



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:17 PM UTC

PDB ID : 7QTT / pdb_00007qtt
EMDB ID : EMD-14146
Title : Structural organization of a late activated human spliceosome (Baqr, core region)
Authors : Cretu, C.; Pena, V.
Deposited on : 2022-01-15
Resolution : 3.10 Å (reported)
Based on initial models : 6FF7, 5Z57, 6FF4, 6QDV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

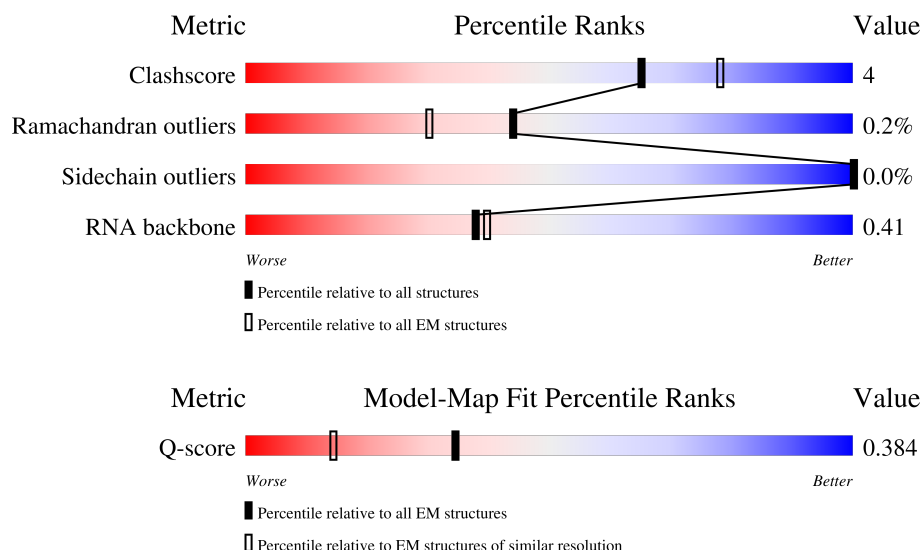
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



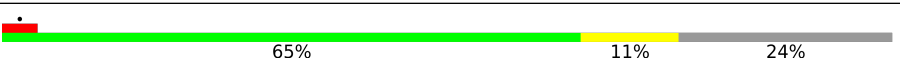
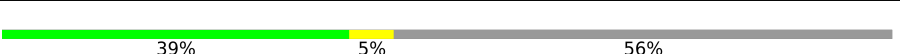
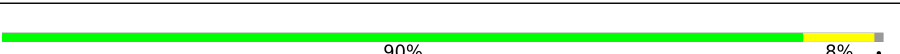
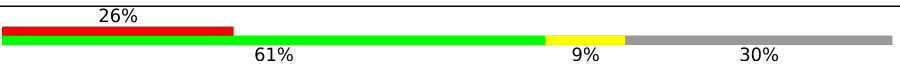
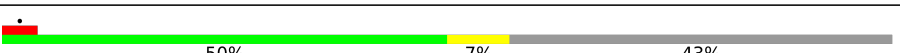
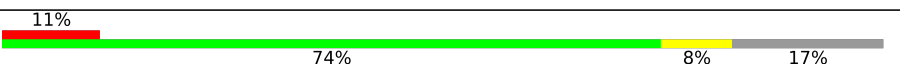
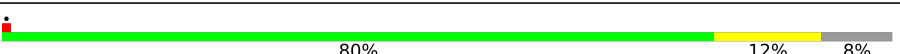
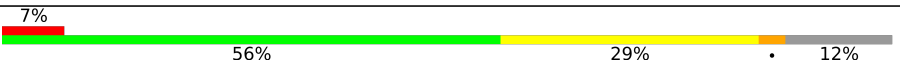
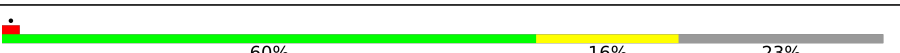
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1217	
2	B	86	
3	C	1304	

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Mol	Chain	Length	Quality of chain
4	D	110	
5	E	895	
6	F	424	
7	G	476	
8	I	464	
9	J	501	
10	L	619	
11	N	1041	
12	O	514	
13	P	802	
14	Q	229	
15	T	144	
16	U	420	
17	V	492	
18	W	908	
19	X	848	
20	Y	536	
21	Z	343	
22	a	2335	
23	b	972	
24	d	106	
25	e	117	
26	f	188	
27	g	319	
28	h	86	

