



Full wwPDB EM Validation Report ⓘ

Jul 3, 2025 – 03:04 am BST

PDB ID : 5MQF / pdb_00005mqf
EMDB ID : EMD-3545
Title : Cryo-EM structure of a human spliceosome activated for step 2 of splicing (C* complex)
Authors : Bertram, K.; Hartmuth, K.; Kastner, B.
Deposited on : 2016-12-20
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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

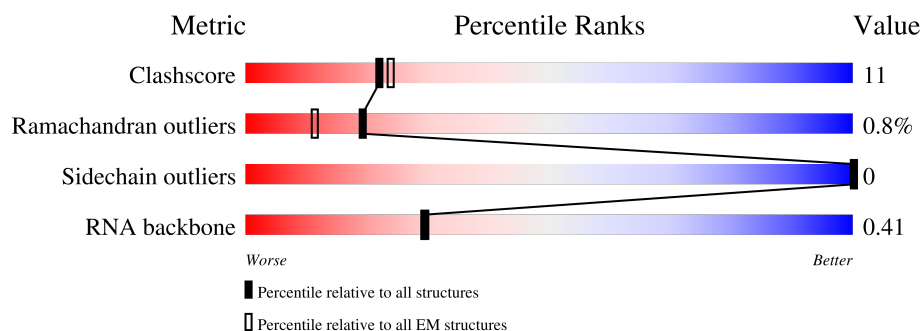
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	2335	
2	B	972	
3	C	536	
4	D	515	
5	E	579	
6	F	357	
7	G	504	


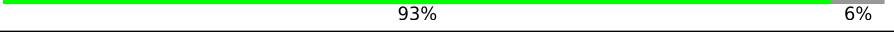
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Mol	Chain	Length	Quality of chain
7	H	504	
7	I	504	
7	J	504	
8	K	225	
9	L	802	
10	M	855	
11	N	243	
12	O	848	
13	P	420	
14	Q	144	
15	R	229	
16	S	2752	
17	T	908	
18	U	1485	
19	V	166	
20	W	255	
21	X	225	
22	a	118	
22	h	118	
23	b	86	
23	i	86	
24	c	92	
24	j	92	
25	d	76	
25	k	76	

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Mol	Chain	Length	Quality of chain
26	e	126	
26	l	126	
27	f	240	
27	m	240	
28	g	119	
28	n	119	
29	o	301	
30	p	411	
31	q	1218	
32	Y	324	
32	Z	324	
33	2	188	
34	5	116	
35	6	106	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 55236 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1965	Total	C	N	O	13	0
			9955	6025	1965	1965		

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	902	Total	C	N	O	0	0
			4566	2762	902	902		

- Molecule 3 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	240	Total	C	N	O	0	0
			1231	751	240	240		

- Molecule 4 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	315	Total	C	N	O	8	0
			1576	946	315	315		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	454	ALA	VAL	conflict	UNP O43660
D	455	VAL	GLN	conflict	UNP O43660
D	456	GLN	PRO	conflict	UNP O43660
D	457	PRO	GLY	conflict	UNP O43660
D	458	GLY	SER	conflict	UNP O43660
D	459	SER	LEU	conflict	UNP O43660
D	460	LEU	ASP	conflict	UNP O43660
D	461	ASP	SER	conflict	UNP O43660
D	492	ASP	-	insertion	UNP O43660

- Molecule 5 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	329	Total	C	N	O	0	0
			1646	988	329	329		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	307	Total	C	N	O	0	0
			1531	917	307	307		

- Molecule 7 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	132	Total	C	N	O	0	0
			679	415	132	132		
7	H	135	Total	C	N	O	0	0
			696	426	135	135		
7	I	134	Total	C	N	O	0	0
			691	423	134	134		
7	J	135	Total	C	N	O	0	0
			696	426	135	135		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	191	Total	C	N	O	0	0
			960	578	191	191		

- Molecule 9 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	336	Total	C	N	O	0	0
			1680	1008	336	336		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	706	Total	C	N	O	0	0
			3553	2141	706	706		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	115	Total	C	N	O	0	0
			579	349	115	115		

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	564	Total	C	N	O	0	0
			2842	1715	564	563		

- Molecule 13 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	277	Total	C	N	O	0	0
			1396	842	277	277		

- Molecule 14 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Q	142	Total	C	N	O	0	0
			713	429	142	142		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	98	Total	C	N	O	0	0
			493	297	98	98		

- Molecule 16 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S	30	Total	C	N	O	0	0
			148	88	30	30		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	395	Total	C	N	O	2	197
			1191	795	198	198		

- Molecule 18 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	U	1287	Total	C		
			1287	1287	6	1287

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	155	Total	C	N	O	0	0
			774	464	155	155		

- Molecule 20 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	W	162	Total	C	N	O	0	0
			816	492	162	162		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	89	ASP	CYS	conflict	UNP P09661
W	119	CYS	SER	conflict	UNP P09661

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	a	99	Total	C	N	O	0	0
			497	299	99	99		
22	h	98	Total	C	N	O	0	0
			493	297	98	98		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	b	76	Total	C	N	O	0	0
			379	227	76	76		
23	i	74	Total	C	N	O	0	0
			369	221	74	74		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	c	79	Total	C	N	O	0	0
			393	235	79	79		
24	j	79	Total	C	N	O	0	0
			393	235	79	79		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	d	74	Total	C	N	O	0	0
			369	221	74	74		
25	k	74	Total	C	N	O	0	0
			369	221	74	74		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	e	84	Total	C	N	O	0	0
			420	252	84	84		
26	l	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	f	71	Total	C	N	O	0	0
			355	213	71	71		
27	m	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	82	Total	C	N	O	0	0
			412	248	82	82		
28	n	82	Total	C	N	O	0	0
			412	248	82	82		

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	o	223	Total	C	0	223
			223	223		

- Molecule 30 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	p	385	Total	C	8	385
			385	385		

- Molecule 31 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	q	627	Total	C	5	627
			627	627		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	MET	deletion	UNP Q14562
q	?	-	ASP	deletion	UNP Q14562
q	948	GLY	ALA	conflict	UNP Q14562
q	949	SER	PRO	conflict	UNP Q14562

- Molecule 32 is a RNA chain called MINX pre-mRNA (intron).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	32	Total	C	N	O	P	0	0
			677	303	115	227	32		
32	Z	12	Total	C	N	O	P	0	0
			256	114	47	83	12		

- Molecule 33 is a RNA chain called Human gene for small nuclear RNA U2 (snRNA U2).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	140	Total	C	N	O	P	0	0
			2968	1327	510	991	140		

- Molecule 34 is a RNA chain called Homo sapiens U5 A small nuclear RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5	114	Total	C	N	O	P	0	0
			2397	1074	399	810	114		

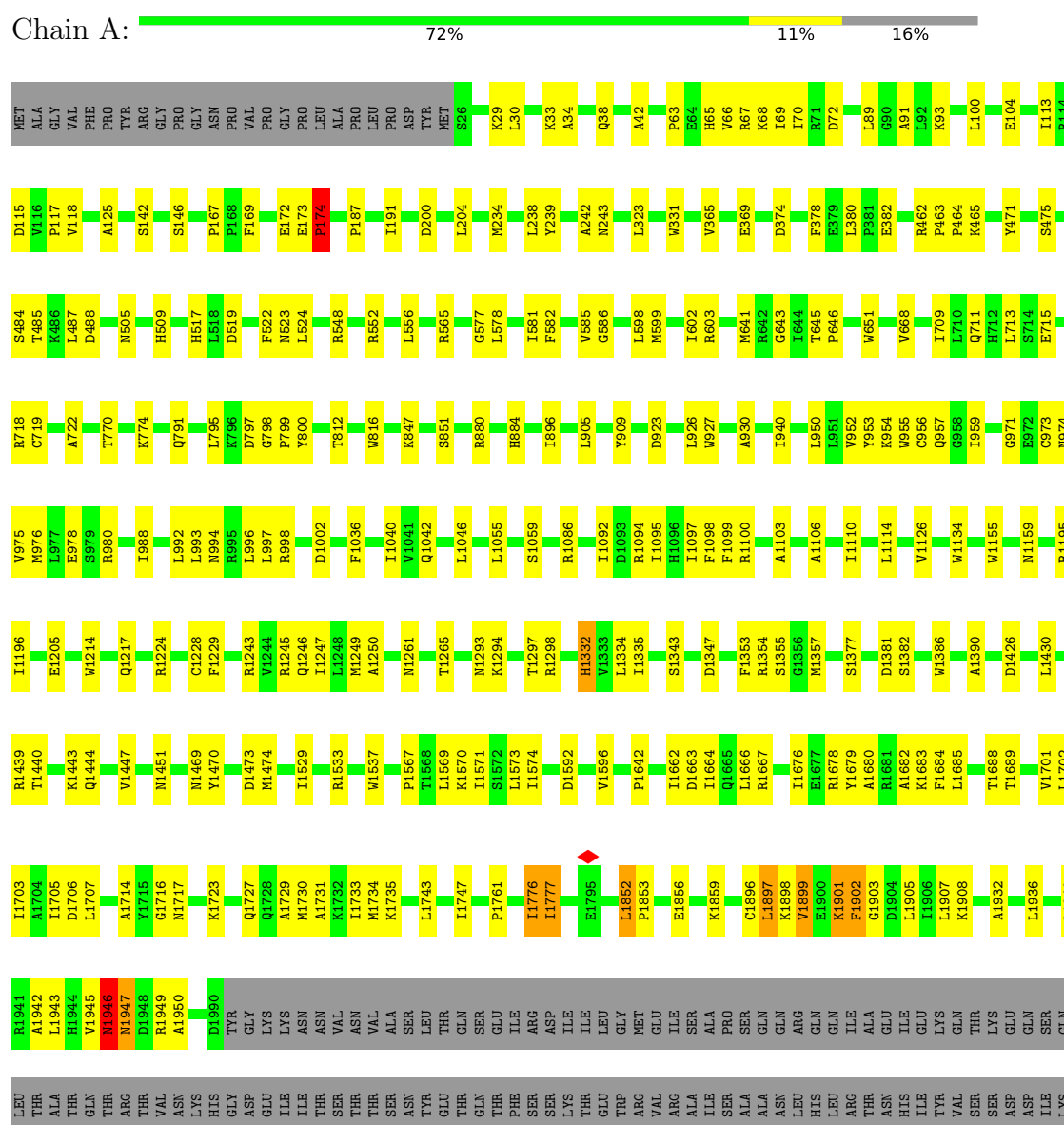
- Molecule 35 is a RNA chain called Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA.

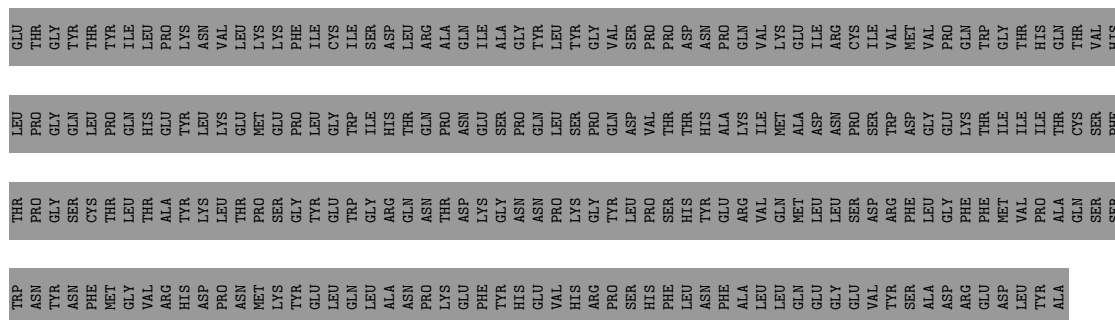
Mol	Chain	Residues	Atoms					AltConf	Trace
35	6	89	Total	C	N	O	P	0	0
			1903	851	350	613	89		

3 Residue-property plots

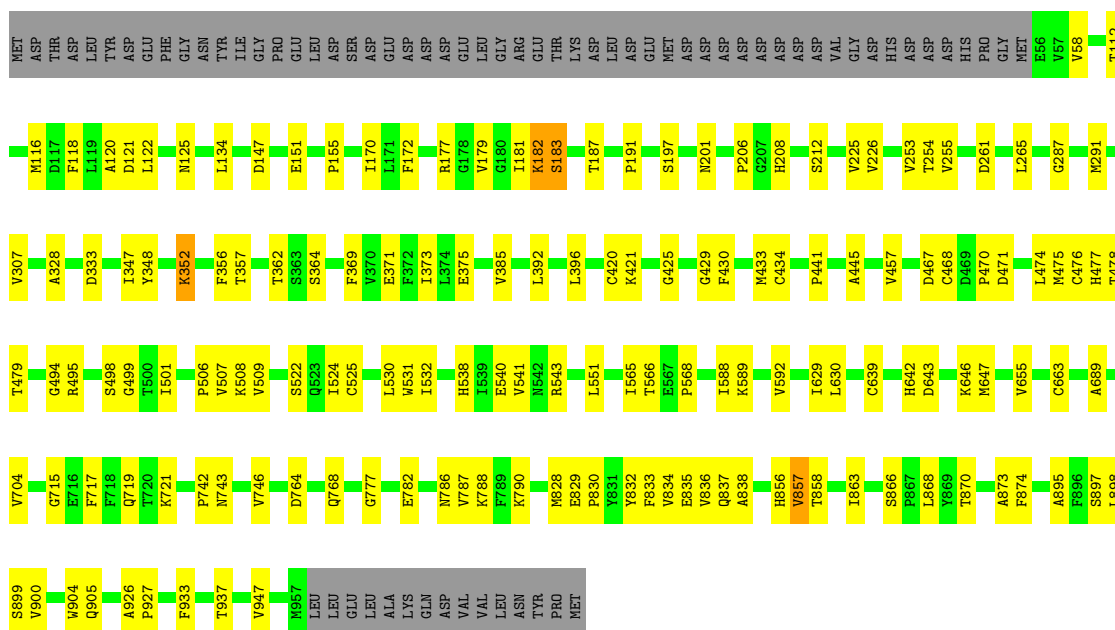
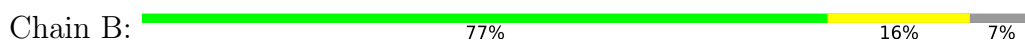
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Pre-mRNA-processing-splicing factor 8

