



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:45 PM UTC

PDB ID : 7OQE / pdb_00007oqe
EMDB ID : EMD-13033
Title : Saccharomyces cerevisiae spliceosomal pre-A complex (delta BS-A ACT1)
Authors : Zhang, Z.; Rigo, N.; Dybkov, O.; Fourmann, J.; Will, C.L.; Kumar, V.; Urlaub, H.; Stark, H.; Luehrmann, R.
Deposited on : 2021-06-03
Resolution : 5.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

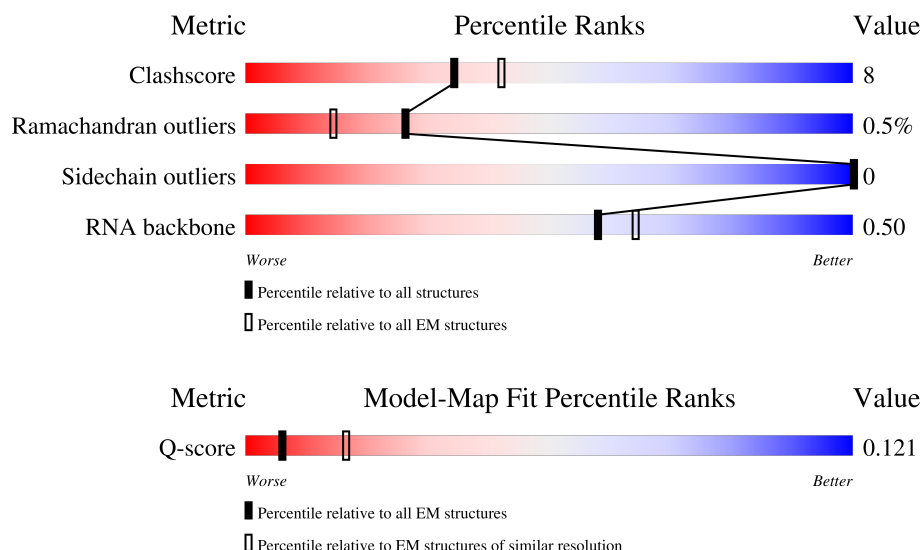
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

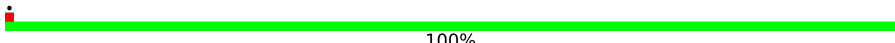
The reported resolution of this entry is 5.90 Å.

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	501 (5.40 - 6.40)

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	F	523	
2	I	373	
3	E	544	

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Mol	Chain	Length	Quality of chain
4	J	620	
5	1	568	
6	G	492	
7	A	298	
8	C	231	
9	b	196	
9	s	196	
10	d	101	
10	v	101	
11	e	94	
11	w	94	
12	f	86	
12	x	86	
13	g	77	
13	y	77	
14	h	146	
14	t	146	
15	i	110	
15	u	110	
16	H	261	
17	D	629	
18	B	300	
19	K	583	
20	O	971	
21	U	282	

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Mol	Chain	Length	Quality of chain
22	V	280	
23	T	530	
24	S	107	
25	Q	436	
26	P	1361	
27	R	213	
28	Z	85	
29	W	238	
30	Y	111	
31	p	849	
32	2	1175	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56606 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 Protein NAM8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	267	Total	C	N	O	0	0
			1335	801	267	267		

- Molecule 2 is a RNA chain called ACT1 pre-mRNA (delta BS-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	86	Total	C	N	O	P	0	0
			1327	575	111	555	86		

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	544	Total	C	N	O	0	0
			2732	1644	544	544		

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	105	Total	C	N	O	0	0
			529	319	105	105		

- Molecule 5 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	558	Total	C	N	O	P	0	0
			11822	5287	2003	3974	558		

- Molecule 6 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	239	Total	C	N	O	0	0
			1202	724	239	239		

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	A	132	Total	C	N	O	0	0
			668	404	132	132		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	195	Total	C	N	O	0	0
			985	595	195	195		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	b	121	Total	C	N	O	0	0
			607	365	121	121		
9	s	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	93	Total	C	N	O	0	0
			473	287	93	93		
10	v	82	Total	C	N	O	0	0
			412	248	82	82		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	77	Total	C	N	O	0	0
			389	235	77	77		
11	w	77	Total	C	N	O	0	0
			389	235	77	77		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	73	Total	C	N	O	0	0
			365	219	73	73		
12	x	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	72	Total	C	N	O	0	0
			356	212	72	72		
13	y	75	Total	C	N	O	0	0
			373	223	75	75		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	h	107	Total	C	N	O	0	0
			535	321	107	107		
14	t	72	Total	C	N	O	0	0
			363	219	72	72		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	i	99	Total	C	N	O	0	0
			501	303	99	99		
15	u	92	Total	C	N	O	0	0
			463	279	92	92		

- Molecule 16 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	192	Total	C	N	O	0	0
			960	576	192	192		

- Molecule 17 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	D	576	Total	C	N	O	0	0
			2892	1740	576	576		

- Molecule 18 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	B	186	Total	C	N	O	0	0
			940	568	186	186		

- Molecule 19 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	406	Total	C	N	O	0	0
			2042	1230	406	406		

- Molecule 20 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	O	812	Total	C	N	O	0	0
			4108	2484	812	812		

- Molecule 21 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	188	Total	C	N	O	0	0
			943	567	188	188		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	121	UNK	-	insertion	UNP Q07350
U	122	UNK	-	insertion	UNP Q07350
U	123	UNK	-	insertion	UNP Q07350
U	124	UNK	-	insertion	UNP Q07350
U	125	UNK	-	insertion	UNP Q07350
U	126	UNK	-	insertion	UNP Q07350
U	127	UNK	-	insertion	UNP Q07350
U	128	UNK	-	insertion	UNP Q07350
U	129	UNK	-	insertion	UNP Q07350
U	130	UNK	-	insertion	UNP Q07350
U	131	UNK	-	insertion	UNP Q07350
U	132	UNK	-	insertion	UNP Q07350
U	133	UNK	-	insertion	UNP Q07350
U	134	UNK	-	insertion	UNP Q07350
U	135	UNK	-	insertion	UNP Q07350
U	136	UNK	-	insertion	UNP Q07350

- Molecule 22 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 23 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	462	Total	C	N	O	0	0
			2318	1394	462	462		

- Molecule 24 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	S	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 25 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Q	220	Total	C	N	O	0	0
			1122	682	220	220		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	P	1186	Total	C	N	O	0	0
			5972	3600	1186	1186		

- Molecule 27 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	R	173	Total	C	N	O	0	0
			868	522	173	173		

- Molecule 28 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Z	83	Total	C	N	O	0	0
			412	246	83	83		

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	170	Total	C	N	O	0	0
			862	522	170	170		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	84	Total	C	N	O	0	0
			418	250	84	84		

- Molecule 31 is a protein called Pre-mRNA-processing ATP-dependent RNA helicase PRP5.

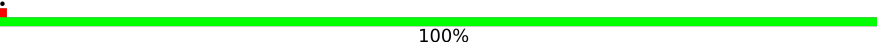
Mol	Chain	Residues	Atoms				AltConf	Trace
31	p	444	Total	C	N	O	5	0
			2239	1351	444	444		

- Molecule 32 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	143	Total	C	N	O	P	0	0
			3021	1351	511	1017	142		

U U U U G U U G C U A U A U U U U U U A G

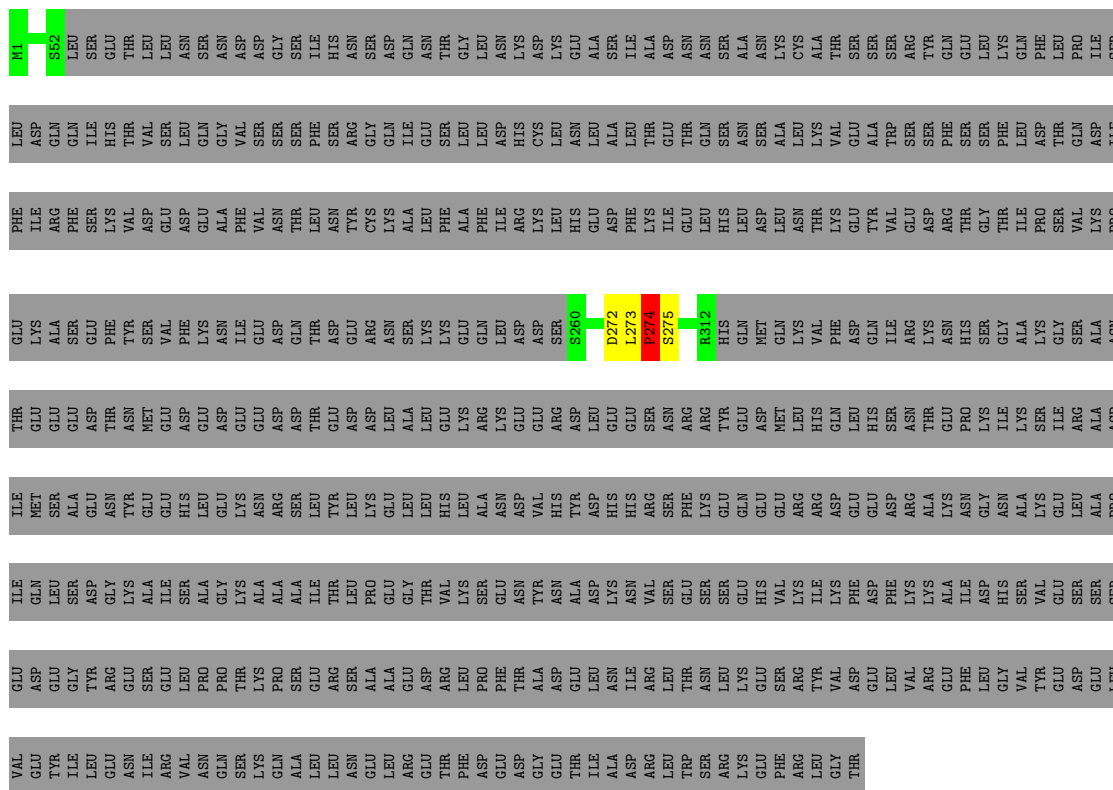
- Molecule 3: U1 small nuclear ribonucleoprotein component PRP42

Chain E:  100%



- Molecule 4: U1 small nuclear ribonucleoprotein component SNU71

Chain J:  16% 83%

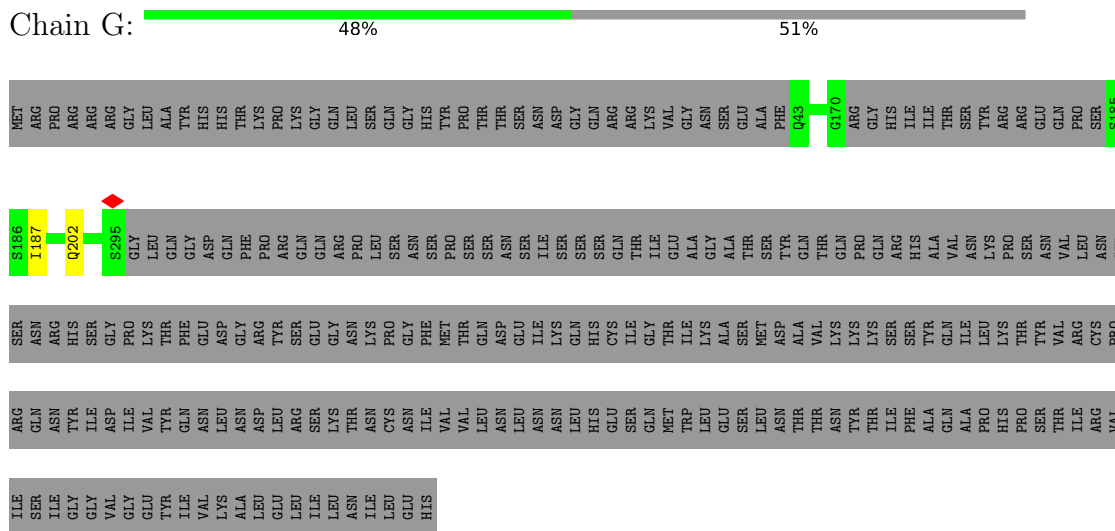


- Molecule 5: U1 snRNA

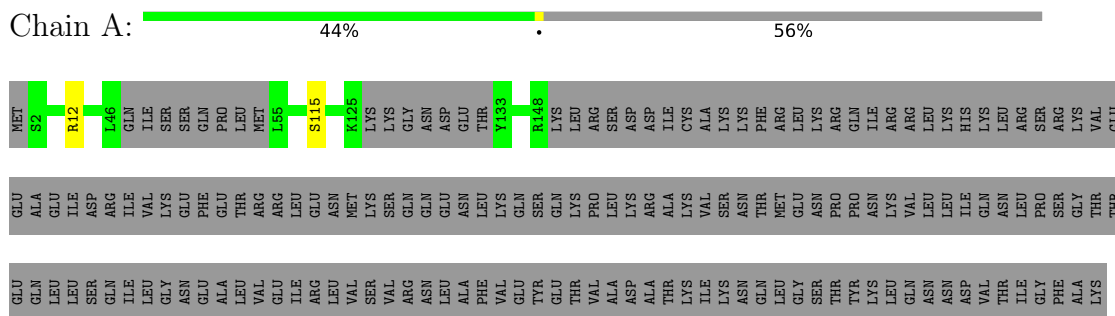
Chain 1:  23% 58% 37%



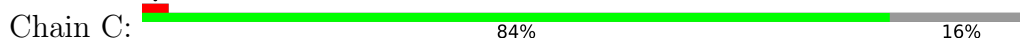
- Molecule 6: 56 kDa U1 small nuclear ribonucleoprotein component



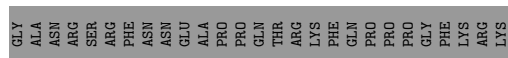
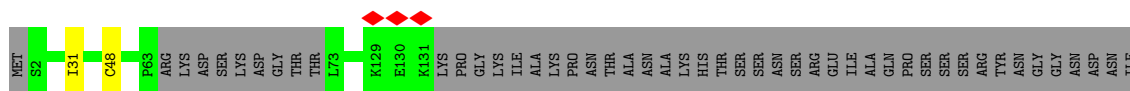
- Molecule 7: U1 small nuclear ribonucleoprotein A



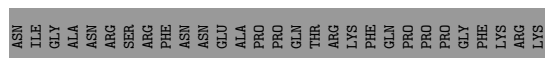
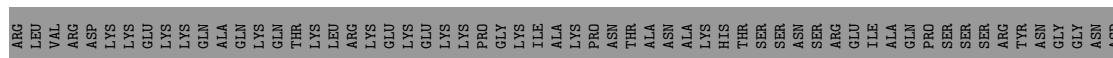
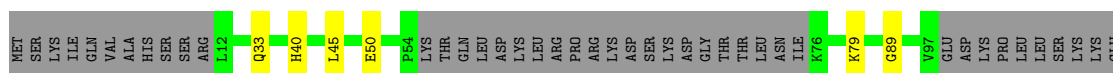
- Molecule 8: U1 small nuclear ribonucleoprotein C



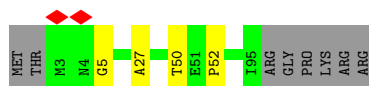
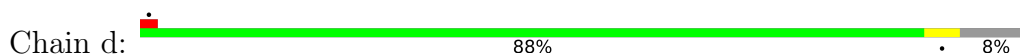
- Molecule 9: Small nuclear ribonucleoprotein-associated protein B



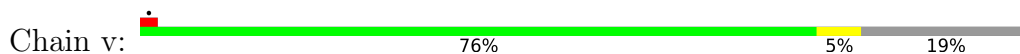
- Molecule 9: Small nuclear ribonucleoprotein-associated protein B



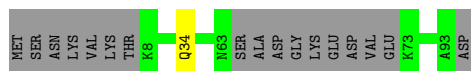
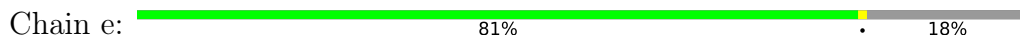
- Molecule 10: Small nuclear ribonucleoprotein Sm D3



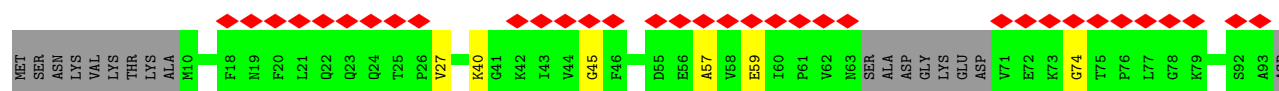
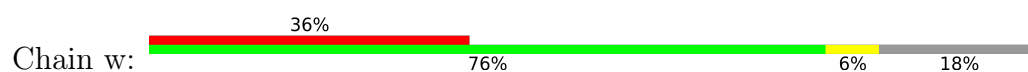
- Molecule 10: Small nuclear ribonucleoprotein Sm D3



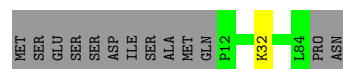
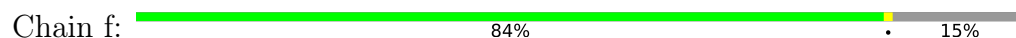
- Molecule 11: Small nuclear ribonucleoprotein E



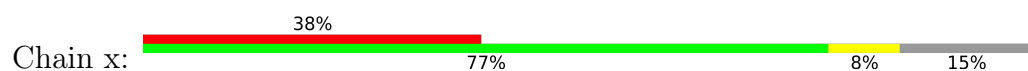
- Molecule 11: Small nuclear ribonucleoprotein E



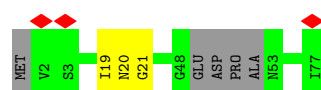
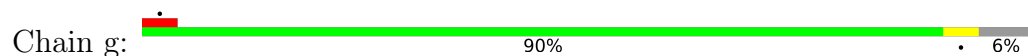
- Molecule 12: Small nuclear ribonucleoprotein F



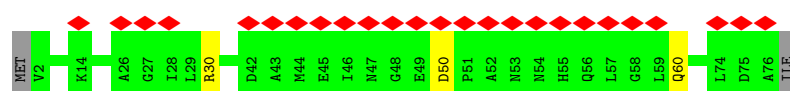
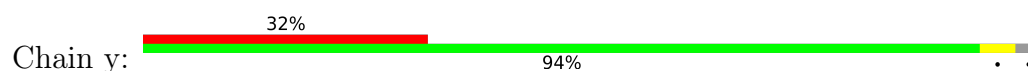
- Molecule 12: Small nuclear ribonucleoprotein F



- Molecule 13: Small nuclear ribonucleoprotein G



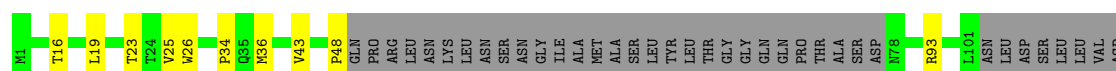
- Molecule 13: Small nuclear ribonucleoprotein G



