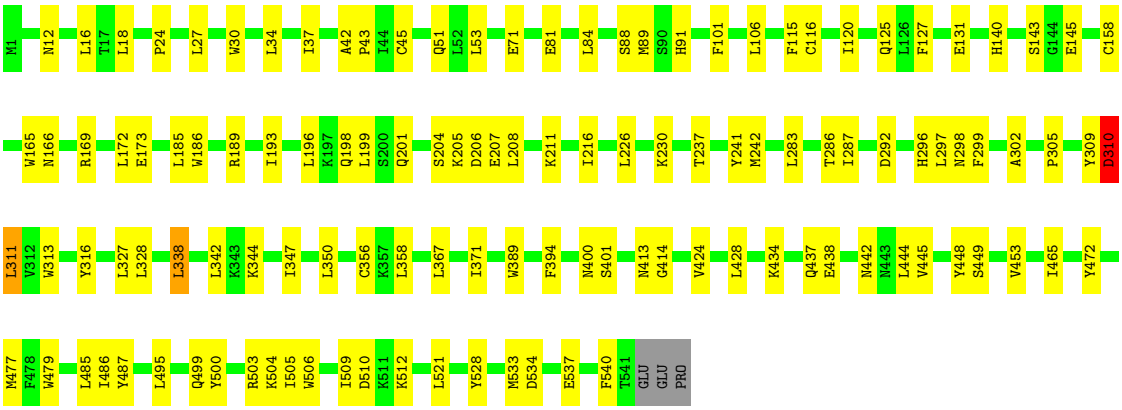
Chain C:





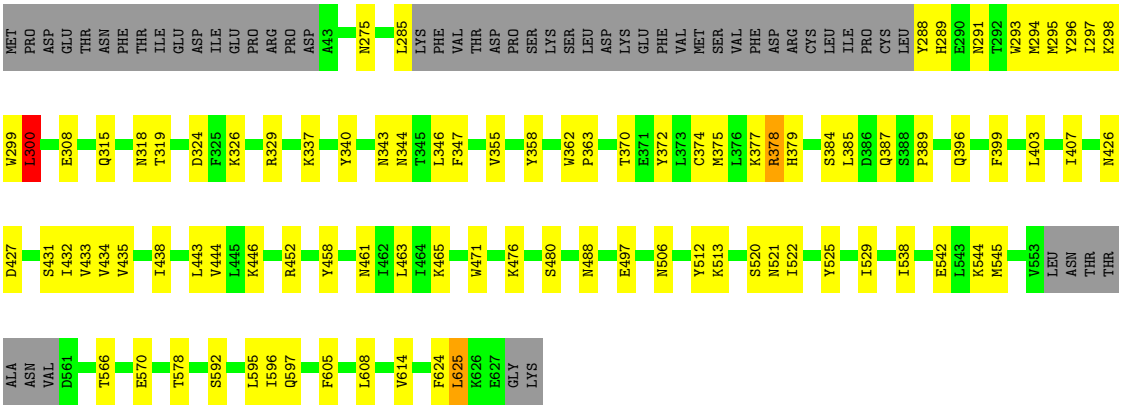
• Molecule 4: U1 small nuclear ribonucleoprotein component PRP42

Chain D:



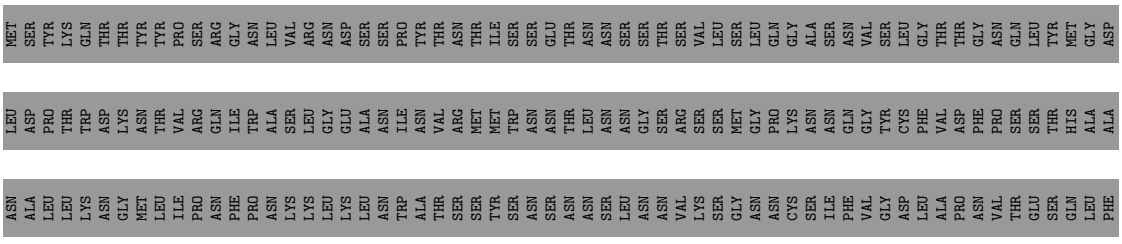
• Molecule 5: Pre-mRNA-processing factor 39

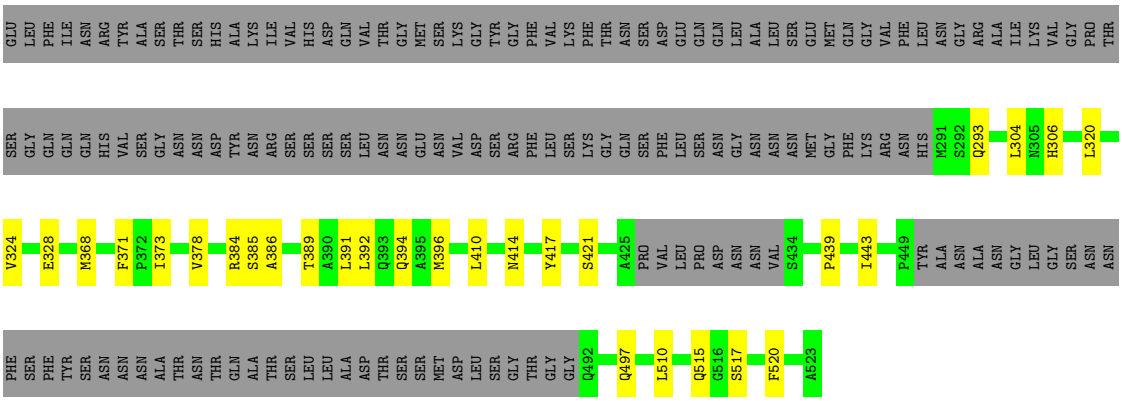
Chain E:



• Molecule 6: Protein NAM8

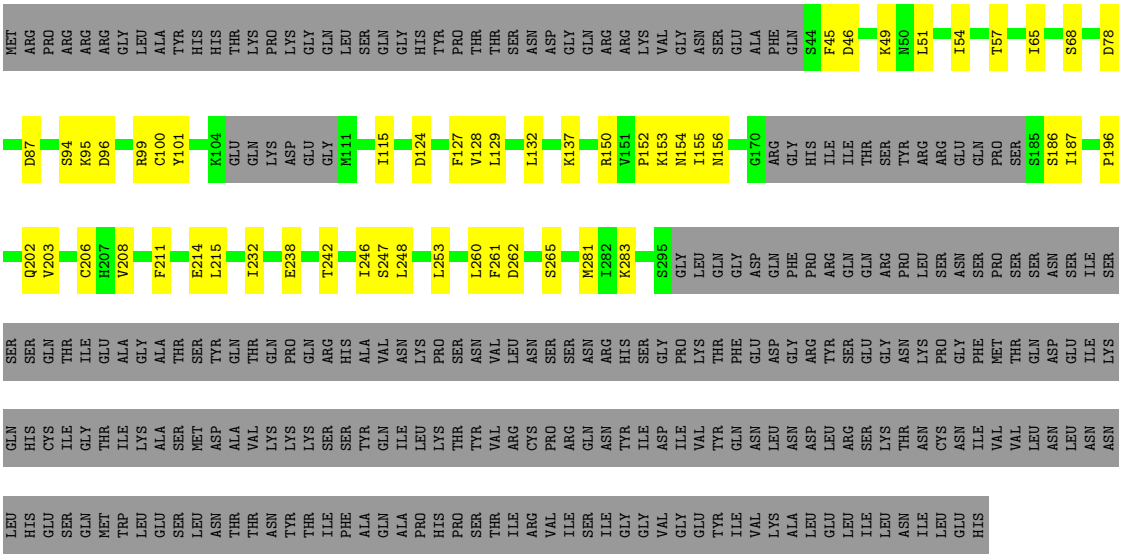
Chain F:





• Molecule 7: 56 kDa U1 small nuclear ribonucleoprotein component

Chain G:

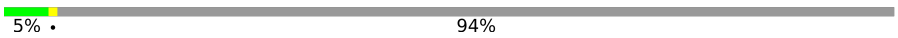


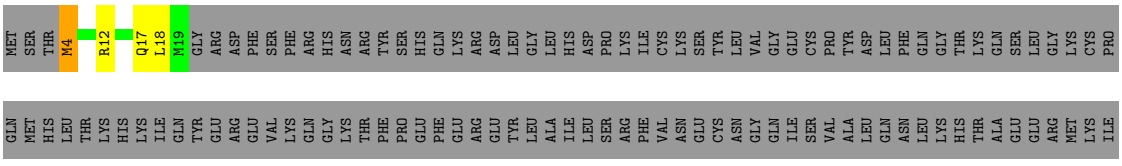
• Molecule 8: U1 small nuclear ribonucleoprotein component SNU71

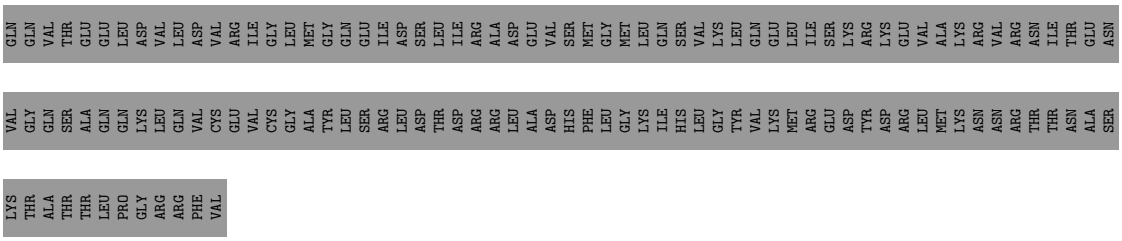
Chain H:

• Molecule 9: Protein LUC7

Chain I:

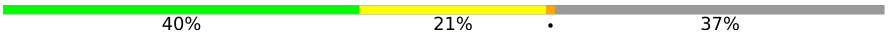


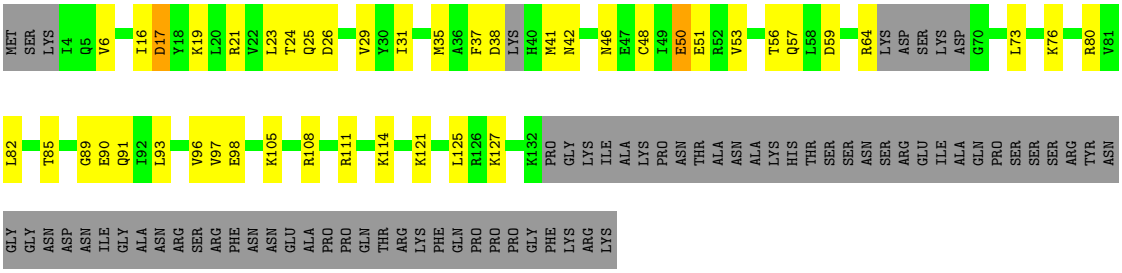




• Molecule 10: Small nuclear ribonucleoprotein-associated protein B

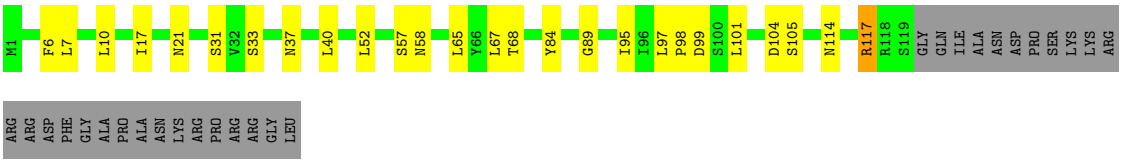
Chain K:





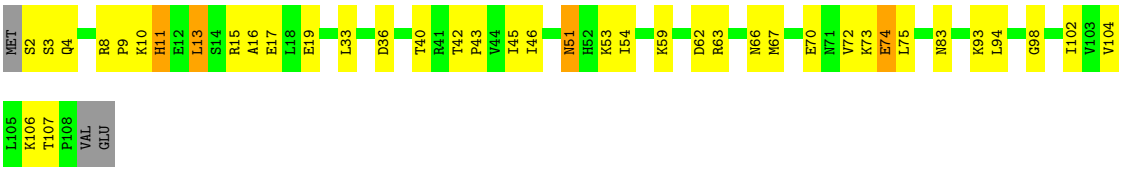
• Molecule 11: Small nuclear ribonucleoprotein Sm D1

Chain L:



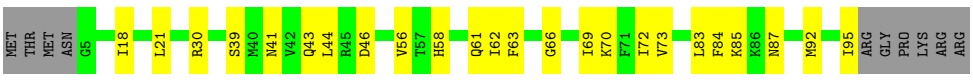
• Molecule 12: Small nuclear ribonucleoprotein Sm D2

Chain M:



• Molecule 13: Small nuclear ribonucleoprotein Sm D3

Chain N:

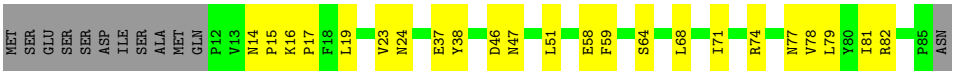


• Molecule 14: Small nuclear ribonucleoprotein E

Chain O:

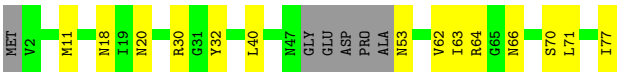
• Molecule 15: Small nuclear ribonucleoprotein F

Chain P:



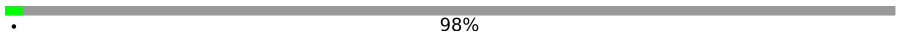
• Molecule 16: Small nuclear ribonucleoprotein G

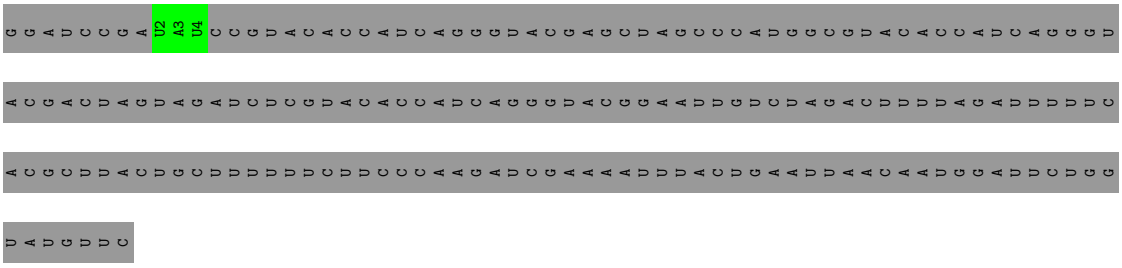
Chain Q:



• Molecule 17: ACT1 pre-mRNA

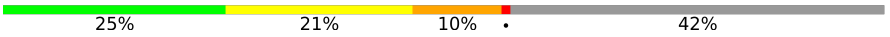
Chain r:

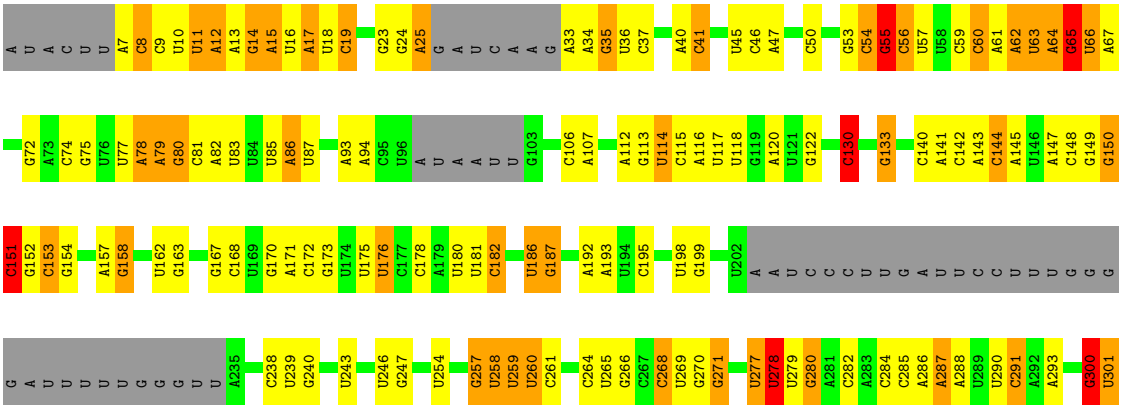


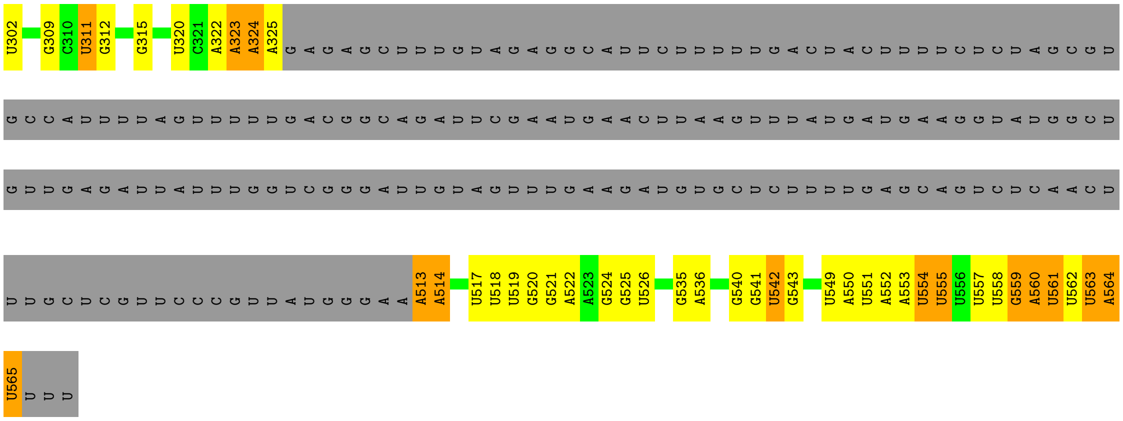


• Molecule 18: U1 snRNA

Chain R:






U302
G309
C310
U311
G312
G315
U320
C321
A322
A323
A324
A325
G A G A G C U U U G U A G A G G C A U U C U U U U U G A C U A C U U U U C U C U A G C G U
G C C A U U U U A G U U U U U G A C G G C A G A U U C G A A U G A A C U U A A G U U U A U G A U G A A G G U A U G G C U
G U U G A G A U U A U U U G G U C G G G A U U G U A G U U U G A A G A U G U G C U C U U U U G A G C A G U C U C A A C U
U U G C U C G U U C C C G U U A U G G G A A
A513
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U558
G559
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U563
A564
U565
U U U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.132	Depositor
Minimum map value	-1.284	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	531.2, 531.2, 531.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.30	0/1107	0.62	1/1514 (0.1%)
2	B	0.25	0/1490	0.49	0/1995
3	C	0.27	0/1055	0.56	0/1416
4	D	0.29	0/4637	0.48	1/6270 (0.0%)
5	E	0.26	0/4050	0.47	1/5543 (0.0%)
6	F	0.29	0/1428	0.49	0/1936
7	G	0.28	0/1938	0.51	1/2605 (0.0%)
8	H	0.28	0/428	0.50	0/575
9	I	0.36	0/125	0.75	1/166 (0.6%)
10	K	0.29	0/1008	0.59	0/1341
11	L	0.27	0/930	0.52	0/1261
12	M	0.29	0/876	0.57	0/1179
13	N	0.27	0/707	0.51	0/959
14	O	0.30	0/583	0.54	0/791
15	P	0.29	0/593	0.52	0/804
16	Q	0.27	0/540	0.60	1/727 (0.1%)
17	r	0.65	0/68	1.17	0/103
18	R	1.34	17/7747 (0.2%)	1.38	114/12053 (0.9%)
All	All	0.73	17/29310 (0.1%)	0.86	120/41238 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	324	A	O3'-P	-23.83	1.32	1.61
18	R	300	G	O3'-P	9.44	1.72	1.61
18	R	301	U	C1'-N1	6.91	1.59	1.48
18	R	72	G	N7-C5	-6.01	1.35	1.39
18	R	564	A	N7-C5	-5.91	1.35	1.39
18	R	559	G	N9-C8	-5.87	1.33	1.37
18	R	559	G	N7-C5	-5.85	1.35	1.39
18	R	553	A	C5-C4	-5.81	1.34	1.38
18	R	563	U	C2-N3	-5.78	1.33	1.37
18	R	561	U	C2-N3	-5.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	254	U	C2-N3	-5.31	1.34	1.37
18	R	560	A	C5-C4	-5.15	1.35	1.38
18	R	157	A	N9-C4	-5.15	1.34	1.37
18	R	86	A	N9-C4	-5.13	1.34	1.37
18	R	62	A	N3-C4	-5.08	1.31	1.34
18	R	559	G	C5-C4	-5.04	1.34	1.38
18	R	60	C	C4-C5	-5.02	1.39	1.43

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	324	A	O3'-P-O5'	19.87	141.74	104.00
18	R	324	A	P-O3'-C3'	-13.68	103.29	119.70
18	R	151	C	N3-C2-O2	-11.54	113.82	121.90
18	R	300	G	O3'-P-O5'	-11.42	82.31	104.00
18	R	324	A	OP1-P-O3'	-10.80	81.44	105.20
1	A	60	PRO	CA-N-CD	-10.70	96.52	111.50
18	R	300	G	P-O3'-C3'	-10.56	107.03	119.70
18	R	56	C	N1-C2-O2	10.44	125.16	118.90
18	R	300	G	OP2-P-O3'	9.84	126.84	105.20
18	R	56	C	C6-N1-C2	-9.53	116.49	120.30
18	R	56	C	C2-N1-C1'	9.39	129.13	118.80
18	R	56	C	N3-C2-O2	-9.14	115.50	121.90
18	R	54	C	C2-N1-C1'	8.54	128.19	118.80
18	R	148	C	N3-C2-O2	-8.42	116.00	121.90
18	R	54	C	C6-N1-C2	-8.18	117.03	120.30
18	R	63	U	N3-C2-O2	-8.01	116.59	122.20
18	R	151	C	C2-N3-C4	-8.00	115.90	119.90
18	R	54	C	C5-C6-N1	7.97	124.98	121.00
18	R	151	C	N1-C2-N3	7.92	124.75	119.20
18	R	80	G	C6-C5-N7	-7.82	125.71	130.40
18	R	56	C	C5-C6-N1	7.81	124.90	121.00
18	R	62	A	C8-N9-C4	-7.80	102.68	105.80
18	R	291	C	N1-C2-O2	7.72	123.53	118.90
18	R	54	C	N1-C2-O2	7.67	123.50	118.90
18	R	80	G	C4-N9-C1'	7.59	136.37	126.50
18	R	62	A	N7-C8-N9	7.56	117.58	113.80
18	R	151	C	C6-N1-C2	-7.54	117.28	120.30
18	R	130	C	C6-N1-C2	-7.47	117.31	120.30
18	R	554	U	N3-C2-O2	-7.43	117.00	122.20
18	R	186	U	C5-C6-N1	7.42	126.41	122.70
18	R	301	U	O3'-P-O5'	7.42	118.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	261	C	C6-N1-C2	-7.38	117.35	120.30
18	R	80	G	C8-N9-C1'	-7.28	117.53	127.00
18	R	41	C	N1-C2-O2	7.10	123.16	118.90
18	R	264	C	C6-N1-C2	-7.09	117.46	120.30
18	R	80	G	N3-C4-N9	7.01	130.21	126.00
18	R	140	C	N3-C2-O2	-6.88	117.08	121.90
18	R	140	C	N1-C2-O2	6.75	122.95	118.90
18	R	83	U	C5-C6-N1	6.74	126.07	122.70
18	R	148	C	N1-C2-O2	6.74	122.94	118.90
18	R	258	U	P-O3'-C3'	6.71	127.75	119.70
18	R	83	U	C2-N1-C1'	6.63	125.66	117.70
18	R	323	A	O3'-P-O5'	-6.60	91.45	104.00
18	R	63	U	P-O3'-C3'	6.55	127.56	119.70
18	R	144	C	C2-N1-C1'	6.38	125.81	118.80
18	R	41	C	N3-C2-O2	-6.34	117.46	121.90
18	R	284	C	C6-N1-C2	-6.27	117.79	120.30
18	R	277	U	P-O3'-C3'	6.24	127.18	119.70
18	R	62	A	C5-N7-C8	-6.16	100.82	103.90
18	R	268	C	P-O3'-C3'	6.16	127.09	119.70
18	R	182	C	C2-N1-C1'	6.12	125.54	118.80
18	R	130	C	C2-N1-C1'	6.09	125.50	118.80
18	R	148	C	C2-N1-C1'	6.09	125.50	118.80
18	R	278	U	N3-C2-O2	-6.02	117.99	122.20
18	R	63	U	C6-N1-C2	-5.94	117.44	121.00
18	R	118	U	C2-N1-C1'	5.93	124.82	117.70
5	E	300	LEU	CA-CB-CG	5.89	128.85	115.30
18	R	118	U	N1-C2-O2	5.88	126.92	122.80
18	R	153	C	C5-C6-N1	5.88	123.94	121.00
18	R	243	U	N3-C2-O2	-5.88	118.08	122.20
18	R	54	C	N3-C2-O2	-5.87	117.79	121.90
18	R	60	C	C5-C6-N1	5.85	123.92	121.00
18	R	118	U	N3-C2-O2	-5.84	118.11	122.20
7	G	78	ASP	CB-CG-OD1	5.83	123.55	118.30
18	R	151	C	P-O3'-C3'	5.83	126.70	119.70
18	R	66	U	P-O3'-C3'	5.79	126.65	119.70
18	R	271	G	C4-N9-C1'	5.76	133.99	126.50
18	R	291	C	N3-C2-O2	-5.70	117.91	121.90
18	R	63	U	N1-C2-O2	5.64	126.75	122.80
18	R	323	A	OP2-P-O3'	5.63	117.59	105.20
18	R	271	G	N7-C8-N9	5.63	115.91	113.10
18	R	277	U	OP2-P-O3'	5.63	117.58	105.20
18	R	311	U	N3-C2-O2	-5.62	118.27	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	554	U	C2-N1-C1'	5.60	124.42	117.70
18	R	261	C	C5-C6-N1	5.59	123.80	121.00
16	Q	40	LEU	CA-CB-CG	5.56	128.09	115.30
18	R	72	G	C4-N9-C1'	5.53	133.69	126.50
18	R	144	C	C6-N1-C1'	-5.53	114.17	120.80
18	R	291	C	C6-N1-C2	-5.52	118.09	120.30
18	R	144	C	N1-C2-O2	5.50	122.20	118.90
18	R	54	C	C6-N1-C1'	-5.46	114.25	120.80
18	R	278	U	C2-N1-C1'	5.45	124.24	117.70
18	R	85	U	C2-N1-C1'	5.45	124.23	117.70
9	I	4	MET	CA-CB-CG	5.43	122.53	113.30
18	R	56	C	C6-N1-C1'	-5.41	114.31	120.80
18	R	80	G	C4-C5-N7	5.40	112.96	110.80
18	R	153	C	C6-N1-C2	-5.39	118.14	120.30
18	R	130	C	C5-C6-N1	5.38	123.69	121.00
18	R	265	U	N3-C2-O2	-5.38	118.44	122.20
18	R	182	C	C6-N1-C2	-5.38	118.15	120.30
18	R	187	G	O5'-P-OP2	5.38	117.15	110.70
18	R	55	G	N1-C2-N3	5.37	127.12	123.90
18	R	271	G	C5-N7-C8	-5.35	101.63	104.30
18	R	271	G	C8-N9-C1'	-5.34	120.06	127.00
18	R	85	U	N3-C2-O2	-5.28	118.50	122.20
18	R	55	G	C6-N1-C2	-5.26	121.94	125.10
18	R	260	U	N3-C2-O2	-5.21	118.55	122.20
18	R	195	C	N1-C2-O2	5.20	122.02	118.90
18	R	565	U	O5'-P-OP2	-5.20	101.02	105.70
18	R	291	C	C5-C6-N1	5.19	123.60	121.00
18	R	65	G	C5-C6-N1	5.19	114.09	111.50
18	R	513	A	P-O3'-C3'	5.17	125.91	119.70
18	R	182	C	N1-C2-O2	5.17	122.00	118.90
18	R	186	U	C6-N1-C2	-5.16	117.91	121.00
4	D	310	ASP	CB-CG-OD1	5.14	122.93	118.30
18	R	178	C	C6-N1-C2	-5.14	118.24	120.30
18	R	120	A	C5-C6-N1	5.14	120.27	117.70
18	R	243	U	N1-C2-O2	5.12	126.39	122.80
18	R	50	C	C6-N1-C2	-5.10	118.26	120.30
18	R	41	C	C2-N1-C1'	5.10	124.41	118.80
18	R	268	C	C2-N1-C1'	5.10	124.41	118.80
18	R	187	G	O5'-P-OP1	-5.09	101.11	105.70
18	R	238	C	C5-C6-N1	5.09	123.54	121.00
18	R	514	A	C2-N3-C4	5.09	113.14	110.60
18	R	62	A	C2-N3-C4	-5.06	108.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	259	U	O5'-P-OP1	-5.05	101.15	105.70
18	R	282	C	C6-N1-C2	-5.05	118.28	120.30
18	R	60	C	C4-C5-C6	-5.03	114.89	117.40
18	R	55	G	N3-C4-N9	-5.01	122.99	126.00
18	R	25	A	C8-N9-C4	-5.01	103.80	105.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1092	0	840	22	0
2	B	1462	0	1466	63	0
3	C	1042	0	1096	23	0
4	D	4523	0	4511	90	0
5	E	3985	0	3293	72	0
6	F	1401	0	1361	20	0
7	G	1897	0	1898	43	0
8	H	420	0	421	8	0
9	I	125	0	131	3	0
10	K	1003	0	1098	42	0
11	L	921	0	970	28	0
12	M	862	0	886	39	0
13	N	695	0	719	33	0
14	O	573	0	604	22	0
15	P	580	0	582	17	0
16	Q	537	0	556	14	0
17	r	62	0	32	0	0
18	R	6937	0	3494	187	0
All	All	28117	0	23958	581	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 11.