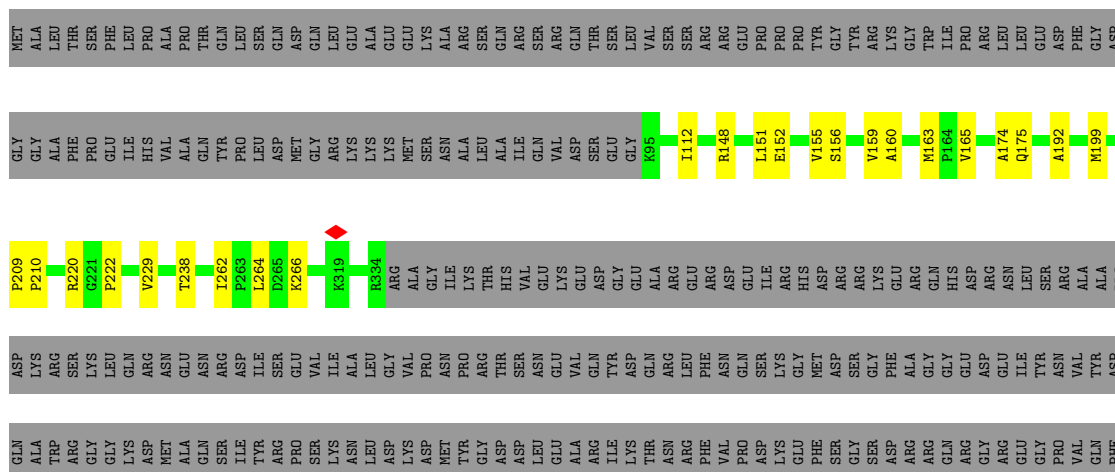


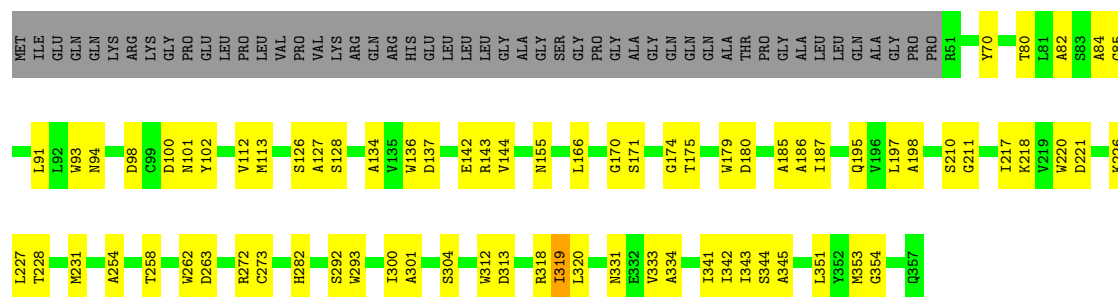


- Molecule 2: 116 kDa U5 small nuclear ribonucleoprotein component

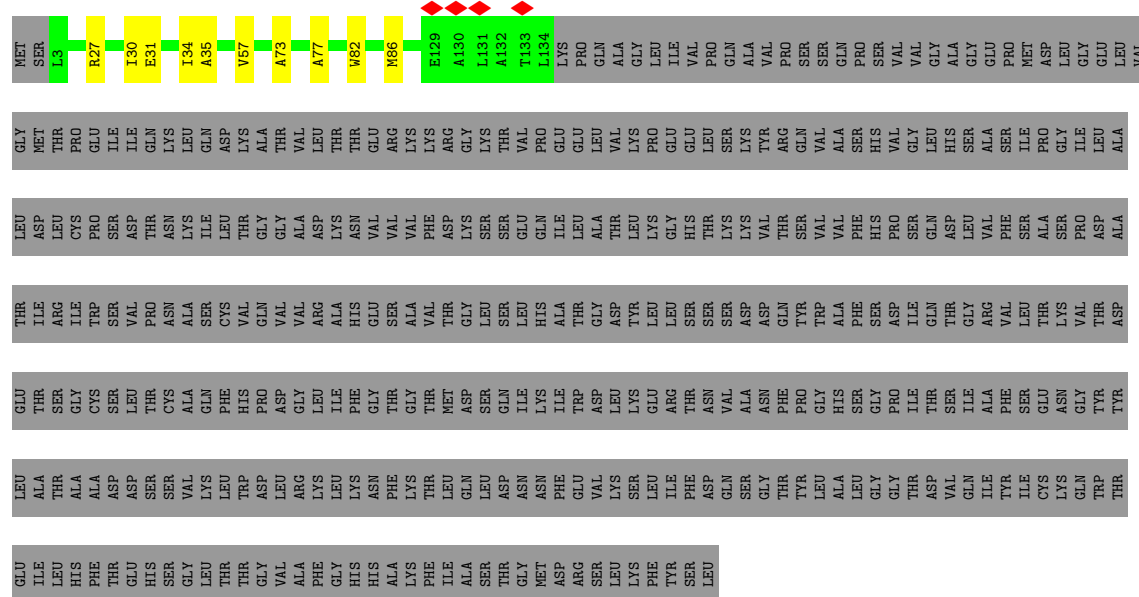


- Molecule 3: SNW domain-containing protein 1

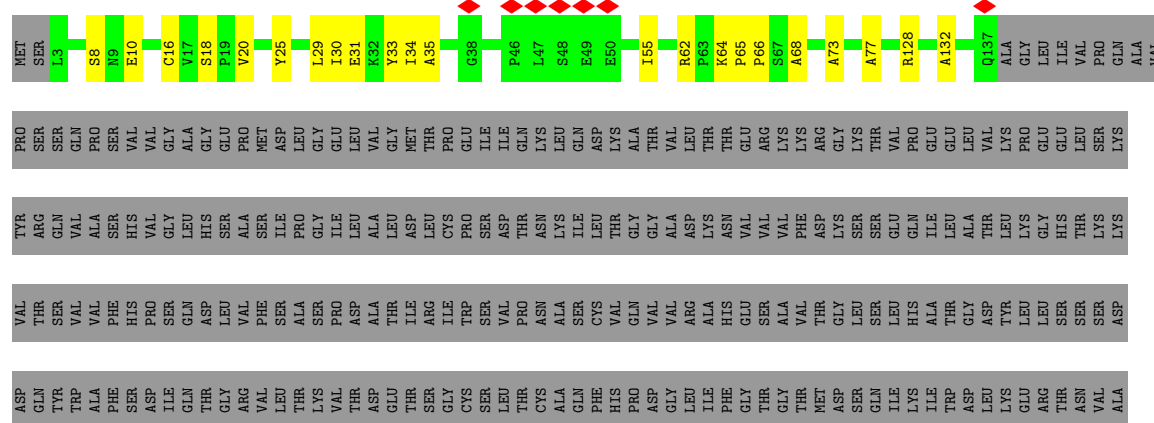


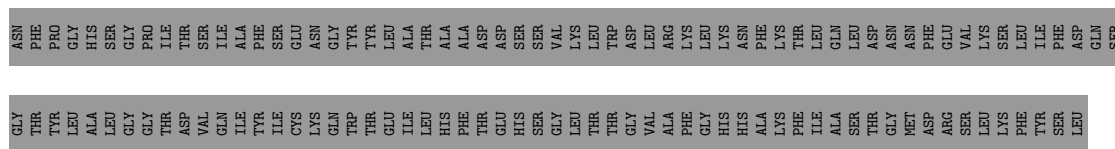


• Molecule 7: Pre-mRNA-processing factor 19

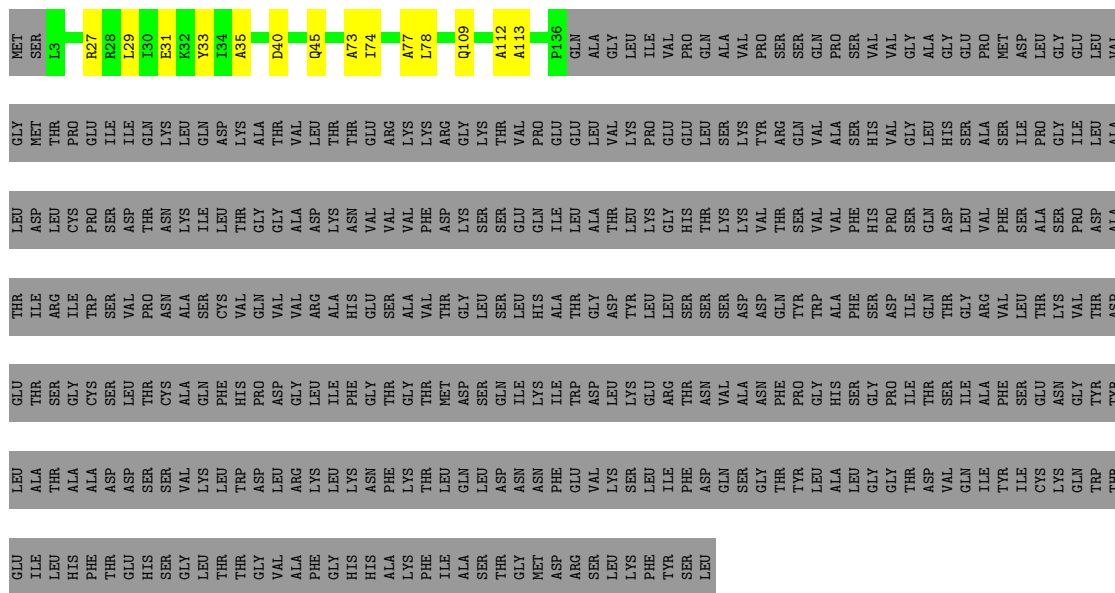


• Molecule 7: Pre-mRNA-processing factor 19

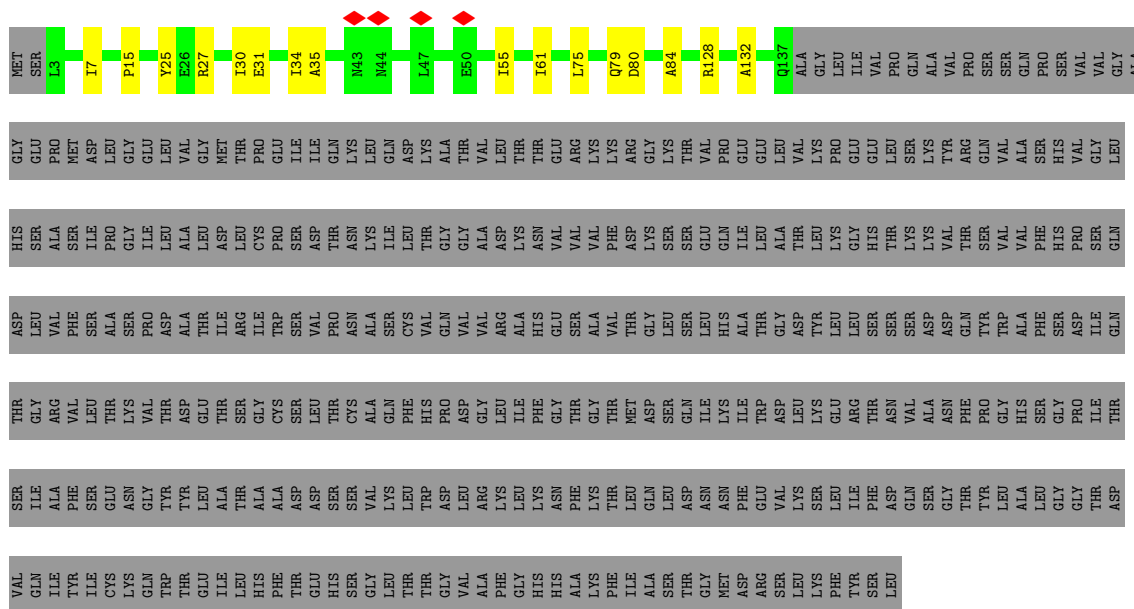




- Molecule 7: Pre-mRNA-processing factor 19

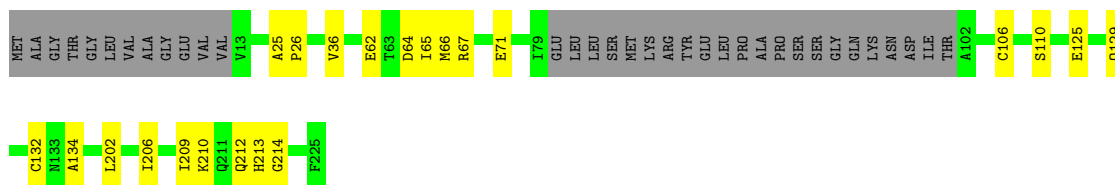


- Molecule 7: Pre-mRNA-processing factor 19



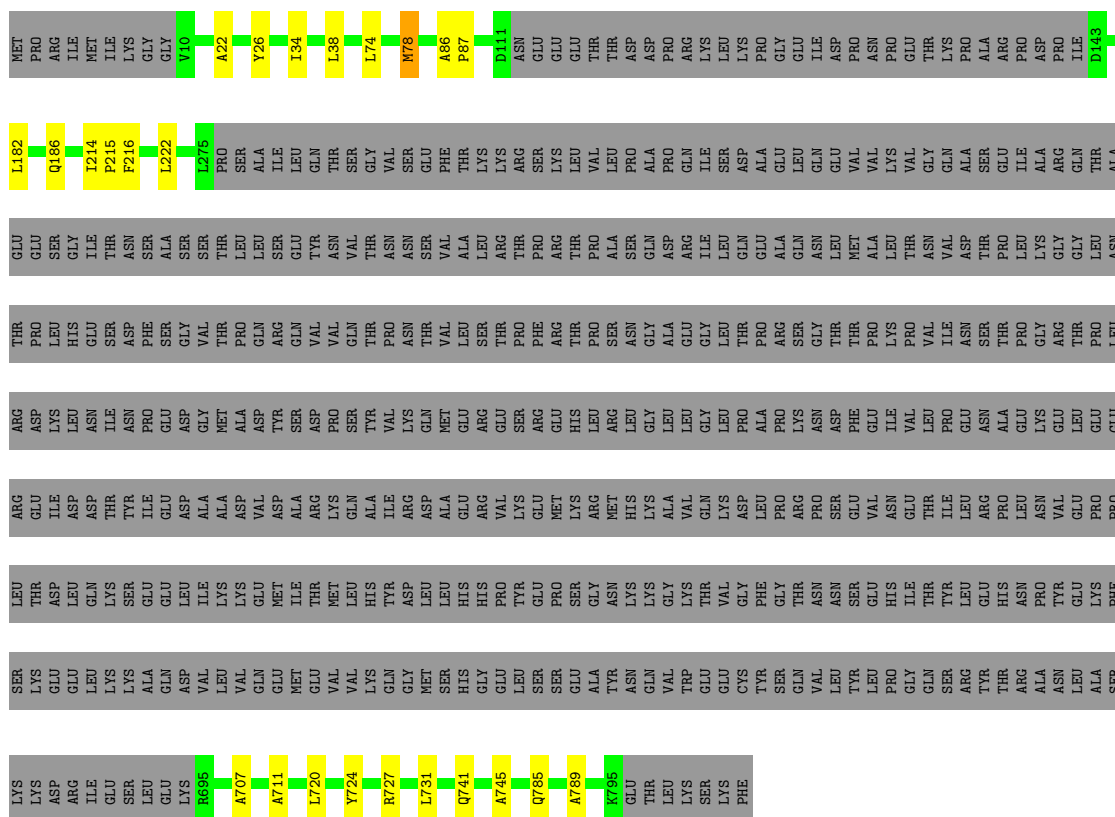
- Molecule 8: Pre-mRNA-splicing factor SPF27

Chain K:  75% 10% 15%



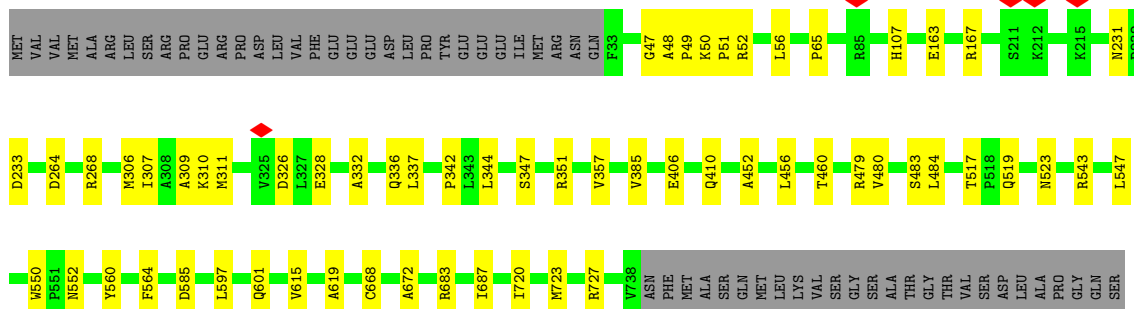
- Molecule 9: Cell division cycle 5-like protein

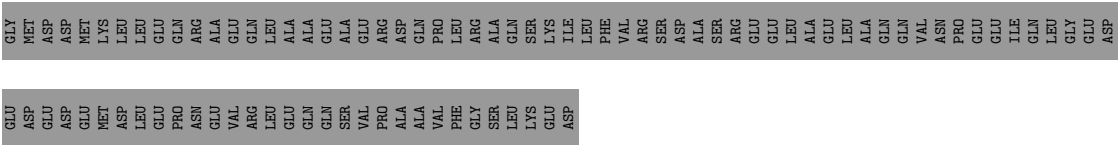
Chain L: 39% 1% 58%



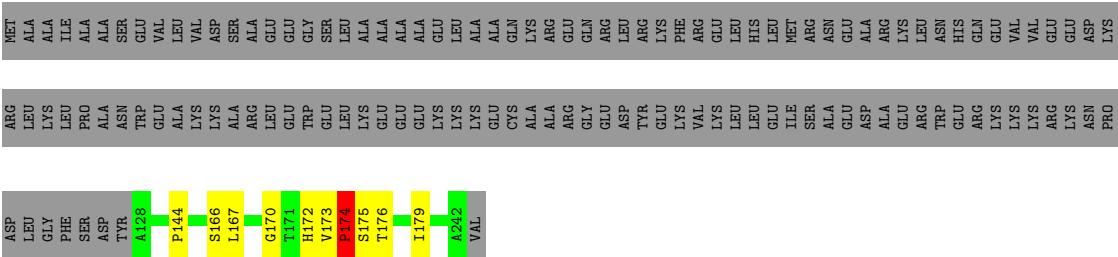
- Molecule 10: Pre-mRNA-splicing factor SYF1

Chain M: 75% 7% 17%

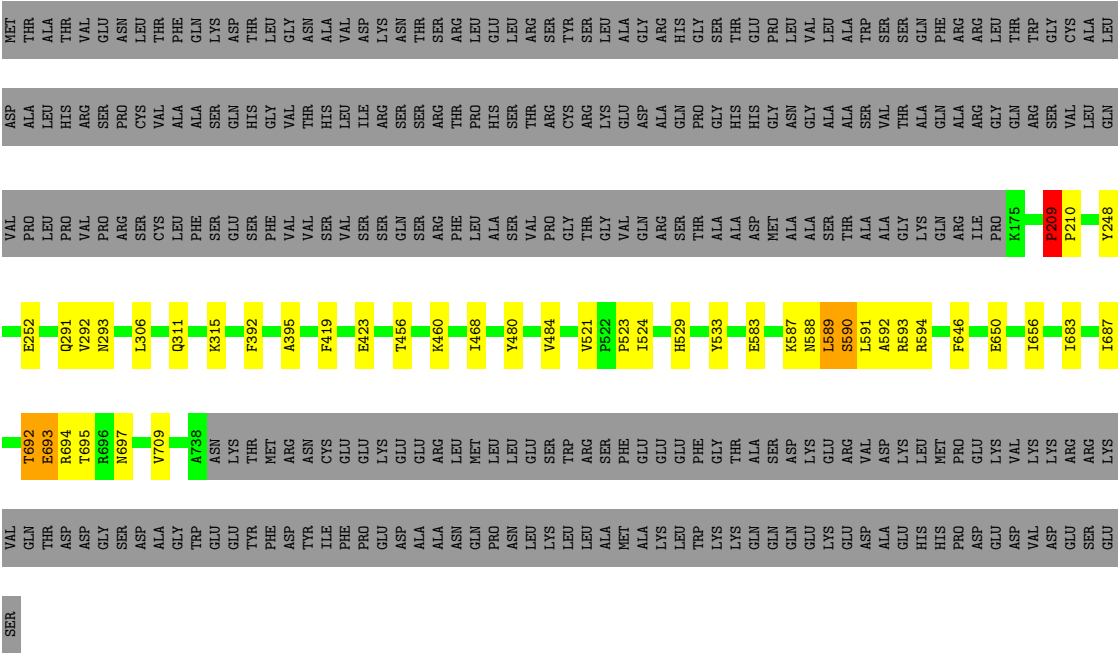




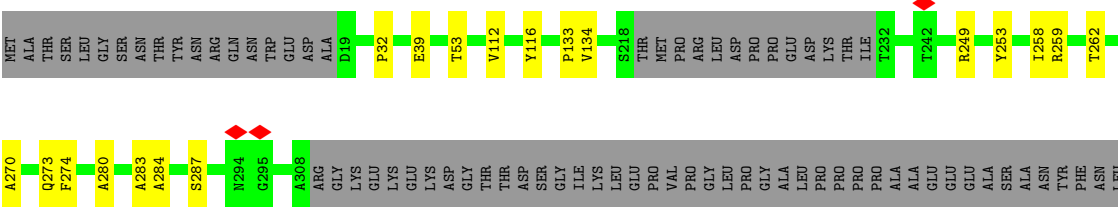
● Molecule 11: Pre-mRNA-splicing factor SYF2



● Molecule 12: Crooked neck-like protein 1

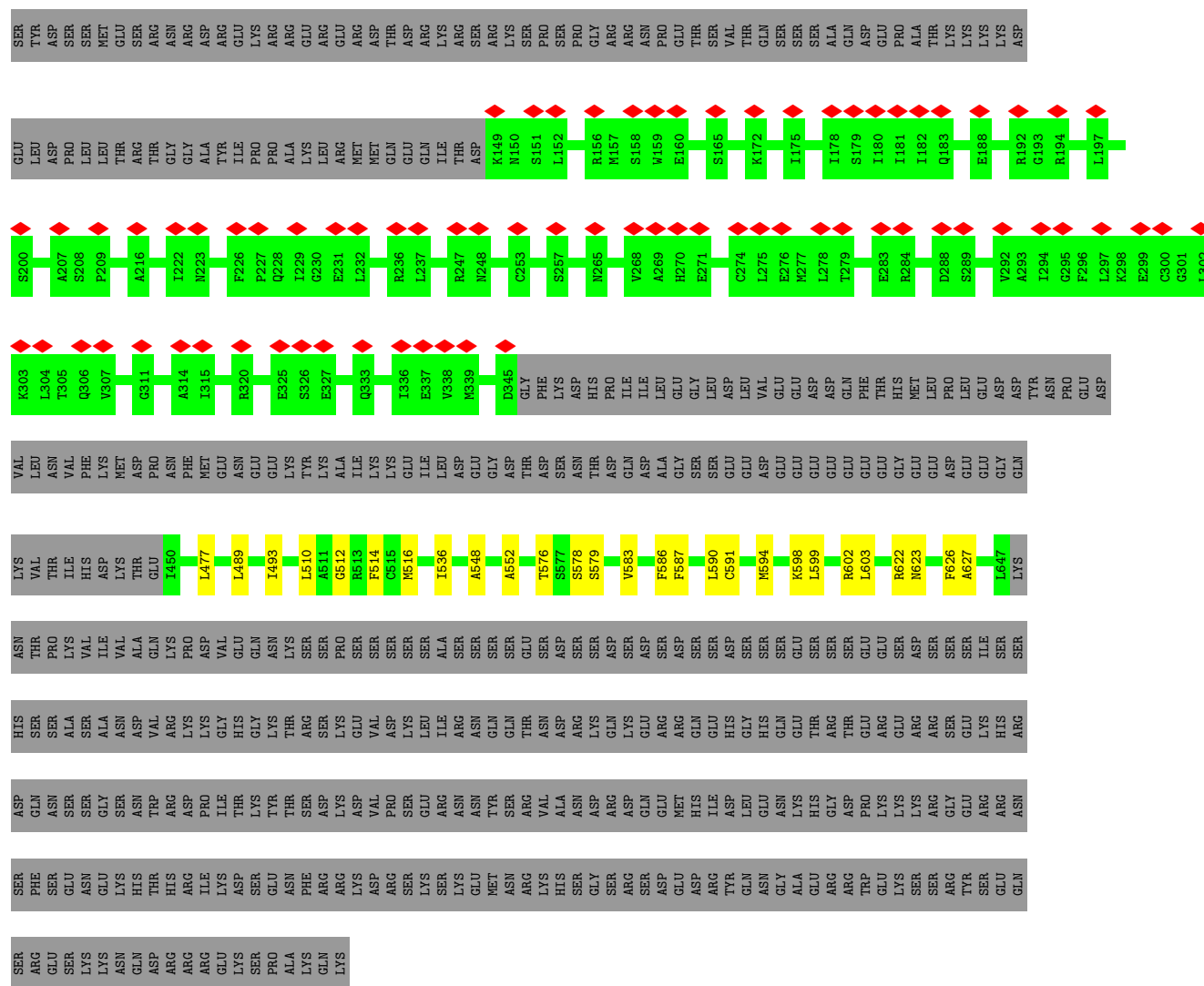


● Molecule 13: Pre-mRNA-splicing factor RBM22

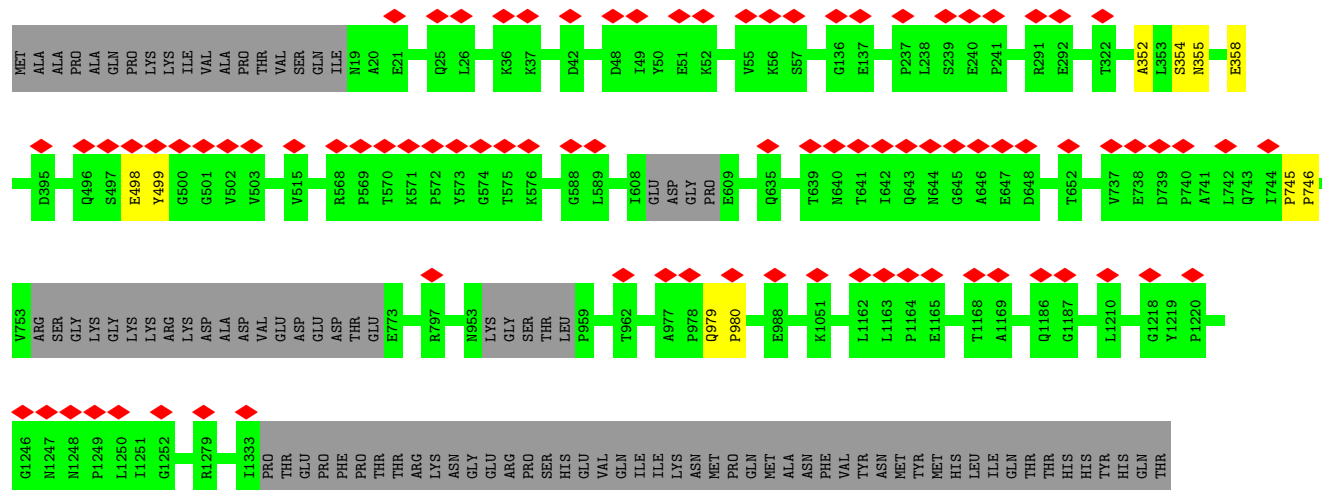
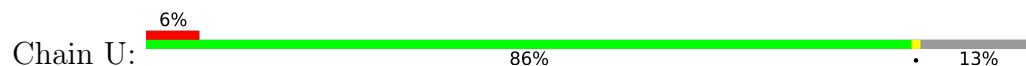


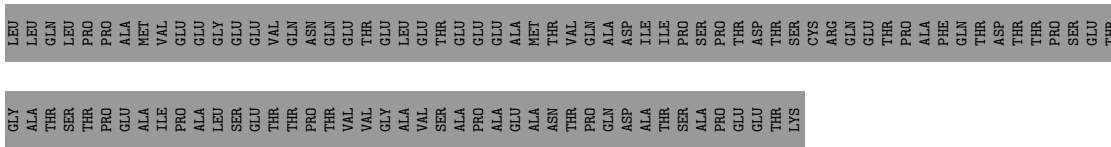


MET	LYS	SER	SER	VAL	ALA	GLN	ILE	LYS	PRO	SER	SER	GLY	HIS	ASP	ARG	ARG	GLU	ASN	ASN	SER	TYR	GLN	ARG	ASN	SER	SER	PRO	GLU	GLU	GLN	GLU	GLU	GLU	GLU	ASP	ASP	ARG	ARG	ASP	ASP	TYR	PHE	ASP	TYR	SER	ARG	ARG	ARG	GLY	PC
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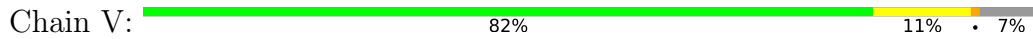


• Molecule 18: Intron-binding protein aquarius

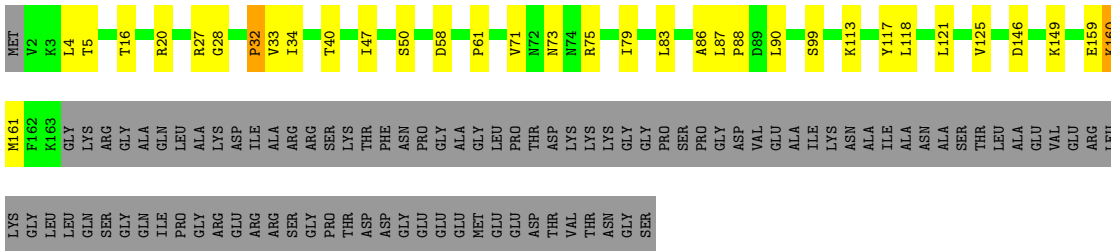




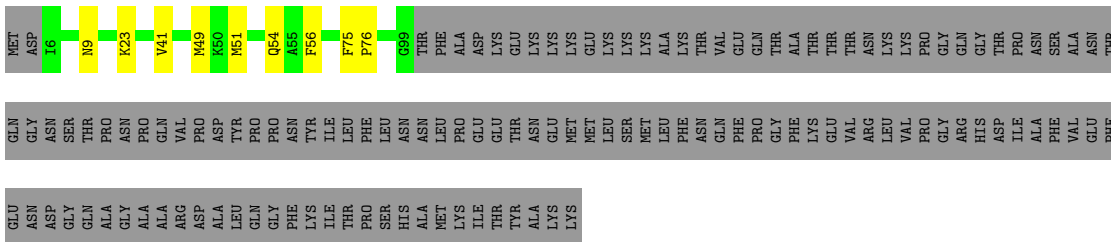
- Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1



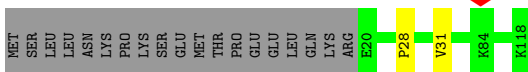
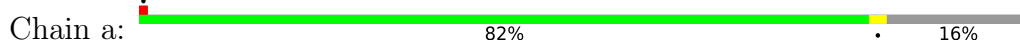
- Molecule 20: U2 small nuclear ribonucleoprotein A'



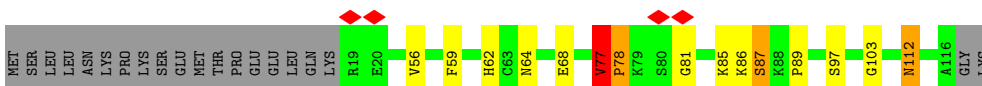
- Molecule 21: U2 small nuclear ribonucleoprotein B''




- Molecule 22: Small nuclear ribonucleoprotein Sm D2

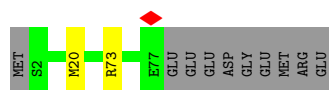


- Molecule 22: Small nuclear ribonucleoprotein Sm D2




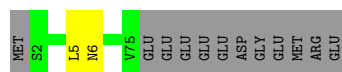
- Molecule 23: Small nuclear ribonucleoprotein F

Chain b:  86% 12%




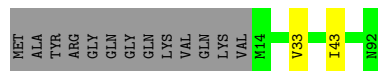
- Molecule 23: Small nuclear ribonucleoprotein F

Chain i:  84% 14%




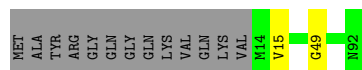
- Molecule 24: Small nuclear ribonucleoprotein E

Chain c:  84% 14%



- Molecule 24: Small nuclear ribonucleoprotein E

Chain j:  84% 14%



- Molecule 25: Small nuclear ribonucleoprotein G

Chain d:  95% 4% 1%



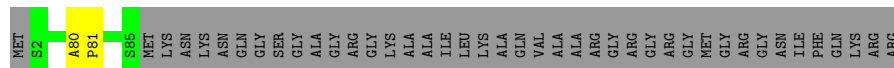
- Molecule 25: Small nuclear ribonucleoprotein G