- Molecule 14: Small nuclear ribonucleoprotein Sm D1



- Molecule 14: Small nuclear ribonucleoprotein Sm D1



GLN
LYS
GLN
GLN
LEU
ASN
SER
SER
LEU
ARG
ARG
GLY
GLY
GLN
TLE
ALA
ASN
ASP
PRO
SER
SER
LYS
LYS
ARG
ARG
ASP
PHE
GLY
ALA
PRO
ASN
LYS
ARG
PRO
ARG
ARG
GLY
LEU

- Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain i:  90% 10%

MET
SER
SER
GLN
ILE
ILE
ASP
R8
K80
GLY
LYS
N83
P108
VAL
GLU

- Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain u:  21% 77% 6% 16%

MET
SER
SER
ILE
ILE
ASP
ARG
PRO
LYS
HIS
GLU
LEU
SER
ARG
ALA
E17
L18
E19
E20
L21
E22
E23
F24
E25
F26
K27
H28
N35
D36
V39
T40
R41
T42
K53
A56
V72
K73
E74
G81
K82
N83
R89
F90
I91
D99
K106
T107
P108
VAL
GLU

- Molecule 16: Protein LUC7

Chain H:  74% 26%

MET
SER
THR
THR
M4
M19
GLY
ARG
ASP
PHE
SER
PHE
PHE
HIS
ASN
TTR
SER
HIS
GLN
LYS
ASP
ASP
LEU
G38
D140
VAL
MET
GLY
GLN
GLU
ILE
ASP
SER
LEU
ILE
ARG
ALA
ASP
GLU
VAL
SER
MET
MET
LEU
GLN
SER
VAL
LYS
LEU
GLN
L172

R244
THR
THR
ASN
ALA
SER
LYS
THR
ALA
THR
THR
LEU
PRO
GLY
ARG
ASP
PHE
VAL

- Molecule 17: Pre-mRNA-processing factor 39

Chain D:  91% 8%

MET
PRO
GLU
ASP
THR
ASN
PHE
THR
ILE
GLU
GLU
PRO
ARG
PRO
PRO
ASP
A43
A61
Y62
R63
G64
L136
A137
T138
R207
I208
I212
D243
I244
V245
L246
R247
L285
LYS
PHE
VAL
THR
PRO
SER
SER
SER
ASP
LYS
GLU
PHE
VAL
MET
SER
VAL
PHE
ASP

ARG
CYS
LEU
ILE
PRO
CYS
LEU
Y288
A417
V553
LEU
ASN
THR
THR
ALA
ASN
VAL
D561
R606
N607
E627
GLY
LYS

- Molecule 18: U1 small nuclear ribonucleoprotein 70 kDa homolog

Chain B:  60% 38%

M1
M2
Y3
R26
P27
N91
TRP
ASN
P94
T108
T133
V154
F155
I176
G188
ARG
THR
VAL
LYS
TYR
PHE
LYS
PRO
ARG
ARG
LEU
GLY
GLY
GLY
LEU
GLY
GLY
TYR
SER
ASN
ARG
PRO
THR
ASP
ALA
ALA
VAL
THR
PRO
GLY
ARG
PHE
TYR
LYS
SER
SER
ALA
SER
THR
SER
ASN
ARG

PRO
ALA
GLU
ARG
ASN
TYR
ALA
PRO
ARG
PRO
ASN
ARG
GLU
THR
SER
SER
SER
ALA
TYR
SER
ASP
ARG
THR
GLY
SER
SER
THR
LEU
LEU
ASP
ALA
TYR
GLY
ASN
ARG
PRO
LEU
LEU
SER
SER
ALA
THR
PRO
THR
THR
ALA
ALA
VAL
THR
SER
VAL
TYR
LYS
SER
SER
ARG
ASN
THR
SER
ARG

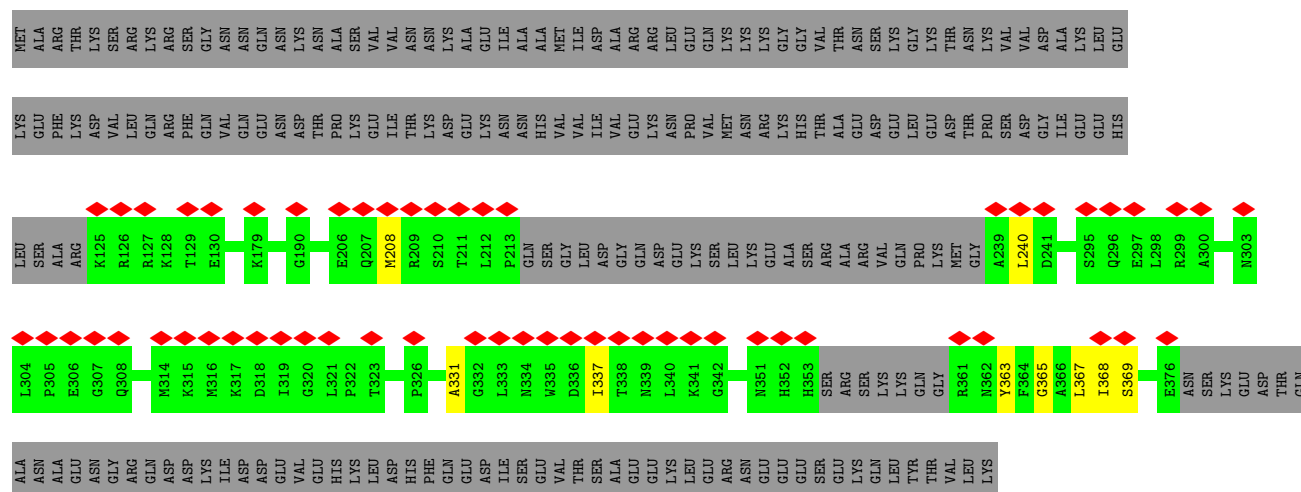
THR
ARG
GLU
SER
GLN
PRO
ALA
PRO
GLU
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PRO
ASP
TYR



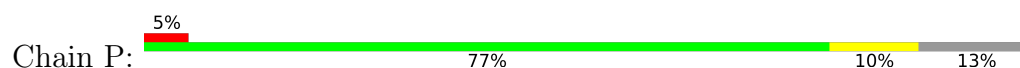
• Molecule 24: Pre-mRNA-splicing factor RDS3



• Molecule 25: Cold sensitive U2 snRNA suppressor 1



• Molecule 26: Pre-mRNA-splicing factor RSE1



G1146	A1147	U1148	G1149	U1150	U1151	U1152	C1153	U1154	C	U	U	C	U1159	C1160	U1161	U1162	C1163	C1164	C1165	C1166	U1167	U1168	C1169	G	C	C	C	C	U
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217460	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size ($\text{\AA}$)	464.0, 464.0, 464.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	F	0.18	0/1342	0.50	0/1868
2	I	0.61	6/768 (0.8%)	0.47	0/1189
3	E	0.19	0/2743	0.48	0/3841
4	J	0.27	0/530	0.74	1/740 (0.1%)
5	1	0.17	0/13201	0.35	2/20553 (0.0%)
6	G	0.19	0/1208	0.52	0/1689
7	A	0.19	0/671	0.59	0/937
8	C	0.20	0/992	0.50	0/1390
9	b	0.20	0/608	0.56	0/848
9	s	0.25	0/322	0.59	0/446
10	d	0.24	0/479	0.61	2/671 (0.3%)
10	v	0.29	0/415	0.57	0/579
11	e	0.21	0/392	0.61	0/546
11	w	0.37	0/392	0.70	0/546
12	f	0.23	0/367	0.60	0/510
12	x	0.29	0/367	0.67	0/510
13	g	0.15	0/355	0.61	2/491 (0.4%)
13	y	0.16	0/374	0.45	0/520
14	h	0.17	0/535	0.46	0/743
14	t	0.31	0/364	0.60	0/507
15	i	0.18	0/503	0.53	0/703
15	u	0.29	0/465	0.59	0/650
16	H	0.13	0/962	0.35	0/1340
17	D	0.18	0/2901	0.41	0/4059
18	B	0.16	0/947	0.44	0/1325
19	K	0.90	0/2050	1.62	12/2870 (0.4%)
20	O	0.42	0/4149	0.85	32/5819 (0.5%)
21	U	0.29	0/867	0.76	1/1208 (0.1%)
22	V	0.57	0/515	0.89	0/719
23	T	0.39	0/2324	0.83	2/3248 (0.1%)
24	S	0.23	0/463	0.64	0/645
25	Q	0.23	0/1137	0.63	0/1593
26	P	0.25	0/6009	0.61	2/8407 (0.0%)
27	R	0.28	0/869	0.54	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	Z	0.22	0/412	0.46	0/573
29	W	0.32	0/869	0.76	0/1219
30	Y	0.19	0/418	0.46	0/582
31	p	0.91	1/2269 (0.0%)	1.04	2/3172 (0.1%)
32	2	4.62	37/3363 (1.1%)	1.80	112/5218 (2.1%)
All	All	1.17	44/57917 (0.1%)	0.78	170/83683 (0.2%)

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
7	A	0	1
13	g	0	1
18	B	0	1
23	T	0	1
26	P	0	2
29	W	0	1
32	2	0	2
All	All	0	9

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	35	U	C1'-N1	151.53	3.75	1.48
32	2	42	U	C1'-N1	151.14	3.75	1.48
32	2	44	U	C1'-N1	150.12	3.73	1.48
31	p	271	THR	C-N	33.66	1.80	1.33
32	2	1161	U	O3'-P	-12.49	1.42	1.61
32	2	1092	A	O3'-P	-11.80	1.43	1.61
32	2	1163	C	O5'-C5'	11.07	1.59	1.42
32	2	1116	A	O3'-P	-9.25	1.47	1.61
32	2	1116	A	C3'-O3'	-8.30	1.29	1.42
32	2	1166	G	O3'-P	8.01	1.73	1.61
32	2	1165	C	O5'-C5'	7.76	1.54	1.42
32	2	1162	U	O5'-C5'	7.75	1.54	1.42
32	2	1154	U	C1'-N1	7.17	1.59	1.48
32	2	1140	U	C1'-N1	7.12	1.59	1.48
32	2	1127	A	O3'-P	-6.98	1.50	1.61
32	2	1167	U	O3'-P	6.89	1.71	1.61
2	I	260	G	C1'-N9	-6.81	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	1169	C	C1'-N1	6.63	1.58	1.48
32	2	1164	C	O3'-P	-6.56	1.51	1.61
2	I	250	U	C1'-N1	6.18	1.57	1.48
2	I	268	U	C1'-N1	6.11	1.56	1.47
32	2	1116	A	O5'-C5'	6.10	1.51	1.42
32	2	1151	U	O5'-C5'	-6.08	1.33	1.42
32	2	1096	C	O5'-C5'	6.06	1.51	1.42
2	I	246	U	C1'-N1	6.01	1.56	1.47
32	2	1166	G	O5'-C5'	6.00	1.51	1.42
2	I	247	U	C1'-N1	5.99	1.56	1.47
32	2	68	U	C1'-N1	5.92	1.57	1.48
2	I	249	C	C1'-N1	5.90	1.57	1.48
32	2	118	U	C1'-N1	5.82	1.57	1.48
32	2	121	C	C1'-N1	5.70	1.57	1.48
32	2	1096	C	O3'-P	5.58	1.69	1.61
32	2	111	C	C1'-N1	5.54	1.56	1.48
32	2	146	A	O5'-C5'	5.52	1.50	1.42
32	2	109	C	C1'-N1	5.51	1.56	1.48
32	2	1128	C	C5'-C4'	-5.48	1.43	1.51
32	2	85	A	C1'-N9	-5.48	1.39	1.48
32	2	1161	U	C3'-O3'	-5.33	1.34	1.42
32	2	1095	U	O3'-P	5.25	1.69	1.61
32	2	1165	C	O3'-P	5.22	1.69	1.61
32	2	1127	A	O5'-C5'	5.08	1.50	1.42
32	2	1162	U	P-O5'	5.06	1.67	1.59
32	2	1117	G	C5'-C4'	5.01	1.58	1.51
32	2	1118	U	O5'-C5'	5.01	1.50	1.42

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	44	U	C6-N1-C1'	-34.73	17.00	121.20
32	2	42	U	C6-N1-C1'	-34.40	17.99	121.20
32	2	35	U	C6-N1-C1'	-34.35	18.16	121.20
31	p	271	THR	O-C-N	-22.11	92.98	122.83
32	2	1151	U	C4'-C3'-O3'	-19.98	83.03	113.00
32	2	1092	A	C2'-C3'-O3'	17.89	140.54	113.70
32	2	1097	G	C3'-C2'-O2'	16.45	135.38	110.70
32	2	1093	C	P-O5'-C5'	15.81	144.62	120.90
32	2	1147	A	C5'-C4'-C3'	-15.12	93.31	116.00
32	2	1168	U	C4'-C3'-O3'	-14.99	90.51	113.00
32	2	44	U	O4'-C1'-N1	-14.87	86.20	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1148	U	C4'-C3'-O3'	-14.36	91.46	113.00
32	2	1092	A	C4'-C3'-O3'	-13.35	92.97	113.00
32	2	1151	U	P-O5'-C5'	12.49	139.64	120.90
32	2	145	G	C5'-C4'-C3'	-11.95	98.08	116.00
32	2	1096	C	C1'-C2'-O2'	-11.90	90.55	108.40
32	2	1117	G	C5'-C4'-C3'	-11.61	98.59	116.00
32	2	42	U	O4'-C1'-N1	-11.42	91.37	108.50
32	2	1162	U	C5'-C4'-O4'	11.39	126.89	109.80
32	2	35	U	O4'-C1'-N1	-11.22	91.67	108.50
32	2	1162	U	C2'-C3'-O3'	-11.21	96.88	113.70
32	2	1097	G	C2'-C3'-O3'	-10.96	97.25	113.70
32	2	1163	C	C5'-C4'-C3'	-10.38	100.43	116.00
32	2	1147	A	C4'-C3'-O3'	10.32	128.48	113.00
32	2	1098	C	N1-C1'-C2'	-10.26	96.61	112.00
32	2	1147	A	P-O5'-C5'	10.25	136.27	120.90
32	2	1165	C	C4'-C3'-O3'	10.07	128.11	113.00
32	2	1162	U	C5'-C4'-C3'	-9.79	101.32	116.00
32	2	1089	G	C4'-C3'-O3'	9.65	127.47	113.00
20	O	238	PRO	CA-N-CD	-9.64	98.50	112.00
20	O	206	PRO	CA-N-CD	-9.64	98.51	112.00
20	O	424	PRO	CA-N-CD	-9.64	98.50	112.00
20	O	284	PRO	CA-N-CD	-9.63	98.51	112.00
20	O	315	PRO	CA-N-CD	-9.59	98.58	112.00
20	O	249	PRO	CA-N-CD	-9.58	98.59	112.00
20	O	399	PRO	CA-N-CD	-9.56	98.61	112.00
20	O	691	PRO	CA-N-CD	-9.56	98.62	112.00
20	O	596	PRO	CA-N-CD	-9.55	98.63	112.00
20	O	687	PRO	CA-N-CD	-9.52	98.67	112.00
20	O	449	PRO	CA-N-CD	-9.51	98.69	112.00
20	O	481	PRO	CA-N-CD	-9.49	98.71	112.00
20	O	656	PRO	CA-N-CD	-9.49	98.71	112.00
20	O	759	PRO	CA-N-CD	-9.46	98.75	112.00
32	2	1115	G	C4'-C3'-O3'	9.38	127.07	113.00
32	2	66	A	C4'-C3'-O3'	9.28	123.31	109.40
32	2	1152	U	P-O5'-C5'	9.26	134.79	120.90
20	O	681	PRO	CA-N-CD	-9.16	99.17	112.00
20	O	428	PRO	CA-N-CD	-9.13	99.22	112.00
32	2	1092	A	P-O5'-C5'	9.10	134.55	120.90
20	O	197	PRO	CA-N-CD	-9.05	99.33	112.00
20	O	525	PRO	CA-N-CD	-9.04	99.35	112.00
20	O	629	PRO	CA-N-CD	-9.01	99.39	112.00
20	O	472	PRO	CA-N-CD	-9.00	99.40	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	O	721	PRO	CA-N-CD	-9.00	99.40	112.00
20	O	680	PRO	CA-N-CD	-8.99	99.42	112.00
20	O	387	PRO	CA-N-CD	-8.98	98.92	111.50
20	O	614	PRO	CA-N-CD	-8.98	99.42	112.00
20	O	600	PRO	CA-N-CD	-8.96	99.46	112.00
20	O	369	PRO	CA-N-CD	-8.95	99.47	112.00
20	O	256	PRO	CA-N-CD	-8.95	99.47	112.00
20	O	532	PRO	CA-N-CD	-8.92	99.51	112.00
4	J	274	PRO	CA-N-CD	-8.88	99.56	112.00
32	2	145	G	C3'-C2'-O2'	-8.88	97.38	110.70
32	2	145	G	P-O5'-C5'	8.88	134.22	120.90
20	O	497	PRO	CA-N-CD	-8.88	99.58	112.00
32	2	148	G	C5'-C4'-C3'	-8.85	102.72	116.00
32	2	1165	C	C5'-C4'-C3'	-8.81	102.79	116.00
32	2	1167	U	C2'-C3'-O3'	8.75	126.83	113.70
32	2	1117	G	C5'-C4'-O4'	8.71	122.86	109.80
5	1	442	U	OP2-P-O3'	-8.61	82.18	108.00
5	1	442	U	OP1-P-O3'	-8.59	82.24	108.00
32	2	1096	C	C2'-C3'-O3'	-8.55	100.87	113.70
20	O	720	PRO	CA-N-CD	-8.54	100.05	112.00
32	2	1168	U	P-O5'-C5'	-8.43	108.25	120.90
32	2	1108	A	C1'-C2'-O2'	-8.32	95.93	108.40
32	2	1161	U	C5'-C4'-C3'	-8.25	103.62	116.00
32	2	1093	C	C5'-C4'-C3'	-8.22	103.67	116.00
32	2	1166	G	O5'-C5'-C4'	8.18	123.77	111.50
32	2	1096	C	C4'-C3'-O3'	8.16	125.25	113.00
32	2	1169	C	P-O5'-C5'	-8.13	108.70	120.90
32	2	1163	C	C5'-C4'-O4'	8.00	121.79	109.80
32	2	1096	C	C3'-C2'-O2'	7.97	122.65	110.70
32	2	1168	U	C2'-C3'-O3'	7.90	125.55	113.70
32	2	1162	U	C4'-C3'-O3'	7.83	124.75	113.00
32	2	145	G	O5'-C5'-C4'	-7.75	99.87	111.50
32	2	141	A	N9-C1'-C2'	-7.73	100.41	112.00
32	2	1168	U	C1'-C2'-O2'	-7.72	96.83	108.40
32	2	1105	C	C4'-C3'-O3'	-7.64	97.94	109.40
32	2	1151	U	O3'-P-O5'	-7.62	92.57	104.00
32	2	141	A	C4'-C3'-O3'	7.58	124.36	113.00
32	2	1128	C	C4'-C3'-O3'	-7.40	101.89	113.00
32	2	1126	G	N9-C1'-C2'	-7.39	100.91	112.00
32	2	1139	G	N9-C1'-C2'	-7.12	101.31	112.00
32	2	1165	C	C2'-C3'-O3'	-6.98	103.23	113.70
32	2	1151	U	C1'-C2'-O2'	-6.86	98.11	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1163	C	C4'-C3'-O3'	6.84	123.27	113.00
32	2	78	G	C2'-C3'-O3'	6.81	123.92	113.70
32	2	145	G	C4'-C3'-O3'	6.80	123.20	113.00
32	2	1168	U	O3'-P-O5'	-6.74	93.89	104.00
32	2	1166	G	C5'-C4'-C3'	6.72	126.09	116.00
32	2	1092	A	N9-C1'-C2'	6.72	122.08	112.00
32	2	44	U	N1-C1'-C2'	6.68	122.03	112.00
32	2	1152	U	C5'-C4'-C3'	-6.56	106.17	116.00
32	2	1147	A	O5'-C5'-C4'	6.53	121.29	111.50
32	2	142	C	N1-C1'-C2'	-6.47	102.29	112.00
32	2	1129	U	C1'-C2'-O2'	6.36	117.94	108.40
32	2	1167	U	C4'-C3'-O3'	-6.32	103.52	113.00
32	2	78	G	C3'-C2'-O2'	6.31	120.16	110.70
32	2	1152	U	O4'-C4'-C3'	6.27	110.27	104.00
32	2	1169	C	O5'-C5'-C4'	-6.27	102.10	111.50
32	2	1097	G	C4'-C3'-O3'	6.23	122.35	113.00
32	2	1117	G	C2'-C3'-O3'	-6.17	104.44	113.70
32	2	1153	C	C4'-C3'-O3'	-6.12	103.83	113.00
32	2	1151	U	N1-C1'-C2'	6.10	121.15	112.00
19	K	211	MET	N-CA-CB	6.04	119.00	110.12
32	2	1151	U	C5'-C4'-O4'	6.04	118.86	109.80
32	2	1093	C	O5'-C5'-C4'	-6.01	102.49	111.50
10	d	5	GLY	CA-C-N	6.01	124.02	120.24
10	d	5	GLY	C-N-CA	6.01	124.02	120.24
32	2	1166	G	O3'-P-O5'	5.98	112.97	104.00
32	2	1167	U	C5'-C4'-C3'	5.95	124.92	116.00
19	K	303	TYR	CA-C-N	5.89	128.53	120.46
19	K	303	TYR	C-N-CA	5.89	128.53	120.46
32	2	1118	U	O5'-C5'-C4'	5.88	120.32	111.50
32	2	1108	A	C4'-C3'-O3'	5.86	121.79	113.00
32	2	1102	C	C3'-C2'-O2'	5.81	119.41	110.70
32	2	1151	U	O5'-C5'-C4'	-5.78	102.83	111.50
32	2	1165	C	C5'-C4'-O4'	5.75	118.42	109.80
32	2	1117	G	C4'-C3'-O3'	5.73	121.59	113.00
32	2	1107	C	N1-C1'-C2'	-5.68	103.48	112.00
32	2	1107	C	C4'-C3'-O3'	-5.66	104.51	113.00
20	O	591	ASP	CB-CA-C	-5.62	109.58	117.23
23	T	28	ASN	CA-C-N	5.62	125.99	119.47
23	T	28	ASN	C-N-CA	5.62	125.99	119.47
20	O	386	TYR	C-N-CD	5.54	132.80	120.60
32	2	46	C	C2'-C3'-O3'	5.50	121.95	113.70
32	2	1148	U	P-O5'-C5'	5.49	129.13	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1139	G	C4'-C3'-O3'	5.43	121.15	113.00
19	K	289	SER	CA-C-N	5.43	128.10	120.28
19	K	289	SER	C-N-CA	5.43	128.10	120.28
32	2	1168	U	C4'-C3'-C2'	-5.42	97.18	102.60
32	2	148	G	C2'-C3'-O3'	-5.42	105.57	113.70
32	2	1162	U	C4'-C3'-C2'	5.42	108.02	102.60
32	2	1092	A	O3'-P-O5'	-5.40	95.90	104.00
32	2	1126	G	C4'-C3'-O3'	5.40	121.10	113.00
19	K	213	GLN	N-CA-C	5.38	117.15	111.28
26	P	961	CYS	CB-CA-C	-5.38	109.39	115.79
32	2	1128	C	C5'-C4'-O4'	5.37	117.86	109.80
32	2	149	A	O5'-C5'-C4'	5.36	119.54	111.50
32	2	146	A	C5'-C4'-C3'	-5.35	107.97	116.00
32	2	1095	U	C3'-C2'-O2'	5.33	118.70	110.70
21	U	229	ASN	N-CA-C	5.32	117.31	107.73
19	K	343	LYS	N-CA-C	5.30	116.75	111.07
19	K	445	THR	N-CA-CB	5.27	117.97	110.06
31	p	273	LYS	N-CA-C	5.26	125.72	111.00
32	2	1089	G	C2'-C3'-O3'	-5.24	105.84	113.70
19	K	528	GLU	CA-C-N	5.23	128.28	120.90
19	K	528	GLU	C-N-CA	5.23	128.28	120.90
32	2	140	G	C3'-C2'-O2'	5.22	118.53	110.70
13	g	19	ILE	CA-C-N	5.21	131.49	121.54
13	g	19	ILE	C-N-CA	5.21	131.49	121.54
32	2	1129	U	O4'-C4'-C3'	5.21	109.21	104.00
32	2	1142	G	C1'-C2'-O2'	-5.21	100.59	108.40
32	2	148	G	C4'-C3'-O3'	5.18	120.77	113.00
32	2	1167	U	C5'-C4'-O4'	-5.16	102.06	109.80
32	2	1167	U	P-O3'-C3'	-5.15	112.48	120.20
19	K	383	TYR	O-C-N	-5.07	115.97	120.48
19	K	286	THR	N-CA-C	5.04	117.17	111.02
32	2	1163	C	C2'-C3'-O3'	-5.02	106.17	113.70
26	P	1233	SER	CB-CA-C	-5.02	109.32	116.34