All (581) 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)
2:B:16:ASP:HB2	2:B:20:VAL:CG1	1.47	1.42
7:G:45:PHE:CD1	7:G:208:VAL:HG21	1.56	1.39
10:K:121:LYS:NZ	18:R:278:U:H6	1.15	1.38
10:K:121:LYS:NZ	18:R:278:U:C6	1.89	1.34
10:K:121:LYS:NZ	18:R:278:U:H1'	1.42	1.33
13:N:92:MET:HE1	18:R:172:C:C4'	1.57	1.33
2:B:15:HIS:CE1	18:R:11:U:H4'	1.70	1.27
5:E:597:GLN:OE1	18:R:77:U:H5'	1.31	1.27
2:B:16:ASP:OD2	2:B:20:VAL:HG13	1.33	1.24
10:K:114:LYS:NZ	18:R:302:U:OP2	1.68	1.23
2:B:16:ASP:CB	2:B:20:VAL:HG11	1.75	1.17
7:G:45:PHE:HD1	7:G:208:VAL:CG2	1.58	1.15
10:K:121:LYS:NZ	18:R:278:U:C1'	2.11	1.13
2:B:17:SER:H	2:B:18:PRO:CD	1.61	1.12
2:B:16:ASP:CB	2:B:20:VAL:CG1	2.28	1.12
13:N:92:MET:CE	18:R:172:C:O4'	1.96	1.12
13:N:92:MET:CE	18:R:172:C:C1'	2.29	1.11
7:G:45:PHE:CD1	7:G:208:VAL:CG2	2.31	1.10
5:E:597:GLN:OE1	18:R:77:U:C5'	1.99	1.10
13:N:92:MET:HE1	18:R:172:C:O4'	1.48	1.09
13:N:92:MET:HE1	18:R:172:C:C1'	1.84	1.08
2:B:15:HIS:HE1	18:R:11:U:H4'	0.95	1.07
12:M:15:ARG:HH12	18:R:549:U:H4'	1.13	1.07
10:K:121:LYS:HZ1	18:R:278:U:C1'	1.67	1.06
2:B:61:ARG:HH12	18:R:64:A:H5"	1.10	1.05
2:B:17:SER:H	2:B:18:PRO:HD2	1.23	1.00
18:R:17:A:N1	18:R:45:U:N3	2.08	0.99
13:N:92:MET:HE1	18:R:172:C:H4'	1.45	0.98
13:N:92:MET:CE	18:R:172:C:C4'	2.42	0.97
13:N:92:MET:HE2	18:R:172:C:H1'	1.49	0.95
18:R:10:U:H6	18:R:10:U:H5"	1.30	0.95
2:B:16:ASP:CG	2:B:20:VAL:HG13	1.86	0.94
10:K:121:LYS:HZ1	18:R:278:U:H1'	0.78	0.93
11:L:117:ARG:HH12	18:R:35:G:H4'	1.36	0.91
11:L:117:ARG:NH1	18:R:35:G:H4'	1.86	0.90
2:B:63:GLU:HB2	18:R:65:G:O6	1.73	0.89
18:R:24:G:O6	18:R:37:C:N4	2.08	0.86
10:K:127:LYS:NZ	18:R:173:G:OP1	2.08	0.86
7:G:45:PHE:CG	7:G:208:VAL:HG21	2.11	0.86
2:B:15:HIS:HE1	18:R:11:U:C4'	1.86	0.85
1:A:52:LEU:HD21	12:M:107:THR:HG23	1.58	0.85
18:R:17:A:N6	18:R:45:U:O4	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:HIS:CE1	18:R:11:U:C4'	2.58	0.84
2:B:61:ARG:HH12	18:R:64:A:C5'	1.91	0.83
18:R:33:A:H8	18:R:33:A:P	2.02	0.83
7:G:45:PHE:HD1	7:G:208:VAL:CB	1.92	0.83
5:E:597:GLN:HE22	18:R:77:U:H5"	1.43	0.83
2:B:16:ASP:HB2	2:B:20:VAL:HG11	0.83	0.82
13:N:92:MET:CE	18:R:172:C:H1'	2.04	0.82
18:R:10:U:H5"	18:R:10:U:C6	2.14	0.81
12:M:15:ARG:NH1	18:R:549:U:H4'	1.95	0.81
12:M:15:ARG:HH22	18:R:549:U:H1'	1.45	0.81
2:B:16:ASP:CB	2:B:20:VAL:HG13	2.04	0.80
5:E:597:GLN:NE2	18:R:77:U:H5"	1.97	0.80
13:N:92:MET:HE1	18:R:172:C:C2'	2.11	0.79
2:B:17:SER:N	2:B:18:PRO:CD	2.39	0.78
12:M:15:ARG:HH12	18:R:549:U:C4'	1.93	0.78
10:K:121:LYS:CE	18:R:278:U:H6	1.96	0.77
18:R:10:U:H6	18:R:10:U:C5'	1.97	0.77
10:K:93:LEU:HD11	11:L:21:ASN:HD21	1.49	0.77
2:B:63:GLU:OE1	18:R:65:G:N1	2.16	0.77
15:P:46:ASP:OD1	15:P:47:ASN:N	2.18	0.77
11:L:37:ASN:OD1	18:R:557:U:O4	2.03	0.76
13:N:92:MET:HE3	18:R:172:C:O4'	1.85	0.76
5:E:396:GLN:HG3	5:E:444:VAL:HG11	1.67	0.76
14:O:12:PRO:HD2	14:O:15:ASN:HD22	1.49	0.76
10:K:56:THR:OG1	18:R:122:G:OP1	2.04	0.75
10:K:121:LYS:NZ	18:R:278:U:N1	2.34	0.75
7:G:45:PHE:HD1	7:G:208:VAL:HG21	1.01	0.74
6:F:373:ILE:HD12	6:F:378:VAL:HG21	1.69	0.74
12:M:62:ASP:OD2	12:M:63:ARG:N	2.19	0.74
2:B:61:ARG:NH1	18:R:64:A:H5"	1.94	0.73
10:K:57:GLN:HE22	10:K:76:LYS:HG2	1.54	0.73
1:A:67:HIS:HE1	12:M:59:LYS:HG3	1.54	0.73
18:R:34:A:H3'	18:R:34:A:N3	2.04	0.73
13:N:95:ILE:CG2	18:R:541:G:N7	2.52	0.72
2:B:63:GLU:CB	18:R:65:G:O6	2.38	0.72
18:R:12:A:H8	18:R:12:A:C5'	2.02	0.71
2:B:16:ASP:HB2	2:B:20:VAL:HG13	1.58	0.71
7:G:45:PHE:HA	7:G:208:VAL:HG11	1.73	0.71
18:R:557:U:H4'	18:R:558:U:H5'	1.72	0.71
18:R:12:A:H8	18:R:12:A:H5'	1.55	0.71
3:C:62:LEU:HD21	3:C:79:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:63:ARG:NH1	18:R:552:A:OP1	2.23	0.71
11:L:117:ARG:HH12	18:R:35:G:C4'	2.04	0.71
18:R:15:A:C8	18:R:15:A:H5"	2.26	0.70
7:G:206:CYS:HB3	7:G:211:PHE:HB2	1.71	0.70
4:D:310:ASP:HA	4:D:313:TRP:HD1	1.54	0.70
2:B:17:SER:N	2:B:18:PRO:HD2	2.02	0.70
11:L:117:ARG:NH1	18:R:35:G:C4'	2.54	0.69
10:K:6:VAL:HG21	10:K:97:VAL:HG11	1.74	0.69
3:C:13:PRO:HG2	3:C:19:TYR:CD1	2.27	0.69
7:G:129:LEU:HD12	7:G:215:LEU:HD11	1.74	0.69
18:R:55:G:N2	18:R:151:C:O2	2.27	0.68
2:B:30:HIS:O	2:B:30:HIS:ND1	2.25	0.68
14:O:29:ILE:HG12	14:O:90:ILE:HG12	1.75	0.68
18:R:57:U:OP1	18:R:150:G:N2	2.25	0.68
5:E:506:ASN:ND2	5:E:545:MET:O	2.27	0.68
5:E:597:GLN:NE2	18:R:77:U:OP1	2.27	0.67
2:B:16:ASP:OD2	2:B:21:ARG:N	2.28	0.67
7:G:153:LYS:O	7:G:154:ASN:ND2	2.28	0.67
13:N:92:MET:CE	18:R:172:C:H4'	2.16	0.67
4:D:534:ASP:OD1	5:E:378:ARG:NH1	2.28	0.67
13:N:46:ASP:OD1	13:N:58:HIS:NE2	2.25	0.67
3:C:12:ARG:N	3:C:13:PRO:HD2	2.09	0.67
4:D:437:GLN:NE2	4:D:472:TYR:OH	2.27	0.66
3:C:29:PRO:O	3:C:30:ASN:ND2	2.29	0.66
2:B:59:ARG:O	2:B:64:ARG:NH1	2.28	0.66
5:E:465:LYS:O	5:E:471:TRP:NE1	2.27	0.66
15:P:23:VAL:HG12	15:P:24:ASN:ND2	2.11	0.66
2:B:18:PRO:HD2	2:B:20:VAL:HG12	1.77	0.66
4:D:127:PHE:O	4:D:131:GLU:HG2	1.96	0.66
7:G:262:ASP:OD1	7:G:265:SER:OG	2.14	0.66
5:E:308:GLU:N	5:E:308:GLU:OE2	2.27	0.65
9:I:12:ARG:HB2	14:O:48:GLU:OE1	1.95	0.65
12:M:98:GLY:O	15:P:74:ARG:NH1	2.30	0.65
18:R:35:G:O5'	18:R:35:G:H8	1.79	0.65
3:C:14:ALA:HB3	18:R:59:C:OP2	1.96	0.65
4:D:401:SER:HB3	5:E:522:ILE:H	1.62	0.65
18:R:8:C:H6	18:R:8:C:O5'	1.80	0.65
5:E:513:LYS:NZ	5:E:538:ILE:O	2.28	0.65
2:B:17:SER:H	2:B:18:PRO:HD3	1.57	0.64
10:K:50:GLU:OE2	10:K:80:ARG:NH2	2.30	0.64
12:M:43:PRO:O	12:M:107:THR:OG1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:199:G:H1	18:R:239:U:H3	1.44	0.64
4:D:533:MET:O	4:D:537:GLU:HG2	1.98	0.64
2:B:186:THR:HG23	4:D:242:MET:HG3	1.79	0.64
5:E:344:ASN:O	5:E:379:HIS:NE2	2.26	0.64
5:E:363:PRO:O	5:E:426:ASN:ND2	2.31	0.64
14:O:29:ILE:HD12	14:O:54:ILE:HD11	1.78	0.64
7:G:46:ASP:HB3	7:G:49:LYS:HG3	1.79	0.63
5:E:597:GLN:CD	18:R:77:U:C5’	2.66	0.63
18:R:320:U:H3	18:R:521:G:H1	1.46	0.63
12:M:15:ARG:HH22	18:R:549:U:C1’	2.11	0.63
4:D:169:ARG:NH2	4:D:173:GLU:OE2	2.28	0.63
7:G:187:ILE:HG12	7:G:203:VAL:HG12	1.81	0.62
18:R:171:A:OP2	18:R:171:A:H8	1.82	0.62
7:G:51:LEU:HD11	7:G:127:PHE:HB2	1.81	0.62
11:L:37:ASN:ND2	18:R:557:U:O4	2.33	0.62
1:A:37:THR:HG22	1:A:38:ASN:H	1.65	0.62
18:R:24:G:H1	18:R:37:C:N4	1.97	0.62
7:G:101:TYR:HE2	7:G:232:ILE:HG21	1.64	0.62
3:C:12:ARG:N	3:C:13:PRO:CD	2.63	0.62
5:E:318:ASN:OD1	5:E:329:ARG:NH2	2.33	0.61
5:E:296:TYR:O	5:E:300:LEU:HD12	1.99	0.61
18:R:324:A:C2	18:R:325:A:C4	2.88	0.61
18:R:17:A:N1	18:R:45:U:C2	2.67	0.61
3:C:144:ARG:O	3:C:144:ARG:NE	2.33	0.61
5:E:337:LYS:NZ	5:E:374:CYS:SG	2.73	0.61
5:E:597:GLN:OE1	18:R:77:U:H5”	1.97	0.61
4:D:328:LEU:HD12	7:G:202:GLN:HB2	1.81	0.61
18:R:19:C:O5’	18:R:19:C:H6	1.84	0.61
2:B:19:SER:O	2:B:23:THR:N	2.34	0.61
7:G:45:PHE:CB	7:G:208:VAL:HG21	2.30	0.61
12:M:73:LYS:HE2	12:M:75:LEU:HD21	1.83	0.61
4:D:486:ILE:HD12	4:D:505:ILE:HD11	1.82	0.61
5:E:597:GLN:CD	18:R:77:U:H5”	2.21	0.61
11:L:98:PRO:HG2	11:L:101:LEU:HD22	1.83	0.61
12:M:73:LYS:HG2	12:M:75:LEU:HD21	1.82	0.61
12:M:4:GLN:O	12:M:8:ARG:HB2	2.01	0.61
13:N:92:MET:HE1	18:R:172:C:C3’	2.29	0.61
3:C:69:ARG:HG3	18:R:150:G:N7	2.16	0.60
8:H:45:HIS:CE1	8:H:46:ILE:HG12	2.36	0.60
4:D:449:SER:O	4:D:453:VAL:HG23	2.01	0.60
5:E:296:TYR:CE2	5:E:300:LEU:HD11	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:368:MET:HE3	6:F:371:PHE:HB3	1.83	0.60
18:R:12:A:H5'	18:R:12:A:C8	2.37	0.60
2:B:82:GLU:OE1	2:B:82:GLU:N	2.34	0.60
15:P:37:GLU:OE2	15:P:82:ARG:NH1	2.35	0.60
18:R:15:A:C8	18:R:15:A:C5'	2.85	0.60
18:R:81:C:O5'	18:R:81:C:H6	1.84	0.60
2:B:18:PRO:HD2	2:B:20:VAL:CG1	2.31	0.59
14:O:31:LEU:HD21	14:O:82:LEU:HD21	1.84	0.59
4:D:453:VAL:HG13	4:D:485:LEU:HD11	1.84	0.59
4:D:165:TRP:NE1	4:D:201:GLN:OE1	2.35	0.59
4:D:309:TYR:HB3	4:D:311:LEU:HD23	1.84	0.59
18:R:14:G:C5'	18:R:14:G:C8	2.85	0.59
1:A:89:LEU:HG	1:A:89:LEU:O	2.02	0.59
11:L:89:GLY:N	18:R:557:U:H5	2.00	0.59
11:L:99:ASP:O	12:M:93:LYS:NZ	2.36	0.58
5:E:488:ASN:ND2	5:E:512:TYR:OH	2.36	0.58
10:K:16:ILE:HG22	10:K:17:ASP:OD1	2.03	0.58
18:R:24:G:H1	18:R:37:C:H42	1.51	0.58
4:D:204:SER:OG	4:D:206:ASP:OD2	2.19	0.58
9:I:18:LEU:HD21	14:O:18:PHE:HB2	1.85	0.58
7:G:137:LYS:NZ	7:G:156:ASN:O	2.34	0.58
7:G:45:PHE:CD1	7:G:208:VAL:CB	2.81	0.58
2:B:70:ASN:OD1	2:B:71:GLU:N	2.36	0.57
18:R:12:A:C5'	18:R:12:A:C8	2.85	0.57
4:D:528:TYR:OH	5:E:476:LYS:NZ	2.37	0.57
4:D:140:HIS:HB3	4:D:143:SER:HB2	1.87	0.57
1:A:84:LEU:HD13	1:A:87:ARG:HH21	1.70	0.57
4:D:24:PRO:HD2	7:G:260:LEU:HB2	1.86	0.57
18:R:17:A:N6	18:R:45:U:C4	2.70	0.57
18:R:36:U:H2'	18:R:36:U:O2	2.05	0.57
10:K:82:LEU:HD13	10:K:85:THR:HG21	1.86	0.56
18:R:323:A:H2'	18:R:324:A:H8	1.70	0.56
7:G:186:SER:HB3	7:G:214:GLU:HG2	1.87	0.56
18:R:198:U:H3	18:R:240:G:H1	1.54	0.56
9:I:17:GLN:N	9:I:17:GLN:OE1	2.38	0.56
4:D:442:ASN:ND2	6:F:510:LEU:HD13	2.22	0.55
4:D:510:ASP:OD2	4:D:512:LYS:NZ	2.24	0.55
10:K:59:ASP:OD2	10:K:59:ASP:N	2.32	0.55
11:L:65:LEU:O	11:L:68:THR:OG1	2.23	0.55
1:A:81:ASN:OD1	1:A:85:LEU:HD23	2.07	0.55
4:D:193:ILE:HG22	4:D:230:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:15:A:H4'	18:R:15:A:OP1	2.06	0.55
4:D:140:HIS:CD2	4:D:297:LEU:HD21	2.41	0.55
5:E:340:TYR:HE1	5:E:379:HIS:HD2	1.53	0.55
10:K:23:LEU:HG	10:K:29:VAL:HG23	1.87	0.55
6:F:443:ILE:HD12	6:F:443:ILE:H	1.70	0.55
13:N:18:ILE:HG21	13:N:30:ARG:HH21	1.72	0.55
4:D:344:LYS:HD2	7:G:253:LEU:HD13	1.89	0.55
11:L:57:SER:OG	11:L:58:ASN:N	2.39	0.55
1:A:53:LYS:HD2	1:A:53:LYS:C	2.27	0.54
4:D:509:ILE:HD11	4:D:540:PHE:CZ	2.42	0.54
5:E:355:VAL:HG11	5:E:372:TYR:HB2	1.88	0.54
5:E:525:TYR:CZ	5:E:529:ILE:HD11	2.42	0.54
11:L:89:GLY:CA	18:R:557:U:H5	2.20	0.54
5:E:427:ASP:OD1	5:E:463:LEU:HD11	2.08	0.54
4:D:81:GLU:HG3	4:D:89:MET:HG2	1.90	0.54
12:M:54:ILE:HG22	12:M:74:GLU:HG2	1.89	0.54
4:D:196:LEU:HD12	4:D:216:ILE:HA	1.90	0.54
14:O:88:THR:HG22	14:O:89:LEU:HD12	1.90	0.54
15:P:16:LYS:HB3	15:P:17:PRO:HD3	1.90	0.54
4:D:186:TRP:HE1	4:D:237:THR:HG1	1.56	0.53
11:L:37:ASN:CG	18:R:557:U:O4	2.47	0.53
13:N:41:ASN:ND2	13:N:66:GLY:H	2.06	0.53
18:R:19:C:H6	18:R:19:C:C5'	2.20	0.53
5:E:426:ASN:OD1	5:E:427:ASP:N	2.39	0.53
8:H:44:LYS:HE2	8:H:44:LYS:HA	1.91	0.53
12:M:10:LYS:HE3	18:R:550:A:H5'	1.90	0.53
3:C:117:LEU:O	3:C:121:ILE:HG12	2.09	0.53
4:D:206:ASP:OD2	4:D:207:GLU:N	2.42	0.53
14:O:35:ILE:HG22	14:O:37:ILE:HG12	1.91	0.53
6:F:320:LEU:HD22	6:F:324:VAL:HG11	1.91	0.53
8:H:35:ASP:OD2	8:H:38:ARG:HD3	2.09	0.53
12:M:40:THR:HG23	12:M:42:THR:HG23	1.90	0.53
18:R:524:G:H2'	18:R:525:G:H8	1.74	0.53
12:M:10:LYS:HA	12:M:13:LEU:CD1	2.39	0.53
13:N:92:MET:HE1	18:R:172:C:O2'	2.08	0.53
18:R:33:A:P	18:R:33:A:C8	2.93	0.53
6:F:417:TYR:HB2	7:G:281:MET:CE	2.39	0.53
5:E:566:THR:O	5:E:570:GLU:HG2	2.09	0.53
5:E:329:ARG:HB3	5:E:358:TYR:CZ	2.44	0.53
13:N:43:GLN:HG2	13:N:63:PHE:HD1	1.72	0.53
2:B:63:GLU:HB2	18:R:65:G:C6	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:36:ASP:O	12:M:40:THR:HG22	2.09	0.52
3:C:115:SER:HA	18:R:144:C:H41	1.75	0.52
4:D:442:ASN:HD22	6:F:510:LEU:HD13	1.75	0.52
5:E:403:LEU:HD12	5:E:433:VAL:HG13	1.92	0.52
5:E:597:GLN:NE2	18:R:77:U:C5'	2.70	0.52
2:B:22:LYS:O	2:B:26:SER:OG	2.22	0.52
4:D:327:LEU:HB3	4:D:358:LEU:HD11	1.91	0.52
1:A:84:LEU:CD1	1:A:87:ARG:HH21	2.23	0.52
4:D:413:ASN:OD1	4:D:413:ASN:N	2.42	0.52
16:Q:64:ARG:HG2	16:Q:66:ASN:H	1.75	0.52
1:A:42:THR:HG22	12:M:51:ASN:HD21	1.74	0.52
11:L:117:ARG:NH1	18:R:35:G:C5'	2.73	0.52
18:R:17:A:C2	18:R:45:U:O2	2.62	0.52
11:L:17:ILE:HD12	11:L:40:LEU:HD11	1.91	0.52
4:D:27:LEU:HA	4:D:30:TRP:HB2	1.91	0.52
5:E:285:LEU:O	5:E:288:TYR:N	2.43	0.52
11:L:89:GLY:H	18:R:557:U:H5	1.57	0.52
16:Q:11:MET:HE1	16:Q:32:TYR:HE2	1.75	0.52
2:B:61:ARG:NH1	18:R:64:A:C5'	2.65	0.52
4:D:499:GLN:OE1	4:D:503:ARG:HG3	2.09	0.52
10:K:108:ARG:HA	10:K:111:ARG:NH1	2.25	0.51
4:D:292:ASP:N	4:D:292:ASP:OD1	2.42	0.51
5:E:294:MET:SD	5:E:294:MET:N	2.84	0.51
13:N:92:MET:CE	18:R:172:C:O2'	2.59	0.51
15:P:38:TYR:CE1	15:P:58:GLU:HG3	2.44	0.51
18:R:14:G:C8	18:R:14:G:H5"	2.45	0.51
4:D:445:VAL:HG13	4:D:485:LEU:HB2	1.93	0.51
10:K:121:LYS:HZ2	18:R:278:U:C1'	2.16	0.51
12:M:46:ILE:HG12	12:M:104:VAL:HG13	1.92	0.51
13:N:83:LEU:HD12	13:N:84:PHE:HD2	1.73	0.51
18:R:7:A:H2'	18:R:8:C:C6	2.46	0.51
5:E:597:GLN:HE22	18:R:77:U:C5'	2.20	0.51
5:E:605:PHE:HB3	5:E:608:LEU:HD23	1.92	0.51
13:N:69:ILE:HD13	13:N:72:ILE:HD11	1.92	0.51
1:A:76:LEU:O	1:A:80:LYS:HB3	2.10	0.51
18:R:18:U:H2'	18:R:19:C:C6	2.46	0.51
18:R:192:A:H2'	18:R:193:A:H8	1.76	0.51
14:O:33:GLU:CD	14:O:33:GLU:H	2.13	0.51
12:M:13:LEU:HD12	12:M:13:LEU:H	1.76	0.50
1:A:72:GLU:O	1:A:76:LEU:HD23	2.11	0.50
3:C:144:ARG:HE	3:C:144:ARG:C	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:338:LEU:O	4:D:344:LYS:NZ	2.42	0.50
18:R:33:A:H2'	18:R:34:A:C4	2.47	0.50
18:R:133:G:N3	18:R:133:G:H2'	2.27	0.50
6:F:324:VAL:HG23	6:F:328:GLU:HG2	1.93	0.50
12:M:59:LYS:HE3	12:M:70:GLU:OE2	2.12	0.50
18:R:300:G:C4	18:R:301:U:C5	2.99	0.50
4:D:88:SER:OG	18:R:115:C:OP1	2.21	0.50
7:G:124:ASP:O	7:G:128:VAL:HG12	2.11	0.50
2:B:32:GLU:HA	2:B:35:LYS:HE3	1.94	0.50
3:C:66:SER:HG	18:R:143:A:H2	1.59	0.50
5:E:544:LYS:O	5:E:544:LYS:HG2	2.10	0.50
18:R:239:U:H2'	18:R:240:G:H8	1.76	0.50
18:R:311:U:H2'	18:R:312:G:H8	1.77	0.50
4:D:196:LEU:HD22	4:D:226:LEU:HD13	1.92	0.49