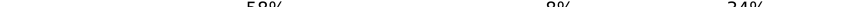

Chain k:  91% 7% 2%



- Molecule 26: Small nuclear ribonucleoprotein Sm D3



Chain e:  65% 33% 2%





- Chain 1: 
- 

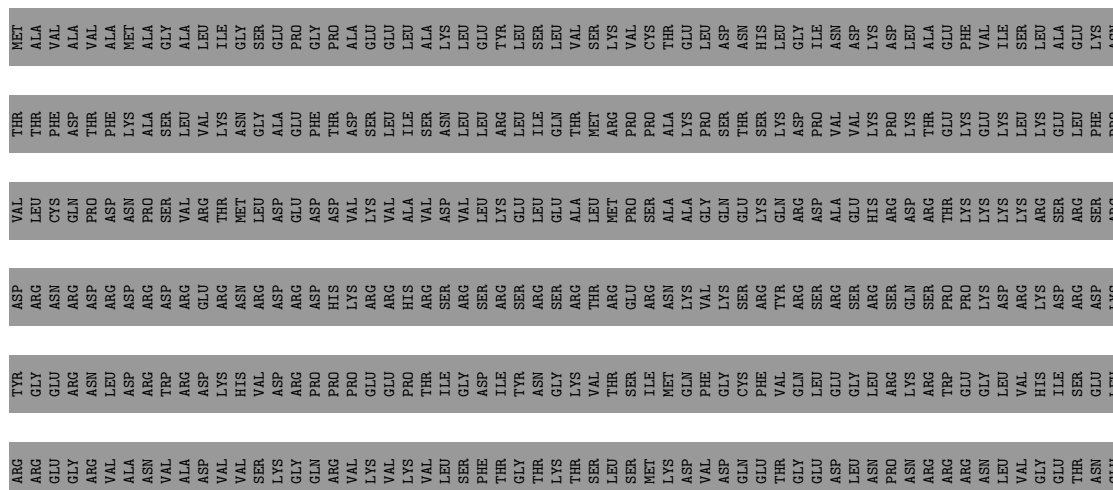
- [illegible]

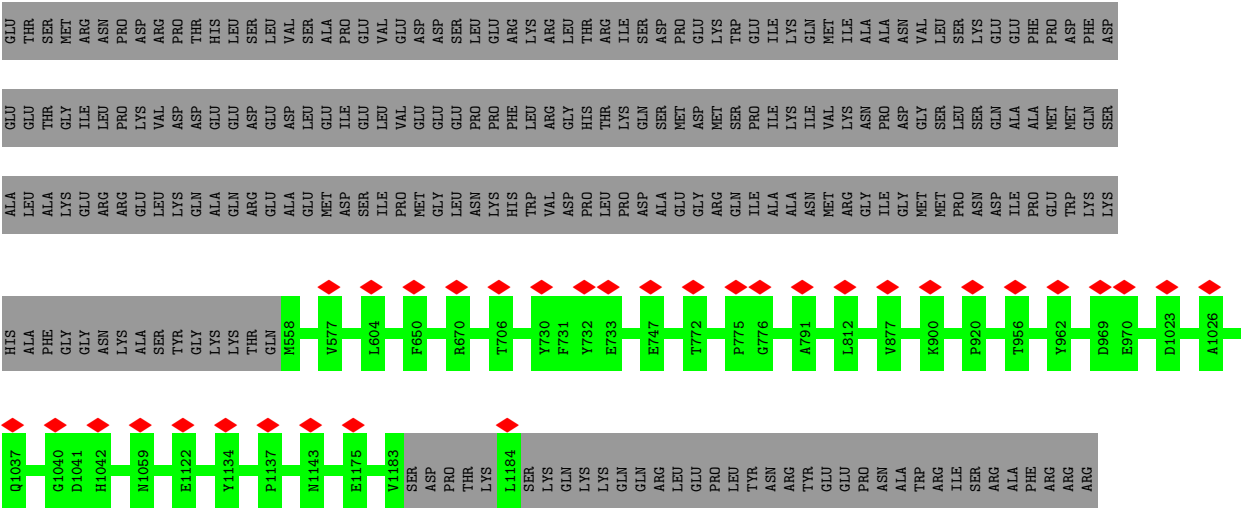
- [illegible]

- Chain g:  65% 31%
- 
- | Amino Acid | Frequency (%) |
|------------|---------------|
| R1 | ~10 |
| Q24 | ~5 |
| K36 | ~5 |
| T46 | ~5 |
| G62 | ~5 |
| L74 | ~5 |
| D82 | ~10 |
| VAL | ~1 |
| GLU | ~1 |
| PRO | ~1 |
| LYS | ~1 |
| VAL | ~1 |
| LYS | ~1 |
| SER | ~1 |
| LYS | ~1 |
| LYS | ~1 |
| ARG | ~1 |
| GLU | ~1 |
| ALA | ~1 |
| VAL | ~1 |
| ALA | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| GLY | ~1 |
| ARG | ~1 |
| PRO | ~1 |
| ARG | ~1 |

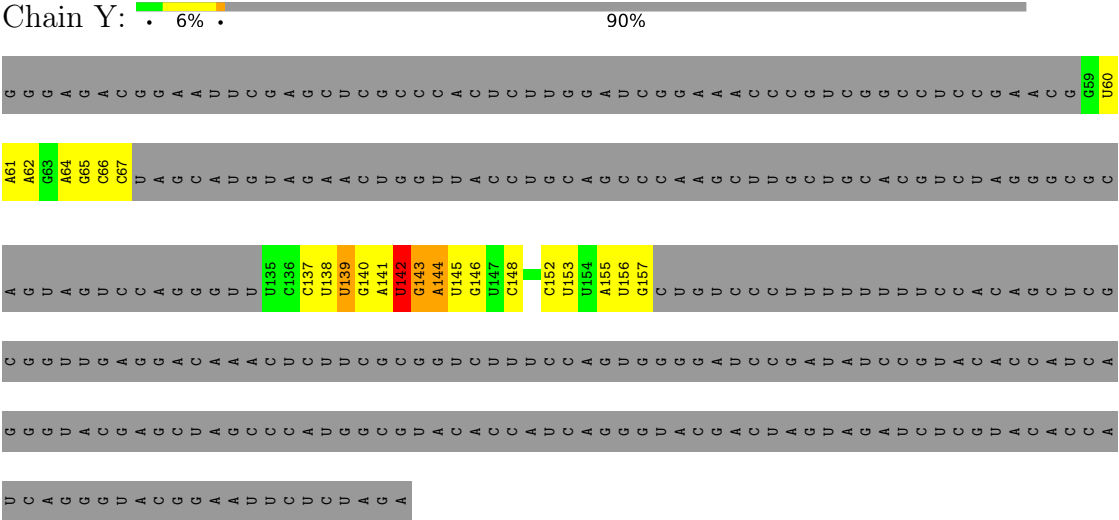
- Chain n:  68% 31%
- 

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

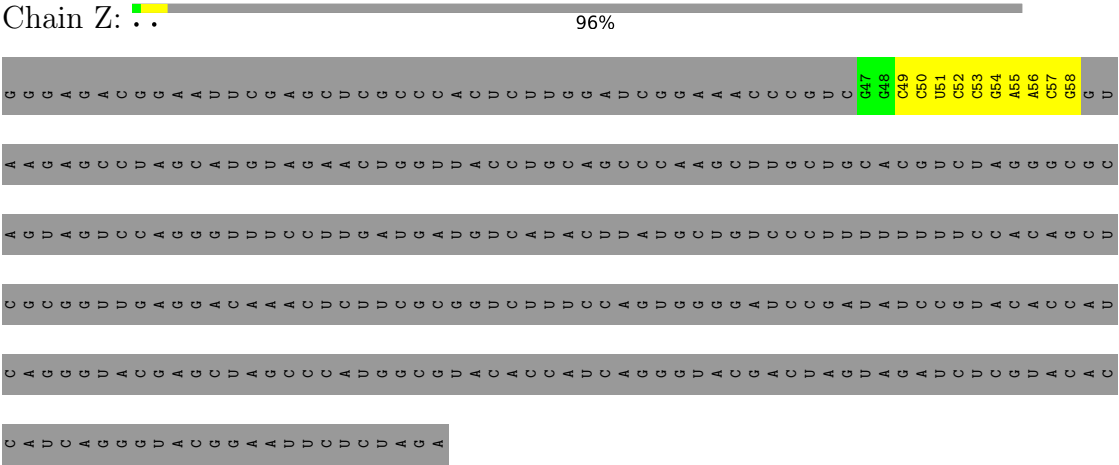




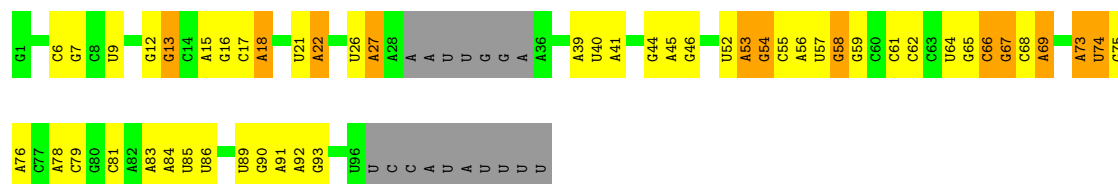
• Molecule 32: MINX pre-mRNA (intron)



• Molecule 32: MINX pre-mRNA (intron)



• Molecule 33: Human gene for small nuclear RNA U2 (snRNA U2)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136534	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 ($e^-/\text{\AA}^2$)	2.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.146	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	572.4, 572.4, 572.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.59, 1.59, 1.59	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	6/10059 (0.1%)	0.40	8/14115 (0.1%)
2	B	0.10	0/4619	0.32	0/6475
3	C	0.22	0/1249	0.54	0/1758
4	D	0.12	0/1587	0.50	3/2215 (0.1%)
5	E	0.11	0/1655	0.43	0/2309
6	F	0.09	0/1540	0.41	0/2148
7	G	0.08	0/688	0.24	0/969
7	H	0.13	0/706	0.28	0/995
7	I	0.07	0/701	0.24	0/988
7	J	0.12	0/706	0.28	0/995
8	K	0.10	0/963	0.30	0/1346
9	L	0.09	0/1683	0.32	1/2349 (0.0%)
10	M	0.09	0/3575	0.35	0/5006
11	N	0.15	0/582	0.51	0/814
12	O	0.37	1/2858 (0.0%)	0.33	0/4007
13	P	0.10	0/1408	0.37	0/1969
14	Q	0.07	0/718	0.26	0/1003
15	R	0.07	0/493	0.30	0/688
16	S	0.41	0/149	0.90	0/205
17	T	0.07	0/999	0.26	0/1397
19	V	0.08	0/782	0.27	0/1088
20	W	0.97	0/821	2.23	43/1149 (3.7%)
21	X	0.94	0/472	1.87	7/658 (1.1%)
22	a	0.13	0/500	0.36	0/698
22	h	0.99	0/496	1.21	3/693 (0.4%)
23	b	0.09	0/382	0.27	0/531
23	i	1.05	0/372	1.20	1/517 (0.2%)
24	c	0.09	0/393	0.30	0/547
24	j	1.03	0/393	1.22	0/547
25	d	0.09	0/371	0.29	0/516
25	k	0.79	0/371	1.03	0/516
26	e	0.10	0/422	0.35	0/588
26	l	0.74	0/417	1.00	0/581
27	f	0.08	0/356	0.29	0/494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	m	0.71	0/356	0.96	0/494
28	g	0.30	1/414 (0.2%)	0.29	0/578
28	n	0.86	0/414	1.06	0/578
32	Y	0.38	2/754 (0.3%)	0.25	0/1169
32	Z	0.07	0/285	0.17	0/442
33	2	0.12	0/3312	0.25	1/5151 (0.0%)
34	5	0.08	0/2672	0.19	0/4154
35	6	0.09	0/2129	0.23	0/3314
All	All	0.31	10/53822 (0.0%)	0.53	67/76754 (0.1%)

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
1	A	0	4
2	B	0	1
4	D	0	1
5	E	0	1
6	F	0	1
9	L	0	1
10	M	0	2
11	N	0	2
12	O	0	2
22	h	0	1
All	All	0	16

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	209	PRO	C-N	19.23	1.78	1.33
1	A	1134	TRP	C-N	12.62	1.63	1.33
1	A	323	LEU	C-N	9.05	1.55	1.33
1	A	369	GLU	C-N	7.95	1.52	1.33
1	A	174	PRO	C-N	7.64	1.51	1.33
32	Y	142	U	C1'-N1	6.09	1.57	1.48
28	g	74	LEU	C-N	5.84	1.47	1.33
32	Y	139	U	C1'-N1	5.71	1.56	1.47
1	A	1451	ASN	C-N	5.19	1.46	1.33
1	A	1946	ASN	N-CA	-5.12	1.39	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1945[A]	VAL	CA-C-N	-10.77	107.23	122.41
1	A	1945[A]	VAL	C-N-CA	-10.77	107.23	122.41
22	h	77	VAL	C-N-CD	-10.51	81.91	125.00
20	W	5	THR	N-CA-CB	-8.48	98.32	111.05
20	W	99	SER	N-CA-C	7.93	122.73	112.26
20	W	16	THR	CA-C-O	-7.86	111.95	120.36
20	W	117	TYR	CA-C-O	7.64	128.42	120.40
33	2	52	G	C2'-C3'-O3'	7.49	120.73	109.50
20	W	71	VAL	CA-C-N	7.13	131.52	120.75
20	W	71	VAL	C-N-CA	7.13	131.52	120.75
20	W	47	ILE	N-CA-CB	7.09	123.07	111.58
20	W	4	LEU	N-CA-C	-6.93	97.93	108.67
20	W	121	LEU	CA-C-O	6.82	128.81	121.44
21	X	56	PHE	CA-C-O	-6.79	112.85	120.32
20	W	58	ASP	N-CA-CB	-6.75	100.57	111.24
20	W	87	LEU	CA-C-N	6.45	126.21	119.05
20	W	87	LEU	C-N-CA	6.45	126.21	119.05
20	W	40	THR	CA-C-N	6.29	131.52	122.40
20	W	40	THR	C-N-CA	6.29	131.52	122.40
1	A	1901	LYS	CA-C-N	-6.18	112.35	122.54
1	A	1901	LYS	C-N-CA	-6.18	112.35	122.54
20	W	73	ASN	N-CA-C	6.12	119.79	111.17
20	W	75	ARG	N-CA-CB	-6.00	102.63	111.51
1	A	1947	ASN	N-CA-C	-5.93	104.21	112.45
21	X	49	MET	N-CA-C	-5.92	104.74	111.07
20	W	79	ILE	CA-C-N	5.91	125.72	120.10
20	W	79	ILE	C-N-CA	5.91	125.72	120.10
20	W	27	ARG	CB-CA-C	-5.89	98.70	109.54
20	W	118	LEU	CA-C-N	-5.88	114.49	122.77
20	W	118	LEU	C-N-CA	-5.88	114.49	122.77
22	h	112	ASN	N-CA-CB	-5.87	105.24	111.29
20	W	113	LYS	N-CA-C	5.81	118.36	111.33
20	W	50	SER	CA-C-O	5.74	127.64	121.55
20	W	149	LYS	CB-CA-C	-5.70	101.96	110.16
20	W	27	ARG	CA-C-N	5.67	128.67	120.11
20	W	27	ARG	C-N-CA	5.67	128.67	120.11
1	A	1205	GLU	CB-CA-C	-5.64	110.05	116.54
20	W	34	ILE	CA-C-O	-5.59	114.14	120.74
20	W	71	VAL	O-C-N	-5.52	115.67	122.57
20	W	159	GLU	N-CA-C	-5.49	104.94	111.69
1	A	1902	PHE	CA-C-N	-5.41	110.81	121.41
1	A	1902	PHE	C-N-CA	-5.41	110.81	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	W	16	THR	O-C-N	5.41	129.38	123.22
23	i	6	ASN	N-CA-C	5.40	116.34	110.13
20	W	40	THR	N-CA-C	-5.38	106.22	112.89
20	W	32	PRO	CA-C-N	5.36	130.44	122.99
20	W	32	PRO	C-N-CA	5.36	130.44	122.99
20	W	125	VAL	CA-C-N	5.33	127.96	120.28
20	W	125	VAL	C-N-CA	5.33	127.96	120.28
20	W	33	VAL	N-CA-CB	-5.33	103.74	111.52
9	L	222	LEU	CB-CA-C	-5.31	110.43	116.54
4	D	400	PHE	CA-C-N	5.31	139.74	127.00
4	D	400	PHE	C-N-CA	5.31	139.74	127.00
21	X	9	ASN	N-CA-CB	-5.28	101.70	111.53
21	X	23	LYS	N-CA-C	5.27	117.44	111.11
20	W	146	ASP	CA-C-N	5.26	130.02	122.40
20	W	146	ASP	C-N-CA	5.26	130.02	122.40
20	W	88	PRO	CB-CA-C	-5.22	104.01	112.62
21	X	54	GLN	N-CA-C	5.20	117.58	109.52
22	h	56	VAL	CB-CA-C	-5.13	104.12	111.31
21	X	51	MET	N-CA-C	5.13	119.54	113.28
21	X	41	VAL	O-C-N	5.13	127.11	121.83
4	D	400	PHE	C-N-CD	-5.11	109.36	120.60
20	W	83	LEU	N-CA-C	5.08	117.48	111.33
20	W	99	SER	N-CA-CB	-5.06	102.87	111.17
20	W	28	GLY	N-CA-C	5.06	120.87	113.48
20	W	90	LEU	CA-C-O	-5.06	113.28	120.51

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	GLU	Peptide
1	A	1852	LEU	Peptide
1	A	1899	VAL	Peptide
1	A	1946	ASN	Peptide
2	B	352	LYS	Peptide
4	D	457	PRO	Peptide
5	E	491	GLN	Peptide
6	F	98	ASP	Peptide
9	L	78	MET	Peptide
10	M	48	ALA	Peptide
10	M	517	THR	Peptide
11	N	173	VAL	Peptide