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	2	141	A	Sidechain
32	2	143	G	Sidechain
7	A	12	ARG	Peptide
18	B	176	ILE	Peptide

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Mol	Chain	Res	Type	Group
26	P	1013	ASP	Peptide
26	P	1014	LYS	Peptide
23	T	458	SER	Peptide
29	W	16	VAL	Peptide
13	g	20	ASN	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	F	1335	0	659	2	0
2	I	1327	0	777	32	0
3	E	2732	0	1201	0	0
4	J	529	0	237	10	0
5	l	11822	0	5939	90	0
6	G	1202	0	549	1	0
7	A	668	0	319	1	0
8	C	985	0	456	0	0
9	b	607	0	271	1	0
9	s	323	0	143	3	0
10	d	473	0	241	2	0
10	v	412	0	204	3	0
11	e	389	0	192	0	0
11	w	389	0	189	5	0
12	f	365	0	173	1	0
12	x	365	0	173	4	0
13	g	356	0	165	0	0
13	y	373	0	180	0	0
14	h	535	0	247	2	0
14	t	363	0	169	5	0
15	i	501	0	230	0	0
15	u	463	0	210	10	0
16	H	960	0	443	0	0
17	D	2892	0	1250	7	0
18	B	940	0	437	3	0
19	K	2042	0	907	4	0
20	O	4108	0	2037	212	0
21	U	943	0	423	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	515	0	224	2	0
23	T	2318	0	1039	32	0
24	S	460	0	217	3	0
25	Q	1122	0	560	5	0
26	P	5972	0	2772	71	0
27	R	868	0	411	10	0
28	Z	412	0	184	0	0
29	W	862	0	401	32	0
30	Y	418	0	188	3	0
31	p	2239	0	1077	14	0
32	2	3021	0	1536	141	0
All	All	56606	0	27030	671	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 8.