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Mol	Chain	Length	Quality of chain
29	i	92	
30	j	126	
31	k	119	
32	l	118	
33	m	76	
34	n	240	
35	p	166	
36	q	2752	
37	u	520	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 73537 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 Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1164	Total	C	N	O	0	0
			5744	3416	1164	1164		

- Molecule 2 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 3 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	815	Total	C	N	O	S	0	0
			5115	3242	928	930	15		

- Molecule 4 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	89	Total	C	N	O	S	0	0
			649	399	117	120	13		

- Molecule 5 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	198	Total	C	N	O	S	0	0
			1350	855	249	241	5		

- Molecule 6 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	78	Total	C	N	O	0	0
			383	227	78	78		

- Molecule 7 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	67	Total	C	N	O	0	0
			364	228	68	68		

- Molecule 8 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	84	Total	C	N	O	S	0	0
			533	321	114	96	2		

- Molecule 9 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	72	Total	C	N	O	S	0	0
			510	325	93	88	4		

- Molecule 10 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	28	Total	C	N	O	S	0	0
			177	111	32	32	2		

- Molecule 11 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	792	Total	C	N	O	S	0	0
			6157	3898	1093	1138	28		

- Molecule 12 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	320	Total	C	N	O	S	0	0
			2517	1592	457	460	8		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	148	Total	C	N	O	S	0	0
			1151	737	202	208	4		

- Molecule 14 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	100	Total	C	N	O	S	0	0
			823	509	161	151	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	142	Total	C	N	O	S	0	0
			1176	741	216	208	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	295	Total	C	N	O	S	0	0
			2080	1290	380	392	18		

- Molecule 17 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	285	Total	C	N	O	S	0	0
			1996	1252	338	396	10		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	459	Total	C	N	O	S	0	0
			2921	1817	533	559	12		

- Molecule 19 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	241	Total	C	N	O	S	0	0
			1587	1017	298	270	2		

- Molecule 20 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	306	Total	C	N	O	S	0	0
			2250	1412	411	417	10		

- Molecule 21 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	95	Total	C	N	O	S	0	0
			607	378	109	117	3		

- Molecule 22 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	1936	Total	C	N	O	S	0	0
			15194	9745	2709	2675	65		

- Molecule 23 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	898	Total	C	N	O	S	0	0
			7046	4513	1172	1327	34		

- Molecule 24 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	93	Total	C	N	O	P	0	0
			1989	889	364	643	93		

- Molecule 25 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	98	Total	C	N	O	P	0	0
			2070	926	347	699	98		

- Molecule 26 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	76	Total	C	N	O	P	0	0
			1600	716	265	543	76		

- Molecule 27 is a RNA chain called MINX.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	76	Total	C	N	O	P	0	0
			1559	697	250	536	76		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	h	66	Total	C	N	O	0	0
			322	190	66	66		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	i	70	Total	C	N	O	0	0
			346	206	70	70		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	j	68	Total	C	N	O	0	0
			335	199	68	68		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	k	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	l	68	Total	C	N	O	0	0
			337	201	68	68		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	63	Total	C	N	O	0	0
			309	183	63	63		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	64	Total	C	N	O	0	0
			315	187	64	64		

- Molecule 35 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	p	159	Total	C	N	O	0	0
			776	457	159	160		

- Molecule 36 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	74	Total	C	N	O	S	0	0
			461	285	89	85	2		

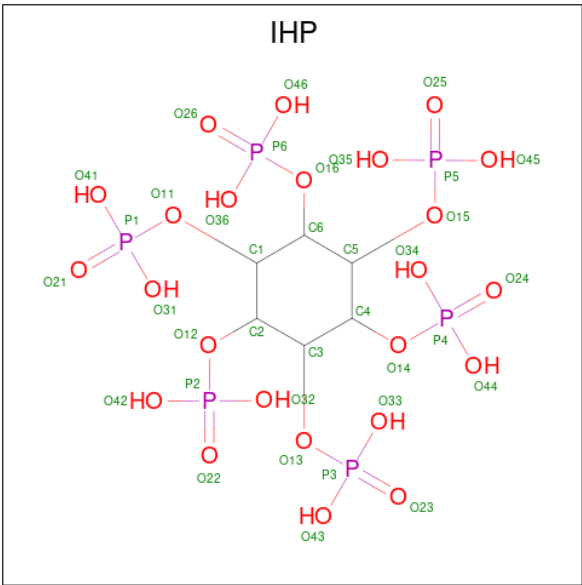
- Molecule 37 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	u	367	Total	C	N	O	S	0	0
			1963	1181	382	399	1		