4:D:310:ASP:HB2	4:D:347:ILE:HD11	1.93	0.49
5:E:343:ASN:ND2	5:E:346:LEU:HB3	2.28	0.49
10:K:38:ASP:HB3	10:K:42:ASN:OD1	2.13	0.49
10:K:125:LEU:HD11	18:R:280:G:OP2	2.12	0.49
11:L:37:ASN:OD1	11:L:89:GLY:N	2.45	0.49
13:N:95:ILE:HG23	18:R:541:G:N7	2.26	0.49
16:Q:64:ARG:NH1	18:R:554:U:N1	2.60	0.49
12:M:13:LEU:HD23	12:M:17:GLU:OE1	2.12	0.49
10:K:41:MET:O	10:K:41:MET:HG2	2.12	0.49
14:O:33:GLU:OE1	16:Q:20:ASN:ND2	2.46	0.49
18:R:11:U:O2	18:R:11:U:O2'	2.25	0.49
4:D:506:TRP:HE1	4:D:521:LEU:HD11	1.77	0.49
10:K:29:VAL:HG12	10:K:51:GLU:HB2	1.93	0.49
11:L:10:LEU:HD11	11:L:97:LEU:HD22	1.94	0.49
18:R:14:G:O5'	18:R:14:G:H8	1.95	0.49
5:E:399:PHE:O	5:E:403:LEU:HD23	2.13	0.49
3:C:33:TYR:OH	3:C:40:PRO:O	2.24	0.48
18:R:521:G:H2'	18:R:522:A:C8	2.47	0.48
5:E:370:THR:HB	5:E:432:ILE:HD11	1.95	0.48
18:R:23:G:H2'	18:R:24:G:H8	1.78	0.48
1:A:82:ALA:O	1:A:85:LEU:HG	2.14	0.48
18:R:24:G:H2'	18:R:25:A:H8	1.78	0.48
13:N:39:SER:O	13:N:39:SER:OG	2.27	0.48
18:R:246:U:H2'	18:R:247:G:H8	1.77	0.48
11:L:117:ARG:NH1	18:R:35:G:O3'	2.39	0.48
4:D:495:LEU:HG	5:E:389:PRO:HB3	1.96	0.48
3:C:13:PRO:HG2	3:C:19:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:73:LYS:HE2	14:O:73:LYS:HA	1.96	0.48
3:C:86:GLU:OE2	3:C:89:ARG:NE	2.45	0.48
4:D:479:TRP:CH2	4:D:509:ILE:HG22	2.49	0.48
5:E:434:VAL:O	5:E:438:ILE:HG12	2.13	0.48
12:M:72:VAL:HG21	12:M:94:LEU:HB3	1.96	0.47
1:A:75:LYS:HE2	1:A:75:LYS:HA	1.95	0.47
18:R:17:A:C6	18:R:45:U:N3	2.69	0.47
2:B:97:LEU:HD11	4:D:185:LEU:HD12	1.96	0.47
12:M:11:HIS:HB3	18:R:550:A:O2'	2.15	0.47
18:R:239:U:H2'	18:R:240:G:C8	2.49	0.47
5:E:315:GLN:O	5:E:319:THR:HG23	2.14	0.47
6:F:392:LEU:O	6:F:396:MET:HG3	2.14	0.47
6:F:385:SER:OG	6:F:386:ALA:N	2.47	0.47
12:M:66:ASN:HB3	12:M:98:GLY:N	2.29	0.47
4:D:205:LYS:HG2	4:D:216:ILE:HD12	1.96	0.47
13:N:56:VAL:HG12	18:R:114:U:H1'	1.95	0.47
2:B:44:ASP:O	2:B:48:LYS:HG2	2.15	0.47
10:K:16:ILE:HD11	10:K:37:PHE:HE1	1.80	0.47
1:A:174:ILE:N	1:A:181:CYS:O	2.43	0.47
4:D:487:TYR:HE2	5:E:443:LEU:HD13	1.80	0.47
8:H:8:SER:OG	8:H:11:LEU:HB2	2.14	0.47
14:O:81:LEU:HD13	15:P:15:PRO:HB3	1.97	0.47
2:B:45:ILE:HA	2:B:48:LYS:HG2	1.97	0.47
13:N:95:ILE:HG22	18:R:541:G:C5	2.50	0.47
4:D:499:GLN:HA	5:E:385:LEU:HD21	1.97	0.46
7:G:196:PRO:HD2	7:G:238:GLU:HG2	1.98	0.46
18:R:10:U:C6	18:R:10:U:C5'	2.85	0.46
18:R:23:G:H2'	18:R:24:G:C8	2.50	0.46
1:A:128:VAL:HA	1:A:131:GLY:O	2.15	0.46
13:N:85:LYS:NZ	13:N:87:ASN:O	2.39	0.46
5:E:434:VAL:HG21	5:E:458:TYR:HD1	1.80	0.46
10:K:85:THR:HG22	13:N:73:VAL:HG13	1.97	0.46
2:B:9:CYS:HB3	2:B:11:THR:HG23	1.98	0.46
2:B:40:ASN:HD21	18:R:285:C:H1'	1.80	0.46
4:D:18:LEU:HD22	8:H:31:ILE:HD11	1.96	0.46
18:R:315:G:H1	18:R:526:U:H3	1.64	0.46
3:C:86:GLU:OE2	3:C:89:ARG:NH2	2.48	0.46
4:D:207:GLU:OE1	4:D:211:LYS:HD2	2.16	0.46
7:G:96:ASP:O	7:G:99:ARG:NH2	2.48	0.46
12:M:9:PRO:HB2	12:M:11:HIS:CE1	2.51	0.46
4:D:166:ASN:ND2	5:E:596:ILE:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:24:THR:HG22	10:K:25:GLN:H	1.80	0.46
12:M:13:LEU:HB3	12:M:17:GLU:HG2	1.97	0.46
1:A:48:LEU:HG	1:A:52:LEU:HD23	1.97	0.46
1:A:52:LEU:HD22	12:M:45:ILE:HD11	1.97	0.46
18:R:518:U:H2'	18:R:519:U:C6	2.51	0.46
2:B:16:ASP:CG	2:B:20:VAL:CG1	2.63	0.45
4:D:165:TRP:CH2	4:D:189:ARG:HG2	2.50	0.45
5:E:295:MET:HA	5:E:298:LYS:HE3	1.98	0.45
7:G:246:ILE:HG13	7:G:247:SER:N	2.31	0.45
13:N:62:ILE:HD11	16:Q:70:SER:HB2	1.97	0.45
4:D:434:LYS:HB2	4:D:437:GLN:OE1	2.15	0.45
7:G:45:PHE:CD1	7:G:208:VAL:HB	2.51	0.45
18:R:521:G:H2'	18:R:522:A:H8	1.81	0.45
2:B:18:PRO:CD	2:B:20:VAL:HG12	2.45	0.45
13:N:61:GLN:HB2	16:Q:77:ILE:HD13	1.97	0.45
18:R:34:A:C2	18:R:34:A:OP2	2.69	0.45
2:B:59:ARG:HH22	2:B:67:SER:HB3	1.81	0.45
4:D:286:THR:OG1	4:D:298:ASN:ND2	2.47	0.45
5:E:521:ASN:OD1	5:E:521:ASN:N	2.50	0.45
1:A:80:LYS:NZ	1:A:84:LEU:HG	2.31	0.45
4:D:287:ILE:HD11	4:D:299:PHE:HZ	1.81	0.45
4:D:424:VAL:HG11	4:D:444:LEU:HD11	1.98	0.45
15:P:14:ASN:HB2	15:P:17:PRO:HD2	1.98	0.45
18:R:246:U:H2'	18:R:247:G:C8	2.51	0.45
5:E:340:TYR:HA	5:E:347:PHE:HD2	1.81	0.45
7:G:283:LYS:O	7:G:283:LYS:HD3	2.16	0.45
18:R:34:A:N3	18:R:34:A:C3'	2.78	0.45
4:D:145:GLU:OE1	4:D:145:GLU:N	2.49	0.45
10:K:31:ILE:O	10:K:48:CYS:HA	2.16	0.45
2:B:15:HIS:O	2:B:15:HIS:CD2	2.70	0.45
4:D:34:LEU:HA	4:D:37:ILE:HG22	1.98	0.45
4:D:487:TYR:CE2	5:E:443:LEU:HD13	2.52	0.45
10:K:90:GLU:OE1	10:K:91:GLN:NE2	2.50	0.45
11:L:7:LEU:HD21	11:L:95:ILE:HD12	1.98	0.45
2:B:6:CYS:SG	2:B:9:CYS:N	2.76	0.44
4:D:367:LEU:O	4:D:371:ILE:HG22	2.17	0.44
8:H:9:PRO:O	8:H:13:LEU:HD12	2.17	0.44
14:O:83:LYS:HG3	15:P:78:VAL:HG23	1.98	0.44
15:P:59:PHE:CE2	15:P:64:SER:HB2	2.52	0.44
3:C:117:LEU:O	3:C:120:SER:OG	2.29	0.44
18:R:24:G:H2'	18:R:25:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:PRO:HG2	2:B:20:VAL:HG12	2.00	0.44
4:D:296:HIS:ND1	4:D:316:TYR:OH	2.49	0.44
4:D:356:CYS:HG	4:D:394:PHE:HE1	1.64	0.44
10:K:53:VAL:HG23	11:L:67:LEU:HD21	1.99	0.44
14:O:31:LEU:HD13	15:P:79:LEU:HD21	2.00	0.44
14:O:59:GLU:O	14:O:74:GLY:HA3	2.16	0.44
16:Q:64:ARG:NH1	18:R:554:U:O4'	2.51	0.44
18:R:24:G:N1	18:R:37:C:N4	2.56	0.44
18:R:33:A:C8	18:R:33:A:OP2	2.70	0.44
2:B:87:MET:CE	18:R:257:G:N7	2.81	0.44
13:N:70:LYS:HB2	13:N:70:LYS:HE3	1.72	0.44
16:Q:18:ASN:OD1	16:Q:18:ASN:N	2.41	0.44
3:C:82:VAL:HG23	3:C:83:THR:HG23	1.99	0.44
5:E:432:ILE:O	5:E:435:VAL:HG12	2.18	0.44
14:O:31:LEU:HD12	14:O:37:ILE:HG13	2.00	0.44
2:B:167:ARG:O	2:B:167:ARG:HG3	2.17	0.44
3:C:65:VAL:HG12	3:C:79:LEU:HD23	2.00	0.44
4:D:53:LEU:HD22	4:D:84:LEU:HD11	2.00	0.44
4:D:428:LEU:HA	4:D:437:GLN:HE22	1.82	0.44
7:G:94:SER:OG	7:G:96:ASP:OD1	2.23	0.44
10:K:105:LYS:NZ	18:R:158:G:OP2	2.49	0.44
16:Q:11:MET:HE1	16:Q:32:TYR:CE2	2.52	0.44
18:R:78:A:H4'	18:R:79:A:H5'	2.00	0.44
18:R:323:A:H2'	18:R:324:A:C8	2.52	0.44
4:D:438:GLU:CD	4:D:477:MET:HG2	2.37	0.44
4:D:465:ILE:HD13	4:D:465:ILE:HA	1.82	0.44
5:E:578:THR:HB	5:E:614:VAL:HG23	1.99	0.44
7:G:65:ILE:HB	7:G:68:SER:HB2	2.00	0.44
2:B:28:ARG:O	2:B:32:GLU:HG3	2.18	0.44
4:D:208:LEU:HD12	4:D:216:ILE:HD11	1.99	0.44
7:G:215:LEU:HD23	7:G:215:LEU:HA	1.79	0.44
11:L:33:SER:HB3	11:L:37:ASN:HB2	1.99	0.44
11:L:52:LEU:HD11	12:M:83:ASN:ND2	2.33	0.44
13:N:41:ASN:HD21	18:R:555:U:H3	1.65	0.44
18:R:33:A:H8	18:R:33:A:OP2	2.00	0.44
4:D:509:ILE:HD11	4:D:540:PHE:HZ	1.83	0.44
14:O:51:ASN:ND2	14:O:84:GLY:H	2.16	0.44
12:M:2:SER:OG	12:M:3:SER:N	2.50	0.43
18:R:557:U:O2	18:R:557:U:O2'	2.28	0.43
2:B:31:LYS:HA	2:B:31:LYS:HD3	1.77	0.43
4:D:71:GLU:HG3	4:D:101:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:384:SER:H	5:E:387:GLN:HE21	1.67	0.43
18:R:519:U:H2'	18:R:520:G:H8	1.83	0.43
4:D:42:ALA:HB3	4:D:43:PRO:HD3	2.01	0.43
7:G:115:ILE:HG13	7:G:132:LEU:HD11	2.00	0.43
10:K:42:ASN:HB3	10:K:89:GLY:H	1.84	0.43
18:R:16:U:H6	18:R:16:U:H2'	1.67	0.43
18:R:162:U:H2'	18:R:163:G:H8	1.82	0.43
4:D:448:TYR:CD2	5:E:480:SER:HA	2.54	0.43
14:O:87:ILE:O	16:Q:64:ARG:HD2	2.18	0.43
14:O:90:ILE:HB	16:Q:62:VAL:HG22	1.99	0.43
18:R:198:U:H2'	18:R:199:G:C8	2.53	0.43
4:D:400:ASN:HD21	4:D:414:GLY:HA2	1.84	0.43
4:D:479:TRP:CZ2	4:D:509:ILE:HG22	2.53	0.43
4:D:116:CYS:SG	4:D:120:ILE:HG13	2.58	0.43
4:D:342:LEU:HD12	6:F:439:PRO:HG2	2.01	0.43
11:L:7:LEU:HD12	11:L:7:LEU:HA	1.86	0.43
11:L:84:TYR:HD1	11:L:84:TYR:O	2.01	0.43
12:M:62:ASP:HB3	12:M:66:ASN:OD1	2.18	0.43
1:A:45:ALA:HB2	15:P:68:LEU:HD11	2.01	0.42
7:G:150:ARG:HA	7:G:150:ARG:HD2	1.74	0.42
18:R:34:A:H2'	18:R:35:G:N9	2.33	0.42
2:B:186:THR:CG2	4:D:242:MET:HG3	2.47	0.42
5:E:326:LYS:HG2	5:E:362:TRP:CZ2	2.54	0.42
10:K:114:LYS:NZ	18:R:302:U:P	2.83	0.42
10:K:127:LYS:NZ	18:R:173:G:P	2.91	0.42
16:Q:71:LEU:O	16:Q:71:LEU:HD23	2.19	0.42
7:G:242:THR:O	7:G:246:ILE:HG23	2.19	0.42
18:R:93:A:H2'	18:R:94:A:C8	2.55	0.42
18:R:175:U:H4'	18:R:176:U:C5	2.54	0.42
3:C:25:LYS:HB2	3:C:34:ALA:HB1	2.01	0.42
18:R:46:C:H2'	18:R:47:A:C8	2.54	0.42
18:R:300:G:H2'	18:R:301:U:H6	1.85	0.42
18:R:517:U:H2'	18:R:518:U:C6	2.55	0.42
2:B:126:ASP:OD1	2:B:127:ILE:N	2.50	0.42
15:P:16:LYS:HD2	15:P:16:LYS:HA	1.81	0.42
18:R:170:G:H2'	18:R:171:A:C8	2.54	0.42
18:R:535:G:H2'	18:R:536:A:H8	1.83	0.42
2:B:181:SER:N	6:F:293:GLN:O	2.44	0.42
18:R:524:G:H2'	18:R:525:G:C8	2.53	0.42
7:G:51:LEU:HA	7:G:54:ILE:HG22	2.02	0.42
15:P:19:LEU:HD23	15:P:19:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:30:ARG:HD3	16:Q:30:ARG:HA	1.79	0.42
2:B:82:GLU:O	2:B:86:ILE:HG12	2.19	0.42
3:C:123:MET:HE2	3:C:135:LEU:HB3	2.01	0.42
6:F:391:LEU:O	6:F:394:GLN:HG3	2.20	0.42
8:H:31:ILE:HA	8:H:31:ILE:HD12	1.79	0.42
12:M:33:LEU:HD11	12:M:106:LYS:HB2	2.02	0.42
5:E:289:HIS:O	5:E:293:TRP:HE3	2.03	0.42
5:E:465:LYS:HD2	5:E:497:GLU:OE1	2.20	0.42
5:E:605:PHE:HB3	5:E:608:LEU:CD2	2.50	0.42
7:G:45:PHE:HB3	7:G:208:VAL:HG21	2.01	0.42
12:M:16:ALA:HA	12:M:19:GLU:OE1	2.20	0.41
4:D:125:GLN:OE1	18:R:116:A:H4'	2.19	0.41
5:E:431:SER:HA	5:E:434:VAL:HG12	2.03	0.41
12:M:102:ILE:HA	15:P:77:ASN:ND2	2.35	0.41
15:P:51:LEU:HD11	15:P:81:ILE:HG12	2.02	0.41
4:D:12:ASN:O	4:D:16:LEU:HD23	2.19	0.41
4:D:302:ALA:O	4:D:305:PRO:HD2	2.19	0.41
7:G:45:PHE:HA	7:G:208:VAL:CG1	2.45	0.41
7:G:57:THR:O	7:G:57:THR:OG1	2.31	0.41
11:L:104:ASP:OD1	11:L:105:SER:N	2.53	0.41
2:B:13:LEU:HD12	2:B:14:THR:N	2.35	0.41
4:D:283:LEU:HD13	4:D:299:PHE:CE1	2.55	0.41
5:E:293:TRP:O	5:E:297:ILE:HG22	2.20	0.41
6:F:410:LEU:HG	6:F:414:ASN:HD22	1.86	0.41
7:G:95:LYS:HA	7:G:95:LYS:HD2	1.78	0.41
10:K:121:LYS:CD	18:R:278:U:H6	2.31	0.41
14:O:21:LEU:HD12	14:O:45:GLY:HA2	2.01	0.41
15:P:68:LEU:HD23	15:P:71:ILE:HG21	2.01	0.41
2:B:40:ASN:ND2	18:R:285:C:H1'	2.35	0.41
4:D:196:LEU:HD13	4:D:199:LEU:HD12	2.02	0.41
7:G:152:PRO:HG2	7:G:155:ILE:HD12	2.03	0.41
10:K:26:ASP:OD1	10:K:26:ASP:N	2.50	0.41
10:K:108:ARG:HA	10:K:111:ARG:HH11	1.83	0.41
18:R:322:A:H2'	18:R:323:A:C8	2.56	0.41
2:B:6:CYS:HG	2:B:9:CYS:H	1.63	0.41
2:B:179:ILE:HB	4:D:241:TYR:OH	2.20	0.41
3:C:6:PHE:CE1	3:C:79:LEU:HD12	2.56	0.41
4:D:91:HIS:CD2	4:D:115:PHE:HE2	2.38	0.41
4:D:500:TYR:O	4:D:504:LYS:HB2	2.21	0.41
5:E:446:LYS:HE3	5:E:446:LYS:HB3	1.78	0.41
10:K:21:ARG:N	10:K:96:VAL:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:19:C:C5'	18:R:19:C:C6	3.02	0.41
5:E:329:ARG:HB3	5:E:358:TYR:OH	2.20	0.41
18:R:81:C:O5'	18:R:81:C:C6	2.70	0.41
5:E:407:ILE:HA	5:E:407:ILE:HD13	1.80	0.41
1:A:42:THR:HG23	12:M:53:LYS:HE2	2.02	0.41
3:C:58:ASP:HB3	3:C:62:LEU:HB3	2.03	0.41
4:D:350:LEU:HD13	5:E:542:GLU:HG2	2.03	0.41
5:E:275:ASN:CB	5:E:299:TRP:HE1	2.34	0.41
5:E:476:LYS:HE2	6:F:517:SER:OG	2.21	0.41
5:E:592:SER:HA	5:E:595:LEU:HB2	2.02	0.41
5:E:625:LEU:HD11	6:F:392:LEU:HG	2.02	0.41
6:F:520:PHE:N	6:F:520:PHE:CD1	2.87	0.41
18:R:557:U:O2	18:R:557:U:C2'	2.68	0.41
7:G:248:LEU:HD12	7:G:248:LEU:O	2.21	0.41
10:K:64:ARG:HH22	10:K:73:LEU:HB3	1.86	0.41
18:R:17:A:N6	18:R:45:U:H3	2.16	0.41
18:R:106:C:H2'	18:R:107:A:C8	2.55	0.41
2:B:105:LEU:HD11	4:D:106:LEU:HG	2.03	0.40
2:B:194:TYR:CE2	6:F:304:LEU:HD22	2.56	0.40
4:D:127:PHE:HD1	4:D:127:PHE:HA	1.77	0.40
5:E:624:PHE:HE2	6:F:389:THR:HG21	1.86	0.40
12:M:54:ILE:CG2	12:M:74:GLU:HG2	2.50	0.40
14:O:83:LYS:HE3	14:O:83:LYS:HB3	1.90	0.40
18:R:14:G:C5'	18:R:14:G:H8	2.31	0.40
1:A:50:THR:OG1	1:A:51:SER:N	2.53	0.40
1:A:75:LYS:O	1:A:75:LYS:HD3	2.20	0.40
2:B:42:ALA:O	2:B:45:ILE:HG13	2.22	0.40
4:D:389:TRP:HA	4:D:389:TRP:CE3	2.57	0.40
6:F:306:HIS:HB3	6:F:384:ARG:HE	1.86	0.40
10:K:35:MET:SD	10:K:46:ASN:HB2	2.60	0.40
18:R:17:A:N6	18:R:45:U:N3	2.68	0.40
18:R:286:A:H2'	18:R:287:A:C8	2.56	0.40
18:R:542:U:H2'	18:R:543:G:H8	1.86	0.40
2:B:118:VAL:O	2:B:124:ARG:NH1	2.55	0.40
4:D:51:GLN:NE2	8:H:2:ARG:HD3	2.37	0.40
4:D:172:LEU:HD11	4:D:186:TRP:CD2	2.56	0.40
5:E:375:MET:HA	5:E:375:MET:CE	2.51	0.40
5:E:461:ASN:O	5:E:465:LYS:HB2	2.21	0.40
10:K:19:LYS:HG2	10:K:98:GLU:OE2	2.21	0.40
18:R:15:A:C5'	18:R:15:A:H8	2.33	0.40
18:R:17:A:N1	18:R:45:U:O2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:LEU:HD23	4:D:172:LEU:HA	1.89	0.40
4:D:198:GLN:HE22	18:R:130:C:H5'	1.87	0.40
7:G:137:LYS:HA	7:G:137:LYS:HD3	1.94	0.40
11:L:37:ASN:OD1	18:R:557:U:C4	2.74	0.40
13:N:21:LEU:HD21	13:N:44:LEU:HD11	2.03	0.40
14:O:89:LEU:HG	16:Q:63:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	165/300 (55%)	159 (96%)	5 (3%)	1 (1%)	25 64
2	B	172/231 (74%)	162 (94%)	8 (5%)	2 (1%)	13 50
3	C	126/350 (36%)	121 (96%)	3 (2%)	2 (2%)	9 43
4	D	539/544 (99%)	518 (96%)	21 (4%)	0	100 100
5	E	570/629 (91%)	542 (95%)	28 (5%)	0	100 100
6	F	177/523 (34%)	170 (96%)	7 (4%)	0	100 100
7	G	226/492 (46%)	212 (94%)	14 (6%)	0	100 100
8	H	50/52 (96%)	50 (100%)	0	0	100 100
9	I	14/261 (5%)	11 (79%)	3 (21%)	0	100 100
10	K	117/196 (60%)	114 (97%)	3 (3%)	0	100 100
11	L	117/146 (80%)	108 (92%)	9 (8%)	0	100 100
12	M	105/110 (96%)	103 (98%)	2 (2%)	0	100 100
13	N	89/101 (88%)	85 (96%)	4 (4%)	0	100 100
14	O	71/94 (76%)	68 (96%)	3 (4%)	0	100 100
15	P	72/86 (84%)	68 (94%)	4 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	Q	67/77 (87%)	65 (97%)	2 (3%)	0	100 100
All	All	2677/4192 (64%)	2556 (96%)	116 (4%)	5 (0%)	50 81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	SER
2	B	18	PRO
1	A	88	ARG
3	C	14	ALA
3	C	13	PRO