All (671) 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)
26:P:626:PRO:HB2	26:P:627:PRO:CD	1.44	1.41
31:p:271:THR:C	31:p:273:LYS:N	1.80	1.38
20:O:644:ASN:CB	20:O:679:GLN:CB	2.07	1.30
32:2:1099:G:O2'	32:2:1100:A:H5'	1.42	1.19
20:O:721:PRO:HD2	20:O:722:LYS:H	1.10	1.16
20:O:197:PRO:HD2	20:O:198:GLU:H	1.12	1.12
20:O:249:PRO:HD2	20:O:250:LEU:H	1.13	1.12
20:O:387:PRO:HD2	20:O:388:TYR:H	1.14	1.11
20:O:497:PRO:HD2	20:O:498:LEU:H	1.12	1.11
20:O:656:PRO:HD2	20:O:657:GLU:H	1.17	1.09
20:O:256:PRO:HD2	20:O:257:MET:H	1.13	1.06
20:O:759:PRO:HD2	20:O:760:HIS:H	1.16	1.06
20:O:399:PRO:HD2	20:O:400:LEU:H	1.14	1.06
20:O:593:ARG:O	20:O:596:PRO:CD	2.03	1.06
20:O:596:PRO:HD2	20:O:597:PHE:H	1.18	1.06
26:P:626:PRO:CB	26:P:627:PRO:HD3	1.85	1.06
20:O:315:PRO:HD2	20:O:316:PHE:H	1.16	1.05
20:O:369:PRO:HD2	20:O:370:VAL:H	1.12	1.05
20:O:525:PRO:HD2	20:O:526:LEU:H	1.18	1.05
20:O:449:PRO:HD2	20:O:450:ASP:H	1.14	1.05
20:O:424:PRO:HD2	20:O:425:LEU:H	1.17	1.02
26:P:626:PRO:CB	26:P:627:PRO:CD	2.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:428:PRO:HD2	20:O:429:GLU:H	1.23	1.01
20:O:472:PRO:HD2	20:O:473:LYS:H	1.20	1.01
20:O:396:VAL:O	20:O:399:PRO:HD2	1.60	1.00
26:P:626:PRO:HB2	26:P:627:PRO:HD3	1.00	0.98
20:O:600:PRO:HD2	20:O:601:ILE:H	1.28	0.97
20:O:687:PRO:HD2	20:O:688:THR:H	1.25	0.97
5:1:384:U:H3	5:1:434:G:H1	1.01	0.97
20:O:530:ALA:C	20:O:532:PRO:HD3	1.90	0.96
20:O:238:PRO:HD2	20:O:239:TYR:H	1.27	0.96
20:O:481:PRO:HD2	20:O:482:GLU:H	1.24	0.96
5:1:380:G:H1	5:1:438:U:H3	1.07	0.96
20:O:629:PRO:HD2	20:O:630:VAL:H	1.28	0.95
20:O:396:VAL:O	20:O:399:PRO:CD	2.15	0.95
20:O:532:PRO:HD2	20:O:533:PHE:H	1.30	0.95
32:2:1099:G:C2'	32:2:1100:A:H5'	1.97	0.94
20:O:684:GLN:O	20:O:687:PRO:HD2	1.66	0.93
23:T:186:HIS:O	23:T:190:LEU:CB	2.17	0.92
23:T:344:ALA:HB3	31:p:261:GLY:HA3	1.51	0.92
25:Q:208:MET:CB	25:Q:240:LEU:CB	2.47	0.92
26:P:827:TRP:HA	26:P:839:ARG:O	1.70	0.92
20:O:206:PRO:HD2	20:O:207:ILE:H	1.32	0.91
21:U:70:LEU:HA	27:R:45:VAL:HA	1.53	0.90
20:O:598:LEU:C	20:O:600:PRO:HD3	1.96	0.90
20:O:691:PRO:HD2	20:O:692:ILE:H	1.36	0.90
4:J:272:ASP:C	4:J:274:PRO:HD3	1.97	0.88
20:O:497:PRO:HD2	20:O:498:LEU:N	1.88	0.88
20:O:721:PRO:HD2	20:O:722:LYS:N	1.88	0.87
4:J:273:LEU:N	4:J:274:PRO:HD3	1.89	0.87
20:O:369:PRO:HD2	20:O:370:VAL:N	1.88	0.87
20:O:593:ARG:O	20:O:596:PRO:HD2	1.74	0.86
20:O:399:PRO:HD2	20:O:400:LEU:N	1.90	0.86
20:O:759:PRO:HD2	20:O:760:HIS:N	1.91	0.85
26:P:379:VAL:O	26:P:390:LYS:HA	1.76	0.85
20:O:387:PRO:HD2	20:O:388:TYR:N	1.89	0.85
20:O:525:PRO:HD2	20:O:526:LEU:N	1.92	0.85
5:1:389:G:H1	5:1:430:U:H3	0.86	0.85
26:P:416:SER:HA	26:P:431:SER:HA	1.56	0.84
26:P:626:PRO:HB2	26:P:627:PRO:HD2	1.52	0.84
20:O:315:PRO:HD2	20:O:316:PHE:N	1.92	0.84
20:O:593:ARG:O	20:O:596:PRO:HD3	1.77	0.83
20:O:600:PRO:HD2	20:O:601:ILE:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:249:PRO:HD2	20:O:250:LEU:N	1.90	0.83
32:2:1099:G:O2'	32:2:1100:A:C5'	2.24	0.83
20:O:424:PRO:HD2	20:O:425:LEU:N	1.93	0.83
20:O:614:PRO:HD2	20:O:615:LEU:H	1.44	0.82
20:O:367:HIS:C	20:O:369:PRO:HD3	2.04	0.82
1:F:162:ASN:HA	1:F:212:PHE:O	1.80	0.81
20:O:532:PRO:HD2	20:O:533:PHE:N	1.94	0.81
26:P:609:HIS:O	26:P:620:ASN:HA	1.80	0.81
20:O:596:PRO:HD2	20:O:597:PHE:N	1.93	0.81
20:O:681:PRO:HG2	20:O:684:GLN:CB	2.11	0.81
20:O:472:PRO:HD2	20:O:473:LYS:N	1.92	0.81
32:2:141:A:H2'	32:2:142:C:C6	2.16	0.81
20:O:531:GLU:N	20:O:532:PRO:HD3	1.96	0.81
20:O:684:GLN:O	20:O:687:PRO:CD	2.30	0.80
20:O:481:PRO:HD2	20:O:482:GLU:N	1.95	0.80
20:O:530:ALA:C	20:O:532:PRO:CD	2.55	0.79
20:O:246:VAL:O	20:O:249:PRO:CD	2.30	0.79
20:O:369:PRO:CD	20:O:370:VAL:H	1.95	0.79
20:O:449:PRO:HD2	20:O:450:ASP:N	1.92	0.79
20:O:629:PRO:HD2	20:O:630:VAL:N	1.96	0.79
20:O:598:LEU:C	20:O:600:PRO:CD	2.56	0.78
20:O:687:PRO:HD2	20:O:688:THR:N	1.96	0.78
23:T:150:PRO:HG3	23:T:154:THR:H	1.46	0.78
20:O:597:PHE:O	20:O:600:PRO:CD	2.31	0.78
20:O:206:PRO:HD2	20:O:207:ILE:N	1.99	0.78
20:O:235:LEU:O	20:O:238:PRO:HD3	1.85	0.77
20:O:197:PRO:HD2	20:O:198:GLU:N	1.90	0.77
20:O:691:PRO:HD2	20:O:692:ILE:N	2.00	0.77
20:O:256:PRO:CD	20:O:257:MET:H	1.97	0.77
20:O:387:PRO:CD	20:O:388:TYR:H	1.97	0.77
20:O:256:PRO:HD2	20:O:257:MET:N	1.90	0.76
23:T:344:ALA:CB	31:p:261:GLY:HA3	2.15	0.76
20:O:497:PRO:CD	20:O:498:LEU:H	1.95	0.76
20:O:656:PRO:HD2	20:O:657:GLU:N	1.92	0.76
23:T:409:TYR:CB	32:2:46:C:C6	2.68	0.76
20:O:614:PRO:HD2	20:O:615:LEU:N	2.01	0.76
20:O:428:PRO:HD2	20:O:429:GLU:N	1.94	0.76
26:P:699:MET:HA	26:P:719:GLN:O	1.85	0.76
20:O:238:PRO:HD2	20:O:239:TYR:N	1.97	0.75
20:O:368:VAL:N	20:O:369:PRO:HD3	2.01	0.75
2:I:8:C:N4	5:1:1:A:N6	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:367:HIS:C	20:O:369:PRO:CD	2.60	0.75
32:2:1138:G:O4'	32:2:1138:G:P	2.45	0.75
20:O:362:CYS:CB	20:O:374:THR:CB	2.64	0.75
20:O:407:HIS:CB	20:O:411:VAL:CB	2.64	0.74
20:O:759:PRO:CD	20:O:760:HIS:H	1.98	0.74
20:O:249:PRO:CD	20:O:250:LEU:H	1.99	0.74
20:O:721:PRO:CD	20:O:722:LYS:H	1.95	0.74
23:T:409:TYR:CB	32:2:46:C:C5	2.70	0.74
20:O:593:ARG:C	20:O:596:PRO:HD3	2.12	0.74
20:O:525:PRO:CD	20:O:526:LEU:H	2.00	0.74
20:O:396:VAL:C	20:O:399:PRO:HD3	2.12	0.73
32:2:140:G:H1	32:2:1168:U:H3	1.37	0.73
32:2:114:U:H5''	32:2:115:U:H5'	1.70	0.72
23:T:150:PRO:HG3	23:T:155:ASN:H	1.55	0.72
31:p:271:THR:O	31:p:273:LYS:N	2.22	0.71
32:2:1093:C:H2'	32:2:1094:G:O4'	1.90	0.71
20:O:197:PRO:CD	20:O:198:GLU:H	1.96	0.71
23:T:191:ASN:CB	15:u:89:ARG:HA	2.21	0.71
26:P:626:PRO:HG2	26:P:630:ILE:H	1.55	0.71
29:W:24:ASN:HA	29:W:32:ARG:O	1.89	0.71
20:O:599:ALA:N	20:O:600:PRO:HD3	2.05	0.71
20:O:449:PRO:CD	20:O:450:ASP:H	1.98	0.70
20:O:246:VAL:O	20:O:249:PRO:HD3	1.90	0.70
20:O:424:PRO:CD	20:O:425:LEU:H	2.01	0.70
4:J:272:ASP:CB	4:J:274:PRO:HD3	2.22	0.70
20:O:600:PRO:CD	20:O:601:ILE:H	2.03	0.70
20:O:171:LEU:O	20:O:175:ASN:N	2.25	0.69
20:O:315:PRO:CD	20:O:316:PHE:H	2.01	0.69
23:T:344:ALA:HB3	31:p:261:GLY:CA	2.21	0.69
4:J:273:LEU:N	4:J:274:PRO:CD	2.56	0.69
2:I:259:U:H3	32:2:41:C:H42	1.40	0.68
20:O:399:PRO:CD	20:O:400:LEU:H	1.99	0.68
20:O:656:PRO:CD	20:O:657:GLU:H	2.02	0.68
32:2:141:A:H2'	32:2:142:C:C5	2.28	0.68
20:O:396:VAL:C	20:O:399:PRO:CD	2.66	0.68
23:T:191:ASN:CB	15:u:89:ARG:CB	2.71	0.68
5:1:512:A:H3'	5:1:513:A:H4'	1.75	0.68
26:P:704:SER:O	26:P:713:LEU:HA	1.94	0.67
21:U:136:UNK:HA	21:U:149:GLY:HA2	1.77	0.67
20:O:472:PRO:CD	20:O:473:LYS:H	2.02	0.67
32:2:1092:A:H3'	32:2:1093:C:H6	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:547:ASN:HA	26:P:563:ILE:O	1.95	0.67
5:1:425:A:H2'	5:1:426:U:H4'	1.76	0.67
20:O:596:PRO:CD	20:O:597:PHE:H	2.01	0.67
2:I:113:N:H4'	17:D:606:ARG:HA	1.77	0.67
20:O:369:PRO:CD	20:O:370:VAL:N	2.57	0.67
20:O:428:PRO:CD	20:O:429:GLU:H	2.04	0.67
20:O:497:PRO:CD	20:O:498:LEU:N	2.56	0.66
2:I:257:C:H6	2:I:257:C:O5'	1.79	0.66
2:I:264:U:C2	32:2:37:G:N2	2.63	0.66
26:P:690:LEU:HA	26:P:703:MET:O	1.96	0.66
20:O:496:ARG:N	20:O:497:PRO:HD3	2.10	0.66
27:R:184:PHE:HA	27:R:188:GLY:HA2	1.76	0.66
15:u:99:ASP:CB	32:2:118:U:C5	2.77	0.66
2:I:113:N:H4'	17:D:607:ASN:H	1.60	0.66
20:O:197:PRO:CD	20:O:198:GLU:N	2.58	0.66
32:2:1138:G:O2'	32:2:1139:G:H8	1.79	0.65
29:W:7:ILE:HA	29:W:27:LYS:H	1.60	0.65
32:2:1120:G:H2'	32:2:1121:U:H6	1.62	0.65
5:1:386:G:H1	5:1:433:U:H3	1.45	0.65
2:I:267:A:N1	32:2:34:G:C6	2.65	0.65
20:O:759:PRO:CD	20:O:760:HIS:N	2.59	0.65
20:O:525:PRO:CD	20:O:526:LEU:N	2.60	0.65
20:O:532:PRO:CD	20:O:533:PHE:H	2.05	0.65
32:2:1115:G:H1	32:2:1130:U:H3	1.43	0.65
20:O:471:THR:CB	20:O:472:PRO:HD3	2.27	0.65
20:O:532:PRO:CD	20:O:533:PHE:N	2.60	0.64
20:O:600:PRO:CD	20:O:601:ILE:N	2.60	0.64
20:O:721:PRO:CD	20:O:722:LYS:N	2.57	0.64
32:2:1138:G:O2'	32:2:1139:G:C8	2.50	0.64
26:P:380:LEU:HA	26:P:389:PHE:O	1.96	0.64
29:W:17:ASP:CB	30:Y:61:VAL:HA	2.26	0.64
20:O:472:PRO:CD	20:O:473:LYS:N	2.60	0.64
25:Q:331:ALA:HB1	25:Q:337:ILE:HA	1.80	0.64
12:x:28:GLY:HA2	12:x:38:TYR:O	1.97	0.64
26:P:540:PRO:HB2	26:P:612:PRO:HG3	1.80	0.64
32:2:1097:G:C2	32:2:1146:G:C4	2.86	0.64
20:O:387:PRO:CD	20:O:388:TYR:N	2.58	0.63
29:W:158:ASN:CB	32:2:1098:C:O3'	2.46	0.63
32:2:1098:C:H2'	32:2:1099:G:H8	1.62	0.63
20:O:238:PRO:CD	20:O:239:TYR:H	2.08	0.63
11:w:40:LYS:O	11:w:57:ALA:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:597:PHE:O	20:O:600:PRO:CG	2.46	0.63
20:O:720:PRO:O	20:O:720:PRO:HD2	1.98	0.63
21:U:70:LEU:HA	27:R:45:VAL:CA	2.27	0.63
20:O:680:PRO:HD2	20:O:680:PRO:O	1.98	0.63
32:2:1099:G:H2'	32:2:1100:A:H5'	1.80	0.63
20:O:629:PRO:CD	20:O:630:VAL:H	2.07	0.62
29:W:31:LEU:CB	29:W:36:LEU:HA	2.29	0.62
20:O:656:PRO:CD	20:O:657:GLU:N	2.61	0.62
2:I:266:C:H6	2:I:266:C:O5'	1.83	0.62
20:O:249:PRO:CD	20:O:250:LEU:N	2.60	0.62
20:O:449:PRO:CD	20:O:450:ASP:N	2.61	0.62
32:2:46:C:O5'	32:2:46:C:H6	1.83	0.62
20:O:629:PRO:CD	20:O:630:VAL:N	2.63	0.62
32:2:1098:C:O5'	32:2:1098:C:H6	1.82	0.62
5:1:326:G:H3'	5:1:327:A:H8	1.63	0.62
20:O:524:THR:N	20:O:525:PRO:HD3	2.15	0.62
20:O:596:PRO:CD	20:O:597:PHE:N	2.62	0.61
29:W:11:ALA:HB3	29:W:25:VAL:N	2.15	0.61
29:W:25:VAL:O	29:W:31:LEU:HA	1.99	0.61
5:1:188:U:H3	5:1:250:G:H1	1.48	0.61
20:O:681:PRO:HD2	20:O:681:PRO:O	1.99	0.61
20:O:687:PRO:CD	20:O:688:THR:H	2.07	0.61
20:O:367:HIS:CB	20:O:369:PRO:HD3	2.31	0.61
20:O:399:PRO:CD	20:O:400:LEU:N	2.60	0.61
20:O:368:VAL:N	20:O:369:PRO:CD	2.64	0.61
2:I:255:C:H6	2:I:255:C:O5'	1.84	0.60
26:P:426:TYR:HA	26:P:439:PHE:O	2.00	0.60
5:1:342:C:H2'	5:1:343:A:H4'	1.82	0.60
32:2:1139:G:H2'	32:2:1140:U:C6	2.36	0.60
32:2:1161:U:O2'	32:2:1162:U:H5'	2.01	0.60
20:O:428:PRO:CD	20:O:429:GLU:N	2.62	0.60
29:W:17:ASP:C	29:W:19:PHE:H	2.09	0.60
20:O:614:PRO:CD	20:O:615:LEU:N	2.65	0.60
26:P:638:SER:HA	26:P:683:GLN:HA	1.84	0.60
20:O:687:PRO:CD	20:O:688:THR:N	2.65	0.60
26:P:156:ASN:HA	26:P:177:GLN:O	2.00	0.60
32:2:65:A:O2'	32:2:66:A:H5'	2.02	0.60
5:1:199:G:H1	5:1:239:U:H3	1.46	0.60
20:O:235:LEU:O	20:O:238:PRO:CD	2.50	0.59
20:O:424:PRO:CD	20:O:425:LEU:N	2.62	0.59
20:O:614:PRO:CD	20:O:615:LEU:H	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:238:PRO:CD	20:O:239:TYR:N	2.66	0.59
31:p:371:MET:CB	32:2:48:U:OP1	2.50	0.59
20:O:684:GLN:C	20:O:687:PRO:HD3	2.26	0.59
32:2:1152:U:H2'	32:2:1153:C:C6	2.38	0.59
10:d:27:ALA:HA	10:d:50:THR:O	2.02	0.59
29:W:158:ASN:CB	32:2:1099:G:OP1	2.50	0.59
20:O:471:THR:CB	20:O:472:PRO:CD	2.81	0.59
2:I:267:A:C6	32:2:34:G:C6	2.91	0.58
20:O:881:MET:O	20:O:884:LEU:N	2.36	0.58
20:O:284:PRO:HD2	20:O:285:ASP:N	2.17	0.58
20:O:481:PRO:CD	20:O:482:GLU:H	2.07	0.58
4:J:272:ASP:C	4:J:274:PRO:CD	2.73	0.58
32:2:1140:U:C2	32:2:1141:C:C5	2.91	0.58
21:U:214:PRO:N	21:U:215:PRO:HD2	2.19	0.58
20:O:481:PRO:CD	20:O:482:GLU:N	2.64	0.58
20:O:691:PRO:CD	20:O:692:ILE:H	2.14	0.58
26:P:1009:LEU:O	26:P:1017:PHE:HA	2.03	0.58
20:O:927:ALA:C	20:O:929:ASN:H	2.11	0.58
26:P:1218:TYR:O	26:P:1225:VAL:HA	2.03	0.58
20:O:256:PRO:CD	20:O:257:MET:N	2.58	0.58
20:O:475:LEU:O	20:O:480:ALA:N	2.37	0.58
20:O:524:THR:H	20:O:525:PRO:HD3	1.68	0.58
20:O:628:ILE:N	20:O:629:PRO:HD3	2.19	0.58
23:T:191:ASN:C	23:T:193:ILE:H	2.12	0.58
5:1:85:U:H3	5:1:117:U:H3	1.52	0.58
29:W:11:ALA:HB2	29:W:25:VAL:C	2.29	0.58
32:2:1141:C:H2'	32:2:1142:G:H8	1.67	0.58
20:O:206:PRO:CD	20:O:207:ILE:N	2.67	0.57
26:P:106:THR:C	26:P:108:ASP:H	2.11	0.57
32:2:66:A:H8	32:2:66:A:OP2	1.87	0.57
5:1:10:U:H5''	5:1:11:U:H5'	1.85	0.57
20:O:496:ARG:N	20:O:497:PRO:CD	2.68	0.57
15:u:99:ASP:CB	32:2:118:U:H5	2.17	0.57
31:p:526:ALA:O	31:p:576:ASN:HA	2.05	0.57
32:2:1097:G:H1'	32:2:1146:G:N2	2.20	0.57
19:K:441:SER:C	19:K:443:GLU:H	2.12	0.57
24:S:23:CYS:HA	24:S:66:GLY:HA2	1.87	0.57
26:P:704:SER:O	26:P:712:PHE:O	2.22	0.57
20:O:493:ALA:HB1	20:O:532:PRO:HB2	1.85	0.57
29:W:17:ASP:O	29:W:19:PHE:N	2.38	0.57
5:1:144:C:H41	7:A:115:SER:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:185:PHE:O	23:T:189:TRP:CB	2.53	0.57
2:I:255:C:H42	32:2:44:U:H3	1.52	0.56
2:I:260:G:N2	32:2:41:C:H1'	2.20	0.56
20:O:284:PRO:HD2	20:O:285:ASP:H	1.70	0.56
20:O:315:PRO:CD	20:O:316:PHE:N	2.61	0.56
4:J:274:PRO:HD2	4:J:275:SER:N	2.19	0.56
20:O:246:VAL:O	20:O:249:PRO:HD2	2.04	0.56
20:O:691:PRO:CD	20:O:692:ILE:N	2.68	0.56
32:2:67:A:O2'	32:2:68:U:H6	1.89	0.56
32:2:1139:G:HO2'	32:2:1140:U:C5'	2.18	0.56
32:2:1098:C:H2'	32:2:1099:G:C8	2.40	0.56
9:s:40:HIS:O	9:s:89:GLY:HA3	2.05	0.56
2:I:113:N:H4'	17:D:606:ARG:CA	2.35	0.56
20:O:522:LEU:C	20:O:525:PRO:HD3	2.31	0.56
20:O:641:ASN:HA	20:O:679:GLN:CB	2.36	0.56
26:P:378:PHE:HA	26:P:391:LEU:O	2.05	0.56
32:2:48:U:H6	32:2:48:U:O5'	1.89	0.56
23:T:508:GLU:H	23:T:513:GLY:HA3	1.70	0.56
32:2:1125:U:O2'	32:2:1126:G:C8	2.57	0.56
5:1:391:C:N4	5:1:423:G:O2'	2.37	0.56
20:O:597:PHE:C	20:O:600:PRO:HD3	2.30	0.56
26:P:207:VAL:O	26:P:237:THR:N	2.39	0.56
32:2:1139:G:C5	32:2:1140:U:C5	2.94	0.56
27:R:139:GLU:O	27:R:151:ALA:HA	2.06	0.55
4:J:272:ASP:CA	4:J:274:PRO:HD3	2.36	0.55
26:P:1117:HIS:O	26:P:1133:ASP:HA	2.06	0.55
32:2:1126:G:O2'	32:2:1127:A:O5'	2.24	0.55
32:2:1139:G:C4	32:2:1140:U:C5	2.95	0.55
5:1:384:U:O4	5:1:434:G:O6	2.25	0.55
5:1:448:G:H2'	5:1:449:G:H8	1.72	0.55
20:O:597:PHE:O	20:O:600:PRO:HD3	2.06	0.55
32:2:141:A:C2'	32:2:142:C:C6	2.87	0.55
20:O:684:GLN:C	20:O:687:PRO:CD	2.79	0.55
26:P:157:LEU:O	26:P:176:ASN:HA	2.07	0.55
29:W:11:ALA:HB2	29:W:26:ASP:N	2.21	0.55
5:1:217:U:O2	5:1:220:G:O6	2.25	0.55
26:P:382:GLN:HA	26:P:387:ASP:O	2.06	0.55
32:2:1126:G:O2'	32:2:1127:A:C5'	2.54	0.55
30:Y:40:ASN:CB	32:2:1097:G:H5'	2.37	0.55
12:x:33:PHE:C	12:x:35:SER:H	2.15	0.55
32:2:1097:G:C5	32:2:1146:G:C6	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:502:C:H2'	5:1:503:G:H8	1.71	0.54
2:I:113:N:C5'	17:D:606:ARG:HA	2.37	0.54
32:2:110:A:H5''	32:2:111:C:OP2	2.07	0.54
20:O:427:ASP:CB	20:O:428:PRO:HD3	2.38	0.54
29:W:158:ASN:CB	32:2:1099:G:P	2.95	0.54
20:O:367:HIS:CB	20:O:369:PRO:CD	2.85	0.54
23:T:147:SER:HA	23:T:155:ASN:O	2.08	0.54
23:T:148:SER:CB	23:T:159:ASP:H	2.20	0.54
26:P:782:GLU:O	26:P:816:MET:N	2.39	0.54
11:w:59:GLU:O	11:w:74:GLY:CA	2.56	0.54
32:2:67:A:C4	32:2:68:U:C5	2.96	0.54
20:O:431:ALA:HB3	20:O:469:SER:CB	2.38	0.54
20:O:484:PHE:HA	20:O:488:TRP:CB	2.38	0.54
25:Q:363:TYR:C	25:Q:365:GLY:H	2.16	0.54
29:W:7:ILE:O	29:W:26:ASP:N	2.40	0.54
31:p:269:LEU:O	31:p:273:LYS:CB	2.56	0.54
9:s:50:GLU:O	9:s:79:LYS:HA	2.08	0.54
31:p:368:GLY:HA2	32:2:46:C:OP1	2.08	0.54
20:O:206:PRO:CD	20:O:207:ILE:H	2.12	0.54
20:O:525:PRO:HB2	20:O:537:ALA:HB2	1.90	0.54
14:t:34:PRO:C	14:t:36:MET:H	2.15	0.54
5:1:313:G:H2'	5:1:314:G:H8	1.73	0.53
2:I:113:N:C4'	17:D:606:ARG:HA	2.37	0.53
2:I:256:U:H6	2:I:256:U:O5'	1.90	0.53
26:P:208:GLU:HA	26:P:236:VAL:HA	1.89	0.53
32:2:1127:A:O2'	32:2:1128:C:H5'	2.08	0.53
20:O:789:ALA:HB1	20:O:794:PRO:HA	1.91	0.53
26:P:154:SER:HA	26:P:182:THR:HA	1.90	0.53
10:v:49:ALA:O	10:v:56:VAL:HA	2.08	0.53
11:w:59:GLU:O	11:w:74:GLY:HA2	2.09	0.53
32:2:1094:G:C6	32:2:1149:G:C6	2.97	0.53
4:J:272:ASP:CB	4:J:274:PRO:CD	2.86	0.53
23:T:191:ASN:CB	15:u:89:ARG:CA	2.87	0.53
29:W:11:ALA:HB3	29:W:24:ASN:CB	2.39	0.53
31:p:270:ILE:C	31:p:274:LEU:H	2.17	0.53
32:2:52:A:N6	32:2:64:G:O6	2.42	0.52
32:2:58:A:H2'	32:2:59:C:O4'	2.09	0.52
27:R:66:ALA:O	27:R:70:MET:CB	2.57	0.52
32:2:139:G:H2'	32:2:140:G:O5'	2.09	0.52
26:P:1201:ASP:O	26:P:1218:TYR:HA	2.10	0.52
26:P:1298:SER:C	26:P:1300:LEU:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:1305:GLN:O	26:P:1309:SER:CB	2.56	0.52
2:I:8:C:N3	5:1:1:A:N1	2.57	0.52
5:1:158:G:H2'	5:1:159:G:H8	1.74	0.52