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

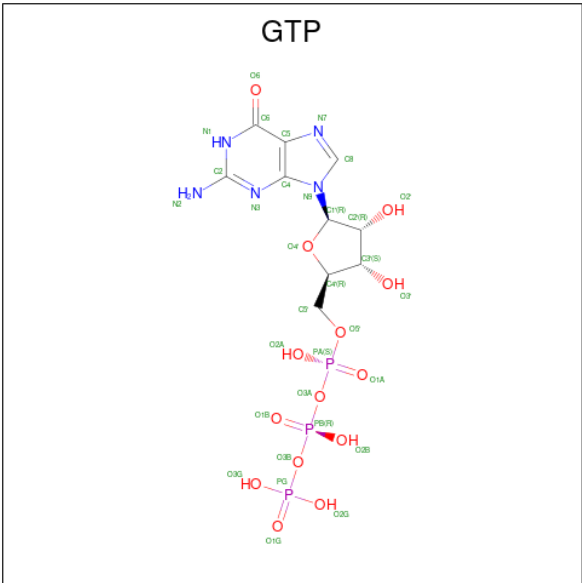
Mol	Chain	Residues	Atoms		AltConf
38	D	3	Total	Zn	0
			3	3	
38	I	1	Total	Zn	0
			1	1	
38	J	1	Total	Zn	0
			1	1	
38	T	3	Total	Zn	0
			3	3	
38	U	3	Total	Zn	0
			3	3	
38	Z	1	Total	Zn	0
			1	1	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	N	O	P	0
			32	10	5	14	3	

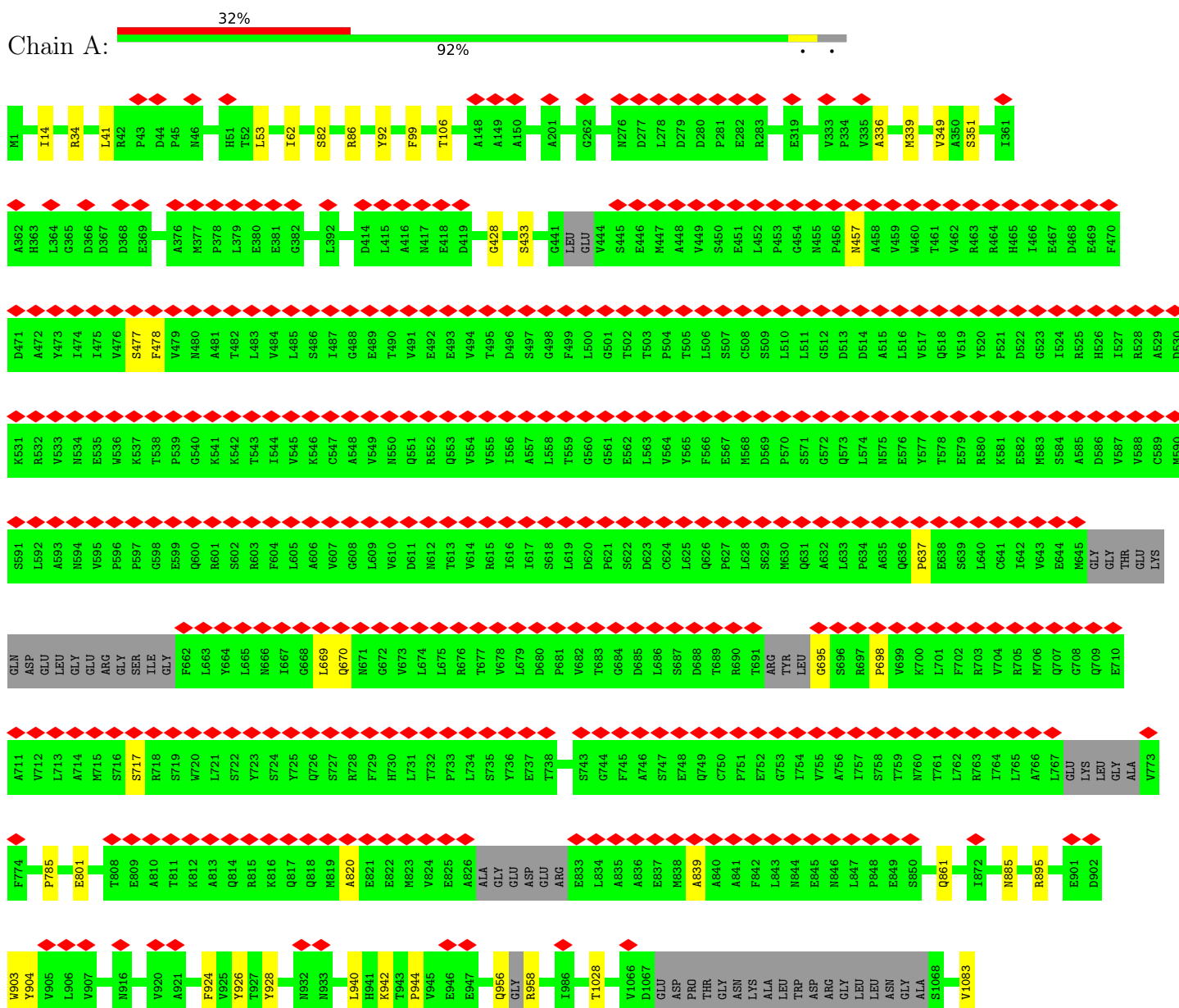
- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