5.3.2 Protein sidechains (i)

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	A	73/265 (28%)	68 (93%)	5 (7%)	16 48
2	B	166/215 (77%)	154 (93%)	12 (7%)	14 45
3	C	115/317 (36%)	108 (94%)	7 (6%)	18 51
4	D	502/519 (97%)	497 (99%)	5 (1%)	76 88
5	E	317/603 (53%)	309 (98%)	8 (2%)	47 75
6	F	155/451 (34%)	152 (98%)	3 (2%)	57 80
7	G	212/448 (47%)	209 (99%)	3 (1%)	67 85
8	H	48/48 (100%)	43 (90%)	5 (10%)	7 31
9	I	14/234 (6%)	13 (93%)	1 (7%)	14 46
10	K	113/176 (64%)	111 (98%)	2 (2%)	59 81
11	L	107/129 (83%)	103 (96%)	4 (4%)	34 65
12	M	96/103 (93%)	91 (95%)	5 (5%)	23 56
13	N	79/89 (89%)	79 (100%)	0	100 100
14	O	63/83 (76%)	61 (97%)	2 (3%)	39 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	P	63/77 (82%)	63 (100%)	0	100 100
16	Q	57/66 (86%)	56 (98%)	1 (2%)	59 81
All	All	2180/3823 (57%)	2117 (97%)	63 (3%)	45 71