26:P:1219:MET:HA	26:P:1224:THR:O	2.10	0.52
29:W:60:THR:HA	29:W:82:GLY:O	2.10	0.52
20:O:246:VAL:C	20:O:249:PRO:HD3	2.35	0.52
20:O:421:SER:O	20:O:424:PRO:CD	2.58	0.52
20:O:599:ALA:N	20:O:600:PRO:CD	2.70	0.52
26:P:924:PHE:HA	26:P:944:ASN:O	2.10	0.52
32:2:73:U:H2'	32:2:74:C:C6	2.45	0.52
32:2:1120:G:H2'	32:2:1121:U:C6	2.45	0.52
32:2:1148:U:H2'	32:2:1149:G:C8	2.45	0.52
20:O:427:ASP:CB	20:O:428:PRO:CD	2.88	0.51
20:O:522:LEU:O	20:O:525:PRO:HD3	2.08	0.51
23:T:191:ASN:HA	15:u:89:ARG:HA	1.92	0.51
14:t:19:LEU:HA	14:t:93:ARG:H	1.76	0.51
20:O:202:ASN:O	20:O:206:PRO:HG3	2.10	0.51
32:2:1140:U:H2'	32:2:1141:C:H6	1.75	0.51
2:I:253:G:O6	23:T:410:TRP:CB	2.58	0.51
2:I:263:C:H2'	2:I:264:U:C6	2.45	0.51
32:2:72:C:H2'	32:2:73:U:C6	2.45	0.51
32:2:1097:G:C2	32:2:1146:G:C5	2.98	0.51
23:T:426:CYS:O	23:T:429:LYS:N	2.37	0.51
5:1:439:U:H2'	5:1:440:A:C8	2.46	0.51
20:O:598:LEU:O	20:O:600:PRO:HD2	2.11	0.51
20:O:530:ALA:CA	20:O:532:PRO:HD3	2.41	0.51
20:O:874:GLU:O	20:O:878:ILE:N	2.36	0.51
26:P:106:THR:O	26:P:108:ASP:N	2.44	0.51
5:1:511:A:H2'	5:1:512:A:C8	2.46	0.51
5:1:516:U:H6	5:1:516:U:O5'	1.94	0.51
27:R:60:GLN:HA	27:R:63:ALA:HB3	1.93	0.51
32:2:1139:G:H2'	32:2:1140:U:H6	1.76	0.51
19:K:342:ASN:O	19:K:346:GLU:O	2.28	0.51
23:T:220:PRO:HB2	23:T:222:MET:O	2.11	0.51
20:O:597:PHE:O	20:O:600:PRO:HG2	2.11	0.50
10:v:28:THR:O	10:v:49:ALA:HA	2.11	0.50
32:2:1097:G:C2	32:2:1098:C:C4	3.00	0.50
5:1:326:G:H3'	5:1:327:A:C8	2.44	0.50
21:U:68:CYS:O	21:U:72:ASN:N	2.43	0.50
23:T:377:VAL:O	23:T:378:ASP:CB	2.60	0.50
27:R:112:ILE:HA	27:R:179:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:264:U:H2'	2:I:265:A:C8	2.46	0.50
29:W:25:VAL:CB	29:W:31:LEU:HA	2.41	0.50
32:2:42:U:C4	32:2:43:G:C8	3.00	0.50
32:2:52:A:H2'	32:2:53:G:H8	1.76	0.50
32:2:67:A:HO2'	32:2:68:U:H6	1.49	0.50
15:u:53:LYS:O	15:u:74:GLU:HA	2.12	0.50
26:P:1234:LYS:O	26:P:1237:VAL:N	2.44	0.50
32:2:43:G:C4	32:2:44:U:C6	3.00	0.50
32:2:1151:U:H2'	32:2:1152:U:C6	2.46	0.50
18:B:133:ILE:HA	18:B:155:PHE:HA	1.94	0.49
24:S:10:MET:HA	24:S:88:ARG:O	2.12	0.49
14:t:23:THR:HA	14:t:48:PRO:HD3	1.93	0.49
32:2:64:G:H2'	32:2:65:A:C8	2.47	0.49
32:2:1139:G:HO2'	32:2:1140:U:H6	1.60	0.49
20:O:214:GLU:O	20:O:218:ARG:N	2.40	0.49
2:I:254:U:O2	2:I:254:U:H2'	2.11	0.49
2:I:264:U:O2	32:2:37:G:N2	2.45	0.49
23:T:191:ASN:C	23:T:193:ILE:N	2.70	0.49
29:W:123:THR:O	29:W:125:LYS:N	2.45	0.49
5:1:547:C:H5''	14:h:34:PRO:HG2	1.94	0.49
26:P:514:THR:O	26:P:886:PHE:HA	2.12	0.49
5:1:401:U:H2'	5:1:402:G:H8	1.78	0.49
14:h:16:THR:HA	14:h:25:VAL:O	2.13	0.49
29:W:11:ALA:HB3	29:W:24:ASN:C	2.37	0.49
20:O:173:ILE:HA	20:O:181:ARG:CB	2.43	0.49
20:O:598:LEU:O	20:O:600:PRO:CD	2.60	0.49
26:P:671:GLU:C	26:P:673:ASP:H	2.21	0.49
5:1:78:A:H4'	5:1:79:A:H3'	1.95	0.48
5:1:389:G:O6	5:1:430:U:O4	2.30	0.48
2:I:267:A:C6	32:2:34:G:N1	2.80	0.48
11:w:27:VAL:O	11:w:40:LYS:HA	2.13	0.48
32:2:67:A:O2'	32:2:68:U:P	2.70	0.48
32:2:1116:A:O2'	32:2:1117:G:H5'	2.13	0.48
20:O:916:MET:O	20:O:919:ILE:N	2.46	0.48
2:I:267:A:H2'	2:I:268:U:C6	2.49	0.48
22:V:119:GLU:C	22:V:121:ARG:H	2.21	0.48
20:O:524:THR:N	20:O:525:PRO:CD	2.77	0.48
2:I:264:U:C2	32:2:37:G:C2	3.02	0.48
5:1:162:U:H2'	5:1:163:G:H8	1.79	0.48
20:O:720:PRO:HD2	20:O:723:GLU:CB	2.44	0.48
32:2:1093:C:C2	32:2:1094:G:C8	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:6:U:H2'	5:1:7:A:H8	1.78	0.48
5:1:392:A:N6	5:1:424:U:O3'	2.46	0.48
26:P:847:LEU:N	26:P:865:ILE:O	2.40	0.48
30:Y:70:GLY:O	30:Y:72:ALA:N	2.45	0.48
5:1:497:G:N2	5:1:498:U:O4	2.46	0.48
26:P:1198:ILE:O	26:P:1221:LEU:N	2.42	0.48
32:2:1152:U:H2'	32:2:1153:C:H6	1.79	0.48
4:J:274:PRO:CD	4:J:275:SER:N	2.77	0.47
5:1:170:G:H2'	5:1:171:A:H8	1.79	0.47
20:O:628:ILE:N	20:O:629:PRO:CD	2.77	0.47
26:P:406:GLN:HA	26:P:455:LEU:O	2.13	0.47
5:1:560:A:N6	12:f:32:LYS:O	2.47	0.47
26:P:632:ILE:HA	26:P:646:LEU:HA	1.95	0.47
32:2:1097:G:C6	32:2:1146:G:C6	3.03	0.47
32:2:1126:G:HO2'	32:2:1127:A:H8	1.62	0.47
32:2:1126:G:O2'	32:2:1127:A:H8	1.97	0.47
26:P:565:ASN:C	26:P:567:SER:H	2.22	0.47
32:2:1097:G:H2'	32:2:1098:C:H5	1.78	0.47
32:2:142:C:H2'	32:2:143:G:C8	2.49	0.47
32:2:1140:U:H2'	32:2:1141:C:C6	2.50	0.47
32:2:1162:U:O2'	32:2:1163:C:H5'	2.14	0.47
2:I:113:N:H5'	17:D:606:ARG:HA	1.97	0.47
23:T:62:PHE:HA	23:T:376:GLN:O	2.14	0.47
26:P:374:LYS:C	26:P:376:ASP:H	2.23	0.47
29:W:51:THR:C	29:W:53:PRO:HD2	2.40	0.47
32:2:38:U:H2'	32:2:39:A:C8	2.50	0.47
32:2:143:G:H2'	32:2:144:G:C8	2.50	0.47
5:1:198:U:H2'	5:1:199:G:H8	1.80	0.47
26:P:831:THR:HA	26:P:836:TRP:HA	1.96	0.47
5:1:249:G:H2'	5:1:250:G:H8	1.80	0.46
5:1:424:U:H2'	5:1:425:A:C8	2.50	0.46
27:R:108:ALA:O	27:R:154:TYR:HA	2.15	0.46
32:2:139:G:C2'	32:2:140:G:O5'	2.62	0.46
5:1:342:C:N4	5:1:480:C:OP2	2.48	0.46
15:u:56:ALA:HB2	15:u:72:VAL:HA	1.96	0.46
2:I:264:U:O2	32:2:37:G:C2	2.68	0.46
26:P:1101:PRO:C	26:P:1103:GLY:H	2.23	0.46
29:W:93:LEU:C	29:W:95:PRO:HD3	2.40	0.46
31:p:396:LEU:O	31:p:401:GLY:HA2	2.15	0.46
32:2:1143:C:H4'	32:2:1144:U:H2'	1.96	0.46
5:1:46:C:H2'	5:1:47:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:912:PRO:O	20:O:916:MET:N	2.23	0.46
32:2:144:G:H2'	32:2:145:G:H8	1.80	0.46
20:O:173:ILE:HA	20:O:181:ARG:HA	1.98	0.46
19:K:185:TYR:HA	19:K:189:ARG:HA	1.98	0.46
20:O:674:ASP:O	20:O:677:LYS:N	2.49	0.46
20:O:720:PRO:O	20:O:720:PRO:CD	2.62	0.46
23:T:219:THR:N	23:T:220:PRO:HD3	2.30	0.46
26:P:1098:ILE:O	26:P:1106:PHE:HA	2.15	0.46
26:P:1199:ILE:HA	26:P:1220:GLY:HA2	1.96	0.46
12:x:27:VAL:O	12:x:39:ARG:HA	2.16	0.46
31:p:462:HIS:O	31:p:463:SER:C	2.58	0.46
32:2:120:G:H2'	32:2:121:C:C6	2.51	0.46
19:K:441:SER:C	19:K:443:GLU:N	2.74	0.46
31:p:469:ILE:O	31:p:470:ASN:C	2.58	0.46
32:2:35:U:O2	32:2:36:A:N6	2.49	0.46
32:2:1139:G:H2'	32:2:1140:U:C5	2.51	0.46
5:1:191:C:H2'	5:1:192:A:H8	1.81	0.46
5:1:529:U:H2'	5:1:530:G:H8	1.81	0.46
26:P:702:ILE:O	26:P:715:VAL:HA	2.15	0.46
32:2:65:A:H2'	32:2:66:A:O4'	2.16	0.46
32:2:144:G:H2'	32:2:145:G:C8	2.51	0.46
23:T:150:PRO:CG	23:T:154:THR:H	2.24	0.45
32:2:1139:G:C6	32:2:1140:U:C4	3.04	0.45
5:1:486:C:H2'	5:1:487:A:C8	2.51	0.45
5:1:535:G:H2'	5:1:536:A:H8	1.81	0.45
32:2:141:A:C2'	32:2:142:C:H6	2.29	0.45
20:O:531:GLU:N	20:O:532:PRO:CD	2.62	0.45
20:O:595:LYS:N	20:O:596:PRO:HD3	2.31	0.45
2:I:258:A:H2'	2:I:259:U:C6	2.52	0.45
20:O:865:ALA:HB3	20:O:905:ALA:HB1	1.97	0.45
32:2:141:A:HO2'	32:2:142:C:H6	1.58	0.45
32:2:1149:G:H2'	32:2:1150:U:C6	2.51	0.45
10:d:27:ALA:HB2	10:d:52:PRO:HD3	1.98	0.45
32:2:143:G:H2'	32:2:144:G:H8	1.81	0.45
20:O:398:GLU:N	20:O:399:PRO:HD3	2.32	0.45
20:O:421:SER:O	20:O:424:PRO:HD3	2.17	0.45
2:I:256:U:H3	32:2:43:G:H1	1.65	0.45
20:O:783:VAL:O	20:O:787:ILE:N	2.50	0.45
5:1:429:C:H2'	5:1:430:U:H6	1.81	0.45
5:1:455:U:H2'	5:1:456:A:H8	1.82	0.45
5:1:538:C:H2'	5:1:539:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:680:PRO:O	20:O:680:PRO:CD	2.63	0.45
26:P:59:TYR:O	26:P:1230:PRO:HA	2.16	0.45
26:P:952:ARG:HA	26:P:972:LYS:O	2.17	0.45
26:P:1249:GLU:O	26:P:1252:ASP:N	2.50	0.45
5:1:334:U:H2'	5:1:335:G:C8	2.52	0.44
20:O:522:LEU:O	20:O:525:PRO:CD	2.66	0.44
15:u:72:VAL:CB	15:u:91:ILE:O	2.66	0.44
20:O:423:ILE:N	20:O:424:PRO:HD3	2.32	0.44
20:O:427:ASP:O	20:O:431:ALA:HB2	2.17	0.44
26:P:443:LYS:C	26:P:445:GLY:H	2.24	0.44
32:2:56:U:H1'	32:2:59:C:H5	1.82	0.44
32:2:67:A:O2'	32:2:68:U:C6	2.65	0.44
32:2:149:A:H2'	32:2:150:G:H8	1.82	0.44
5:1:328:G:H2'	5:1:329:A:H8	1.83	0.44
5:1:403:A:H2'	5:1:404:A:H8	1.81	0.44
6:G:187:ILE:HA	6:G:202:GLN:O	2.17	0.44
20:O:716:PRO:O	20:O:756:ALA:HB1	2.18	0.44
32:2:52:A:H2'	32:2:53:G:C8	2.51	0.44
5:1:380:G:O6	5:1:438:U:O4	2.36	0.44
26:P:62:HIS:HA	26:P:1227:CYS:O	2.18	0.44
9:b:31:ILE:O	9:b:48:CYS:HA	2.17	0.44
20:O:480:ALA:N	20:O:481:PRO:HD3	2.33	0.44
20:O:593:ARG:O	20:O:596:PRO:CG	2.65	0.44
11:w:45:GLY:HA3	12:x:13:VAL:O	2.18	0.44
32:2:59:C:H3'	32:2:60:A:H8	1.82	0.44
5:1:478:A:H2'	5:1:479:G:H8	1.81	0.44
20:O:284:PRO:CD	20:O:285:ASP:N	2.81	0.44
21:U:235:GLU:O	21:U:239:LYS:CB	2.65	0.44
32:2:45:U:O5'	32:2:45:U:H6	2.00	0.44
32:2:1138:G:C6	32:2:1139:G:O6	2.71	0.44
21:U:87:GLY:HA2	32:2:44:U:OP1	2.18	0.44
26:P:361:LYS:C	26:P:363:VAL:H	2.25	0.44
9:s:33:GLN:O	9:s:45:LEU:HA	2.16	0.44
32:2:1094:G:H2'	32:2:1095:U:H6	1.83	0.44
5:1:73:A:O2'	5:1:75:G:OP1	2.28	0.44
26:P:393:VAL:HA	26:P:404:LEU:O	2.18	0.44
5:1:73:A:H2'	5:1:75:G:C8	2.53	0.43
5:1:94:A:N6	5:1:105:U:O4	2.51	0.43
5:1:307:G:H2'	5:1:308:A:H8	1.84	0.43
21:U:200:VAL:HA	21:U:209:ILE:O	2.17	0.43
32:2:64:G:C2	32:2:65:A:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:449:HIS:O	23:T:453:LEU:CB	2.66	0.43
14:t:26:TRP:O	14:t:43:VAL:HA	2.17	0.43
5:1:521:G:H2'	5:1:522:A:H8	1.83	0.43
29:W:11:ALA:HB2	29:W:26:ASP:CB	2.48	0.43
5:1:396:U:H5	5:1:416:G:H1	1.65	0.43
20:O:367:HIS:CA	20:O:369:PRO:HD3	2.48	0.43
24:S:15:PRO:HB3	24:S:44:ARG:O	2.19	0.43
32:2:1099:G:H2'	32:2:1100:A:H8	1.82	0.43
23:T:191:ASN:CA	15:u:89:ARG:HA	2.48	0.43
26:P:826:THR:O	26:P:840:GLN:HA	2.18	0.43
32:2:140:G:H2'	32:2:141:A:H8	1.83	0.43
5:1:192:A:H2'	5:1:193:A:H8	1.83	0.43
20:O:927:ALA:C	20:O:929:ASN:N	2.77	0.43
26:P:776:SER:O	26:P:821:CYS:HA	2.18	0.43
5:1:64:A:N6	5:1:140:C:O2	2.52	0.43
32:2:1094:G:H2'	32:2:1095:U:C6	2.54	0.43
2:I:253:G:N3	2:I:253:G:H2'	2.34	0.43
25:Q:367:LEU:C	25:Q:369:SER:H	2.26	0.43
26:P:704:SER:O	26:P:712:PHE:C	2.62	0.43
29:W:8:VAL:HA	29:W:25:VAL:CB	2.49	0.43
5:1:350:U:H1'	5:1:351:U:H5	1.84	0.43
5:1:556:U:H3'	5:1:557:U:H2'	2.00	0.43
20:O:675:LEU:HA	20:O:676:ASP:HA	1.55	0.43
23:T:185:PHE:O	23:T:189:TRP:N	2.51	0.43
26:P:155:GLY:HA3	26:P:179:LEU:O	2.19	0.43
32:2:78:G:H2'	32:2:79:A:H5''	2.01	0.43
5:1:325:A:H3'	5:1:326:G:H8	1.83	0.42
5:1:328:G:H2'	5:1:329:A:C8	2.55	0.42
29:W:13:GLN:CB	29:W:24:ASN:H	2.32	0.42
29:W:23:TYR:H	29:W:33:ASP:CB	2.32	0.42
1:F:197:HIS:HA	1:F:204:SER:HA	2.01	0.42
5:1:171:A:H61	5:1:540:G:H1	1.67	0.42
5:1:321:C:H2'	5:1:322:A:H8	1.84	0.42
5:1:418:U:H2'	5:1:419:G:C8	2.55	0.42
20:O:842:LEU:HA	20:O:845:ALA:HB3	2.01	0.42
29:W:52:LYS:O	29:W:54:THR:N	2.52	0.42
32:2:1153:C:H2'	32:2:1154:U:H6	1.84	0.42
5:1:403:A:H2'	5:1:404:A:C8	2.55	0.42
20:O:927:ALA:O	20:O:929:ASN:N	2.52	0.42
29:W:11:ALA:CB	29:W:25:VAL:N	2.79	0.42
23:T:33:TYR:O	23:T:34:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:496:SER:CB	26:P:497:PRO:HD3	2.49	0.42
32:2:1146:G:H2'	32:2:1147:A:H8	1.84	0.42
18:B:108:THR:HA	18:B:154:VAL:HA	2.00	0.42
20:O:431:ALA:CB	20:O:469:SER:CB	2.98	0.42
32:2:66:A:OP2	32:2:66:A:C8	2.70	0.42
5:1:337:A:H2'	5:1:338:G:H8	1.84	0.42
5:1:52:U:H2'	5:1:53:G:C8	2.55	0.42
5:1:444:G:H2'	5:1:445:G:C8	2.55	0.42
20:O:681:PRO:O	20:O:681:PRO:CD	2.65	0.42
23:T:453:LEU:HA	27:R:200:ARG:CB	2.49	0.42
26:P:879:PHE:HA	26:P:880:PRO:HD3	1.83	0.42
20:O:595:LYS:N	20:O:596:PRO:CD	2.83	0.42
21:U:213:LEU:C	21:U:215:PRO:HD2	2.45	0.42
27:R:10:THR:HA	27:R:56:GLU:HA	2.02	0.42
29:W:5:PRO:O	29:W:8:VAL:N	2.52	0.42
29:W:66:MET:C	29:W:68:PRO:HD3	2.45	0.42
14:t:16:THR:HA	14:t:25:VAL:O	2.20	0.42
5:1:323:A:H2'	5:1:324:A:C8	2.55	0.41
5:1:443:U:H2'	5:1:444:G:H8	1.84	0.41
32:2:1097:G:C4	32:2:1146:G:C2	3.07	0.41
32:2:141:A:H2'	32:2:142:C:H6	1.78	0.41
32:2:1089:G:H2'	32:2:1090:A:C8	2.55	0.41
32:2:1097:G:N1	32:2:1146:G:C5	2.88	0.41
32:2:1143:C:H4'	32:2:1144:U:H3'	2.01	0.41
5:1:21:G:H2'	5:1:22:A:H8	1.86	0.41
5:1:413:U:H2'	5:1:414:A:C8	2.56	0.41
26:P:1046:GLY:O	26:P:1073:LYS:HA	2.21	0.41
29:W:17:ASP:C	29:W:19:PHE:N	2.74	0.41
32:2:1092:A:H3'	32:2:1093:C:C6	2.47	0.41
5:1:91:U:H2'	5:1:92:G:C8	2.56	0.41
5:1:389:G:N2	5:1:430:U:O2	2.33	0.41
5:1:444:G:H2'	5:1:445:G:H8	1.86	0.41
5:1:498:U:H1'	5:1:514:A:N1	2.35	0.41
32:2:60:A:H3'	32:2:61:A:H8	1.84	0.41
32:2:74:C:H6	32:2:74:C:O5'	2.02	0.41
5:1:443:U:H2'	5:1:444:G:C8	2.55	0.41
26:P:298:LEU:HA	26:P:299:PRO:HD3	1.93	0.41
32:2:1098:C:O5'	32:2:1098:C:C6	2.69	0.41
5:1:438:U:H2'	5:1:439:U:C6	2.56	0.41
5:1:453:U:H2'	5:1:454:G:C8	2.56	0.41
10:v:30:ARG:O	10:v:47:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:195:C:H42	5:1:243:U:H3	1.68	0.41
20:O:237:LYS:N	20:O:238:PRO:HD3	2.36	0.41
4:J:274:PRO:HD2	4:J:275:SER:H	1.84	0.41
5:1:327:A:H8	5:1:327:A:O5'	2.03	0.41
18:B:26:ARG:HA	18:B:27:PRO:HD3	1.97	0.41
20:O:916:MET:O	20:O:917:ASN:C	2.63	0.41
23:T:149:ASP:N	23:T:150:PRO:HD2	2.35	0.41
26:P:978:ASP:O	26:P:998:ALA:HA	2.20	0.41
26:P:1007:LYS:O	26:P:1019:ILE:HA	2.21	0.41
26:P:1056:LYS:C	26:P:1058:GLN:H	2.28	0.41
32:2:118:U:O2'	32:2:120:G:OP1	2.25	0.41
2:I:113:N:H4'	17:D:607:ASN:N	2.31	0.41
5:1:510:G:H2'	5:1:511:A:C8	2.56	0.41
22:V:157:LYS:O	22:V:158:ARG:C	2.64	0.41
29:W:99:GLN:HA	29:W:123:THR:O	2.21	0.41
5:1:454:G:H2'	5:1:455:U:H6	1.86	0.40
32:2:45:U:H2'	32:2:46:C:C6	2.56	0.40
32:2:1101:C:O2	32:2:1101:C:C2'	2.70	0.40
32:2:1118:U:H2'	32:2:1119:C:H6	1.86	0.40
5:1:125:A:H2'	5:1:126:A:C8	2.56	0.40
5:1:416:G:H4'	5:1:417:A:H5'	2.03	0.40
20:O:839:THR:N	20:O:840:PRO:HD2	2.36	0.40
25:Q:363:TYR:O	25:Q:365:GLY:N	2.53	0.40
29:W:7:ILE:HA	29:W:27:LYS:N	2.30	0.40
32:2:47:U:O2	32:2:47:U:H2'	2.21	0.40
32:2:83:U:H2'	32:2:84:C:C6	2.56	0.40
32:2:1125:U:O2'	32:2:1126:G:H8	2.00	0.40
32:2:1145:U:O2	32:2:1145:U:C2'	2.69	0.40
26:P:672:LEU:C	26:P:674:THR:H	2.29	0.40
2:I:8:C:C4	5:1:1:A:N6	2.89	0.40
23:T:367:ASP:C	23:T:369:THR:H	2.29	0.40
20:O:421:SER:C	20:O:424:PRO:HD3	2.46	0.40
26:P:190:ILE:C	26:P:192:TYR:H	2.30	0.40
31:p:530:ILE:HA	31:p:598:ILE:O	2.22	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	F	259/523 (50%)	251 (97%)	8 (3%)	0	100	100
3	E	542/544 (100%)	521 (96%)	21 (4%)	0	100	100
4	J	101/620 (16%)	92 (91%)	8 (8%)	1 (1%)	12	48
6	G	235/492 (48%)	222 (94%)	13 (6%)	0	100	100
7	A	126/298 (42%)	116 (92%)	10 (8%)	0	100	100
8	C	193/231 (84%)	183 (95%)	10 (5%)	0	100	100
9	b	117/196 (60%)	110 (94%)	7 (6%)	0	100	100
9	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
10	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
10	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
11	e	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	9	40
11	w	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
12	f	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
12	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
13	g	68/77 (88%)	62 (91%)	5 (7%)	1 (2%)	8	39
13	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	2	17
14	h	101/146 (69%)	98 (97%)	3 (3%)	0	100	100
14	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
15	i	95/110 (86%)	91 (96%)	4 (4%)	0	100	100
15	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
16	H	186/261 (71%)	180 (97%)	6 (3%)	0	100	100
17	D	570/629 (91%)	554 (97%)	16 (3%)	0	100	100
18	B	182/300 (61%)	169 (93%)	13 (7%)	0	100	100
19	K	402/583 (69%)	379 (94%)	19 (5%)	4 (1%)	12	48
20	O	810/971 (83%)	772 (95%)	35 (4%)	3 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	166/282 (59%)	141 (85%)	24 (14%)	1 (1%)	21	59
22	V	101/280 (36%)	90 (89%)	10 (10%)	1 (1%)	12	48
23	T	454/530 (86%)	414 (91%)	40 (9%)	0	100	100
24	S	90/107 (84%)	79 (88%)	11 (12%)	0	100	100
25	Q	214/436 (49%)	202 (94%)	11 (5%)	1 (0%)	24	63
26	P	1170/1361 (86%)	1055 (90%)	105 (9%)	10 (1%)	14	50
27	R	165/213 (78%)	161 (98%)	3 (2%)	1 (1%)	21	59
28	Z	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	43
29	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	12
30	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	10	43
31	p	445/849 (52%)	431 (97%)	13 (3%)	1 (0%)	43	77
All	All	7874/11564 (68%)	7373 (94%)	460 (6%)	41 (0%)	26	63