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Mol	Chain	Res	Type	Group
11	N	174	PRO	Peptide
12	O	589	LEU	Peptide
12	O	692	THR	Peptide
22	h	112	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	A	9955	0	4850	177	0
2	B	4566	0	2269	91	0
3	C	1231	0	665	18	0
4	D	1576	0	774	80	0
5	E	1646	0	787	85	0
6	F	1531	0	747	77	0
7	G	679	0	356	7	0
7	H	696	0	367	14	0
7	I	691	0	365	10	0
7	J	696	0	367	11	0
8	K	960	0	461	15	0
9	L	1680	0	807	12	0
10	M	3553	0	1738	50	0
11	N	579	0	277	6	0
12	O	2842	0	1355	22	0
13	P	1396	0	684	11	0
14	Q	713	0	337	3	0
15	R	493	0	220	5	0
16	S	148	0	78	29	0
17	T	1191	0	457	16	0
18	U	1287	0	0	20	0
19	V	774	0	404	17	0
20	W	816	0	386	3	0
21	X	470	0	223	1	0
22	a	497	0	229	1	0
22	h	493	0	226	15	0
23	b	379	0	186	1	0
23	i	369	0	182	1	0
24	c	393	0	169	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	j	393	0	169	2	0
25	d	369	0	178	1	0
25	k	369	0	178	5	0
26	e	420	0	200	1	0
26	l	415	0	196	26	0
27	f	355	0	164	1	0
27	m	355	0	164	1	0
28	g	412	0	188	2	0
28	n	412	0	188	1	0
29	o	223	0	0	13	0
30	p	385	0	0	1	0
31	q	627	0	0	0	0
32	Y	677	0	342	8	0
32	Z	256	0	132	11	0
33	2	2968	0	1494	82	0
34	5	2397	0	1216	30	0
35	6	1903	0	964	29	0
All	All	55236	0	25739	905	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 (905) 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)
10:M:107:HIS:H	29:o:263:VAL:CA	1.04	1.58
1:A:1355:SER:CB	16:S:17:GLY:HA3	1.26	1.57
30:p:85:GLY:CA	30:p:371:TYR:CA	1.83	1.54
1:A:1355:SER:CB	16:S:17:GLY:CA	1.88	1.49
10:M:309:ALA:HB3	18:U:358:GLU:CA	1.42	1.48
10:M:309:ALA:CB	18:U:358:GLU:CA	1.91	1.45
1:A:1355:SER:CA	16:S:17:GLY:HA3	1.43	1.43
12:O:209:PRO:C	12:O:210:PRO:N	1.78	1.39
22:h:85:LYS:CB	33:2:137:U:H1'	1.49	1.39
26:l:52:ASP:CA	33:2:181:G:C4	1.99	1.37
10:M:107:HIS:N	29:o:263:VAL:CA	1.90	1.34
1:A:1776:ILE:CB	1:A:1859:LYS:H	1.43	1.31
22:h:77:VAL:CB	22:h:78:PRO:CD	2.10	1.29
10:M:310:LYS:CB	18:U:354:SER:CA	2.11	1.28
26:l:54:ARG:N	33:2:151:C:O2	1.65	1.26
10:M:310:LYS:N	18:U:354:SER:CA	1.99	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:65:PRO:HG3	29:o:242:ASN:CA	1.64	1.26
10:M:310:LYS:CA	18:U:354:SER:CA	2.13	1.25
1:A:1355:SER:CB	16:S:17:GLY:N	1.98	1.23
22:h:77:VAL:CB	22:h:78:PRO:HD2	1.66	1.23
33:2:53:U:O2'	33:2:54:U:H5'	1.40	1.22
29:o:53:GLU:CA	29:o:151:LYS:CA	2.18	1.22
22:h:87:SER:CB	33:2:137:U:H5'	1.68	1.22
26:l:52:ASP:N	33:2:181:G:C4	1.92	1.22
10:M:306:MET:N	18:U:355:ASN:CA	2.08	1.17
16:S:11:ARG:HA	32:Z:51:U:H1'	1.18	1.11
26:l:52:ASP:N	33:2:181:G:N3	1.82	1.10
1:A:1355:SER:CB	16:S:17:GLY:H	1.60	1.08
5:E:489:GLY:H	5:E:498:LYS:C	1.61	1.08
5:E:489:GLY:H	5:E:499:LYS:N	1.53	1.06
10:M:306:MET:CB	18:U:355:ASN:CA	2.34	1.05
4:D:440:ASP:H	4:D:447:PHE:N	1.53	1.05
32:Y:143:G:N2	32:Y:144:A:H62	1.52	1.04
1:A:1853:PRO:O	1:A:1856:GLU:N	1.90	1.04
16:S:11:ARG:CA	32:Z:51:U:H1'	1.88	1.04
4:D:440:ASP:H	4:D:446:ASN:C	1.66	1.03
20:W:20:ARG:CB	27:m:66:VAL:CB	2.37	1.02
4:D:274:ASP:H	4:D:281:ILE:N	1.57	1.02
4:D:274:ASP:H	4:D:280:VAL:C	1.65	1.02
10:M:65:PRO:CG	29:o:242:ASN:CA	2.37	1.01
10:M:306:MET:CA	18:U:355:ASN:CA	2.38	1.01
6:F:137:ASP:H	6:F:143:ARG:C	1.69	1.00
22:h:77:VAL:CB	22:h:78:PRO:HD3	1.87	1.00
6:F:94:ASN:H	6:F:101:ASN:C	1.68	1.00
6:F:221:ASP:H	6:F:227:LEU:C	1.70	1.00
26:l:52:ASP:HA	33:2:181:G:C5	1.96	1.00
1:A:1946:ASN:O	1:A:1950:ALA:HB2	1.59	0.99
33:2:94:A:H5''	33:2:94:A:H8	1.26	0.99
26:l:29:ARG:CB	33:2:168:A:H1'	1.93	0.99
26:l:52:ASP:CA	33:2:181:G:C5	2.40	0.99
26:l:52:ASP:HA	33:2:181:G:C4	1.90	0.98
26:l:66:SER:CB	33:2:101:U:O4'	2.12	0.97
6:F:313:ASP:H	6:F:319:ILE:C	1.72	0.97
4:D:399:LYS:H	4:D:405:PHE:C	1.71	0.97
5:E:360:ASP:H	5:E:366:CYS:C	1.72	0.97
5:E:317:GLU:H	5:E:324:CYS:C	1.72	0.97
5:E:536:ASP:H	5:E:542:LEU:C	1.70	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:ASP:H	4:D:238:LEU:C	1.73	0.97
6:F:180:ASP:H	6:F:186:ALA:C	1.72	0.97
1:A:1776:ILE:CB	1:A:1859:LYS:N	2.28	0.96
19:V:100:MET:H	19:V:128:ILE:C	1.74	0.96
7:I:73:ALA:O	7:I:77:ALA:HB3	1.64	0.96
2:B:225:VAL:O	2:B:253:VAL:HA	1.66	0.96
33:2:53:U:O2'	33:2:54:U:C5'	2.14	0.96
4:D:316:ASP:O	4:D:321:ALA:O	1.83	0.95
34:5:12:U:H3	34:5:65:G:H1	1.03	0.95
1:A:1943:LEU:O	1:A:1947:ASN:CB	2.14	0.95
1:A:976:MET:HA	1:A:1097:ILE:O	1.67	0.94
22:h:85:LYS:CB	33:2:137:U:C1'	2.45	0.93
2:B:501:ILE:O	2:B:543:ARG:HA	1.68	0.93
4:D:440:ASP:N	4:D:447:PHE:N	2.16	0.93
8:K:210:LYS:HA	8:K:214:GLY:HA3	1.50	0.93
1:A:974:ASN:HA	1:A:1099:PHE:O	1.67	0.92
4:D:426:VAL:HA	4:D:439:TRP:O	1.69	0.92
2:B:746:VAL:O	2:B:790:LYS:HA	1.70	0.91
29:o:274:VAL:CA	33:2:59:A:H4'	2.00	0.91
1:A:117:PRO:HA	1:A:485:THR:O	1.70	0.91
4:D:358:ASP:H	4:D:364:THR:C	1.78	0.91
4:D:476:ARG:HA	4:D:489:TYR:O	1.71	0.91
5:E:489:GLY:N	5:E:499:LYS:N	2.18	0.90
2:B:255:VAL:O	2:B:307:VAL:HA	1.72	0.90
6:F:263:ASP:H	6:F:273:CYS:C	1.79	0.90
5:E:404:ASP:H	5:E:410:ILE:C	1.79	0.90
1:A:118:VAL:O	1:A:484:SER:HA	1.72	0.89
1:A:1666:LEU:HA	1:A:1705:ILE:O	1.72	0.89
25:k:50:THR:CB	33:2:183:G:O2'	2.20	0.89
2:B:347:ILE:HA	2:B:357:THR:O	1.72	0.88
4:D:479:THR:O	4:D:486:ILE:HA	1.71	0.88
16:S:11:ARG:HA	32:Z:51:U:C1'	2.04	0.88
10:M:309:ALA:HB2	18:U:358:GLU:CA	2.04	0.88
4:D:316:ASP:O	4:D:321:ALA:C	2.17	0.87
33:2:150:U:H3	33:2:181:G:H1	1.20	0.87
6:F:94:ASN:H	6:F:102:TYR:N	1.73	0.87
2:B:857:VAL:C	2:B:874:PHE:H	1.82	0.86
4:D:274:ASP:O	4:D:279:LYS:O	1.93	0.86
5:E:446:GLU:H	5:E:452:ASP:C	1.82	0.86
22:h:87:SER:CB	33:2:136:G:O2'	2.22	0.86
34:5:17:U:H3	34:5:60:G:H1	0.86	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:LYS:C	4:D:490:ARG:O	2.18	0.86
10:M:306:MET:H	18:U:355:ASN:CA	1.83	0.86
1:A:1897:LEU:O	1:A:1902:PHE:N	2.08	0.86
1:A:1355:SER:HA	16:S:17:GLY:HA3	1.54	0.86
16:S:11:ARG:HA	32:Z:51:U:O2	1.75	0.86
1:A:1355:SER:CA	16:S:17:GLY:CA	2.35	0.86
1:A:1355:SER:C	16:S:17:GLY:HA3	2.01	0.86
19:V:100:MET:H	19:V:129:PHE:N	1.74	0.85
10:M:309:ALA:HB1	18:U:358:GLU:CA	2.06	0.85
32:Y:143:G:H21	32:Y:144:A:N6	1.73	0.85
32:Y:142:U:HO2'	32:Y:143:G:H8	0.91	0.85
8:K:209:ILE:O	8:K:212:GLN:O	1.94	0.85
8:K:210:LYS:O	8:K:213:HIS:O	1.94	0.84
29:o:273:ASP:CA	33:2:58:U:O2'	2.25	0.84
2:B:134:LEU:HA	2:B:226:VAL:O	1.78	0.84
1:A:1899:VAL:O	1:A:1901:LYS:N	2.10	0.83
13:P:280:ALA:O	13:P:284:ALA:HB2	1.77	0.83
2:B:530:LEU:O	2:B:540:GLU:HA	1.77	0.82
2:B:833:PHE:HA	2:B:873:ALA:O	1.80	0.82
34:5:43:U:H4'	35:6:67:G:H1	1.43	0.82
4:D:399:LYS:O	4:D:404:SER:O	1.98	0.82
26:l:53:GLY:HA3	33:2:152:G:C4	2.15	0.82
5:E:360:ASP:H	5:E:367:ILE:N	1.78	0.82
32:Y:143:G:H21	32:Y:144:A:H62	0.87	0.82
6:F:137:ASP:H	6:F:144:VAL:N	1.78	0.81
6:F:254:ALA:HB3	6:F:258:THR:O	1.80	0.81
6:F:180:ASP:H	6:F:187:ILE:N	1.79	0.81
5:E:554:ILE:H	5:E:571:TRP:HA	1.44	0.81
6:F:292:SER:O	6:F:301:ALA:HB3	1.82	0.80
4:D:274:ASP:N	4:D:281:ILE:N	2.28	0.80
6:F:313:ASP:H	6:F:320:LEU:N	1.79	0.80
2:B:589:LYS:HA	2:B:629:ILE:O	1.82	0.79
4:D:399:LYS:O	4:D:404:SER:C	2.26	0.79
5:E:404:ASP:H	5:E:411:VAL:N	1.80	0.79
6:F:221:ASP:H	6:F:228:THR:N	1.80	0.79
29:o:23:HIS:CA	29:o:31:ASP:CA	2.60	0.79
6:F:342:ILE:O	6:F:353:MET:HA	1.82	0.79
32:Y:143:G:N2	32:Y:144:A:N6	2.30	0.78
26:l:29:ARG:CB	33:2:168:A:C1'	2.62	0.78
6:F:82:ALA:HA	6:F:91:LEU:O	1.84	0.78
1:A:973:CYS:O	1:A:1100:ARG:HA	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1896:CYS:O	1:A:1899:VAL:O	2.02	0.78
10:M:310:LYS:H	18:U:354:SER:CA	1.91	0.78
33:2:94:A:H5''	33:2:94:A:C8	2.17	0.78
1:A:1898[A]:LYS:O	1:A:1903:GLY:N	2.14	0.78
4:D:440:ASP:O	4:D:445:TYR:O	2.01	0.78
5:E:317:GLU:O	5:E:323:ARG:O	2.03	0.77
33:2:53:U:C6	33:2:54:U:C5	2.73	0.77
1:A:517:HIS:O	1:A:524:LEU:HA	1.84	0.77
1:A:1776:ILE:O	1:A:1777:ILE:CB	2.33	0.76
2:B:856:HIS:O	2:B:874:PHE:O	2.03	0.76
2:B:181:ILE:C	2:B:183:SER:H	1.94	0.76
5:E:404:ASP:O	5:E:409:GLU:O	2.03	0.76
1:A:994:ASN:O	1:A:998:ARG:CB	2.34	0.76
12:O:590:SER:O	12:O:594:ARG:CB	2.34	0.76
2:B:441:PRO:O	2:B:445:ALA:HB2	1.85	0.76
5:E:446:GLU:O	5:E:451:VAL:O	2.03	0.75
1:A:115:ASP:H	1:A:488:ASP:HA	1.51	0.75
19:V:98:LEU:HA	19:V:115:THR:O	1.86	0.75
19:V:100:MET:HA	19:V:113:PHE:O	1.86	0.75
2:B:507:VAL:O	2:B:524:ILE:HA	1.87	0.75
5:E:536:ASP:H	5:E:543:TYR:N	1.85	0.75
19:V:99:ALA:H	19:V:115:THR:H	1.34	0.75
2:B:834:VAL:HA	2:B:898:LEU:O	1.87	0.74
5:E:446:GLU:H	5:E:453:PHE:N	1.84	0.74
6:F:344:SER:O	6:F:351:LEU:HA	1.87	0.74
3:C:174:ALA:O	3:C:199:MET:O	2.05	0.74
10:M:310:LYS:HA	18:U:354:SER:CA	2.15	0.74
4:D:232:ASP:O	4:D:237:LYS:C	2.30	0.74
22:h:87:SER:CB	33:2:137:U:C5'	2.58	0.74
6:F:221:ASP:O	6:F:226:LYS:O	2.06	0.74
7:J:31:GLU:O	7:J:35:ALA:HB2	1.87	0.73
4:D:232:ASP:O	4:D:237:LYS:O	2.06	0.73
5:E:536:ASP:O	5:E:541:LYS:O	2.04	0.73
33:2:53:U:HO2'	33:2:54:U:H5'	1.52	0.73
1:A:1246:GLN:O	1:A:1250:ALA:HB3	1.88	0.73
1:A:980:ARG:HA	1:A:1094:ARG:HA	1.70	0.73
1:A:1946:ASN:O	1:A:1950:ALA:CB	2.34	0.73
6:F:313:ASP:O	6:F:318:ARG:O	2.06	0.73
5:E:360:ASP:O	5:E:365:GLN:O	2.06	0.73
4:D:250:ARG:H	4:D:265:GLY:HA2	1.54	0.72
5:E:489:GLY:N	5:E:498:LYS:C	2.45	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:ARG:H	1:A:1099:PHE:HA	1.54	0.72
6:F:180:ASP:O	6:F:185:ALA:O	2.07	0.72
12:O:692:THR:O	12:O:694:ARG:N	2.21	0.72
6:F:137:ASP:O	6:F:142:GLU:O	2.07	0.72
33:2:53:U:H2'	33:2:54:U:H6	1.53	0.72
4:D:274:ASP:O	4:D:279:LYS:C	2.32	0.72
17:T:590:LEU:O	17:T:594:MET:CB	2.38	0.72
19:V:100:MET:O	19:V:127:THR:O	2.08	0.72
33:2:53:U:H2'	33:2:54:U:C6	2.25	0.72
7:H:31:GLU:O	7:H:35:ALA:HB2	1.90	0.71
1:A:582:PHE:O	1:A:586:GLY:HA3	1.91	0.71
4:D:316:ASP:H	4:D:322:SER:C	1.98	0.71
5:E:445:TRP:HA	5:E:453:PHE:H	1.56	0.70
19:V:16:LEU:O	19:V:22:ILE:HA	1.90	0.70
29:O:277:GLN:CA	33:2:59:A:O2'	2.39	0.70
4:D:358:ASP:O	4:D:363:LYS:C	2.34	0.70
22:h:86:LYS:H	33:2:136:G:H21	1.39	0.70
6:F:126:SER:O	6:F:134:ALA:HB3	1.91	0.70
4:D:195:LYS:O	4:D:490:ARG:O	2.08	0.70
9:L:214:ILE:O	9:L:216:PHE:N	2.24	0.70
29:O:274:VAL:CA	33:2:59:A:C4'	2.69	0.69
33:2:53:U:C5	33:2:54:U:C5	2.80	0.69
2:B:191:PRO:HA	2:B:197:SER:HA	1.74	0.69
4:D:292:TYR:N	4:D:306:CYS:O	2.25	0.69
6:F:94:ASN:O	6:F:100:ASP:O	2.11	0.69
2:B:182:LYS:O	2:B:183:SER:CB	2.40	0.69
33:2:12:G:H1	35:6:86:U:H3	1.39	0.69
1:A:896:ILE:HA	1:A:909:TYR:HA	1.75	0.68
33:2:46:U:H2'	33:2:47:U:O4'	1.93	0.68
4:D:334:ALA:N	4:D:348:GLY:O	2.25	0.68
4:D:440:ASP:H	4:D:446:ASN:CA	2.07	0.68
16:S:14:GLY:O	32:Z:51:U:C4	2.46	0.68
15:R:68:ARG:O	15:R:72:ARG:CB	2.42	0.68
1:A:599:MET:O	1:A:603:ARG:CB	2.42	0.68
1:A:1676:ILE:O	1:A:1680:ALA:HB3	1.93	0.68
2:B:863:ILE:CB	2:B:868:LEU:O	2.42	0.68
2:B:181:ILE:O	2:B:183:SER:N	2.27	0.68
2:B:477:HIS:O	2:B:495:ARG:O	2.10	0.68
6:F:94:ASN:O	6:F:101:ASN:HA	1.94	0.68
5:E:317:GLU:H	5:E:325:LEU:N	1.90	0.68
1:A:847:LYS:O	1:A:851:SER:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1896:CYS:O	1:A:1899:VAL:C	2.37	0.68
6:F:155:ASN:H	6:F:171:SER:HA	1.59	0.67
2:B:837:GLN:O	2:B:895:ALA:HA	1.94	0.67
4:D:382:PRO:HG3	4:D:423:SER:HA	1.76	0.67
6:F:93:TRP:HA	6:F:102:TYR:H	1.59	0.67
16:S:11:ARG:CA	32:Z:51:U:O2	2.42	0.67
2:B:371:GLU:O	2:B:375:GLU:CB	2.43	0.67
10:M:347:SER:O	10:M:351:ARG:CB	2.43	0.67
33:2:53:U:C4	33:2:95:A:N6	2.63	0.67
4:D:358:ASP:O	4:D:363:LYS:O	2.12	0.67
8:K:209:ILE:O	8:K:212:GLN:C	2.38	0.67
1:A:1730:MET:O	1:A:1734:MET:CB	2.43	0.66
1:A:1908:LYS:HA	5:E:450:PRO:HD2	1.77	0.66
12:O:589:LEU:O	12:O:591:LEU:N	2.28	0.66
1:A:1195:ARG:CB	1:A:1229:PHE:O	2.43	0.66
33:2:46:U:H5'	33:2:47:U:OP2	1.95	0.66
2:B:478:THR:C	2:B:495:ARG:H	2.03	0.66
2:B:858:THR:N	2:B:874:PHE:H	1.93	0.66
19:V:99:ALA:HA	19:V:129:PHE:H	1.60	0.66
2:B:832:TYR:HA	2:B:900:VAL:O	1.97	0.65
7:I:31:GLU:O	7:I:35:ALA:HB2	1.96	0.65
26:I:54:ARG:N	33:2:151:C:C2	2.57	0.65
1:A:1946:ASN:HA	1:A:1949:ARG:H	1.60	0.65
28:n:35:SER:CB	33:2:103:U:O2	2.45	0.65
33:2:42:G:OP2	33:2:42:G:N2	2.30	0.65
1:A:791:GLN:O	1:A:795:LEU:CB	2.44	0.65
4:D:440:ASP:O	4:D:445:TYR:C	2.41	0.64
1:A:1664:ILE:HA	1:A:1703:ILE:O	1.98	0.64
5:E:390:LEU:HA	5:E:403:TRP:O	1.96	0.64
13:P:283:ALA:O	13:P:287:SER:CB	2.45	0.64
2:B:836:VAL:O	2:B:870:THR:HA	1.98	0.64
1:A:1743:LEU:O	1:A:1747:ILE:CB	2.46	0.64
2:B:689:ALA:HA	2:B:788:LYS:O	1.97	0.64
5:E:489:GLY:O	5:E:497:ASN:HA	1.96	0.64
1:A:91:ALA:HB2	1:A:125:ALA:HB1	1.80	0.63
12:O:480:TYR:O	12:O:484:VAL:CB	2.46	0.63
1:A:950:LEU:O	1:A:954:LYS:CB	2.47	0.63
1:A:1903:GLY:O	1:A:1907:LEU:CB	2.47	0.63
10:M:332:ALA:O	10:M:336:GLN:CB	2.46	0.63
5:E:535:TRP:HA	5:E:543:TYR:H	1.62	0.63
11:N:166:SER:O	11:N:170:GLY:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:6:57:U:H2'	35:6:58:G:C8	2.34	0.63
33:2:101:U:H5''	33:2:102:U:H5'	1.81	0.63
5:E:359:TRP:HA	5:E:367:ILE:H	1.63	0.63
26:l:53:GLY:HA3	33:2:152:G:N3	2.14	0.62
1:A:1897:LEU:O	1:A:1899:VAL:O	2.15	0.62
4:D:196:LEU:C	4:D:490:ARG:H	2.07	0.62
6:F:179:TRP:HA	6:F:187:ILE:H	1.64	0.62
1:A:1377:SER:O	1:A:1381:ASP:CB	2.47	0.62
2:B:441:PRO:O	2:B:445:ALA:CB	2.47	0.62
33:2:94:A:H8	33:2:94:A:C5'	2.06	0.62
6:F:197:LEU:N	6:F:211:GLY:O	2.33	0.61
4:D:477:LEU:O	4:D:488:VAL:HA	2.00	0.61
1:A:798:GLY:O	1:A:800:TYR:N	2.31	0.61
2:B:858:THR:H	2:B:873:ALA:HA	1.64	0.61
4:D:342:GLU:O	4:D:344:GLN:N	2.34	0.61
5:E:489:GLY:O	5:E:497:ASN:CA	2.48	0.61
9:L:22:ALA:O	9:L:26:TYR:CB	2.49	0.61
33:2:53:U:C6	33:2:54:U:C6	2.88	0.61
13:P:259:ARG:N	13:P:273:GLN:O	2.33	0.61
1:A:167:PRO:O	1:A:169:PHE:N	2.34	0.61
1:A:374:ASP:O	1:A:378:PHE:CB	2.49	0.61
10:M:306:MET:C	18:U:355:ASN:CA	2.74	0.61
5:E:340:PHE:HA	5:E:347:PHE:HA	1.83	0.60
1:A:1355:SER:HA	16:S:17:GLY:O	2.00	0.60
34:5:12:U:O4	34:5:65:G:O6	2.18	0.60
34:5:12:U:O2	34:5:65:G:N2	2.32	0.60
5:E:516:PHE:HA	5:E:523:VAL:HA	1.83	0.60
2:B:926:ALA:HB1	2:B:927:PRO:HD2	1.83	0.60
4:D:440:ASP:N	4:D:447:PHE:H	1.96	0.60
16:S:11:ARG:HA	32:Z:51:U:C2	2.35	0.60
4:D:457:PRO:HG2	15:R:211:VAL:HA	1.83	0.60
16:S:11:ARG:CB	32:Z:51:U:O2'	2.50	0.60
34:5:94:U:O2	34:5:95:G:N2	2.35	0.60
7:H:16:CYS:O	7:H:25:TYR:CB	2.50	0.60
4:D:436:MET:O	4:D:450:VAL:CB	2.49	0.60
33:2:49:U:C4	33:2:50:C:C5	2.90	0.60
19:V:18:THR:HA	19:V:160:ILE:H	1.67	0.59
2:B:866:SER:O	2:B:868:LEU:N	2.34	0.59
4:D:440:ASP:N	4:D:446:ASN:HA	2.17	0.59
6:F:70:TYR:H	6:F:85:GLY:HA2	1.66	0.59
1:A:1355:SER:HA	16:S:17:GLY:C	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:ASP:H	4:D:239:LYS:N	1.99	0.59
8:K:206:ILE:O	8:K:210:LYS:CB	2.51	0.59
2:B:509:VAL:O	2:B:522:SER:HA	2.02	0.59
4:D:390:GLY:HA2	4:D:395:ILE:HA	1.85	0.59
1:A:975:VAL:O	1:A:1098:PHE:HA	2.03	0.59
34:5:42:U:H2'	34:5:43:U:C6	2.38	0.59
6:F:312:TRP:HA	6:F:320:LEU:H	1.68	0.59
22:h:85:LYS:CB	33:2:137:U:O2	2.50	0.59
2:B:181:ILE:C	2:B:183:SER:N	2.61	0.59
1:A:926:LEU:O	1:A:930:ALA:HB2	2.03	0.58
1:A:953:TYR:O	1:A:957:GLN:CB	2.51	0.58
10:M:107:HIS:CB	29:o:263:VAL:CA	2.81	0.58
10:M:723:MET:O	10:M:727:ARG:CB	2.51	0.58
1:A:1382:SER:O	1:A:1386:TRP:CB	2.52	0.58
1:A:1470:TYR:O	1:A:1474:MET:CB	2.51	0.58
4:D:274:ASP:H	4:D:280:VAL:CA	2.14	0.58
18:U:498:GLU:CA	18:U:499:TYR:CA	2.81	0.58
1:A:1386:TRP:O	1:A:1390:ALA:HB2	2.04	0.58
1:A:1662:ILE:HA	1:A:1701:VAL:O	2.03	0.58
5:E:403:TRP:HA	5:E:411:VAL:H	1.67	0.58
1:A:797:ASP:C	1:A:799:PRO:HD3	2.28	0.58
1:A:1217:GLN:HA	1:A:1224:ARG:HA	1.85	0.58
1:A:1355:SER:HA	16:S:17:GLY:CA	2.19	0.58
5:E:356:LEU:O	5:E:370:PHE:CB	2.52	0.58
5:E:525:SER:O	5:E:533:ASN:CB	2.52	0.58
7:J:80:ASP:O	7:J:84:ALA:HB2	2.03	0.58
1:A:1533:ARG:O	1:A:1537:TRP:CB	2.52	0.58
33:2:161:U:O2	33:2:163:G:N2	2.36	0.58
34:5:43:U:H5'	35:6:69:A:H1'	1.84	0.58
1:A:926:LEU:O	1:A:930:ALA:CB	2.52	0.58
1:A:1942:ALA:O	1:A:1946:ASN:C	2.46	0.58
2:B:643:ASP:O	2:B:647:MET:CB	2.52	0.58
5:E:446:GLU:O	5:E:452:ASP:HA	2.04	0.58
5:E:515:ASP:CB	5:E:524:ILE:O	2.51	0.58
7:H:73:ALA:O	7:H:77:ALA:HB3	2.03	0.58
2:B:287:GLY:O	2:B:291:MET:CB	2.52	0.58
5:E:296:LEU:HA	5:E:304:LEU:HA	1.86	0.58
33:2:46:U:C2'	33:2:47:U:O4'	2.51	0.58
10:M:307:ILE:O	18:U:352:ALA:CA	2.51	0.57
5:E:489:GLY:H	5:E:498:LYS:CA	2.18	0.57
1:A:1569:LEU:O	1:A:1573:LEU:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1729:ALA:O	1:A:1733:ILE:CB	2.52	0.57
6:F:220:TRP:HA	6:F:228:THR:H	1.70	0.57
10:M:668:CYS:O	10:M:672:ALA:HB2	2.04	0.57
32:Y:142:U:O2'	32:Y:143:G:H8	1.73	0.57
1:A:715:GLU:O	1:A:719:CYS:CB	2.53	0.57
1:A:1245:ARG:O	1:A:1249:MET:CB	2.53	0.57
5:E:336:ARG:N	5:E:350:ALA:O	2.38	0.57
1:A:115:ASP:C	1:A:487:LEU:O	2.48	0.57
1:A:978:GLU:HA	1:A:1095:ILE:O	2.04	0.57
1:A:1567:PRO:O	1:A:1571:ILE:CB	2.52	0.57
1:A:1676:ILE:O	1:A:1680:ALA:CB	2.53	0.57
3:C:209:PRO:HG2	3:C:210:PRO:HD3	1.86	0.57
4:D:206:TRP:O	4:D:224:ALA:N	2.34	0.57
5:E:292:SER:N	5:E:307:CYS:O	2.36	0.57
7:I:73:ALA:O	7:I:77:ALA:CB	2.47	0.57
33:2:49:U:O4	33:2:50:C:C5	2.58	0.57
35:6:15:A:H2'	35:6:16:G:H8	1.70	0.57
4:D:307:SER:CB	4:D:311:THR:O	2.52	0.57
6:F:94:ASN:N	6:F:102:TYR:N	2.49	0.57
12:O:248:TYR:O	12:O:252:GLU:CB	2.53	0.57
1:A:651:TRP:HA	35:6:66:C:H1'	1.87	0.56
10:M:480:VAL:O	10:M:484:LEU:CB	2.53	0.56
17:T:586:PHE:O	17:T:590:LEU:CB	2.53	0.56
3:C:220:ARG:C	3:C:222:PRO:HD2	2.31	0.56
4:D:260:TYR:HA	4:D:273:TRP:O	2.05	0.56
6:F:136:TRP:HA	6:F:144:VAL:H	1.70	0.56
1:A:641:MET:O	1:A:645:THR:CB	2.53	0.56
12:O:583:GLU:O	12:O:587:LYS:N	2.38	0.56
26:l:80:ALA:HB1	26:l:81:PRO:HA	1.86	0.56
10:M:107:HIS:CA	29:o:263:VAL:CA	2.83	0.56
10:M:479:ARG:O	10:M:483:SER:CB	2.53	0.56
26:l:52:ASP:HA	33:2:181:G:N9	2.20	0.56
4:D:477:LEU:H	4:D:489:TYR:H	1.54	0.56
6:F:94:ASN:N	6:F:101:ASN:C	2.51	0.56
9:L:182:LEU:O	9:L:186:GLN:CB	2.53	0.56
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	1.87	0.56
5:E:523:VAL:O	5:E:535:TRP:CB	2.53	0.56
10:M:163:GLU:O	10:M:167:ARG:CB	2.53	0.56
2:B:856:HIS:C	2:B:874:PHE:O	2.49	0.56
6:F:282:HIS:HA	6:F:304:SER:HA	1.88	0.56
7:J:31:GLU:O	7:J:35:ALA:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:489:GLY:O	5:E:497:ASN:C	2.48	0.56
1:A:68:LYS:O	1:A:72:ASP:CB	2.55	0.55
4:D:399:LYS:CB	4:D:405:PHE:O	2.54	0.55
7:J:75:LEU:O	7:J:79:GLN:CB	2.55	0.55
16:S:17:GLY:O	16:S:19:VAL:N	2.39	0.55
1:A:1667:ARG:O	1:A:1707:LEU:N	2.39	0.55
1:A:1679:TYR:O	1:A:1683:LYS:CB	2.54	0.55
2:B:506:PRO:HA	2:B:525:CYS:O	2.05	0.55
2:B:830:PRO:HA	2:B:904:TRP:HA	1.88	0.55
4:D:274:ASP:N	4:D:280:VAL:HA	2.22	0.55
1:A:1214:TRP:CB	1:A:1228:CYS:O	2.54	0.55
26:I:52:ASP:HA	33:2:181:G:C8	2.41	0.55
1:A:1684:PHE:O	1:A:1688:THR:CB	2.54	0.55
2:B:764:ASP:O	2:B:768:GLN:CB	2.54	0.55
5:E:479:GLN:HA	5:E:485:ILE:HA	1.87	0.55
6:F:113:MET:N	6:F:127:ALA:O	2.40	0.55
10:M:52:ARG:O	10:M:56:LEU:CB	2.54	0.55
19:V:100:MET:N	19:V:128:ILE:C	2.54	0.55
1:A:1155:TRP:O	1:A:1159:ASN:CB	2.55	0.55
1:A:1570:LYS:O	1:A:1574:ILE:CB	2.55	0.55
1:A:1702:LEU:H	1:A:1716:GLY:HA3	1.72	0.55
17:T:512:GLY:O	17:T:516:MET:CB	2.55	0.55
7:G:31:GLU:O	7:G:35:ALA:HB2	2.07	0.55
7:H:64:LYS:O	7:H:66:PRO:HD3	2.07	0.55
13:P:280:ALA:O	13:P:284:ALA:CB	2.50	0.55
24:c:33:VAL:N	24:c:43:ILE:O	2.39	0.55
1:A:709:ILE:O	1:A:713:LEU:CB	2.55	0.54
3:C:175:GLN:CB	3:C:199:MET:O	2.54	0.54
4:D:358:ASP:H	4:D:364:THR:CA	2.19	0.54
1:A:598:LEU:O	1:A:602:ILE:CB	2.55	0.54
1:A:1731:ALA:O	1:A:1735:LYS:CB	2.56	0.54
2:B:532:ILE:O	2:B:538:HIS:HA	2.08	0.54
4:D:440:ASP:H	4:D:446:ASN:HA	1.71	0.54
10:M:47:GLY:HA3	10:M:50:LYS:H	1.72	0.54
1:A:1901:LYS:O	1:A:1905:LEU:CB	2.55	0.54
6:F:217:ILE:CB	6:F:231:MET:O	2.54	0.54
6:F:254:ALA:CB	6:F:258:THR:O	2.54	0.54
10:M:406:GLU:HA	10:M:410:GLN:HA	1.89	0.54
6:F:341:ILE:HA	6:F:354:GLY:O	2.07	0.54
7:J:27:ARG:O	7:J:31:GLU:CB	2.55	0.54
34:5:17:U:O4	34:5:60:G:O6	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:316:TRP:HA	5:E:325:LEU:H	1.73	0.54
5:E:446:GLU:N	5:E:452:ASP:C	2.60	0.54
16:S:23:LEU:CB	17:T:477:LEU:CB	2.86	0.54
1:A:1426:ASP:O	1:A:1430:LEU:CB	2.56	0.54
7:J:128:ARG:O	7:J:132:ALA:CB	2.55	0.54
34:5:78:U:O2'	34:5:80:U:OP1	2.26	0.54
9:L:74:LEU:O	9:L:78:MET:N	2.37	0.54
16:S:22:ASN:C	16:S:24:SER:H	2.16	0.54
26:l:55:VAL:N	33:2:152:G:H5'	2.23	0.54
1:A:581:ILE:O	1:A:585:VAL:CB	2.56	0.54
1:A:711:GLN:O	1:A:715:GLU:CB	2.56	0.54
1:A:1246:GLN:O	1:A:1250:ALA:CB	2.55	0.54
2:B:829:GLU:O	2:B:905:GLN:N	2.37	0.53
8:K:67:ARG:O	8:K:71:GLU:CB	2.56	0.53
12:O:683:ILE:O	12:O:687:ILE:CB	2.57	0.53
1:A:955:TRP:O	1:A:959:ILE:CB	2.56	0.53
12:O:693:GLU:O	12:O:697:ASN:CB	2.56	0.53
17:T:510:LEU:O	17:T:514:PHE:CB	2.56	0.53
10:M:342:PRO:C	10:M:344:LEU:H	2.16	0.53
12:O:590:SER:H	12:O:593:ARG:CB	2.21	0.53
1:A:65:HIS:O	1:A:69:ILE:CB	2.57	0.53
9:L:720:LEU:O	9:L:724:TYR:CB	2.57	0.53
3:C:192:ALA:H	13:P:32:PRO:HB3	1.74	0.53
6:F:70:TYR:N	6:F:84:ALA:O	2.41	0.53
1:A:1469:ASN:O	1:A:1473:ASP:CB	2.56	0.53
19:V:97:ILE:O	19:V:115:THR:O	2.27	0.53
4:D:345:ILE:CB	4:D:357:TRP:O	2.57	0.53
7:I:27:ARG:O	7:I:31:GLU:CB	2.56	0.52
19:V:11:PRO:HB3	19:V:29:TRP:H	1.74	0.52
1:A:142:SER:O	1:A:146:SER:CB	2.58	0.52
1:A:1293:ASN:O	1:A:1297:THR:CB	2.58	0.52
4:D:219:PHE:CB	4:D:231:TRP:O	2.57	0.52
1:A:1946:ASN:HA	1:A:1949:ARG:N	2.23	0.52
3:C:155:VAL:O	3:C:159:VAL:CB	2.57	0.52