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	38	ASN
1	A	53	LYS
1	A	87	ARG
1	A	89	LEU
2	B	3	LYS
2	B	4	PHE
2	B	5	TYR
2	B	6	CYS
2	B	12	TYR
2	B	15	HIS
2	B	36	ASP
2	B	49	HIS
2	B	77	CYS
2	B	78	LEU
2	B	80	ASN
2	B	132	LYS
3	C	28	ASN
3	C	30	ASN
3	C	33	TYR
3	C	44	ASN
3	C	89	ARG
3	C	108	MET
3	C	144	ARG
4	D	45	CYS
4	D	158	CYS
4	D	310	ASP
4	D	311	LEU
4	D	338	LEU
5	E	291	ASN
5	E	300	LEU
5	E	324	ASP
5	E	377	LYS
5	E	378	ARG

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Mol	Chain	Res	Type
5	E	452	ARG
5	E	520	SER
5	E	625	LEU
6	F	421	SER
6	F	497	GLN
6	F	515	GLN
7	G	87	ASP
7	G	100	CYS
7	G	261	PHE
8	H	22	ASP
8	H	25	LYS
8	H	34	ASN
8	H	45	HIS
8	H	51	ASN
9	I	4	MET
10	K	17	ASP
10	K	50	GLU
11	L	6	PHE
11	L	31	SER
11	L	114	ASN
11	L	117	ARG
12	M	11	HIS
12	M	13	LEU
12	M	51	ASN
12	M	67	MET
12	M	74	GLU
14	O	32	PHE
14	O	59	GLU
16	Q	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	40	ASN
1	A	66	ASN
1	A	67	HIS
2	B	40	ASN
2	B	51	HIS
2	B	80	ASN
2	B	94	GLN
2	B	163	ASN

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Mol	Chain	Res	Type
2	B	170	ASN
3	C	28	ASN
3	C	30	ASN
4	D	51	GLN
4	D	122	HIS
4	D	153	GLN
4	D	298	ASN
4	D	332	ASN
4	D	400	ASN
4	D	437	GLN
4	D	442	ASN
4	D	462	GLN
5	E	383	ASN
5	E	387	GLN
5	E	488	ASN
5	E	506	ASN
5	E	533	ASN
6	F	354	GLN
6	F	412	GLN
6	F	515	GLN
7	G	81	GLN
7	G	90	HIS
7	G	292	ASN
10	K	74	ASN
11	L	21	ASN
11	L	90	ASN
11	L	114	ASN
12	M	51	ASN
13	N	12	ASN
13	N	15	GLN
13	N	41	ASN
14	O	15	ASN
14	O	51	ASN
15	P	24	ASN
15	P	50	ASN
15	P	77	ASN
16	Q	20	ASN
16	Q	53	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	r	2/187 (1%)	0	0
18	R	323/568 (56%)	85 (26%)	18 (5%)
All	All	325/755 (43%)	85 (26%)	18 (5%)

All (85) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	8	C
18	R	9	C
18	R	11	U
18	R	12	A
18	R	13	A
18	R	14	G
18	R	15	A
18	R	17	A
18	R	19	C
18	R	35	G
18	R	40	A
18	R	41	C
18	R	53	G
18	R	54	C
18	R	55	G
18	R	56	C
18	R	60	C
18	R	61	A
18	R	62	A
18	R	63	U
18	R	64	A
18	R	65	G
18	R	66	U
18	R	67	A
18	R	74	C
18	R	75	G
18	R	78	A
18	R	79	A
18	R	80	G
18	R	82	A
18	R	87	U
18	R	113	G
18	R	114	U
18	R	117	U
18	R	130	C
18	R	133	G

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Mol	Chain	Res	Type
18	R	141	A
18	R	142	C
18	R	145	A
18	R	147	A
18	R	149	G
18	R	150	G
18	R	151	C
18	R	152	G
18	R	153	C
18	R	154	G
18	R	158	G
18	R	167	G
18	R	168	C
18	R	176	U
18	R	180	U
18	R	181	U
18	R	182	C
18	R	186	U
18	R	187	G
18	R	257	G
18	R	258	U
18	R	259	U
18	R	260	U
18	R	266	G
18	R	269	U
18	R	270	G
18	R	271	G
18	R	278	U
18	R	279	U
18	R	280	G
18	R	287	A
18	R	288	A
18	R	290	U
18	R	291	C
18	R	293	A
18	R	300	G
18	R	309	G
18	R	514	A
18	R	540	G
18	R	542	U
18	R	551	U
18	R	555	U

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Mol	Chain	Res	Type
18	R	559	G
18	R	560	A
18	R	561	U
18	R	562	U
18	R	563	U
18	R	564	A
18	R	565	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	11	U
18	R	12	A
18	R	14	G
18	R	63	U
18	R	64	A
18	R	66	U
18	R	79	A
18	R	86	A
18	R	112	A
18	R	113	G
18	R	151	C
18	R	152	G
18	R	186	U
18	R	258	U
18	R	268	C
18	R	277	U
18	R	279	U
18	R	513	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	324:A	O3'	325:A	P	1.32

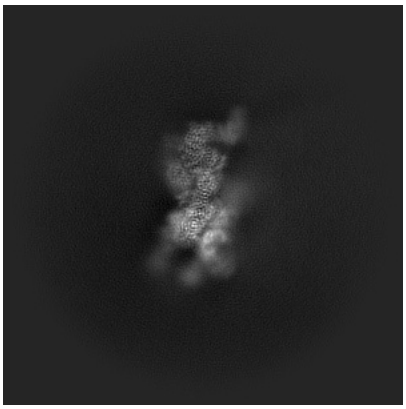
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43753. These allow visual inspection of the internal detail of the map and identification of artifacts.

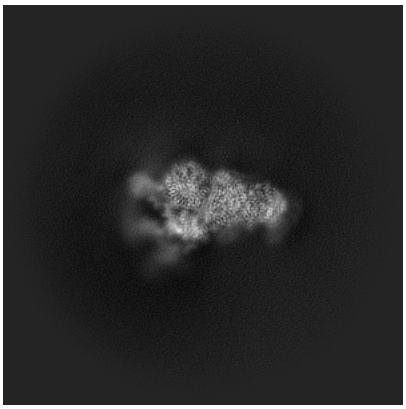
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

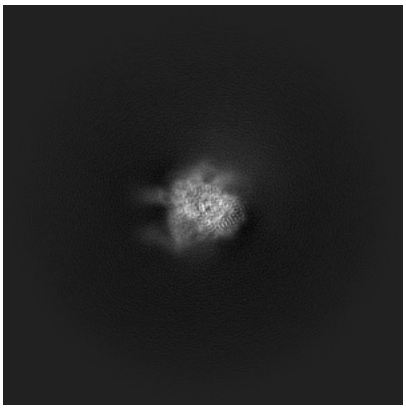
6.1.1 Primary map



X

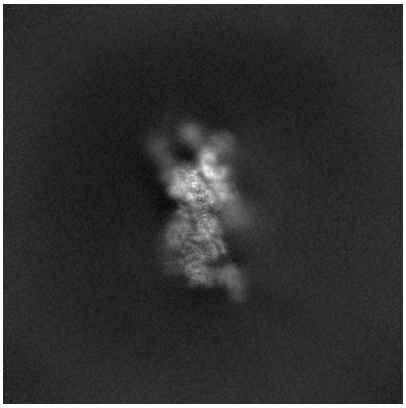


Y

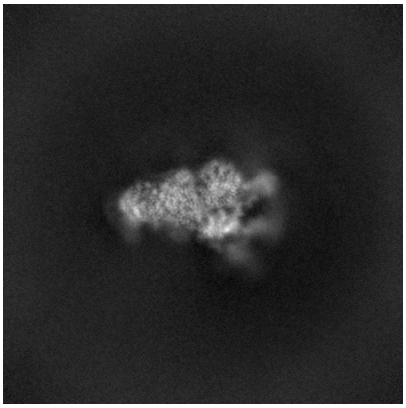


Z

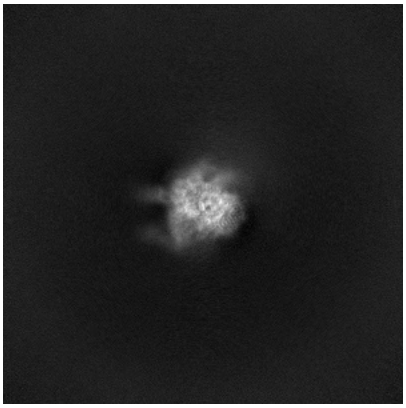
6.1.2 Raw map



X



Y

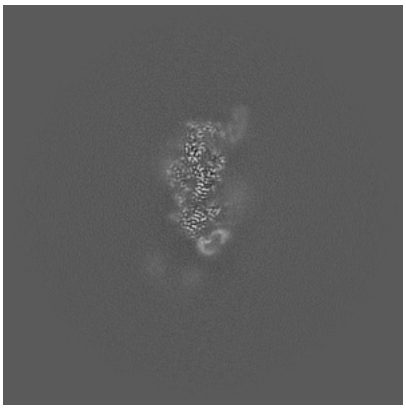


Z

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

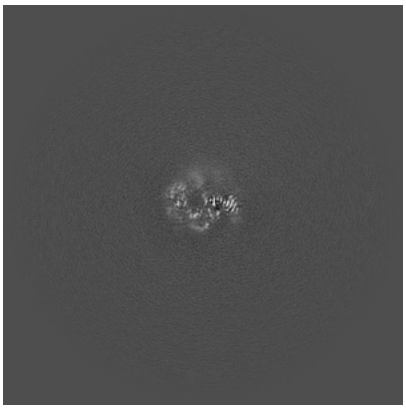
6.2 Central slices (i)

6.2.1 Primary map



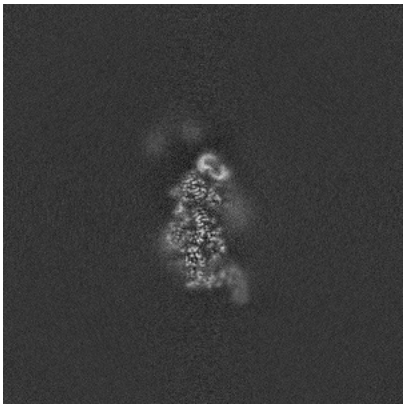
X Index: 320

Y Index: 320



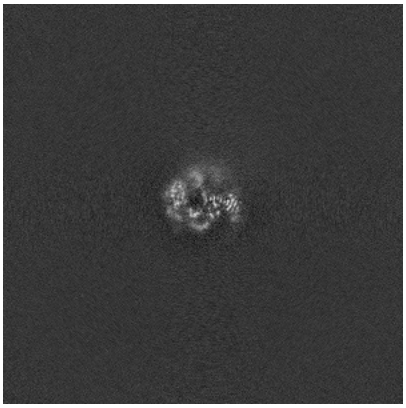
Z Index: 320

6.2.2 Raw map



X Index: 320

Y Index: 320

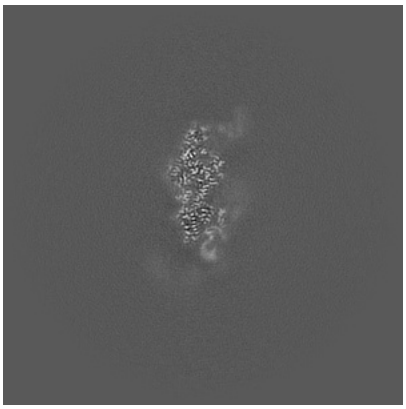


Z Index: 320

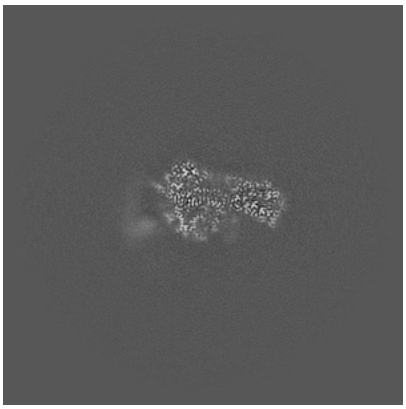
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

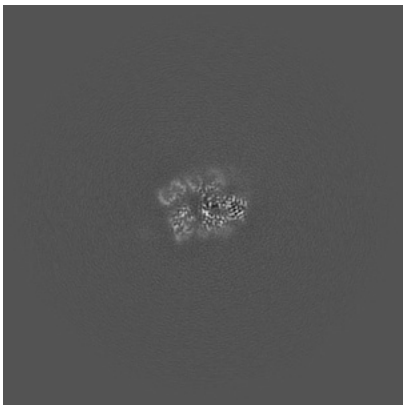
6.3.1 Primary map



X Index: 330

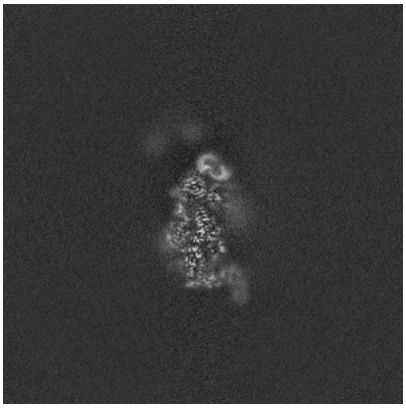


Y Index: 309

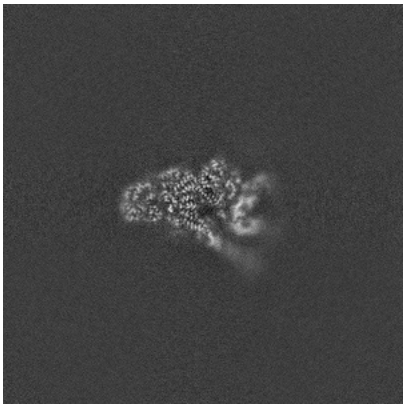


Z Index: 303

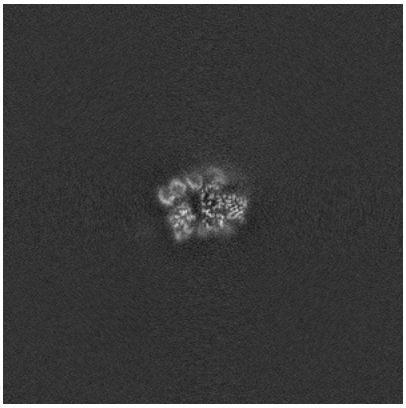
6.3.2 Raw map



X Index: 319



Y Index: 323

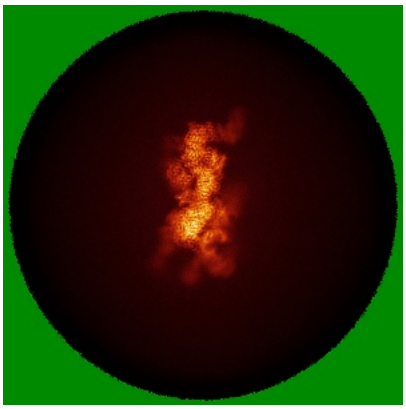


Z Index: 335

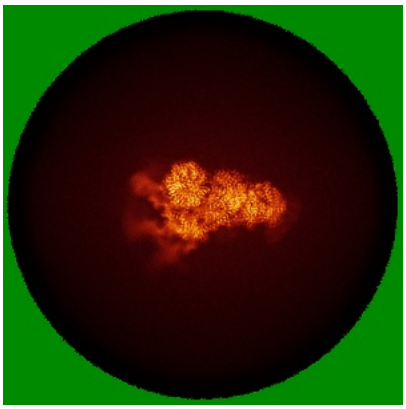
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