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	Q	368	ILE
26	P	1299	ILE
29	W	34	LEU
29	W	52	LYS
13	y	50	ASP
4	J	274	PRO
19	K	356	ARG
19	K	370	PRO
26	P	363	VAL
26	P	413	ILE
26	P	626	PRO
26	P	629	GLY
29	W	17	ASP
29	W	18	HIS
29	W	51	THR
29	W	68	PRO
29	W	121	PRO
29	W	124	LEU
30	Y	71	GLN
11	e	34	GLN
27	R	48	ALA
29	W	29	VAL

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Mol	Chain	Res	Type
31	p	273	LYS
13	g	21	GLY
19	K	353	THR
19	K	442	ASP
20	O	713	LYS
20	O	717	THR
26	P	107	ALA
26	P	628	ALA
28	Z	19	ILE
29	W	12	PRO
21	U	232	GLY
22	V	181	HIS
13	y	30	ARG
13	y	60	GLN
26	P	364	THR
26	P	486	PRO
29	W	159	VAL
20	O	614	PRO
26	P	1031	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	11/451 (2%)	11 (100%)	0	100	100
3	E	12/519 (2%)	12 (100%)	0	100	100
4	J	3/568 (0%)	3 (100%)	0	100	100
6	G	8/448 (2%)	8 (100%)	0	100	100
7	A	6/273 (2%)	6 (100%)	0	100	100
8	C	8/214 (4%)	8 (100%)	0	100	100
9	b	3/176 (2%)	3 (100%)	0	100	100
9	s	1/176 (1%)	1 (100%)	0	100	100
10	d	7/89 (8%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	v	4/89 (4%)	4 (100%)	0	100	100
11	e	5/83 (6%)	5 (100%)	0	100	100
11	w	5/83 (6%)	5 (100%)	0	100	100
12	f	3/77 (4%)	3 (100%)	0	100	100
12	x	3/77 (4%)	3 (100%)	0	100	100
13	g	1/66 (2%)	1 (100%)	0	100	100
13	y	2/66 (3%)	2 (100%)	0	100	100
14	h	3/129 (2%)	3 (100%)	0	100	100
14	t	3/129 (2%)	3 (100%)	0	100	100
15	i	4/103 (4%)	4 (100%)	0	100	100
15	u	3/103 (3%)	3 (100%)	0	100	100
16	H	5/234 (2%)	5 (100%)	0	100	100
17	D	12/603 (2%)	12 (100%)	0	100	100
18	B	9/265 (3%)	9 (100%)	0	100	100
19	K	10/538 (2%)	10 (100%)	0	100	100
20	O	42/867 (5%)	42 (100%)	0	100	100
21	U	7/236 (3%)	7 (100%)	0	100	100
22	V	1/259 (0%)	1 (100%)	0	100	100
23	T	10/492 (2%)	10 (100%)	0	100	100
24	S	4/97 (4%)	4 (100%)	0	100	100
25	Q	18/392 (5%)	18 (100%)	0	100	100
26	P	45/1244 (4%)	45 (100%)	0	100	100
27	R	5/189 (3%)	5 (100%)	0	100	100
28	Z	1/77 (1%)	1 (100%)	0	100	100
29	W	8/219 (4%)	8 (100%)	0	100	100
30	Y	1/100 (1%)	1 (100%)	0	100	100
31	p	17/768 (2%)	17 (100%)	0	100	100
All	All	290/10499 (3%)	290 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	31/373 (8%)	11 (35%)	0
32	2	138/1175 (11%)	53 (38%)	27 (19%)
5	1	556/568 (97%)	118 (21%)	9 (1%)
All	All	725/2116 (34%)	182 (25%)	36 (4%)

All (182) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	247	U
2	I	248	A
2	I	249	C
2	I	250	U
2	I	251	A
2	I	252	A
2	I	253	G
2	I	254	U
2	I	258	A
2	I	265	A
2	I	267	A
5	1	11	U
5	1	12	A
5	1	40	A
5	1	41	C
5	1	55	G
5	1	56	C
5	1	62	A
5	1	63	U
5	1	64	A
5	1	65	G
5	1	66	U
5	1	67	A
5	1	74	C
5	1	75	G
5	1	79	A
5	1	80	G
5	1	87	U
5	1	97	A
5	1	98	U
5	1	100	A
5	1	101	U
5	1	103	G

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Mol	Chain	Res	Type
5	1	107	A
5	1	113	G
5	1	114	U
5	1	117	U
5	1	133	G
5	1	134	G
5	1	141	A
5	1	142	C
5	1	147	A
5	1	149	G
5	1	150	G
5	1	151	C
5	1	152	G
5	1	153	C
5	1	154	G
5	1	167	G
5	1	171	A
5	1	176	U
5	1	180	U
5	1	181	U
5	1	182	C
5	1	186	U
5	1	187	G
5	1	205	U
5	1	206	C
5	1	218	U
5	1	219	U
5	1	220	G
5	1	227	U
5	1	228	U
5	1	230	G
5	1	254	U
5	1	255	U
5	1	257	G
5	1	258	U
5	1	259	U
5	1	260	U
5	1	269	U
5	1	270	G
5	1	271	G
5	1	272	A
5	1	278	U

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Mol	Chain	Res	Type
5	1	279	U
5	1	280	G
5	1	287	A
5	1	290	U
5	1	326	G
5	1	327	A
5	1	328	G
5	1	343	A
5	1	352	G
5	1	365	U
5	1	369	G
5	1	377	U
5	1	378	U
5	1	385	U
5	1	386	G
5	1	389	G
5	1	393	G
5	1	394	A
5	1	395	U
5	1	399	A
5	1	400	A
5	1	407	U
5	1	409	A
5	1	416	G
5	1	418	U
5	1	422	G
5	1	424	U
5	1	426	U
5	1	427	G
5	1	443	U
5	1	460	U
5	1	466	U
5	1	468	U
5	1	477	G
5	1	482	G
5	1	493	G
5	1	504	U
5	1	505	U
5	1	506	A
5	1	508	G
5	1	513	A
5	1	515	A

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Mol	Chain	Res	Type
5	1	540	G
5	1	542	U
5	1	551	U
5	1	553	A
5	1	554	U
5	1	555	U
5	1	559	G
5	1	560	A
5	1	562	U
5	1	563	U
5	1	564	A
5	1	565	U
32	2	33	U
32	2	41	C
32	2	46	C
32	2	47	U
32	2	48	U
32	2	49	U
32	2	50	U
32	2	66	A
32	2	67	A
32	2	68	U
32	2	79	A
32	2	83	U
32	2	111	C
32	2	112	A
32	2	113	U
32	2	117	U
32	2	140	G
32	2	141	A
32	2	142	C
32	2	143	G
32	2	144	G
32	2	1094	G
32	2	1095	U
32	2	1096	C
32	2	1097	G
32	2	1098	C
32	2	1100	A
32	2	1101	C
32	2	1102	C
32	2	1103	C

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Mol	Chain	Res	Type
32	2	1104	U
32	2	1105	C
32	2	1106	G
32	2	1107	C
32	2	1108	A
32	2	1119	C
32	2	1120	G
32	2	1121	U
32	2	1122	U
32	2	1123	C
32	2	1124	U
32	2	1125	U
32	2	1126	G
32	2	1130	U
32	2	1139	G
32	2	1141	C
32	2	1142	G
32	2	1143	C
32	2	1144	U
32	2	1145	U
32	2	1146	G
32	2	1150	U
32	2	1151	U

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	1	86	A
5	1	100	A
5	1	113	G
5	1	151	C
5	1	152	G
5	1	258	U
5	1	268	C
5	1	399	A
5	1	505	U
32	2	32	G
32	2	46	C
32	2	66	A
32	2	67	A
32	2	78	G
32	2	110	A

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Mol	Chain	Res	Type
32	2	1095	U
32	2	1096	C
32	2	1097	G
32	2	1100	A
32	2	1101	C
32	2	1102	C
32	2	1105	C
32	2	1107	C
32	2	1119	C
32	2	1120	G
32	2	1121	U
32	2	1122	U
32	2	1123	C
32	2	1124	U
32	2	1125	U
32	2	1138	G
32	2	1141	C
32	2	1142	G
32	2	1144	U
32	2	1145	U
32	2	1150	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

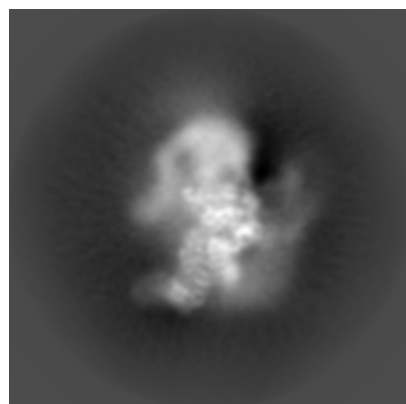
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13033. These allow visual inspection of the internal detail of the map and identification of artifacts.

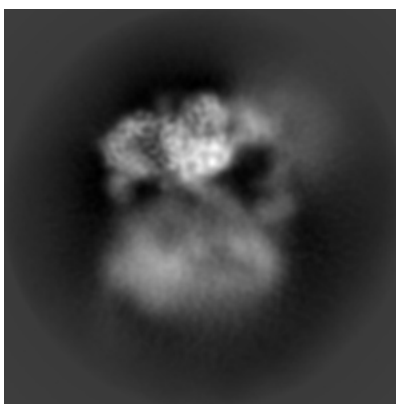
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

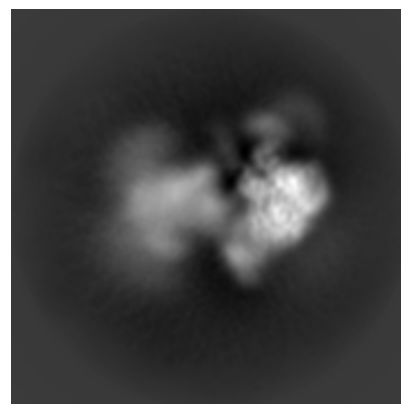
6.1.1 Primary map



X

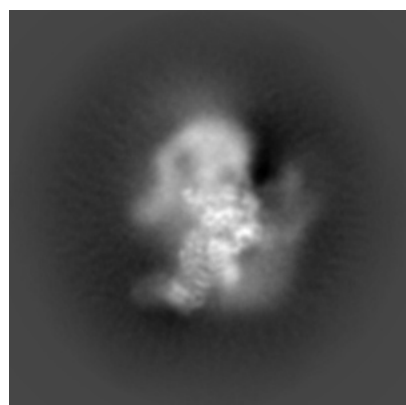


Y

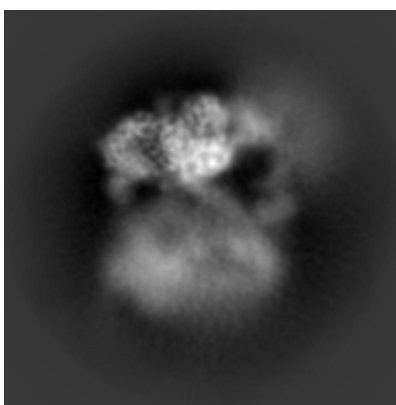


Z

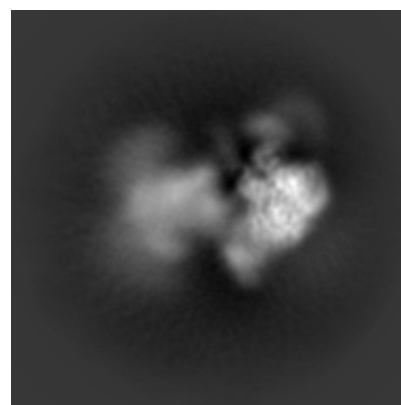
6.1.2 Raw map



X



Y

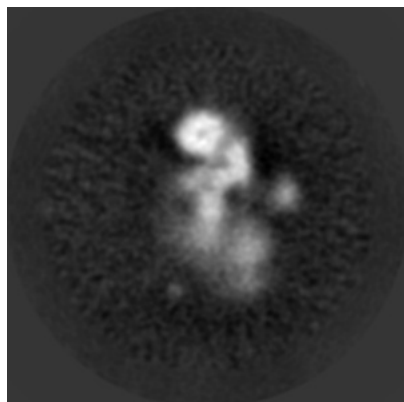


Z

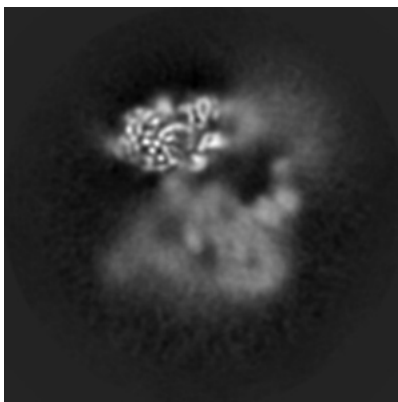
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