4:D:262:PHE:HA	4:D:272:CYS:HA	1.89	0.52
33:2:53:U:O4	33:2:95:A:N6	2.43	0.52
34:5:21:A:O2'	34:5:23:C:OP1	2.27	0.52
1:A:519:ASP:O	1:A:522:PHE:N	2.42	0.52
1:A:1529:ILE:O	1:A:1533:ARG:N	2.42	0.52
24:j:15:VAL:O	25:k:33:GLY:HA3	2.09	0.52
1:A:1261:ASN:O	1:A:1265:THR:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:HIS:C	2:B:495:ARG:O	2.53	0.52
7:G:82:TRP:O	7:G:86:MET:CB	2.58	0.52
8:K:25:ALA:HB3	8:K:26:PRO:HD3	1.90	0.52
6:F:170:GLY:HA2	6:F:175:THR:O	2.09	0.52
4:D:399:LYS:H	4:D:406:ILE:N	2.04	0.51
5:E:404:ASP:N	5:E:410:ILE:C	2.59	0.51
16:S:11:ARG:N	32:Z:51:U:H1'	2.24	0.51
1:A:577:GLY:O	1:A:581:ILE:CB	2.58	0.51
1:A:1106:ALA:O	1:A:1110:ILE:CB	2.58	0.51
7:H:30:ILE:O	7:H:34:ILE:CB	2.58	0.51
17:T:599:LEU:O	17:T:603:LEU:CB	2.58	0.51
1:A:880:ARG:O	1:A:884:HIS:CB	2.59	0.51
2:B:369:PHE:O	2:B:373:ILE:CB	2.58	0.51
2:B:833:PHE:O	2:B:899:SER:HA	2.10	0.51
5:E:445:TRP:HA	5:E:453:PHE:N	2.25	0.51
2:B:429:GLY:O	2:B:433:MET:CB	2.59	0.51
17:T:587:PHE:O	17:T:591:CYS:CB	2.59	0.51
1:A:238:LEU:O	1:A:242:ALA:HB3	2.10	0.51
5:E:422:ASN:H	5:E:437:SER:HA	1.75	0.51
1:A:1703:ILE:HA	1:A:1714:ALA:HA	1.93	0.51
10:M:456:LEU:O	10:M:460:THR:CB	2.59	0.51
33:2:53:U:C2'	33:2:54:U:C5'	2.89	0.51
3:C:238:THR:HA	11:N:144:PRO:HG3	1.92	0.51
26:I:66:SER:CB	33:2:101:U:C4'	2.89	0.51
34:5:5:U:H2'	34:5:6:C:C6	2.45	0.50
2:B:187:THR:HA	2:B:201:ASN:HA	1.93	0.50
4:D:358:ASP:CB	4:D:364:THR:O	2.59	0.50
7:J:80:ASP:O	7:J:84:ALA:CB	2.60	0.50
2:B:530:LEU:CB	2:B:541:VAL:O	2.59	0.50
10:M:231:ASN:O	10:M:233:ASP:N	2.41	0.50
2:B:430:PHE:O	2:B:434:CYS:CB	2.59	0.50
2:B:508:LYS:N	2:B:566:THR:O	2.38	0.50
33:2:49:U:C5	33:2:50:C:C5	3.00	0.50
7:G:73:ALA:O	7:G:77:ALA:CB	2.60	0.50
10:M:328:GLU:O	10:M:332:ALA:CB	2.60	0.50
16:S:14:GLY:O	32:Z:51:U:N3	2.45	0.50
1:A:100:LEU:O	1:A:104:GLU:CB	2.60	0.50
1:A:239:TYR:O	1:A:243:ASN:CB	2.60	0.50
6:F:137:ASP:N	6:F:144:VAL:N	2.53	0.50
1:A:238:LEU:O	1:A:242:ALA:CB	2.60	0.50
2:B:742:PRO:HG2	2:B:786:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:112:VAL:O	13:P:116:TYR:N	2.44	0.50
35:6:73:A:N6	35:6:76:A:H5'	2.27	0.50
6:F:180:ASP:O	6:F:186:ALA:HA	2.11	0.50
11:N:174:PRO:O	11:N:176:THR:N	2.45	0.50
13:P:259:ARG:H	13:P:274:PHE:HA	1.77	0.50
34:5:87:A:N6	34:5:93:U:OP1	2.45	0.50
13:P:39:GLU:O	13:P:53:THR:HA	2.12	0.49
19:V:100:MET:O	19:V:127:THR:C	2.54	0.49
1:A:812:THR:O	1:A:816:TRP:CB	2.60	0.49
2:B:208:HIS:O	2:B:212:SER:N	2.45	0.49
7:H:31:GLU:O	7:H:35:ALA:CB	2.58	0.49
26:l:52:ASP:CB	33:2:151:C:N3	2.75	0.49
1:A:1343:SER:O	1:A:1347:ASP:N	2.31	0.49
2:B:116:MET:O	2:B:120:ALA:HB3	2.12	0.49
2:B:478:THR:HA	2:B:495:ARG:O	2.12	0.49
2:B:838:ALA:HB2	2:B:895:ALA:HA	1.95	0.49
4:D:252:VAL:HA	4:D:262:PHE:O	2.12	0.49
5:E:351:ALA:HB3	5:E:355:TYR:O	2.12	0.49
8:K:106:CYS:O	8:K:110:SER:CB	2.61	0.49
10:M:615:VAL:O	10:M:619:ALA:CB	2.60	0.49
17:T:579:SER:O	17:T:583:VAL:CB	2.60	0.49
2:B:717:PHE:O	2:B:721:LYS:CB	2.60	0.49
6:F:263:ASP:O	6:F:272:ARG:C	2.55	0.49
1:A:1110:ILE:O	1:A:1114:LEU:CB	2.61	0.49
3:C:156:SER:O	3:C:160:ALA:CB	2.60	0.49
6:F:221:ASP:N	6:F:227:LEU:C	2.55	0.49
22:h:87:SER:N	33:2:136:G:O2'	2.46	0.49
5:E:355:TYR:HA	5:E:371:THR:HA	1.95	0.49
19:V:35:THR:O	19:V:39:PHE:CB	2.60	0.49
33:2:177:A:H2	33:2:178:A:H62	1.61	0.49
4:D:273:TRP:HA	4:D:281:ILE:H	1.76	0.49
6:F:137:ASP:O	6:F:143:ARG:HA	2.13	0.49
8:K:132:CYS:C	8:K:134:ALA:H	2.20	0.49
16:S:22:ASN:O	16:S:24:SER:N	2.46	0.49
1:A:578:LEU:O	1:A:582:PHE:CB	2.61	0.49
1:A:1899:VAL:C	1:A:1901:LYS:H	2.16	0.49
4:D:315:TRP:HA	4:D:323:VAL:N	2.28	0.49
7:H:128:ARG:O	7:H:132:ALA:HB2	2.13	0.49
7:I:31:GLU:O	7:I:35:ALA:CB	2.60	0.49
1:A:1332:HIS:HA	1:A:1357:MET:CB	2.43	0.49
3:C:151:LEU:O	3:C:155:VAL:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:333:VAL:HA	6:F:343:ILE:O	2.12	0.49
7:H:73:ALA:O	7:H:77:ALA:CB	2.61	0.49
12:O:419:PHE:O	12:O:423:GLU:CB	2.60	0.49
1:A:1685:LEU:O	1:A:1689:THR:CB	2.61	0.48
2:B:261:ASP:O	2:B:265:LEU:CB	2.61	0.48
2:B:642:HIS:O	2:B:646:LYS:CB	2.61	0.48
6:F:80:THR:HA	6:F:93:TRP:O	2.12	0.48
34:5:100:U:H2'	34:5:101:U:C6	2.48	0.48
17:T:622:ARG:O	17:T:626:PHE:CB	2.61	0.48
1:A:718:ARG:O	1:A:722:ALA:HB3	2.13	0.48
1:A:1723:LYS:O	1:A:1727:GLN:CB	2.61	0.48
2:B:475:MET:O	2:B:498:SER:N	2.46	0.48
7:G:73:ALA:O	7:G:77:ALA:HB3	2.13	0.48
16:S:13:SER:O	16:S:14:GLY:C	2.55	0.48
26:l:52:ASP:C	33:2:151:C:O2	2.57	0.48
35:6:17:C:H2'	35:6:18:A:C8	2.48	0.48
1:A:463:PRO:O	1:A:465:LYS:N	2.47	0.48
7:H:128:ARG:O	7:H:132:ALA:CB	2.62	0.48
33:2:53:U:O2'	33:2:54:U:C4'	2.61	0.48
7:G:31:GLU:O	7:G:35:ALA:CB	2.61	0.48
7:H:68:ALA:H	8:K:66:MET:HA	1.78	0.48
8:K:202:LEU:O	8:K:206:ILE:CB	2.61	0.48
18:U:979:GLN:CA	18:U:980:PRO:CA	2.92	0.48
27:f:7:SER:O	27:f:11:GLN:N	2.43	0.48
15:R:32:SER:C	15:R:34:ASP:H	2.21	0.48
4:D:305:THR:O	4:D:312:ALA:HA	2.13	0.48
6:F:137:ASP:H	6:F:143:ARG:CA	2.26	0.48
8:K:210:LYS:O	8:K:213:HIS:C	2.56	0.48
1:A:1055:LEU:O	1:A:1059:SER:CB	2.61	0.48
1:A:1196:ILE:HA	1:A:1228:CYS:HA	1.96	0.48
2:B:588:ILE:O	2:B:630:LEU:HA	2.14	0.48
26:l:54:ARG:HA	33:2:152:G:O4'	2.14	0.48
34:5:97:G:H2'	34:5:98:C:H6	1.79	0.48
34:5:101:U:H2'	34:5:102:G:C8	2.49	0.48
2:B:474:LEU:HA	2:B:499:GLY:HA3	1.96	0.47
2:B:476:CYS:O	2:B:565:ILE:N	2.40	0.47
4:D:439:TRP:C	4:D:447:PHE:H	2.22	0.47
6:F:221:ASP:H	6:F:227:LEU:CA	2.27	0.47
17:T:623:ASN:O	17:T:627:ALA:CB	2.62	0.47
1:A:923:ASP:O	1:A:927:TRP:CB	2.62	0.47
5:E:536:ASP:H	5:E:542:LEU:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:536:ASP:N	5:E:543:TYR:N	2.60	0.47
1:A:29:LYS:O	1:A:33:LYS:CB	2.62	0.47
1:A:1439:ARG:O	1:A:1443:LYS:CB	2.62	0.47
1:A:1663:ASP:O	1:A:1703:ILE:CB	2.62	0.47
5:E:360:ASP:O	5:E:366:CYS:HA	2.14	0.47
17:T:598:LYS:O	17:T:602:ARG:CB	2.62	0.47
1:A:1334:LEU:CB	1:A:1353:PHE:O	2.63	0.47
5:E:360:ASP:N	5:E:367:ILE:N	2.56	0.47
1:A:173:GLU:N	1:A:174:PRO:HD3	2.30	0.47
5:E:317:GLU:H	5:E:324:CYS:CA	2.26	0.47
7:I:29:LEU:O	7:I:33:TYR:CB	2.62	0.47
8:K:125:GLU:O	8:K:129:GLN:CB	2.63	0.47
26:e:80:ALA:HB1	26:e:81:PRO:HA	1.95	0.47
33:2:25:G:H2'	33:2:26:A:H5'	1.96	0.47
35:6:15:A:H2'	35:6:16:G:C8	2.48	0.47
1:A:1592:ASP:O	1:A:1596:VAL:CB	2.63	0.47
5:E:469:LEU:HA	5:E:476:LEU:HA	1.96	0.47
6:F:180:ASP:N	6:F:186:ALA:C	2.57	0.47
7:G:30:ILE:O	7:G:34:ILE:CB	2.63	0.47
7:I:74:ILE:O	7:I:78:LEU:CB	2.63	0.47
7:J:30:ILE:O	7:J:34:ILE:CB	2.63	0.47
1:A:519:ASP:CB	1:A:523:ASN:O	2.63	0.47
1:A:952:VAL:O	1:A:956:CYS:CB	2.63	0.47
1:A:1667:ARG:H	1:A:1706:ASP:HA	1.78	0.47
2:B:506:PRO:HG2	2:B:568:PRO:HG3	1.97	0.47
5:E:349:SER:CB	5:E:357:LYS:O	2.63	0.47
6:F:263:ASP:CB	6:F:273:CYS:O	2.62	0.47
16:S:22:ASN:C	16:S:24:SER:N	2.73	0.47
19:V:100:MET:N	19:V:129:PHE:N	2.55	0.47
4:D:429:SER:O	4:D:436:MET:HA	2.15	0.47
7:H:62:ARG:O	7:H:65:PRO:HD2	2.14	0.47
12:O:392:PHE:HA	12:O:395:ALA:HB3	1.96	0.47
12:O:529:HIS:O	12:O:533:TYR:N	2.40	0.47
14:Q:40:LYS:O	35:6:27:A:O2'	2.33	0.47
1:A:971:GLY:HA2	1:A:1103:ALA:HB2	1.97	0.47
2:B:348:TYR:O	2:B:356:PHE:HA	2.14	0.47
5:E:404:ASP:O	5:E:409:GLU:C	2.57	0.47
5:E:536:ASP:O	5:E:542:LEU:HA	2.15	0.46
9:L:785:GLN:O	9:L:789:ALA:HB2	2.16	0.46
25:k:24:GLY:HA3	33:2:183:G:H5''	1.97	0.46
1:A:552:ARG:O	1:A:556:LEU:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:352:TYR:C	5:E:354:ARG:H	2.24	0.46
6:F:221:ASP:N	6:F:228:THR:N	2.56	0.46
10:M:306:MET:O	18:U:355:ASN:CA	2.63	0.46
1:A:1899:VAL:C	1:A:1901:LYS:N	2.66	0.46
6:F:180:ASP:N	6:F:187:ILE:N	2.56	0.46
1:A:993:LEU:O	1:A:997:LEU:CB	2.63	0.46
33:2:53:U:H2'	33:2:54:U:O4'	2.14	0.46
1:A:581:ILE:O	1:A:586:GLY:N	2.48	0.46
7:J:128:ARG:O	7:J:132:ALA:HB2	2.16	0.46
25:k:50:THR:CB	33:2:184:C:H5'	2.45	0.46
1:A:770:THR:O	1:A:774:LYS:CB	2.63	0.46
5:E:317:GLU:N	5:E:325:LEU:N	2.62	0.46
5:E:570:GLY:HA2	5:E:575:ILE:HA	1.97	0.46
6:F:334:ALA:O	6:F:342:ILE:HA	2.15	0.46
10:M:683:ARG:O	10:M:687:ILE:CB	2.63	0.46
34:5:10:U:H2'	34:5:11:U:C6	2.51	0.46
2:B:121:ASP:O	2:B:125:ASN:CB	2.64	0.46
33:2:46:U:C5'	33:2:47:U:OP2	2.64	0.46
15:R:39:THR:N	34:5:53:U:OP1	2.48	0.46
33:2:3:C:H2'	33:2:4:G:C8	2.51	0.46
5:E:317:GLU:O	5:E:323:ARG:C	2.59	0.46
1:A:38:GLN:O	1:A:42:ALA:CB	2.64	0.46
3:C:174:ALA:C	3:C:199:MET:O	2.58	0.46
3:C:175:GLN:O	3:C:199:MET:CB	2.64	0.46
6:F:293:TRP:HA	6:F:300:ILE:HA	1.97	0.46
6:F:313:ASP:N	6:F:320:LEU:N	2.57	0.46
7:J:15:PRO:HA	7:J:25:TYR:O	2.16	0.46
34:5:11:U:H2'	34:5:12:U:C6	2.50	0.46
2:B:508:LYS:O	2:B:566:THR:N	2.42	0.45
4:D:399:LYS:H	4:D:405:PHE:CA	2.27	0.45
12:O:209:PRO:C	12:O:210:PRO:CA	2.82	0.45
17:T:623:ASN:O	17:T:627:ALA:HB2	2.15	0.45
34:5:101:U:H2'	34:5:102:G:H8	1.81	0.45
1:A:1335:ILE:H	1:A:1354:ARG:CB	2.29	0.45
5:E:536:ASP:N	5:E:542:LEU:C	2.56	0.45
6:F:221:ASP:O	6:F:227:LEU:HA	2.17	0.45
1:A:200:ASP:O	1:A:204:LEU:N	2.46	0.45
1:A:1678:ARG:O	1:A:1682:ALA:HB3	2.17	0.45
1:A:1243:ARG:O	1:A:1247:ILE:CB	2.64	0.45
5:E:360:ASP:O	5:E:365:GLN:C	2.60	0.45
1:A:1932:ALA:O	1:A:1936:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:ASP:CB	4:D:238:LEU:O	2.64	0.45
4:D:294:LEU:HA	4:D:304:VAL:O	2.17	0.45
6:F:198:ALA:O	6:F:210:SER:HA	2.17	0.45
6:F:313:ASP:N	6:F:319:ILE:C	2.56	0.45
7:G:27:ARG:O	7:G:31:GLU:CB	2.65	0.45
7:H:29:LEU:O	7:H:33:TYR:CB	2.64	0.45
20:W:61:PRO:O	20:W:86:ALA:HB1	2.16	0.45
26:I:51:ARG:O	33:2:180:G:N3	2.49	0.45
1:A:992:LEU:O	1:A:996:LEU:CB	2.64	0.45
2:B:147:ASP:O	2:B:151:GLU:CB	2.64	0.45
2:B:392:LEU:O	2:B:396:LEU:CB	2.64	0.45
1:A:234:MET:O	1:A:238:LEU:CB	2.65	0.45
2:B:420:CYS:O	2:B:425:GLY:N	2.50	0.45
3:C:264:LEU:C	3:C:266:LYS:H	2.24	0.45
4:D:200:ILE:CB	4:D:486:ILE:O	2.65	0.45
5:E:554:ILE:N	5:E:571:TRP:HA	2.23	0.45
6:F:174:GLY:HA2	6:F:195:GLN:HA	1.99	0.45
7:I:40:ASP:N	7:I:45:GLN:O	2.45	0.45
1:A:63:PRO:O	1:A:67:ARG:CB	2.65	0.45
4:D:439:TRP:HA	4:D:446:ASN:HA	1.98	0.45
11:N:172:HIS:C	11:N:174:PRO:HD3	2.42	0.45
12:O:311:GLN:O	12:O:315:LYS:CB	2.65	0.45
35:6:90:G:H2'	35:6:91:A:H8	1.82	0.45
1:A:1897:LEU:O	1:A:1898[A]:LYS:C	2.60	0.45
10:M:519:GLN:O	10:M:523:ASN:N	2.33	0.45
1:A:89:LEU:O	1:A:93:LYS:CB	2.65	0.45
1:A:1294:LYS:O	1:A:1298:ARG:CB	2.65	0.45
3:C:262:ILE:O	3:C:264:LEU:N	2.50	0.45
4:D:420:THR:O	4:D:427:LEU:HA	2.17	0.45
34:5:109:C:H2'	34:5:110:A:C8	2.52	0.45
1:A:795:LEU:HA	1:A:799:PRO:HG3	1.99	0.44
2:B:182:LYS:HA	2:B:206:PRO:HG3	1.99	0.44
2:B:858:THR:N	2:B:873:ALA:HA	2.31	0.44
1:A:1042:GLN:O	1:A:1046:LEU:CB	2.64	0.44
26:I:51:ARG:O	33:2:181:G:C8	2.68	0.44
35:6:91:A:H2'	35:6:92:A:H8	1.82	0.44
1:A:471:TYR:O	1:A:475:SER:N	2.46	0.44
2:B:116:MET:O	2:B:120:ALA:CB	2.65	0.44
2:B:592:VAL:HA	2:B:655:VAL:HA	1.99	0.44
5:E:292:SER:H	5:E:308:SER:HA	1.82	0.44
10:M:65:PRO:HG2	29:o:242:ASN:CA	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:167:LEU:C	11:N:170:GLY:H	2.26	0.44
33:2:53:U:O2'	33:2:54:U:O4'	2.34	0.44
1:A:1664:ILE:CA	1:A:1703:ILE:O	2.65	0.44
5:E:465:PRO:HG2	5:E:481:MET:N	2.32	0.44
9:L:727:ARG:O	9:L:731:LEU:CB	2.66	0.44
14:Q:77:TYR:O	14:Q:81:GLU:CB	2.66	0.44
16:S:1:MET:HA	16:S:6:GLY:HA3	1.98	0.44
26:I:53:GLY:N	33:2:151:C:O2	2.50	0.44
5:E:536:ASP:O	5:E:541:LYS:C	2.60	0.44
6:F:313:ASP:O	6:F:319:ILE:HA	2.17	0.44
8:K:62:GLU:C	8:K:64:ASP:H	2.25	0.44
12:O:588:ASN:O	12:O:592:ALA:HB3	2.18	0.44
19:V:36:CYS:O	19:V:40:ALA:CB	2.66	0.44
35:6:91:A:H2'	35:6:92:A:C8	2.53	0.44
1:A:1940:LEU:O	1:A:1943:LEU:N	2.50	0.44
6:F:137:ASP:O	6:F:142:GLU:C	2.61	0.44
6:F:166:LEU:HA	6:F:179:TRP:O	2.18	0.44
35:6:40:U:H2'	35:6:41:A:C8	2.52	0.44
5:E:360:ASP:N	5:E:366:CYS:C	2.56	0.44
10:M:550:TRP:O	10:M:552:ASN:N	2.48	0.44
34:5:42:U:H2'	34:5:43:U:H6	1.79	0.44
1:A:1440:THR:O	1:A:1444:GLN:CB	2.66	0.44
3:C:163:MET:O	3:C:165:VAL:N	2.51	0.44
6:F:221:ASP:O	6:F:226:LYS:C	2.60	0.44
10:M:560:TYR:O	10:M:564:PHE:CB	2.66	0.44
33:2:51:A:H4'	33:2:52:G:OP1	2.18	0.44
2:B:328:ALA:HB1	2:B:333:ASP:HA	1.98	0.44
2:B:835:GLU:O	2:B:897:SER:HA	2.17	0.44
5:E:317:GLU:O	5:E:324:CYS:HA	2.17	0.44
5:E:532:LEU:CB	5:E:546:PHE:O	2.65	0.44
7:I:109:GLN:O	7:I:113:ALA:CB	2.66	0.44
2:B:112:THR:N	2:B:155:PRO:HD3	2.33	0.43
5:E:489:GLY:N	5:E:499:LYS:H	2.11	0.43
6:F:112:VAL:HA	6:F:128:SER:HA	1.99	0.43
10:M:47:GLY:HA3	10:M:51:PRO:HD3	1.99	0.43
1:A:462:ARG:O	1:A:464:PRO:HD3	2.19	0.43
1:A:1947:ASN:HA	1:A:1950:ALA:HB3	2.00	0.43
4:D:274:ASP:N	4:D:280:VAL:C	2.51	0.43
9:L:707:ALA:O	9:L:711:ALA:CB	2.66	0.43
33:2:53:U:C2'	33:2:54:U:O4'	2.66	0.43
2:B:118:PHE:O	2:B:122:LEU:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:427:LEU:O	4:D:439:TRP:CB	2.66	0.43
4:D:439:TRP:CA	4:D:447:PHE:H	2.31	0.43
13:P:258:ILE:HA	13:P:274:PHE:HA	2.00	0.43
35:6:16:G:H2'	35:6:17:C:C6	2.54	0.43
2:B:857:VAL:HA	2:B:874:PHE:O	2.17	0.43
5:E:421:VAL:HA	5:E:437:SER:HA	2.00	0.43
10:M:264:ASP:O	10:M:268:ARG:CB	2.66	0.43
11:N:167:LEU:O	11:N:170:GLY:N	2.51	0.43
1:A:380:LEU:O	1:A:382:GLU:N	2.51	0.43
5:E:536:ASP:N	5:E:542:LEU:HA	2.33	0.43
17:T:489:LEU:O	17:T:493:ILE:CB	2.67	0.43
35:6:17:C:H2'	35:6:18:A:H8	1.84	0.43
1:A:187:PRO:HG3	1:A:565:ARG:HA	2.01	0.43
4:D:230:ILE:CB	4:D:240:LEU:O	2.67	0.43
5:E:290:GLY:HA2	5:E:573:GLY:H	1.84	0.43
1:A:998:ARG:HA	1:A:1002:ASP:O	2.17	0.43
2:B:639:CYS:O	2:B:643:ASP:CB	2.66	0.43
4:D:274:ASP:N	4:D:280:VAL:CA	2.80	0.43
4:D:316:ASP:H	4:D:323:VAL:N	2.16	0.43
6:F:263:ASP:H	6:F:273:CYS:CA	2.29	0.43
6:F:313:ASP:O	6:F:318:ARG:C	2.61	0.43
21:X:75:PHE:HA	21:X:76:PRO:HD3	1.83	0.43
22:a:28:PRO:O	22:a:31:VAL:N	2.51	0.43
25:d:18:SER:N	25:d:71:GLU:O	2.35	0.43
26:l:38:ASN:CB	33:2:101:U:O2	2.66	0.43
35:6:89:U:H2'	35:6:90:G:C8	2.53	0.43
1:A:582:PHE:O	1:A:586:GLY:CA	2.65	0.43
13:P:262:THR:O	13:P:270:ALA:HA	2.19	0.43
1:A:30:LEU:O	1:A:34:ALA:HB2	2.19	0.43
1:A:905:LEU:N	15:R:227:TYR:O	2.52	0.43
1:A:1335:ILE:N	1:A:1354:ARG:CB	2.82	0.43
2:B:531:TRP:N	2:B:551:LEU:O	2.46	0.43
4:D:263:SER:CB	4:D:271:LYS:O	2.67	0.43
9:L:707:ALA:O	9:L:711:ALA:HB2	2.19	0.43
35:6:89:U:H2'	35:6:90:G:H8	1.84	0.43
1:A:1776:ILE:CB	1:A:1859:LYS:CB	2.97	0.42
3:C:209:PRO:CG	3:C:210:PRO:HD3	2.48	0.42
4:D:357:TRP:HA	4:D:364:THR:HA	1.99	0.42
12:O:646:PHE:O	12:O:650:GLU:CB	2.67	0.42
35:6:12:G:H3'	35:6:13:G:H8	1.84	0.42
6:F:137:ASP:N	6:F:143:ARG:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:331:ASN:N	6:F:345:ALA:O	2.52	0.42
19:V:100:MET:N	19:V:128:ILE:HA	2.34	0.42
34:5:9:G:OP2	34:5:9:G:N2	2.52	0.42
1:A:505:ASN:O	1:A:509:HIS:CB	2.67	0.42
3:C:156:SER:O	3:C:160:ALA:HB2	2.18	0.42
5:E:278:LYS:O	5:E:579:ASP:N	2.38	0.42
6:F:179:TRP:HA	6:F:186:ALA:HB1	2.01	0.42
34:5:72:U:H2'	34:5:73:C:C6	2.54	0.42
35:6:92:A:H2'	35:6:93:G:H8	1.84	0.42
2:B:170:ILE:C	2:B:172:PHE:H	2.27	0.42
7:H:18:SER:O	7:H:20:VAL:N	2.50	0.42
9:L:86:ALA:HB3	9:L:87:PRO:HD3	2.02	0.42
32:Y:142:U:O2'	32:Y:143:G:C8	2.57	0.42
35:6:64:U:H2'	35:6:65:G:O4'	2.18	0.42
6:F:313:ASP:H	6:F:319:ILE:CA	2.31	0.42
18:U:745:PRO:CA	18:U:746:PRO:CA	2.97	0.42
4:D:315:TRP:HA	4:D:323:VAL:H	1.84	0.42
5:E:404:ASP:CB	5:E:410:ILE:O	2.68	0.42
6:F:180:ASP:O	6:F:185:ALA:C	2.62	0.42
17:T:576:THR:C	17:T:578:SER:H	2.28	0.42
28:g:36:MET:O	28:g:62:GLY:HA2	2.20	0.42
35:6:53:A:H5'	35:6:54:G:H5''	2.02	0.42
1:A:1852:LEU:O	1:A:1856:GLU:C	2.63	0.42
1:A:1897:LEU:O	1:A:1902:PHE:CA	2.68	0.42
2:B:467:ASP:HA	2:B:471:ASP:O	2.19	0.42
5:E:360:ASP:H	5:E:366:CYS:CA	2.32	0.42
7:H:8:SER:C	7:H:10:GLU:H	2.28	0.42
10:M:311:MET:H	18:U:355:ASN:CA	2.33	0.42
33:2:3:C:H2'	33:2:4:G:H8	1.84	0.42
34:5:76:A:H2'	34:5:77:G:C8	2.55	0.42
2:B:421:LYS:HA	2:B:425:GLY:HA3	2.01	0.42
33:2:94:A:C8	33:2:94:A:C5'	2.92	0.42
35:6:92:A:H2'	35:6:93:G:C8	2.54	0.42
4:D:207:VAL:HA	4:D:223:SER:HA	2.01	0.42
5:E:446:GLU:CB	5:E:452:ASP:O	2.68	0.42
22:h:68:GLU:HA	22:h:97:SER:O	2.20	0.42
34:5:98:C:H2'	34:5:99:C:H6	1.85	0.42
2:B:715:GLY:O	2:B:719:GLN:CB	2.68	0.42
2:B:777:GLY:H	2:B:782:GLU:N	2.17	0.42
35:6:53:A:H3'	35:6:54:G:H5''	2.02	0.42
4:D:308:ARG:HA	4:D:332:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:452:ALA:O	10:M:456:LEU:CB	2.68	0.41
22:h:87:SER:CA	33:2:136:G:O2'	2.68	0.41
33:2:23:A:O2'	33:2:24:A:OP1	2.32	0.41
33:2:173:C:H2'	33:2:174:A:C8	2.55	0.41
35:6:55:C:OP2	35:6:74:U:O2'	2.32	0.41
3:C:229:VAL:H	12:O:306:LEU:HA	1.85	0.41
5:E:398:LYS:HA	5:E:420:ALA:HA	2.01	0.41
35:6:53:A:H3'	35:6:54:G:O4'	2.19	0.41
1:A:643:GLY:O	1:A:646:PRO:HD2	2.20	0.41
9:L:34:ILE:O	9:L:38:LEU:N	2.53	0.41
10:M:543:ARG:O	10:M:547:LEU:CB	2.68	0.41
12:O:521:VAL:O	12:O:523:PRO:HD3	2.20	0.41
23:b:20:MET:N	23:b:73:ARG:O	2.51	0.41
23:i:5:LEU:O	24:j:49:GLY:HA3	2.20	0.41
12:O:291:GLN:C	12:O:293:ASN:H	2.28	0.41
12:O:456:THR:O	12:O:460:LYS:CB	2.68	0.41
35:6:54:G:H2'	35:6:55:C:C6	2.55	0.41
1:A:66:VAL:O	1:A:70:ILE:CB	2.68	0.41
2:B:933:PHE:O	2:B:937:THR:CB	2.68	0.41
6:F:221:ASP:N	6:F:227:LEU:HA	2.35	0.41
25:k:35:ASP:CB	25:k:36:PRO:HD2	2.51	0.41
1:A:1036:PHE:O	1:A:1040:ILE:N	2.41	0.41
2:B:226:VAL:HA	2:B:254:THR:H	1.85	0.41
5:E:535:TRP:HA	5:E:543:TYR:N	2.31	0.41
17:T:583:VAL:O	17:T:587:PHE:CB	2.68	0.41
5:E:360:ASP:N	5:E:366:CYS:HA	2.36	0.41
10:M:597:LEU:O	10:M:601:GLN:CB	2.68	0.41
1:A:331:TRP:HA	2:B:177:ARG:CB	2.51	0.41
1:A:1898[A]:LYS:O	1:A:1899:VAL:O	2.38	0.41
4:D:253:ILE:O	4:D:261:LEU:HA	2.20	0.41
7:J:128:ARG:O	7:J:132:ALA:HB3	2.21	0.41
17:T:548:ALA:O	17:T:552:ALA:CB	2.69	0.41
2:B:362:THR:C	2:B:364:SER:H	2.28	0.41
5:E:349:SER:O	5:E:356:LEU:HA	2.21	0.41
5:E:471:PRO:HG2	5:E:518:PRO:HB3	2.03	0.41
5:E:506:MET:O	5:E:528:GLY:N	2.43	0.41
6:F:94:ASN:H	6:F:101:ASN:CA	2.30	0.41
6:F:179:TRP:HA	6:F:187:ILE:N	2.34	0.41
14:Q:135:THR:H	35:6:22:A:H2	1.69	0.41
32:Y:152:C:H2'	32:Y:153:U:C6	2.56	0.41
34:5:78:U:O2'	34:5:79:C:O5'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:5:97:G:H2'	34:5:98:C:C6	2.55	0.41
1:A:1642:PRO:HA	1:A:1717:ASN:HA	2.02	0.41
2:B:479:THR:N	2:B:494:GLY:HA2	2.36	0.41
2:B:743:ASN:HA	2:B:787:VAL:O	2.21	0.41
6:F:210:SER:O	6:F:218:LYS:CB	2.69	0.41
10:M:326:ASP:C	10:M:328:GLU:H	2.29	0.41
28:g:24:GLN:N	28:g:46:THR:O	2.49	0.41
35:6:40:U:H2'	35:6:41:A:H8	1.85	0.41
1:A:548:ARG:O	1:A:552:ARG:CB	2.70	0.40
10:M:615:VAL:O	10:M:619:ALA:HB3	2.21	0.40
13:P:249:ARG:O	13:P:253:TYR:CB	2.69	0.40
20:W:160:LYS:O	20:W:161:MET:C	2.63	0.40
33:2:49:U:O4	33:2:50:C:C4	2.74	0.40
3:C:148:ARG:O	3:C:152:GLU:CB	2.69	0.40
34:5:98:C:H2'	34:5:99:C:C6	2.57	0.40
5:E:359:TRP:HA	5:E:367:ILE:N	2.33	0.40
7:I:112:ALA:HB1	8:K:36:VAL:HA	2.02	0.40
16:S:11:ARG:O	32:Z:51:U:O2	2.38	0.40
22:h:59:PHE:HA	22:h:64:ASN:O	2.22	0.40
26:l:52:ASP:HA	33:2:181:G:N7	2.34	0.40
2:B:663:CYS:CB	2:B:828:MET:O	2.69	0.40
6:F:262:TRP:HA	6:F:273:CYS:HA	2.03	0.40
9:L:741:GLN:O	9:L:745:ALA:HB2	2.21	0.40
4:D:358:ASP:N	4:D:364:THR:C	2.61	0.40
12:O:692:THR:O	12:O:695:THR:N	2.55	0.40
22:h:62:HIS:O	22:h:103:GLY:HA3	2.21	0.40
33:2:20:G:H2'	33:2:21:C:C6	2.56	0.40
34:5:76:A:H2'	34:5:77:G:H8	1.86	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	1961/2335 (84%)	1618 (82%)	328 (17%)	15 (1%)	16	55
2	B	898/972 (92%)	778 (87%)	108 (12%)	12 (1%)	10	42
3	C	238/536 (44%)	193 (81%)	44 (18%)	1 (0%)	30	68
4	D	313/515 (61%)	282 (90%)	30 (10%)	1 (0%)	37	73
5	E	325/579 (56%)	287 (88%)	37 (11%)	1 (0%)	37	73
6	F	305/357 (85%)	274 (90%)	30 (10%)	1 (0%)	37	73
7	G	130/504 (26%)	120 (92%)	9 (7%)	1 (1%)	16	55
7	H	133/504 (26%)	120 (90%)	12 (9%)	1 (1%)	16	55
7	I	132/504 (26%)	122 (92%)	10 (8%)	0	100	100
7	J	133/504 (26%)	116 (87%)	14 (10%)	3 (2%)	5	28
8	K	187/225 (83%)	167 (89%)	19 (10%)	1 (0%)	25	65
9	L	330/802 (41%)	297 (90%)	32 (10%)	1 (0%)	37	73
10	M	703/855 (82%)	600 (85%)	97 (14%)	6 (1%)	14	51
11	N	113/243 (46%)	87 (77%)	23 (20%)	3 (3%)	4	25
12	O	562/848 (66%)	476 (85%)	78 (14%)	8 (1%)	9	40
13	P	273/420 (65%)	232 (85%)	39 (14%)	2 (1%)	19	57
14	Q	140/144 (97%)	127 (91%)	12 (9%)	1 (1%)	19	57
15	R	94/229 (41%)	84 (89%)	10 (11%)	0	100	100
16	S	28/2752 (1%)	20 (71%)	5 (18%)	3 (11%)	0	6
17	T	196/908 (22%)	177 (90%)	18 (9%)	1 (0%)	25	65
19	V	153/166 (92%)	145 (95%)	7 (5%)	1 (1%)	19	57
20	W	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10	42
21	X	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
22	a	97/118 (82%)	95 (98%)	2 (2%)	0	100	100
22	h	96/118 (81%)	83 (86%)	8 (8%)	5 (5%)	1	15
23	b	74/86 (86%)	72 (97%)	2 (3%)	0	100	100
23	i	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
24	c	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
24	j	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
25	d	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
25	k	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
26	e	82/126 (65%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	l	81/126 (64%)	80 (99%)	1 (1%)	0	100	100
27	f	67/240 (28%)	63 (94%)	4 (6%)	0	100	100
27	m	67/240 (28%)	66 (98%)	1 (2%)	0	100	100
28	g	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
28	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
All	All	8693/17096 (51%)	7611 (88%)	1012 (12%)	70 (1%)	19	55