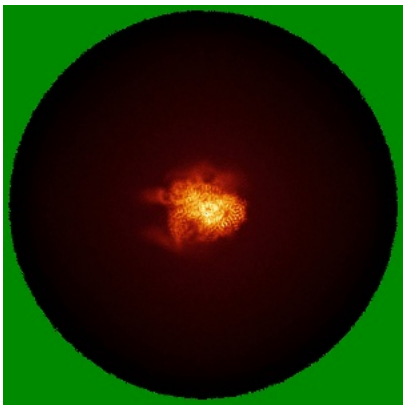
6.4.1 Primary map



X

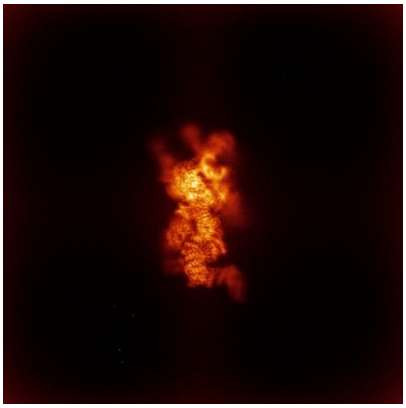


Y

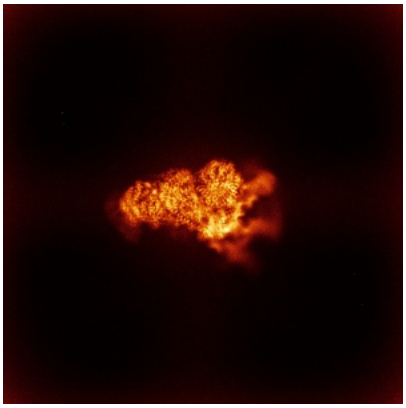


Z

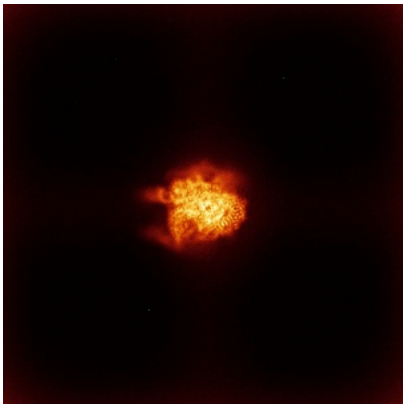
6.4.2 Raw map



X



Y

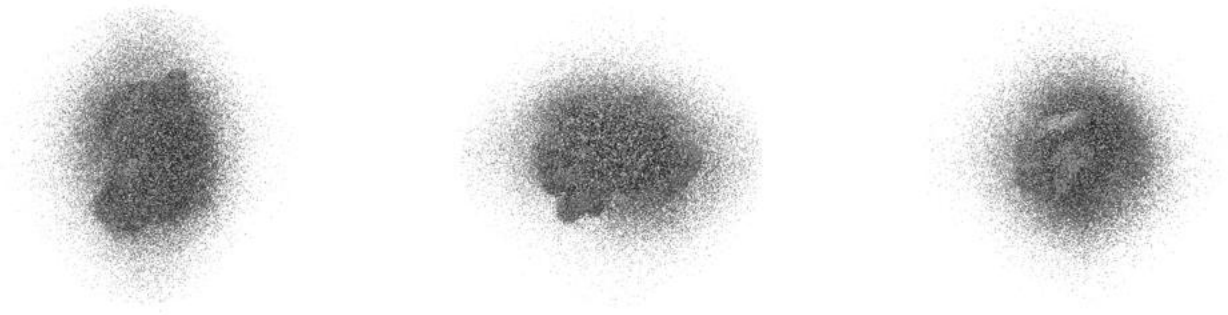


Z

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

6.5 Orthogonal surface views (i)

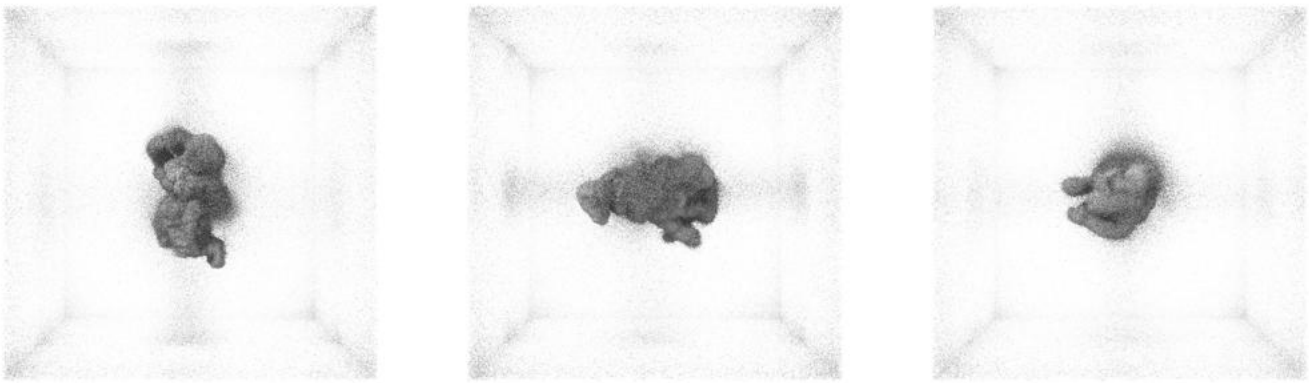
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



X Y Z

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.

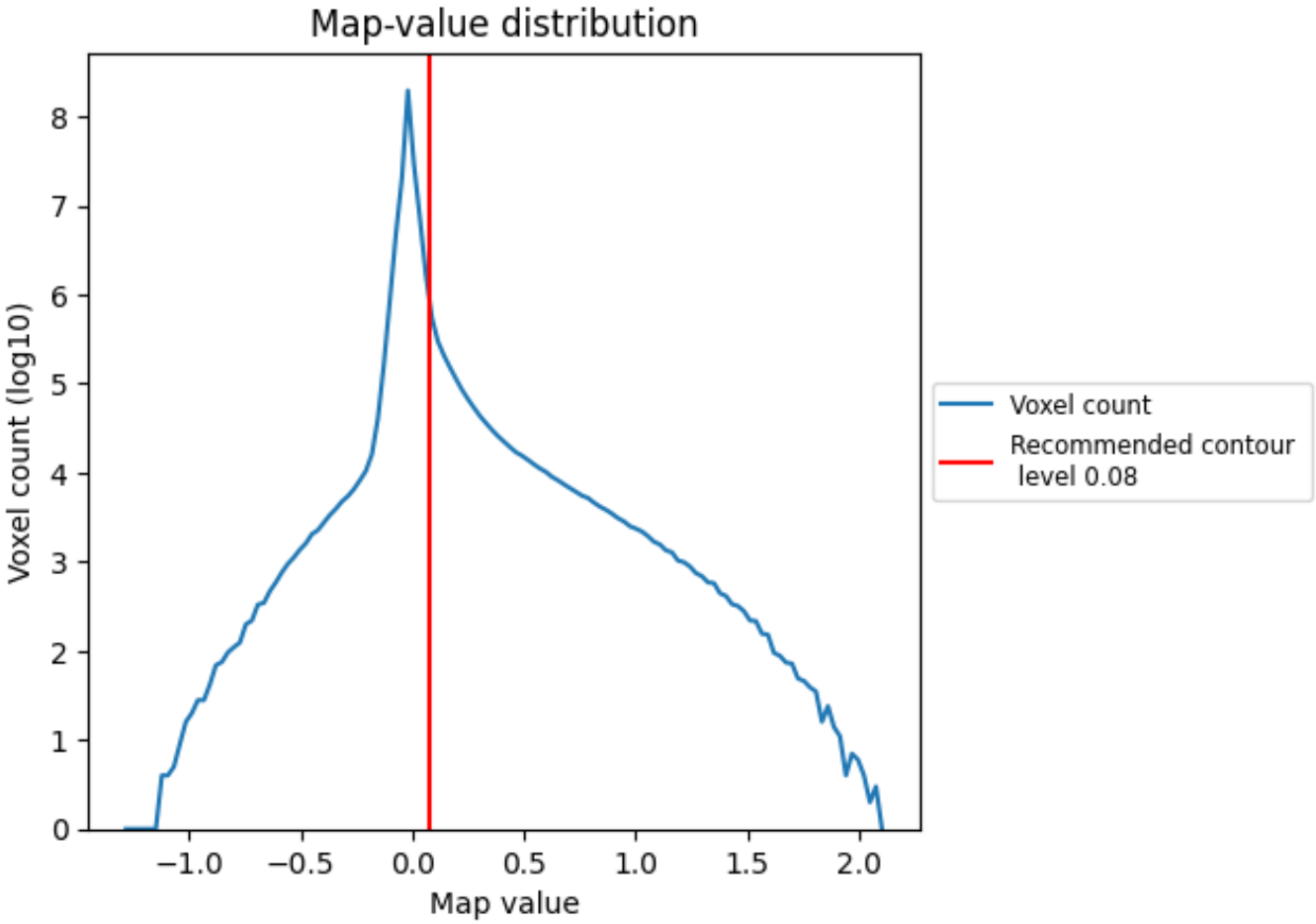
6.6 Mask visualisation (i)

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

7 Map analysis

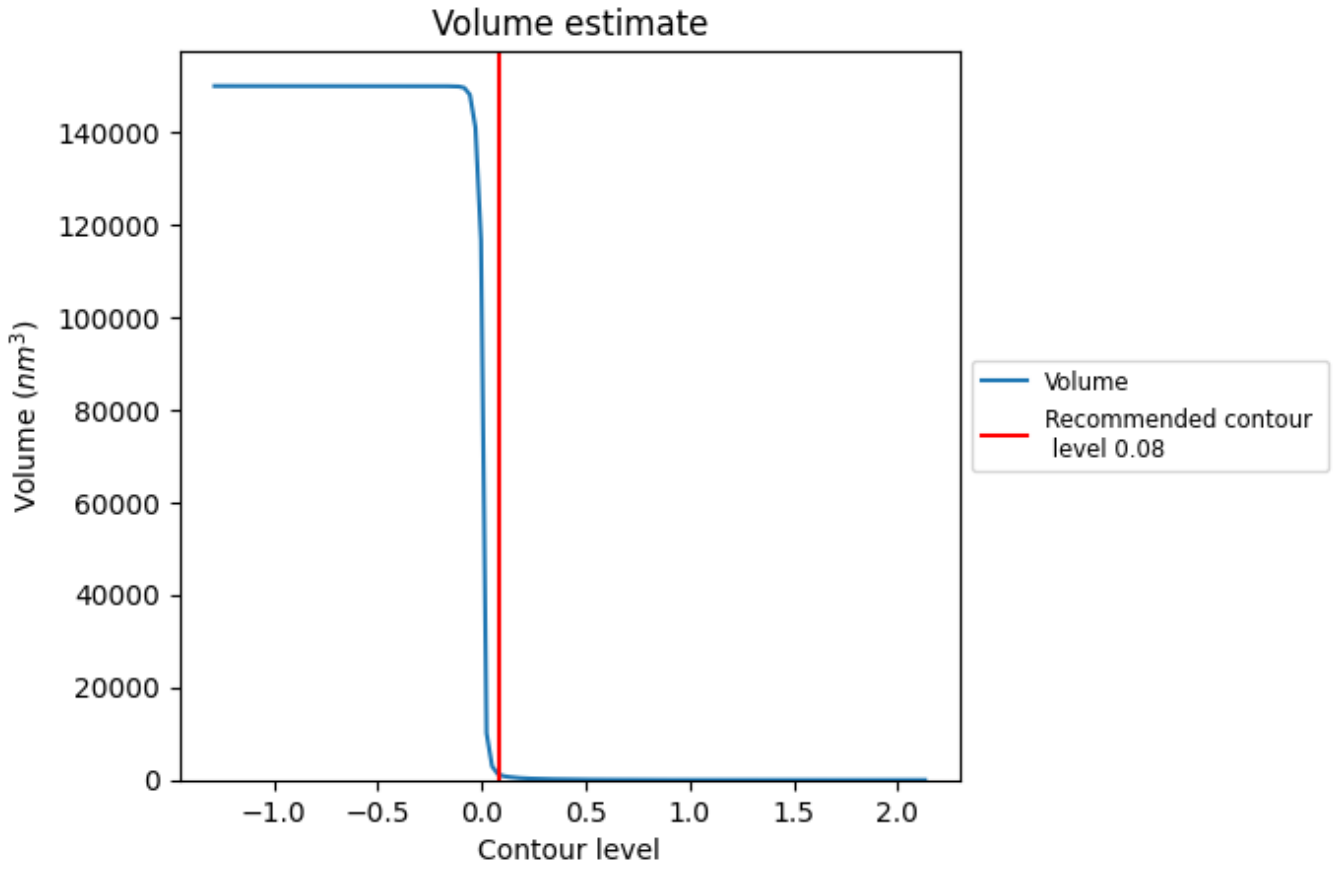
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