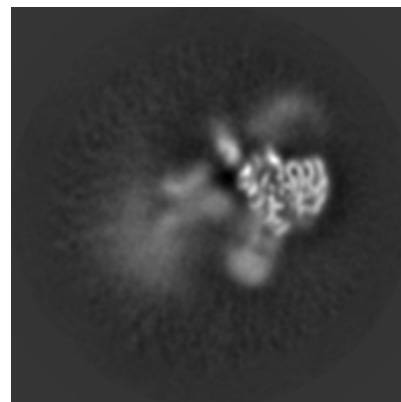
6.2.1 Primary map



X Index: 200

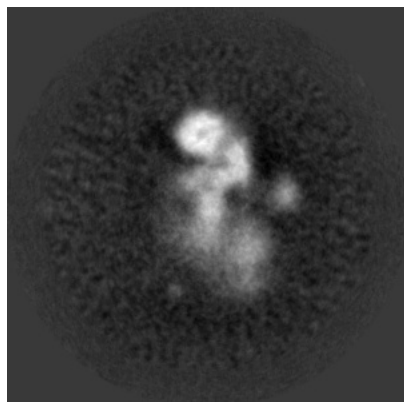


Y Index: 200

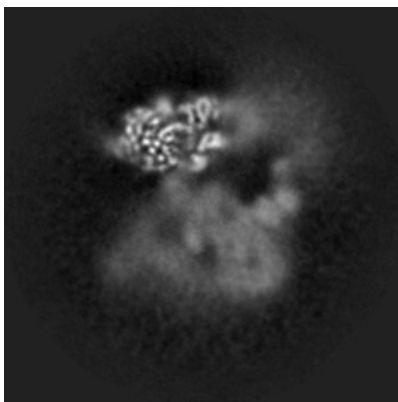


Z Index: 200

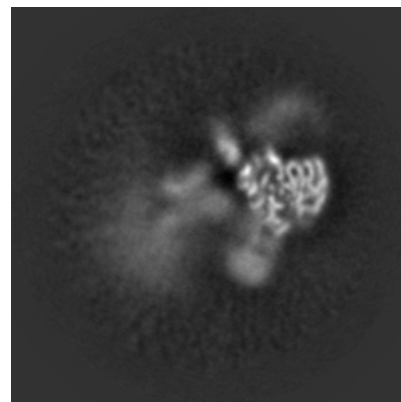
6.2.2 Raw map



X Index: 200



Y Index: 200

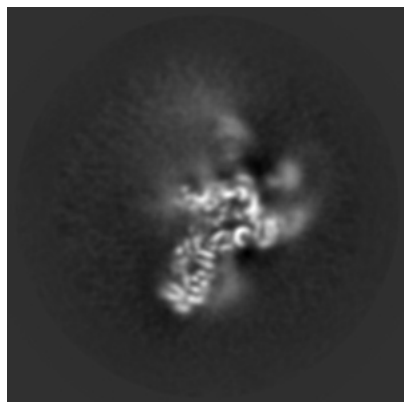


Z Index: 200

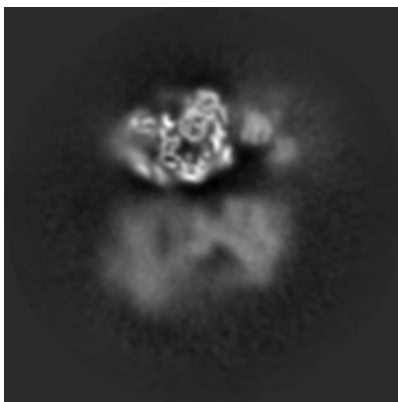
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

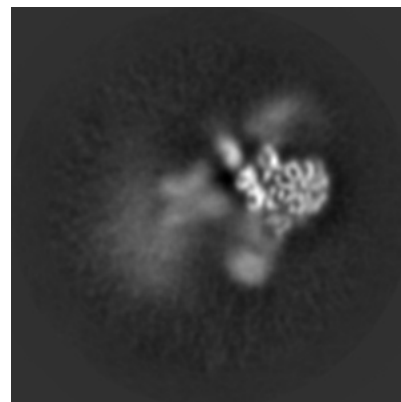
6.3.1 Primary map



X Index: 263

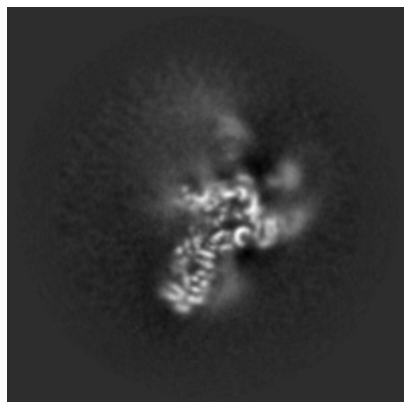


Y Index: 222

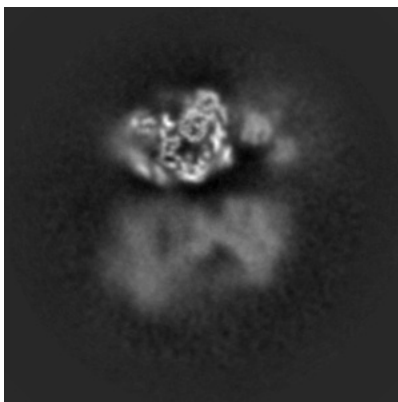


Z Index: 196

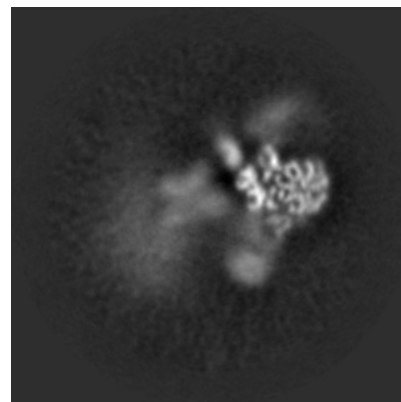
6.3.2 Raw map



X Index: 263



Y Index: 222



Z Index: 196

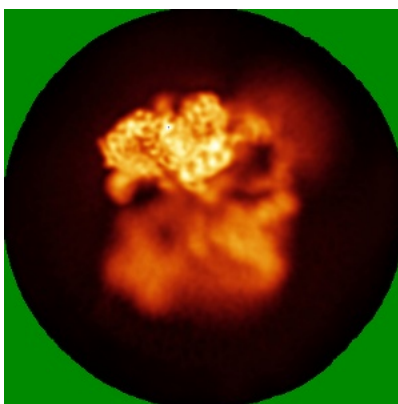
The images above show the largest variance slices of the map in three orthogonal directions.

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

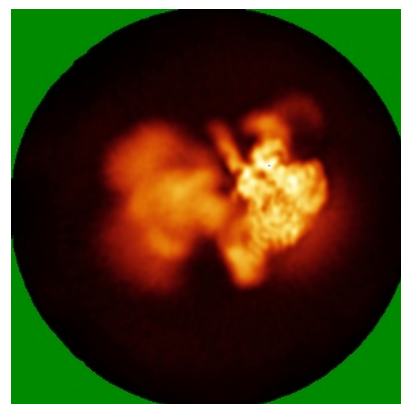
6.4.1 Primary map



X



Y

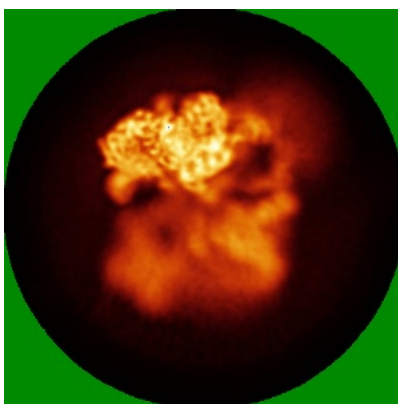


Z

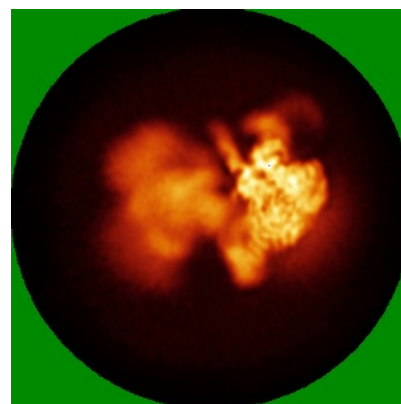
6.4.2 Raw map



X



Y

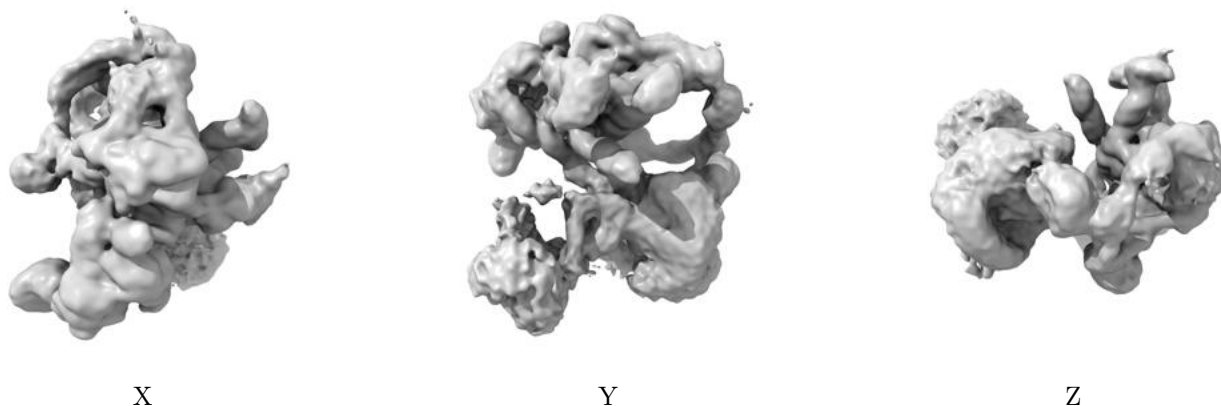


Z

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 0.0125. 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.

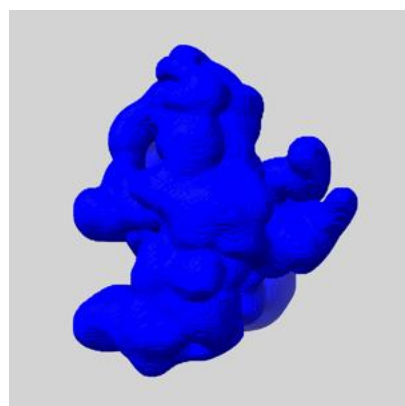
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

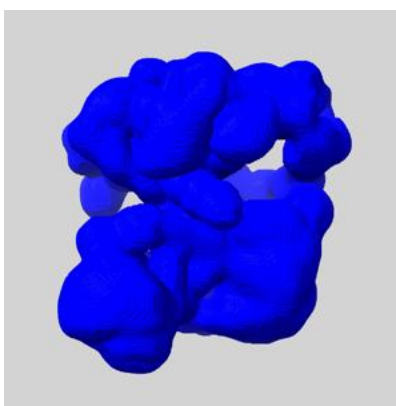
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

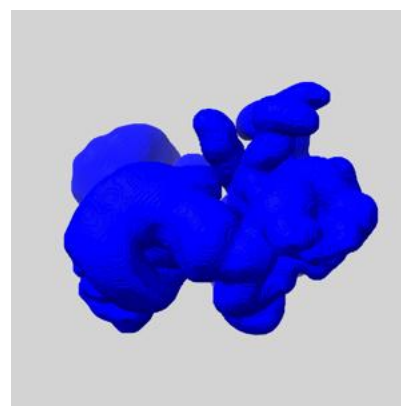
6.6.1 emd_13033_msk_1.map [i](#)



X



Y

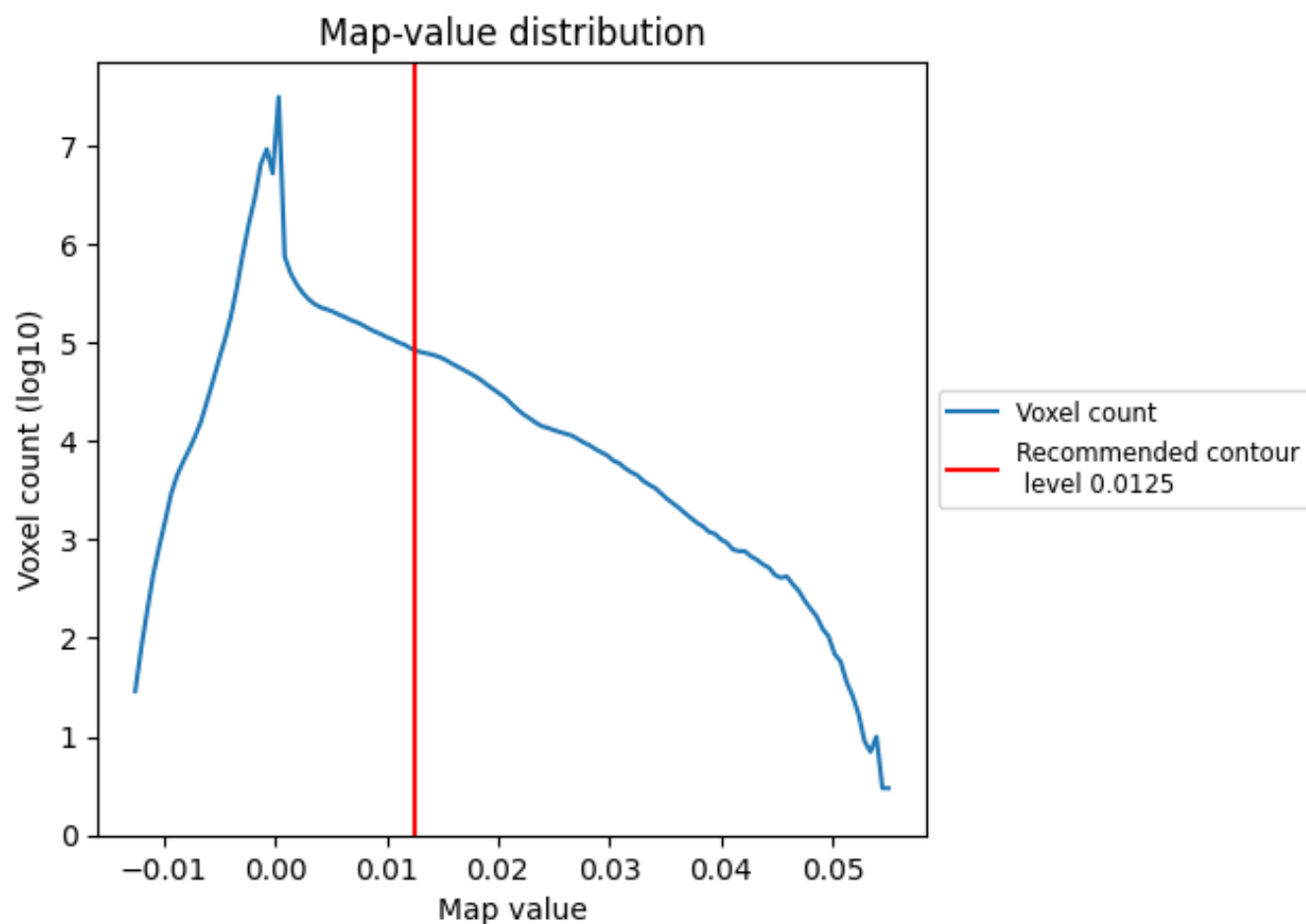


Z

7 Map analysis [i](#)

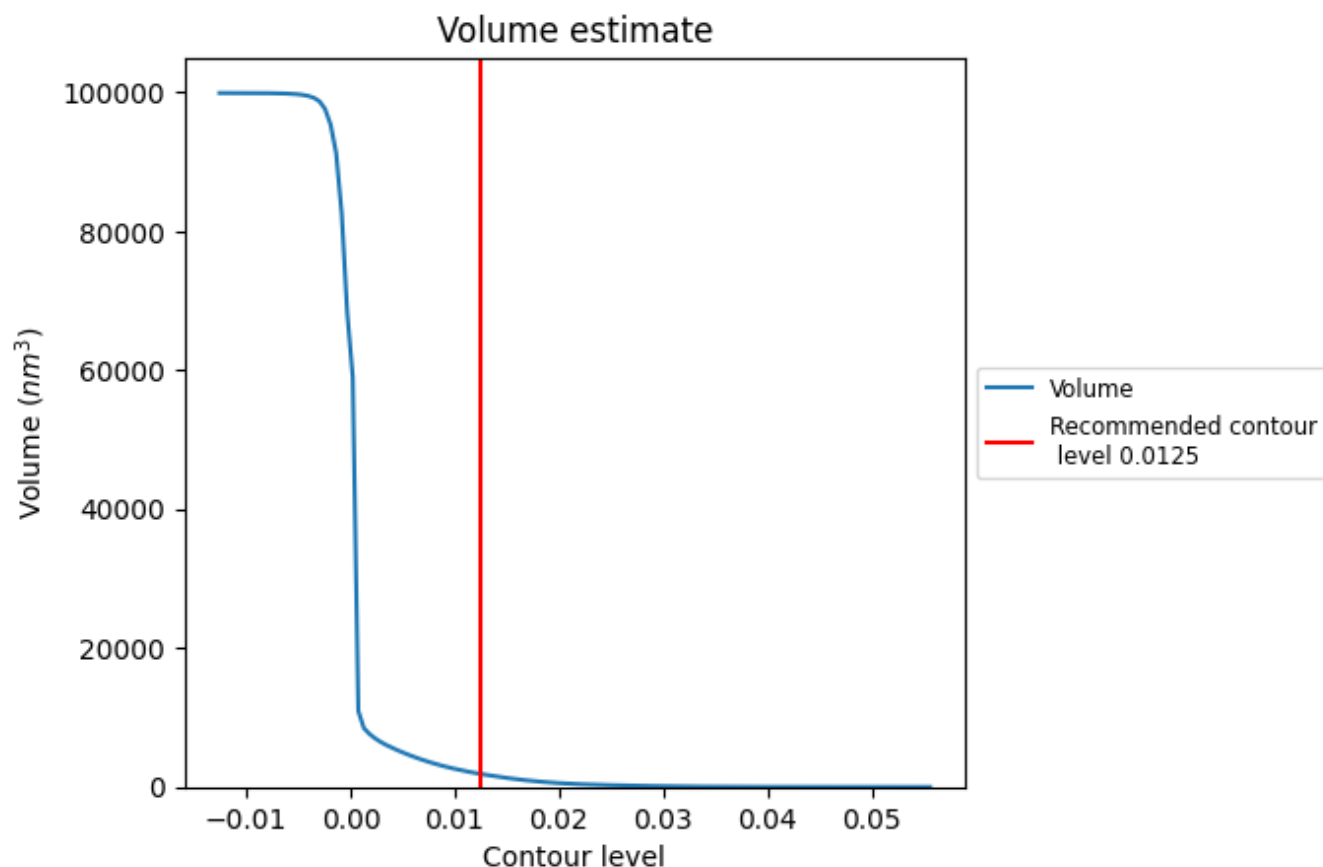
This section contains the results of statistical analysis of the map.