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	988	ILE
1	A	1777	ILE
2	B	182	LYS
2	B	947	VAL
10	M	720	ILE
12	O	292	VAL
12	O	693	GLU
16	S	18	TYR
22	h	78	PRO
1	A	1332	HIS
1	A	1447	VAL
2	B	179	VAL
2	B	183	SER
7	G	57	VAL
10	M	49	PRO
12	O	590	SER
20	W	160	LYS
22	h	87	SER
1	A	113	ILE
1	A	1126	VAL
7	H	55	ILE
7	J	7	ILE
7	J	55	ILE
7	J	61	ILE
10	M	385	VAL
11	N	174	PRO
11	N	175	SER
16	S	23	LEU
1	A	191	ILE
1	A	668	VAL

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Mol	Chain	Res	Type
1	A	940	ILE
1	A	1092	ILE
2	B	385	VAL
2	B	457	VAL
5	E	410	ILE
10	M	357	VAL
10	M	585	ASP
12	O	468	ILE
14	Q	132	ILE
16	S	22	ASN
17	T	536	ILE
20	W	32	PRO
22	h	81	GLY
1	A	174	PRO
1	A	1897	LEU
2	B	704	VAL
2	B	857	VAL
6	F	319	ILE
8	K	65	ILE
10	M	337	LEU
12	O	524	ILE
12	O	709	VAL
13	P	133	PRO
19	V	128	ILE
22	h	77	VAL
2	B	352	LYS
2	B	468	CYS
2	B	470	PRO
1	A	1776	ILE
12	O	209	PRO
12	O	656	ILE
13	P	134	VAL
1	A	365	VAL
1	A	1761	PRO
4	D	457	PRO
11	N	179	ILE
3	C	112	ILE
9	L	215	PRO
2	B	58	VAL
22	h	89	PRO