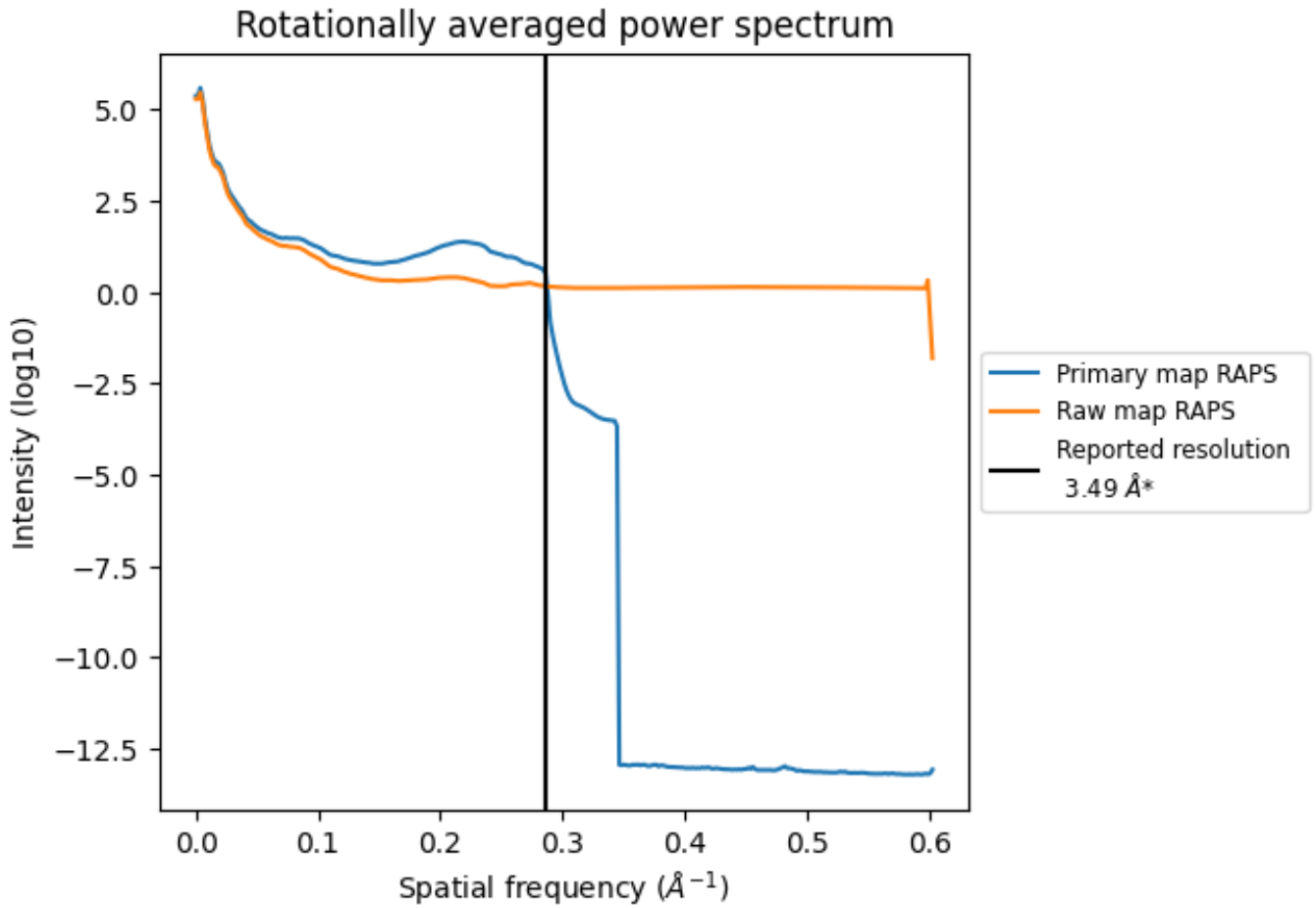
7.2 Volume estimate



The volume at the recommended contour level is 1260 nm^3; this corresponds to an approximate mass of 1138 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 (i)

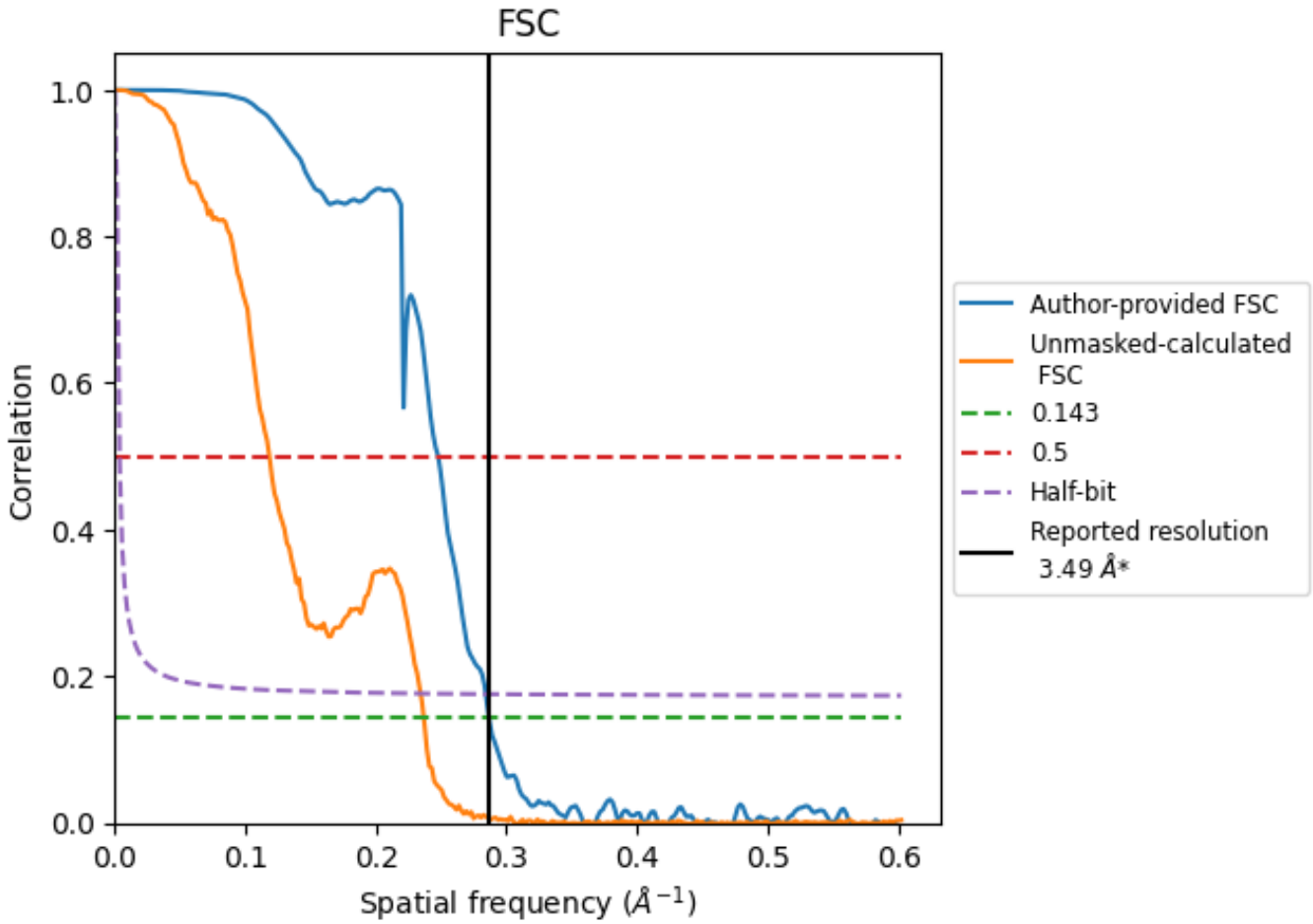


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

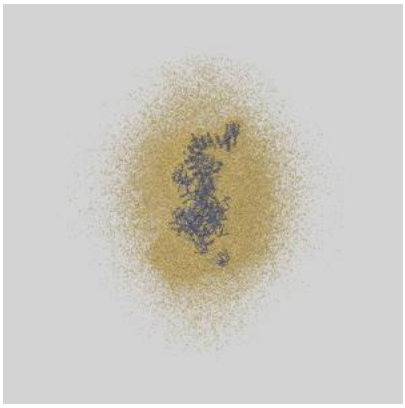
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.04	3.52
Unmasked-calculated*	4.22	8.44	4.27

*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 4.22 differs from the reported value 3.49 by more than 10 %

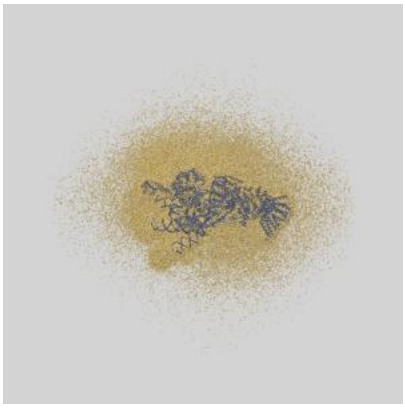
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43753 and PDB model 8W2O. Per-residue inclusion information can be found in section 3 on page 9.

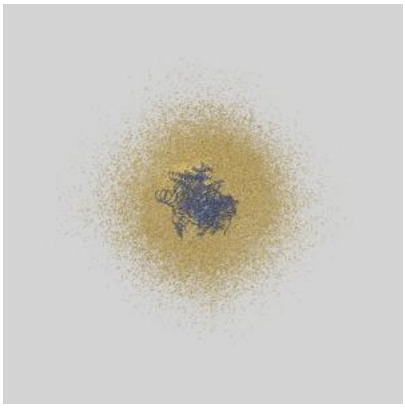
9.1 Map-model overlay



X



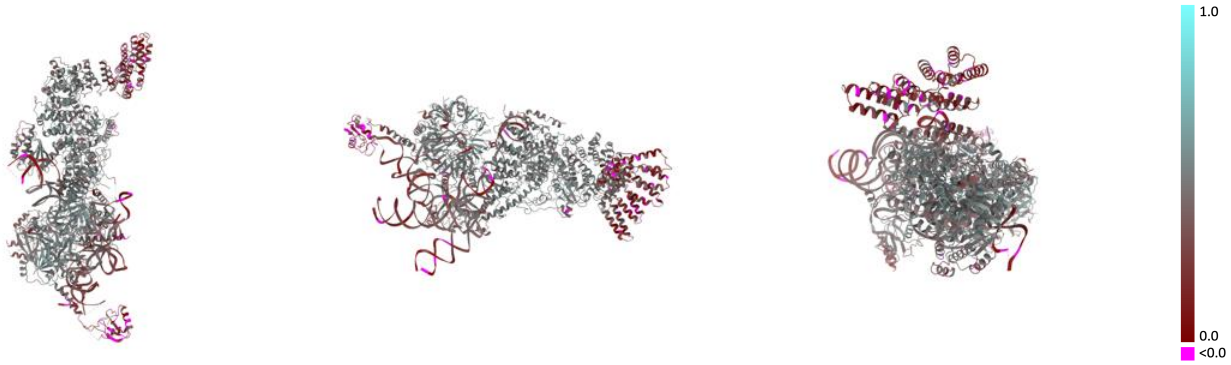
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

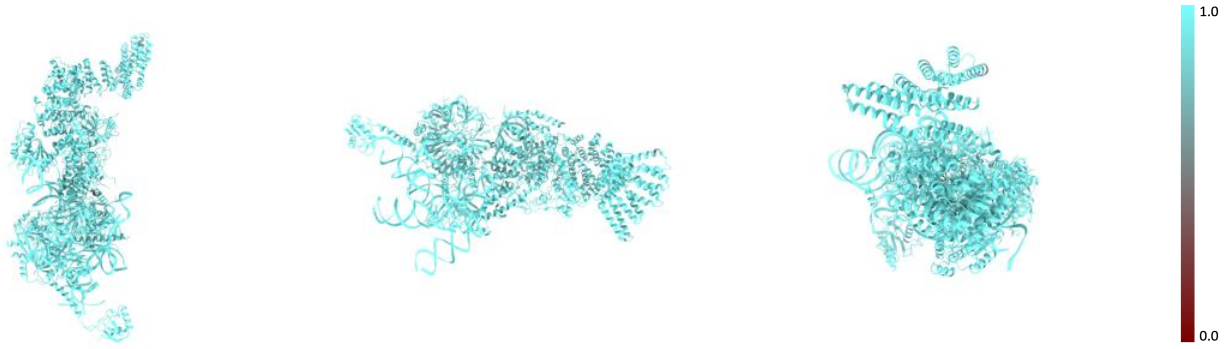
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

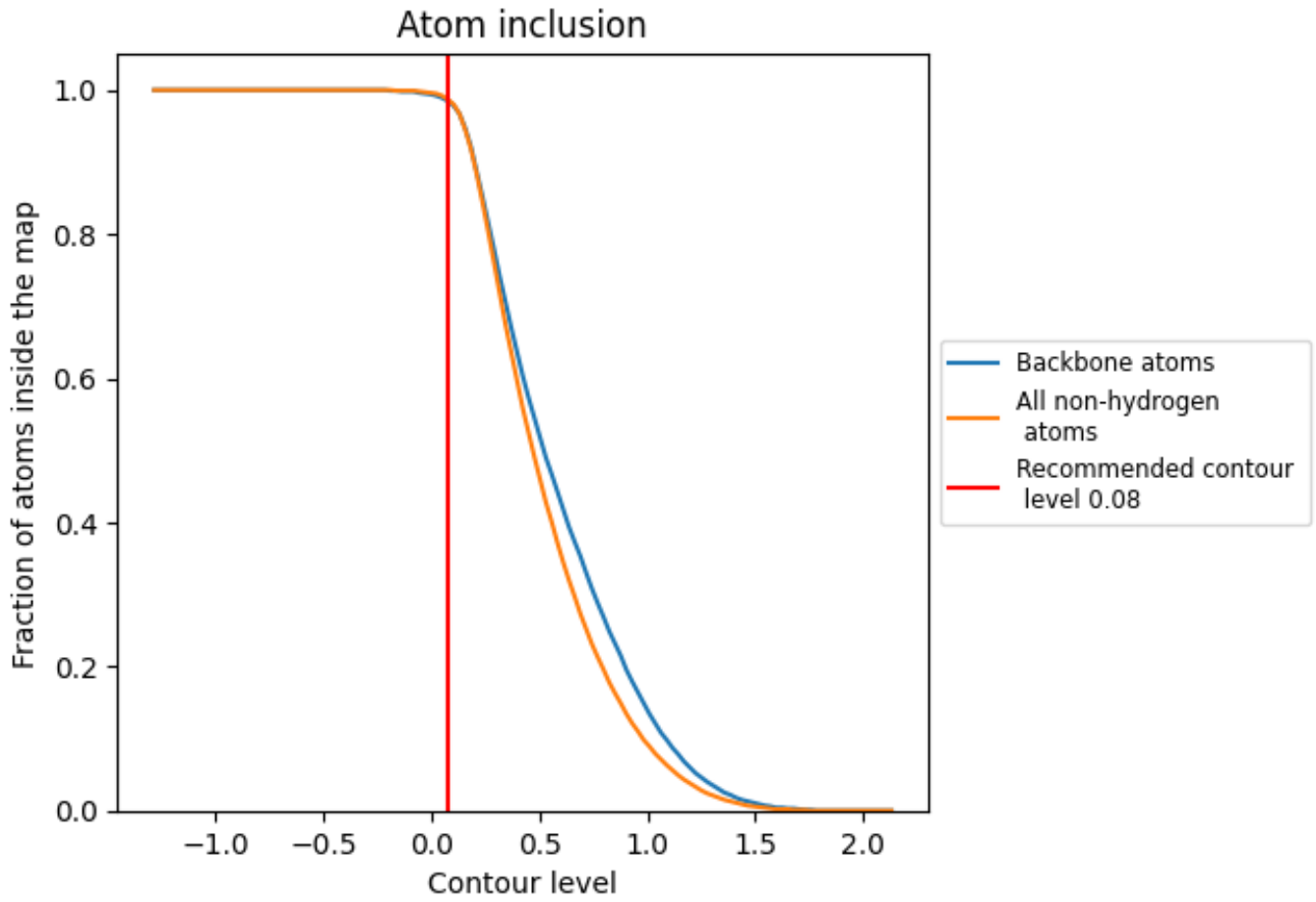
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9860	0.4170
A	0.9950	0.3290
B	0.9780	0.4520
C	0.9990	0.3780
D	0.9810	0.4960
E	0.9860	0.3810
F	0.9750	0.4870
G	0.9940	0.4470
H	0.9850	0.4600
I	0.8860	0.3330
K	0.9750	0.4760
L	0.9850	0.4930
M	0.9810	0.4770
N	0.9560	0.4960
O	0.9910	0.4950
P	0.9900	0.5070
Q	0.9770	0.5120
R	0.9970	0.3220
r	0.9840	0.2080