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.

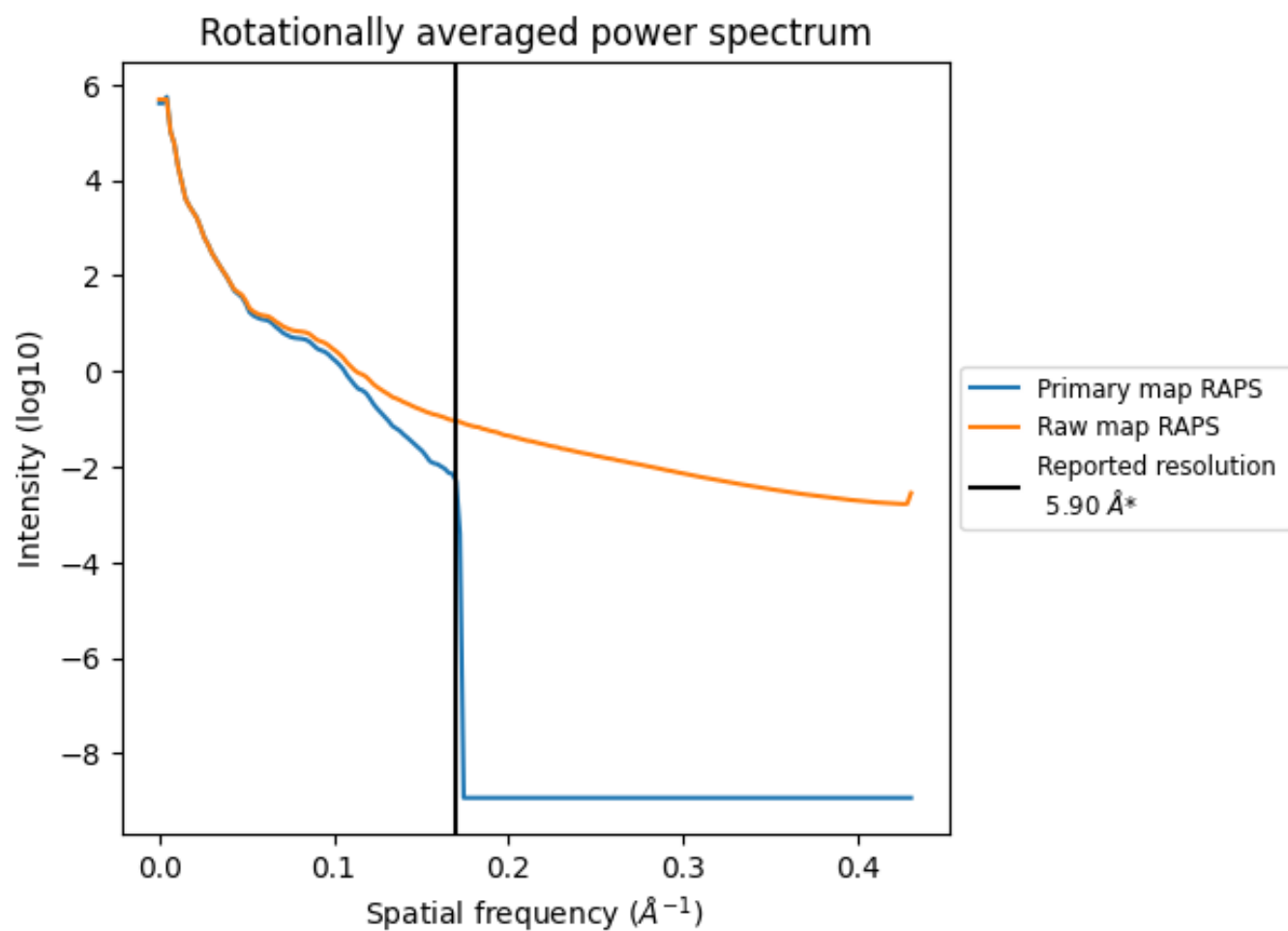
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1867 nm^3 ; this corresponds to an approximate mass of 1686 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 ⓘ

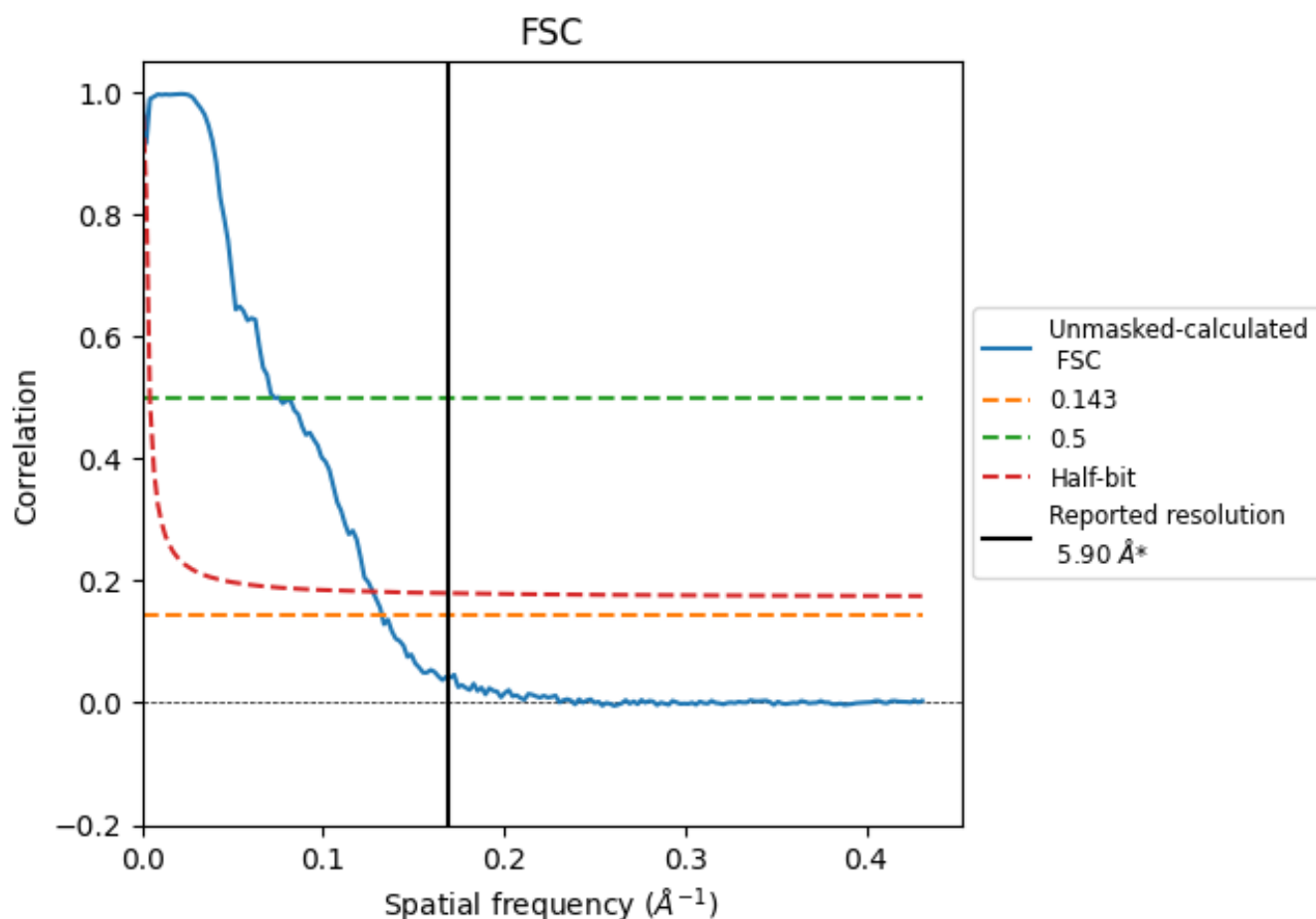


*Reported resolution corresponds to spatial frequency of 0.169 $\text{\AA}^{-1}$

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 0.169 Å⁻¹

8.2 Resolution estimates [i](#)

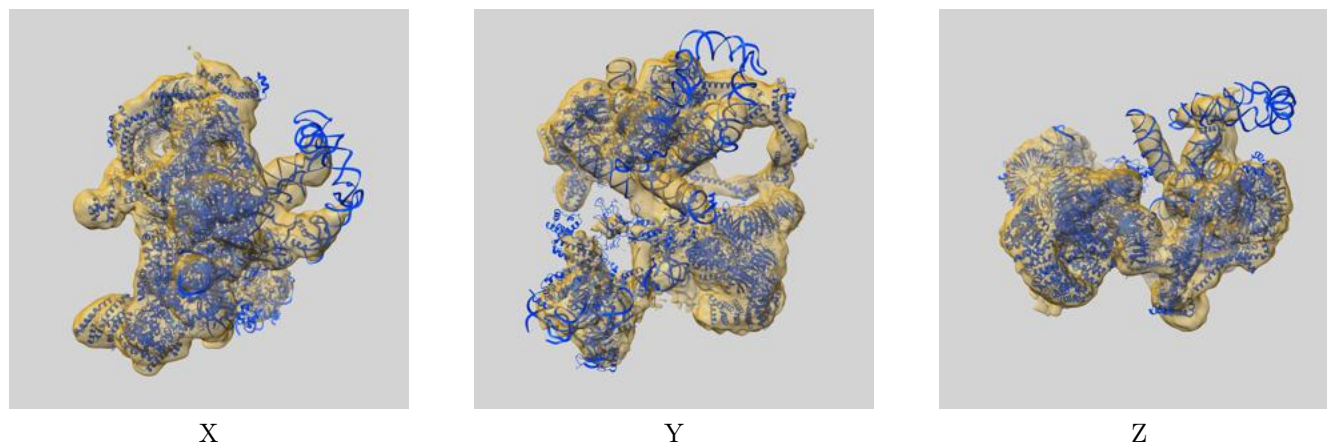
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.55	13.74	7.85

*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 7.55 differs from the reported value 5.9 by more than 10 %

9 Map-model fit [i](#)

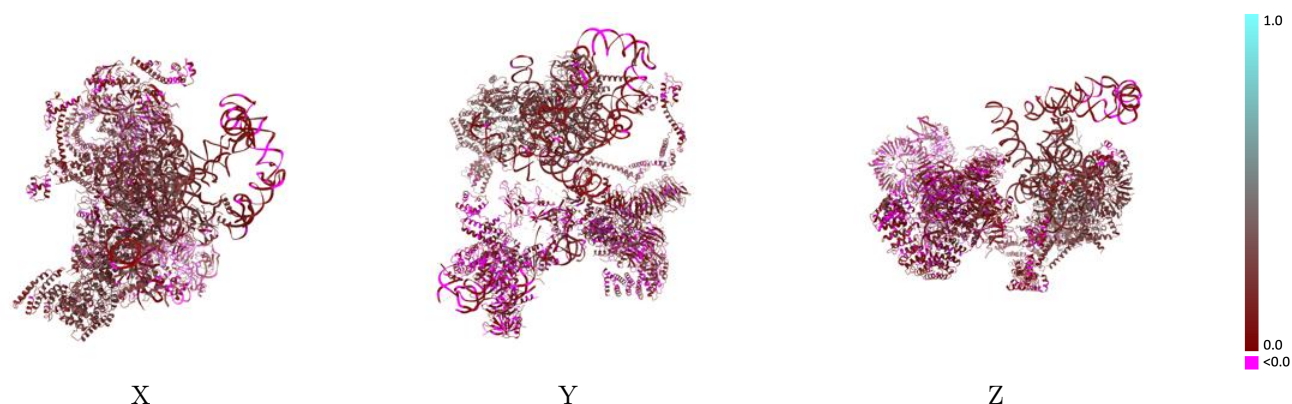
This section contains information regarding the fit between EMDB map EMD-13033 and PDB model 7OQE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



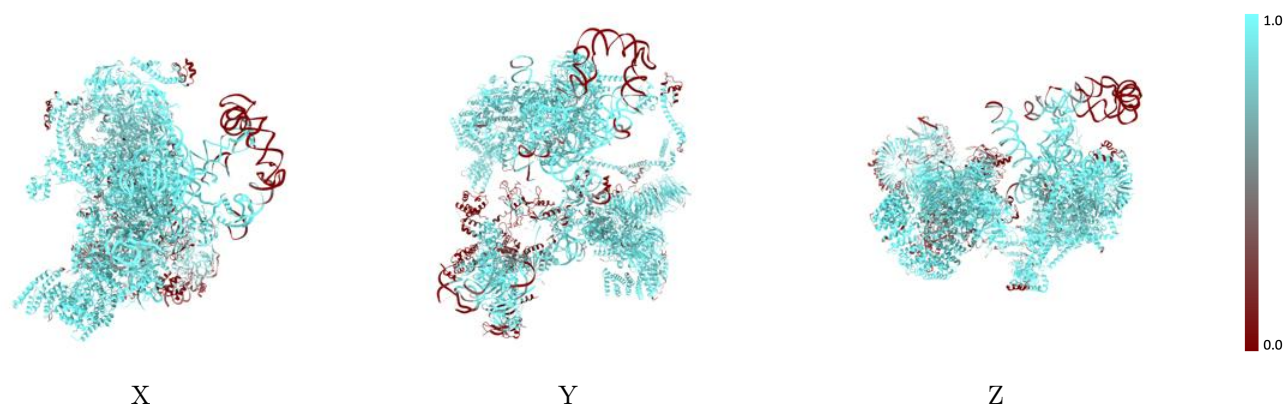
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



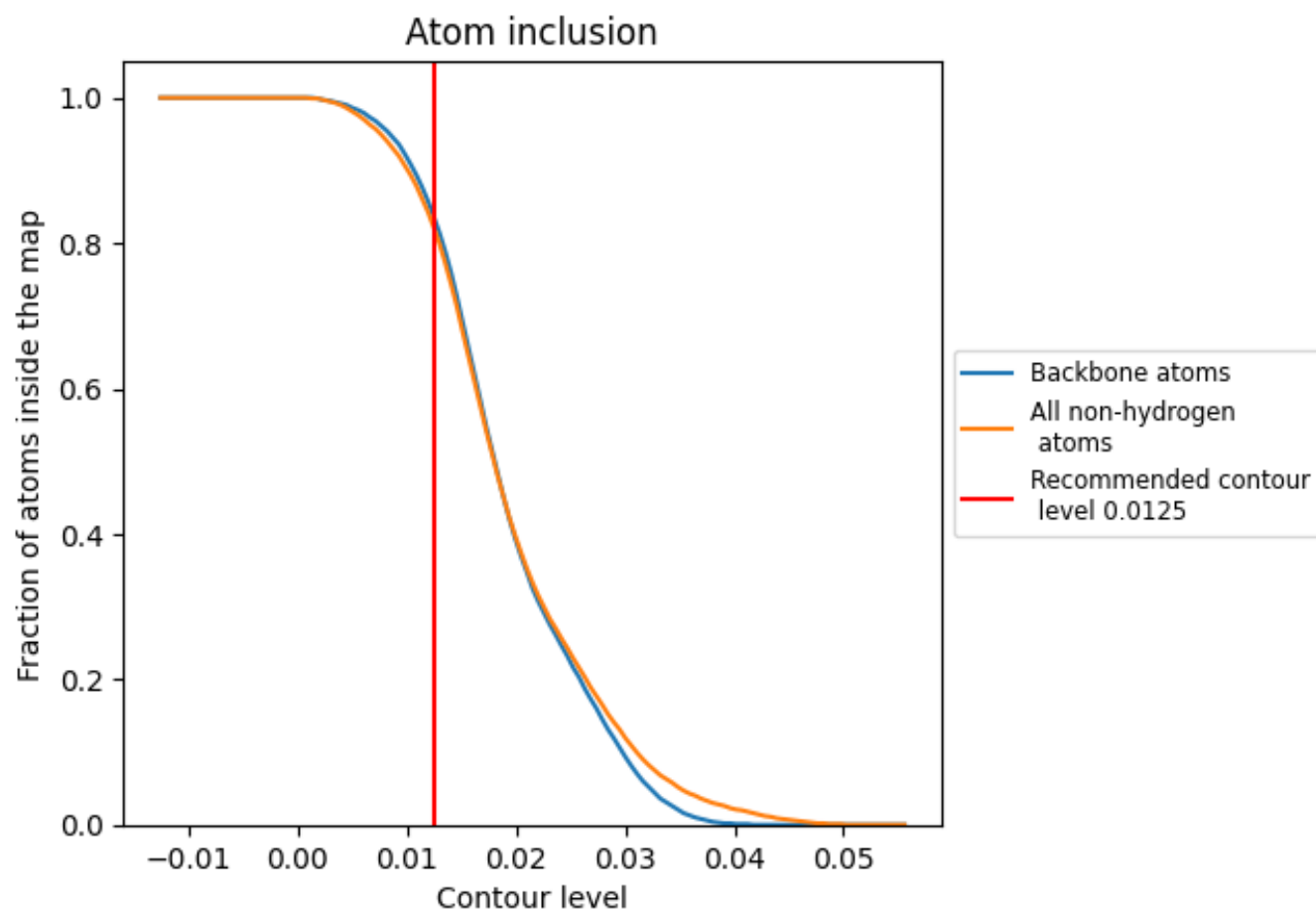
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.1210
1	 0.7420	 0.1300
2	 0.6690	 0.0610
A	 0.9910	 0.1800
B	 0.9770	 0.1860
C	 0.9590	 0.2280
D	 0.9720	 0.1980
E	 0.9920	 0.2430
F	 0.9440	 0.1570
G	 0.9950	 0.2430
H	 0.9920	 0.2090
I	 0.9190	 0.0980
J	 0.9790	 0.2140
K	 0.8150	 0.0850
O	 0.9740	 0.0760
P	 0.9430	 0.0950
Q	 0.7480	 0.0690
R	 0.6610	 0.0790
S	 0.9260	 0.0800
T	 0.6110	 0.0560
U	 0.3130	 0.0370
V	 0.1360	 0.0200
W	 0.6530	 0.0130
Y	 0.8920	 0.0610
Z	 0.9660	 0.0870
b	 0.9650	 0.2430
d	 0.9790	 0.2480
e	 0.9970	 0.2280
f	 1.0000	 0.2090
g	 0.9610	 0.2290
h	 0.9960	 0.2440
i	 0.9960	 0.2420
p	 0.3890	 0.0390
s	 1.0000	 0.0790
t	 1.0000	 0.0240



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Chain	Atom inclusion	Q-score
u	 0.7650	 -0.0010
v	 0.9780	 0.0050
w	 0.5710	 0.0440
x	 0.5750	 0.0590
y	 0.6680	 0.0550