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	A	106/2108 (5%)	106 (100%)	0	100	100
2	B	55/866 (6%)	55 (100%)	0	100	100
3	C	19/459 (4%)	19 (100%)	0	100	100
4	D	12/441 (3%)	12 (100%)	0	100	100
5	E	11/502 (2%)	11 (100%)	0	100	100
6	F	10/300 (3%)	10 (100%)	0	100	100
7	G	10/435 (2%)	10 (100%)	0	100	100
7	H	11/435 (2%)	11 (100%)	0	100	100
7	I	11/435 (2%)	11 (100%)	0	100	100
7	J	11/435 (2%)	11 (100%)	0	100	100
8	K	5/196 (3%)	5 (100%)	0	100	100
9	L	6/709 (1%)	6 (100%)	0	100	100
10	M	24/749 (3%)	24 (100%)	0	100	100
11	N	4/209 (2%)	4 (100%)	0	100	100
12	O	17/751 (2%)	17 (100%)	0	100	100
13	P	14/361 (4%)	14 (100%)	0	100	100
14	Q	6/130 (5%)	6 (100%)	0	100	100
15	R	2/203 (1%)	2 (100%)	0	100	100
16	S	2/2432 (0%)	2 (100%)	0	100	100
17	T	6/838 (1%)	6 (100%)	0	100	100
19	V	9/134 (7%)	9 (100%)	0	100	100
20	W	6/218 (3%)	6 (100%)	0	100	100
21	X	3/195 (2%)	3 (100%)	0	100	100
22	a	4/110 (4%)	4 (100%)	0	100	100
22	h	4/110 (4%)	4 (100%)	0	100	100
23	b	4/74 (5%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	i	4/74 (5%)	4 (100%)	0	100	100
24	c	1/84 (1%)	1 (100%)	0	100	100
24	j	1/84 (1%)	1 (100%)	0	100	100
25	d	3/66 (4%)	3 (100%)	0	100	100
25	k	3/66 (4%)	3 (100%)	0	100	100
26	e	3/101 (3%)	3 (100%)	0	100	100
26	l	3/101 (3%)	3 (100%)	0	100	100
27	f	3/177 (2%)	3 (100%)	0	100	100
27	m	3/177 (2%)	3 (100%)	0	100	100
28	g	3/101 (3%)	3 (100%)	0	100	100
28	n	3/101 (3%)	3 (100%)	0	100	100
All	All	402/14967 (3%)	402 (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
32	Y	30/324 (9%)	21 (70%)	1 (3%)
32	Z	11/324 (3%)	9 (81%)	0
33	2	137/188 (72%)	34 (24%)	2 (1%)
34	5	113/116 (97%)	42 (37%)	2 (1%)
35	6	87/106 (82%)	34 (39%)	1 (1%)
All	All	378/1058 (35%)	140 (37%)	6 (1%)

All (140) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	Y	60	U
32	Y	61	A
32	Y	62	A
32	Y	64	A
32	Y	65	G
32	Y	66	C

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Mol	Chain	Res	Type
32	Y	67	C
32	Y	137	C
32	Y	138	U
32	Y	139	U
32	Y	140	G
32	Y	141	A
32	Y	142	U
32	Y	143	G
32	Y	144	A
32	Y	145	U
32	Y	146	G
32	Y	148	C
32	Y	155	A
32	Y	156	U
32	Y	157	G
32	Z	49	C
32	Z	50	C
32	Z	52	C
32	Z	53	C
32	Z	54	G
32	Z	55	A
32	Z	56	A
32	Z	57	C
32	Z	58	G
33	2	17	U
33	2	18	U
33	2	19	G
33	2	20	G
33	2	22	U
33	2	23	A
33	2	24	A
33	2	25	G
33	2	26	A
33	2	29	A
33	2	30	A
33	2	31	G
33	2	39	U
33	2	42	G
33	2	43	U
33	2	44	U
33	2	45	C
33	2	47	U

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Mol	Chain	Res	Type
33	2	48	A
33	2	49	U
33	2	50	C
33	2	51	A
33	2	52	G
33	2	53	U
33	2	95	A
33	2	96	U
33	2	97	G
33	2	111	G
33	2	116	A
33	2	117	U
33	2	146	C
33	2	147	G
33	2	157	G
33	2	177	A
34	5	8	G
34	5	10	U
34	5	11	U
34	5	20	G
34	5	21	A
34	5	22	U
34	5	23	C
34	5	24	G
34	5	25	C
34	5	27	U
34	5	33	U
34	5	34	U
34	5	36	C
34	5	37	G
34	5	38	C
34	5	41	U
34	5	44	A
34	5	45	C
34	5	47	A
34	5	48	A
34	5	52	U
34	5	53	U
34	5	54	U
34	5	57	G
34	5	68	C
34	5	69	A

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Mol	Chain	Res	Type
34	5	70	A
34	5	76	A
34	5	79	C
34	5	80	U
34	5	81	U
34	5	83	A
34	5	85	C
34	5	88	A
34	5	90	U
34	5	91	U
34	5	93	U
34	5	94	U
34	5	95	G
34	5	96	A
34	5	115	U
34	5	116	A
35	6	6	C
35	6	7	G
35	6	9	U
35	6	13	G
35	6	18	A
35	6	21	U
35	6	22	A
35	6	26	U
35	6	27	A
35	6	39	A
35	6	44	G
35	6	45	A
35	6	46	G
35	6	52	U
35	6	53	A
35	6	54	G
35	6	56	A
35	6	58	G
35	6	59	G
35	6	61	C
35	6	62	C
35	6	66	C
35	6	67	G
35	6	68	C
35	6	69	A
35	6	73	A

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Mol	Chain	Res	Type
35	6	74	U
35	6	75	G
35	6	78	A
35	6	79	C
35	6	81	C
35	6	83	A
35	6	84	A
35	6	85	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	Y	65	G
33	2	23	A
33	2	52	G
34	5	78	U
34	5	93	U
35	6	53	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
10	M	1
2	B	1
12	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	33:PHE	C	34:SER	N	4.52
1	B	797:ALA	C	798:GLN	N	3.21
1	A	1914:MET	C	1915:VAL	N	3.11
1	O	209:PRO	C	210:PRO	N	1.78
1	A	1134:TRP	C	1135:PRO	N	1.63

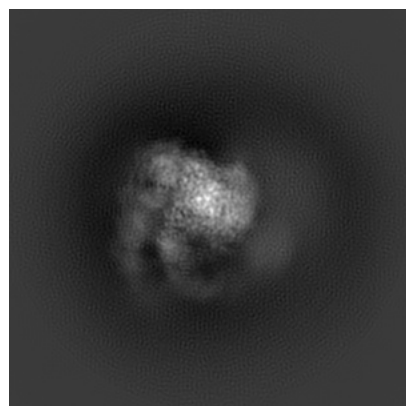
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3545. These allow visual inspection of the internal detail of the map and identification of artifacts.

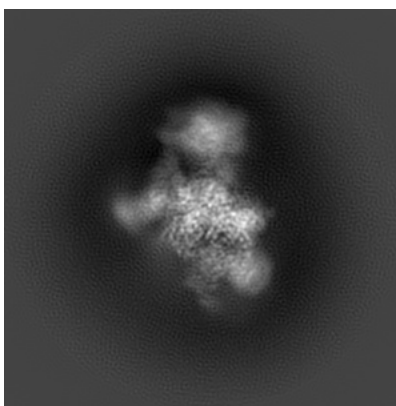
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

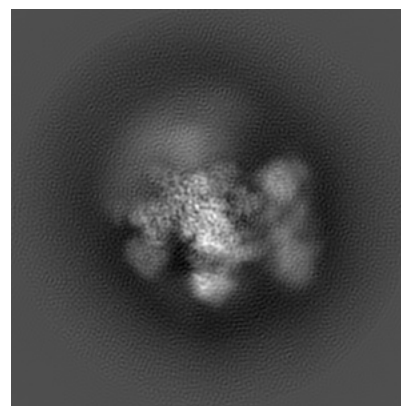
6.1.1 Primary map



X

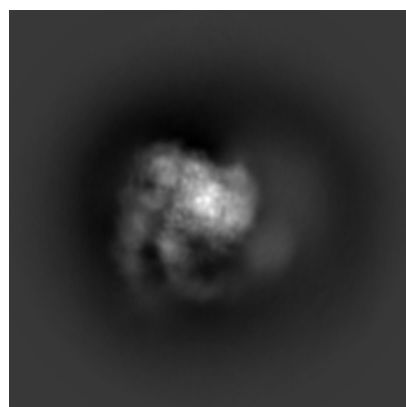


Y

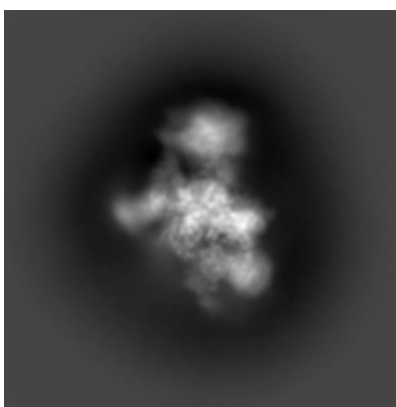


Z

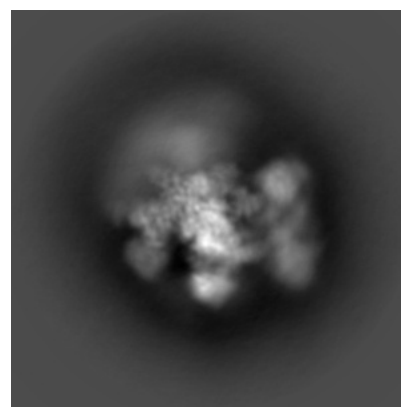
6.1.2 Raw map



X



Y

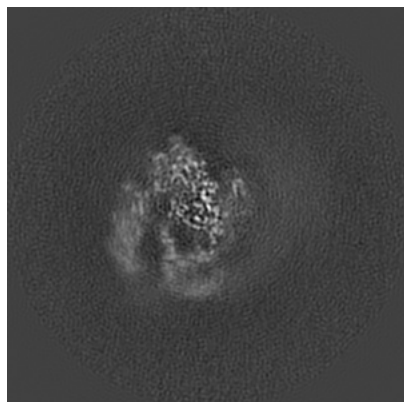


Z

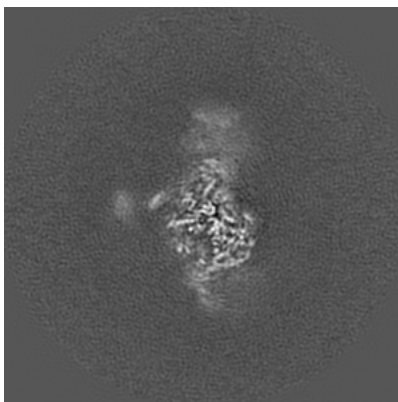
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

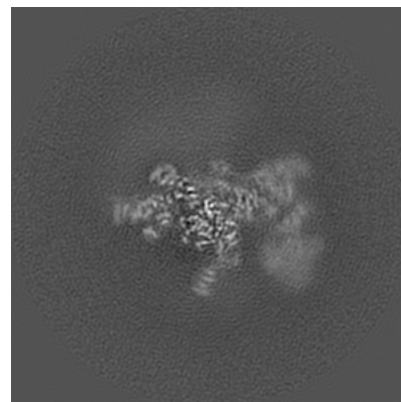
6.2.1 Primary map



X Index: 180

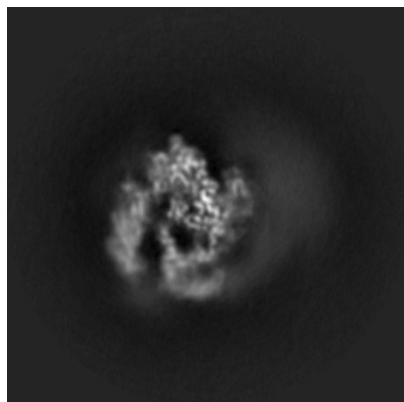


Y Index: 180

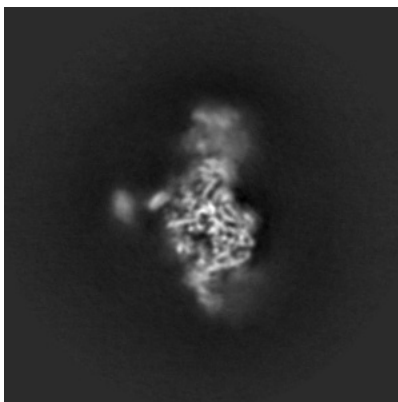


Z Index: 180

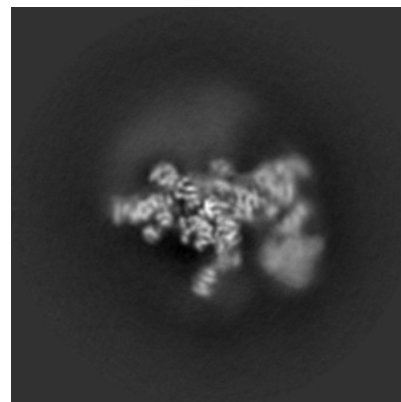
6.2.2 Raw map



X Index: 180



Y Index: 180

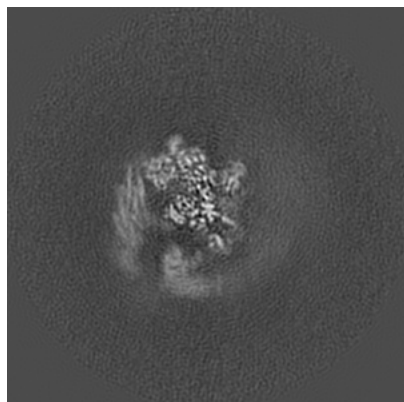


Z Index: 180

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

6.3 Largest variance slices [i](#)

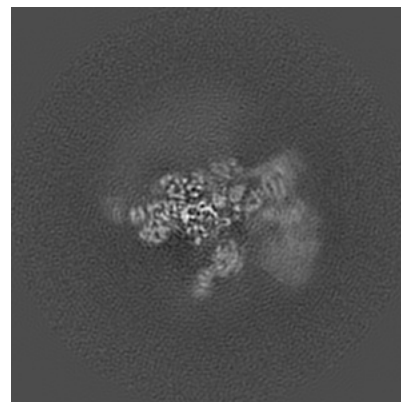
6.3.1 Primary map



X Index: 175

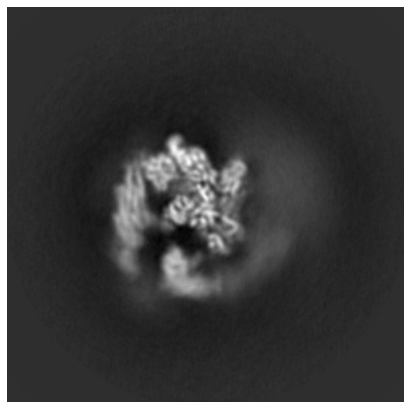


Y Index: 171

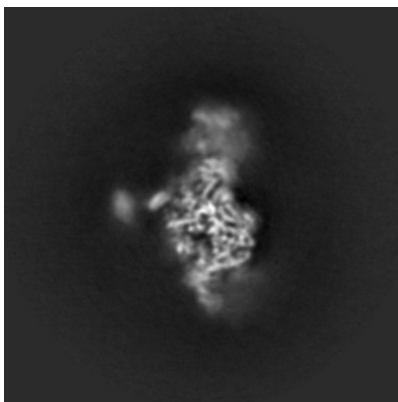


Z Index: 189

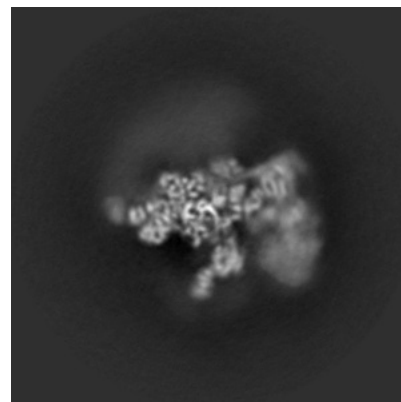
6.3.2 Raw map



X Index: 174



Y Index: 180

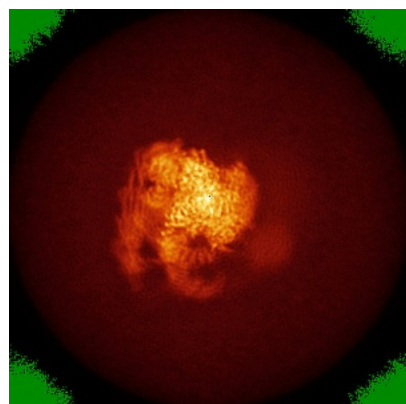


Z Index: 188

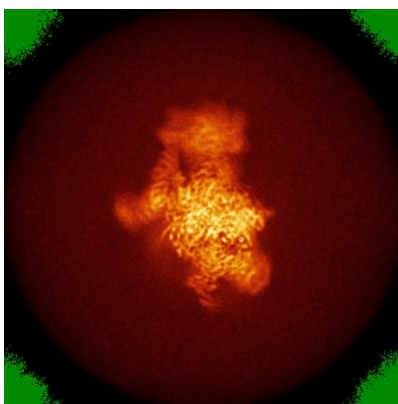
The images above show the largest variance slices of the map in three orthogonal directions.

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

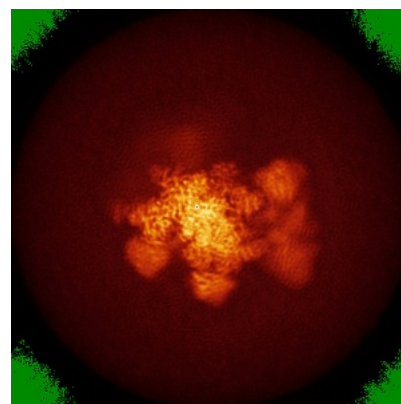
6.4.1 Primary map



X

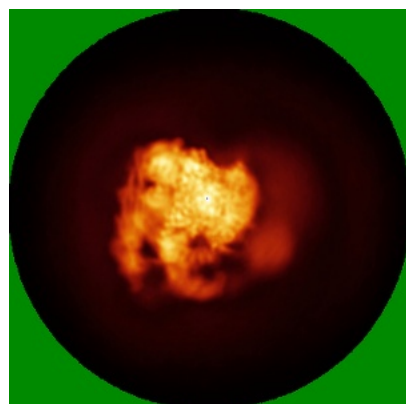


Y

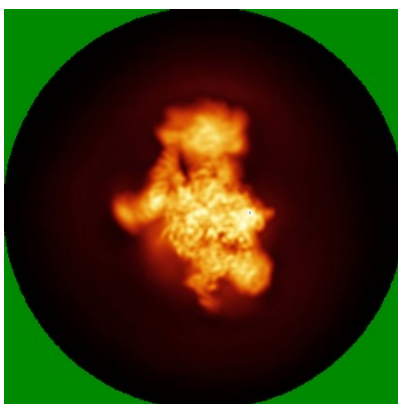


Z

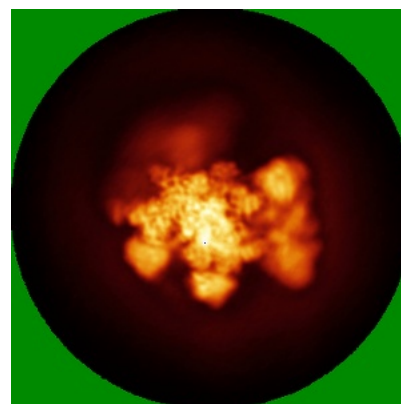
6.4.2 Raw map



X



Y

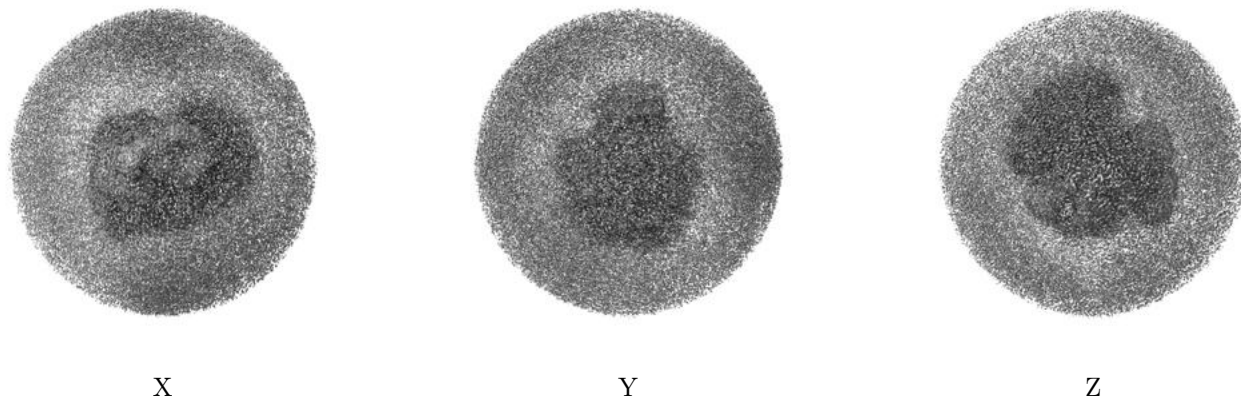


Z

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.

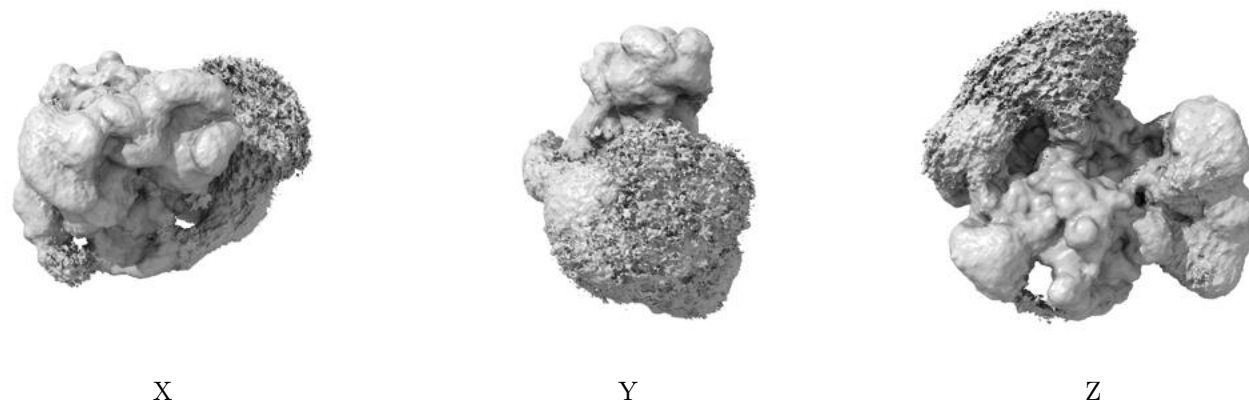
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

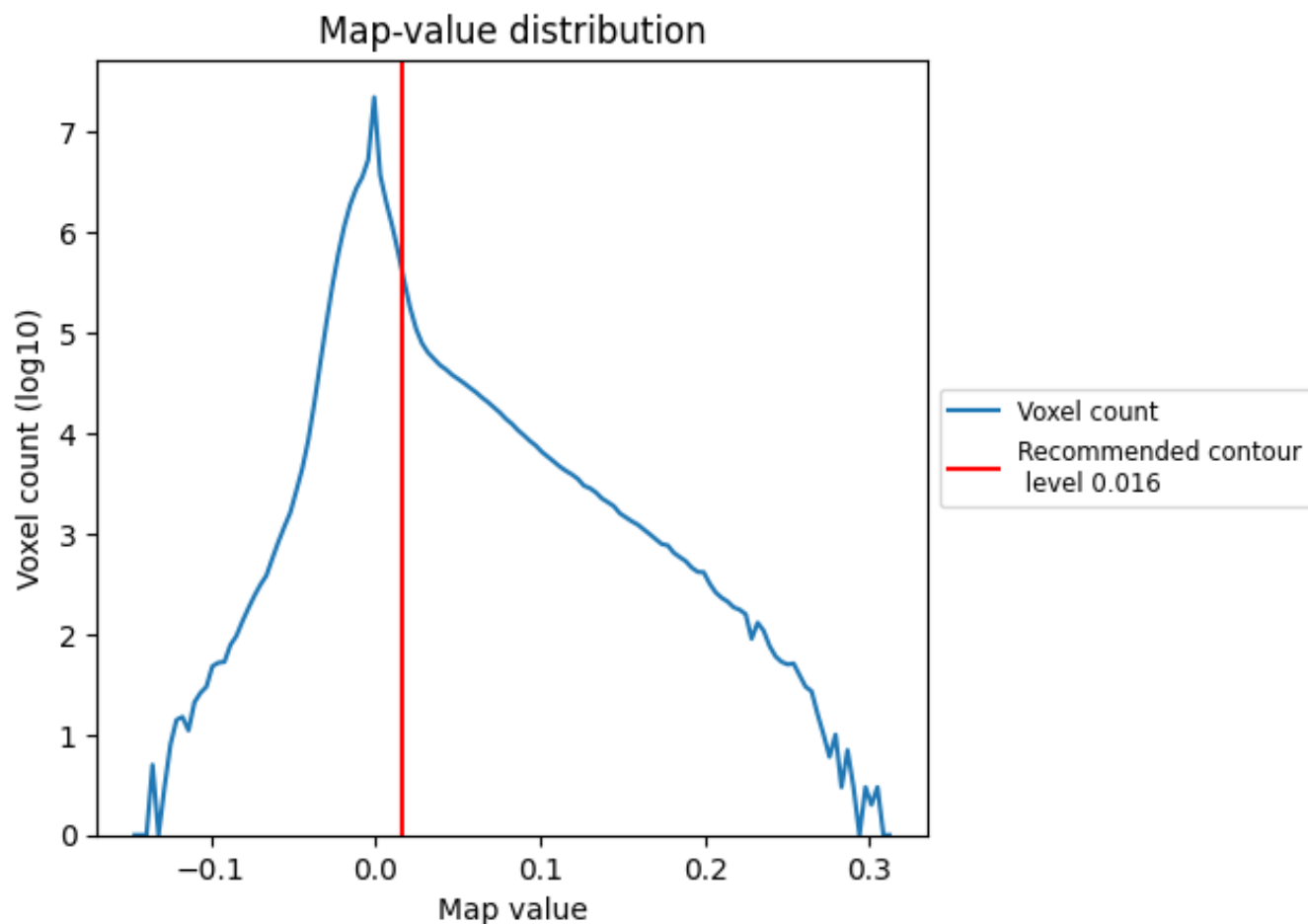
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

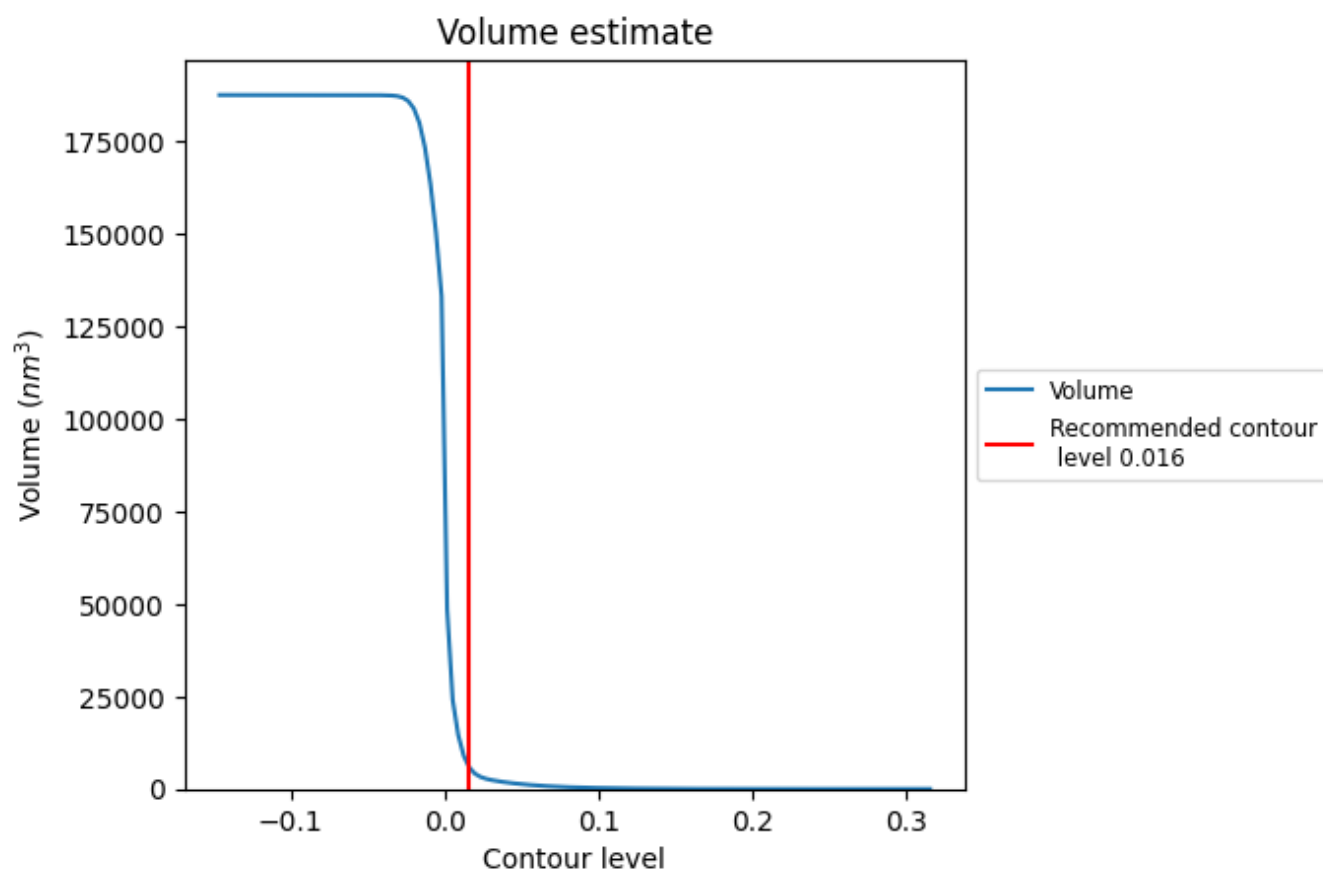
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

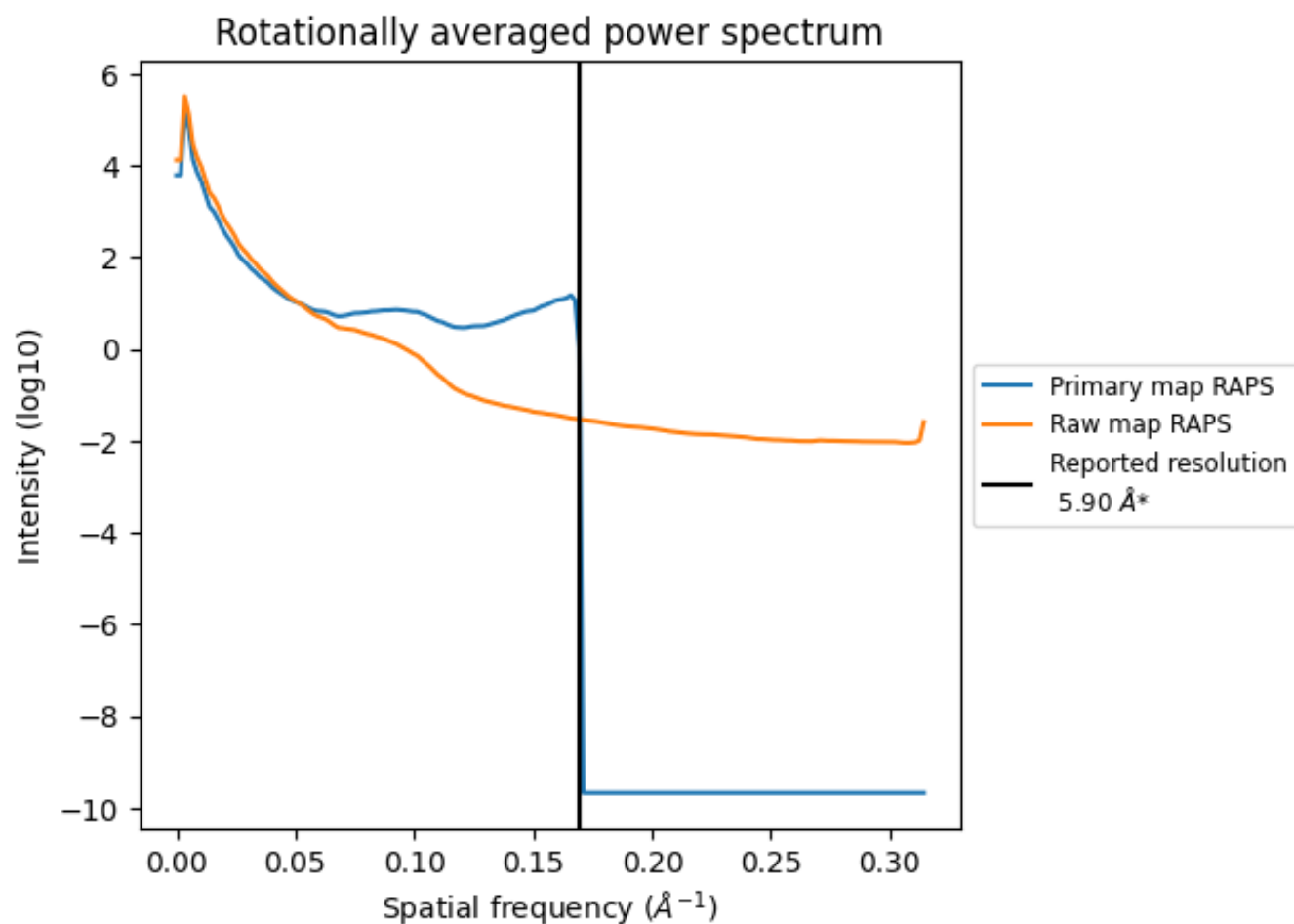
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5939 nm^3 ; this corresponds to an approximate mass of 5364 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 ⓘ

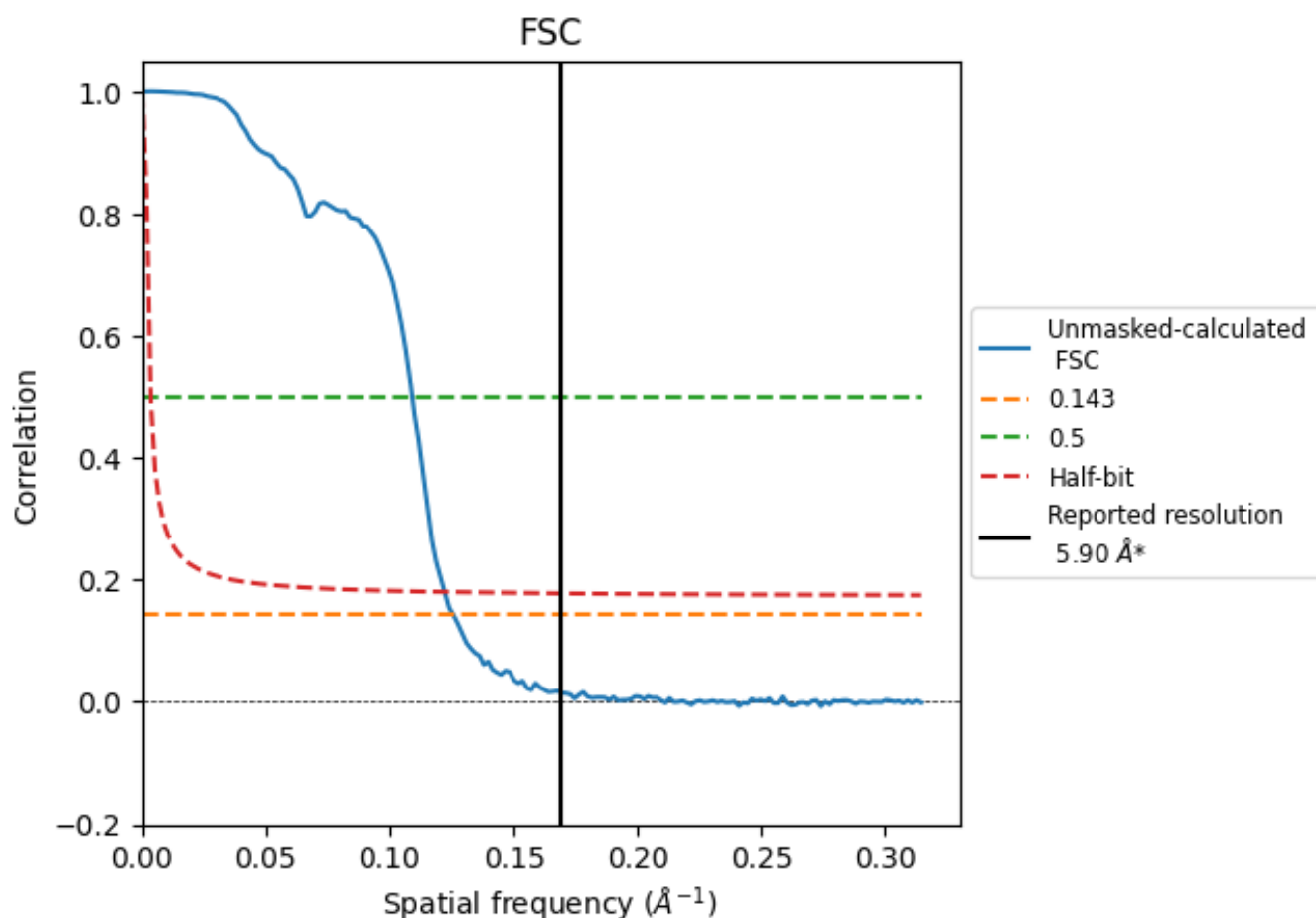


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

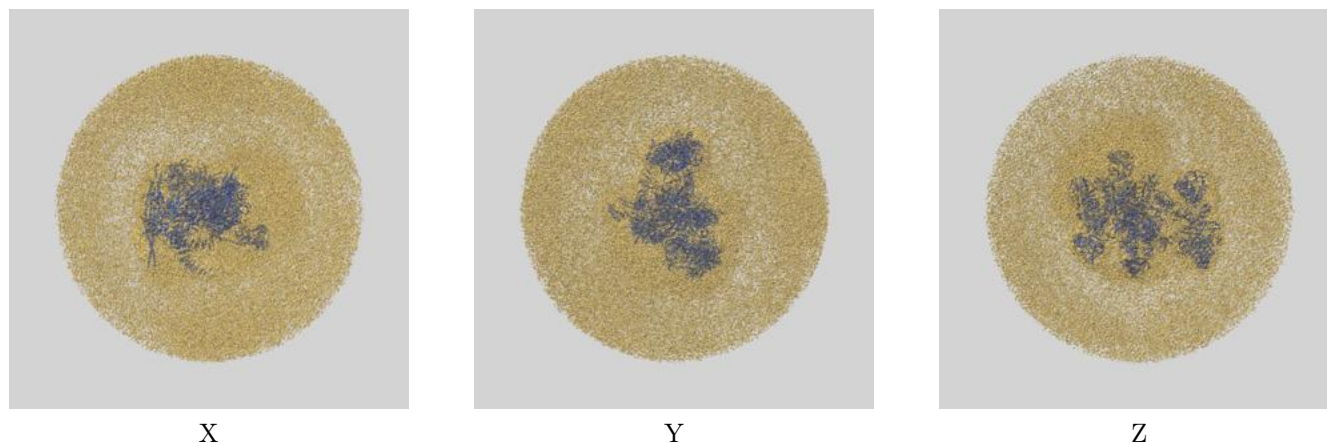
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.96	9.16	8.18

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

9 Map-model fit [i](#)

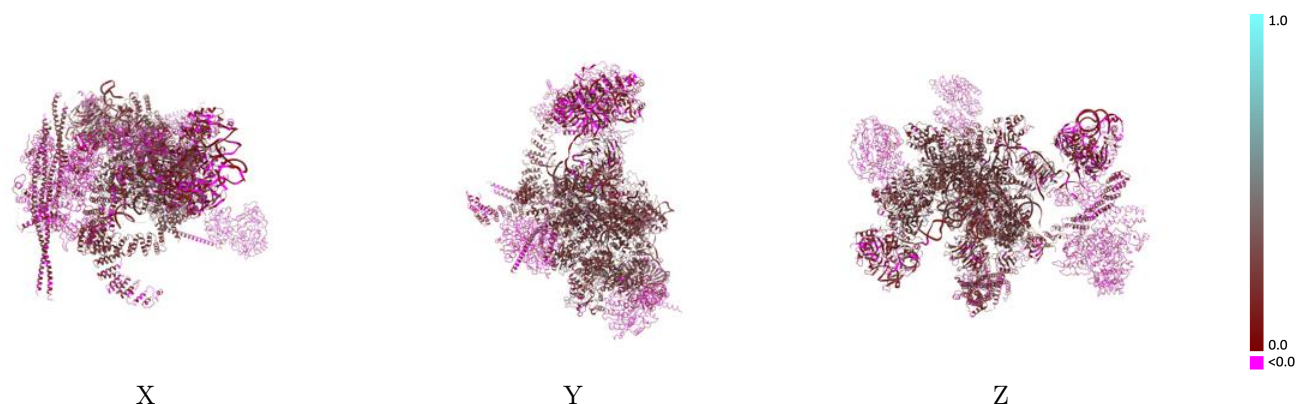
This section contains information regarding the fit between EMDB map EMD-3545 and PDB model 5MQF. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



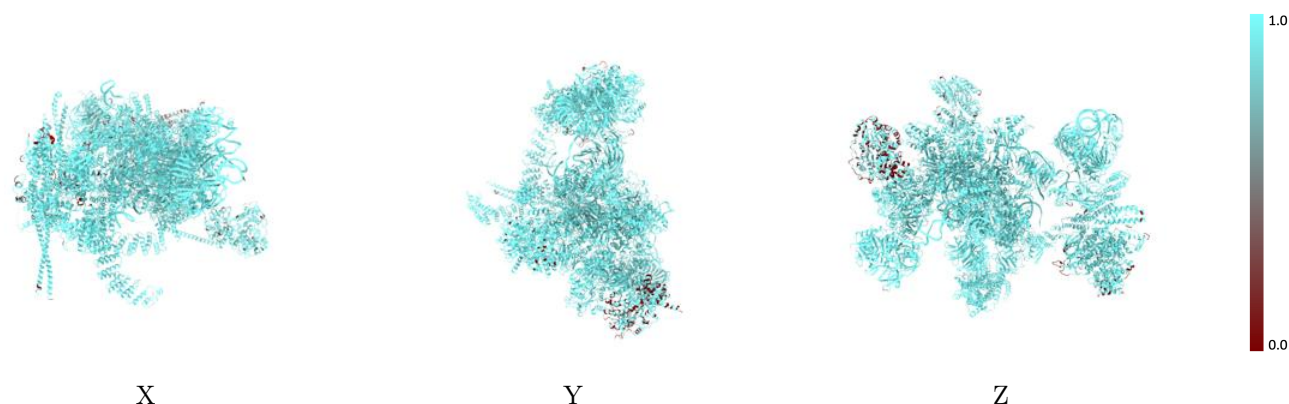
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



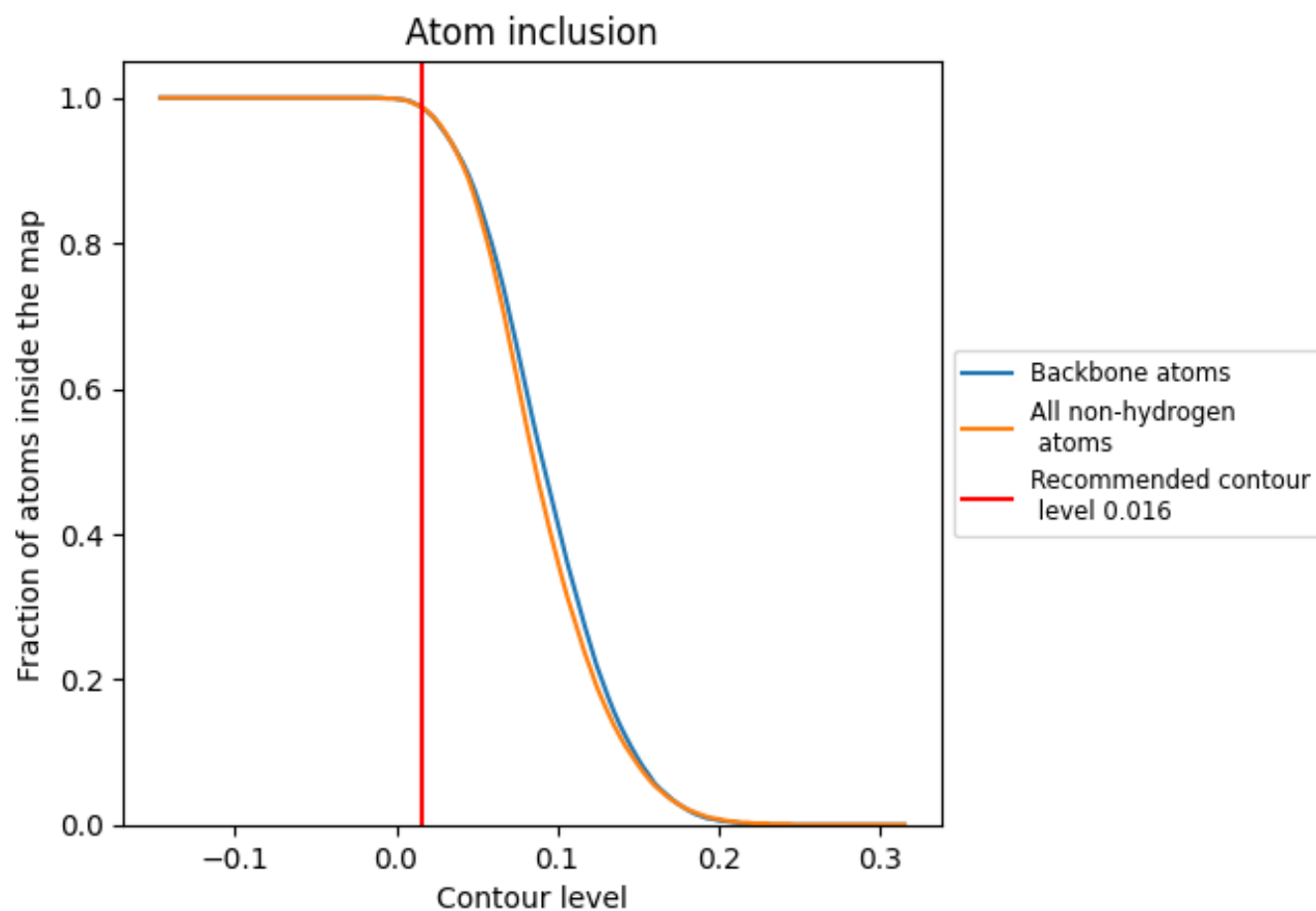
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9870	 0.2020
2	 0.9840	 0.1140
5	 0.9950	 0.2160
6	 0.9960	 0.2300
A	 0.9950	 0.2760
B	 0.9990	 0.2670
C	 0.9850	 0.2710
D	 0.9920	 0.2840
E	 0.9980	 0.2420
F	 1.0000	 0.2340
G	 0.9570	 0.1250
H	 0.9350	 0.0670
I	 0.9990	 0.1550
J	 0.9670	 0.1200
K	 0.9990	 0.1880
L	 0.9950	 0.2530
M	 0.9920	 0.1740
N	 1.0000	 0.2930
O	 0.9990	 0.1990
P	 0.9890	 0.2280
Q	 1.0000	 0.2610
R	 0.9840	 0.2630
S	 1.0000	 0.2700
T	 0.9370	 0.2110
U	 0.9320	 0.0170
V	 1.0000	 0.2380
W	 1.0000	 0.0650
X	 1.0000	 0.1190
Y	 0.9850	 0.1590
Z	 0.9920	 0.2530
a	 0.9780	 0.1460
b	 0.9870	 0.1210
c	 1.0000	 0.1090
d	 0.9970	 0.1450
e	 0.9950	 0.1930



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Chain	Atom inclusion	Q-score
f	 1.0000	 0.1710
g	 1.0000	 0.1660
h	 0.9590	 0.0760
i	 0.9890	 0.0740
j	 0.9980	 0.0650
k	 0.9950	 0.0200
l	 0.9980	 0.1370
m	 1.0000	 0.1100
n	 0.9980	 0.1280
o	 0.9730	 0.0280
p	 0.6650	 0.0040
q	 0.9470	 0.0080