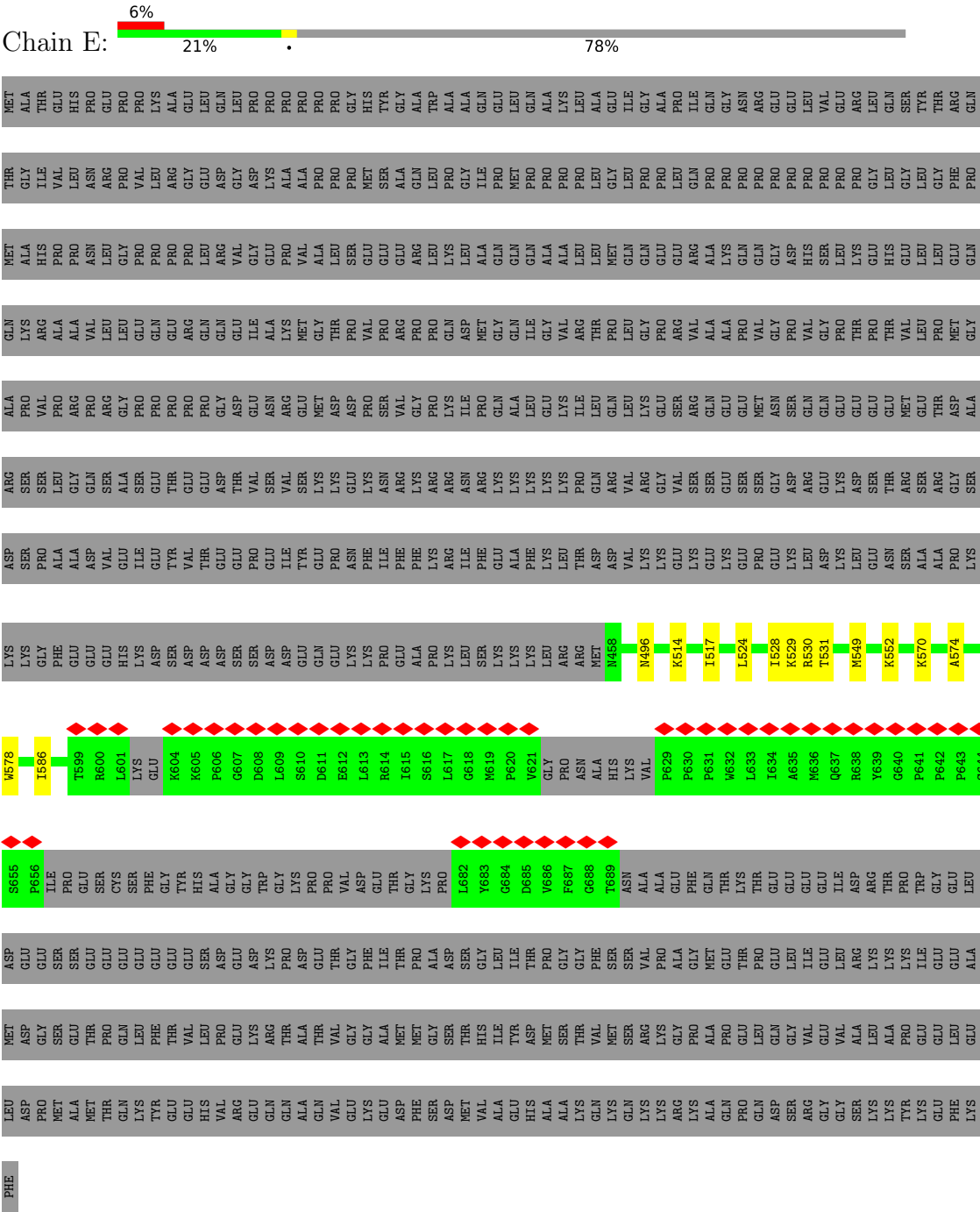
Mol	Chain	Residues	Atoms		AltConf
41	b	1	Total 1	Mg 1	0
41	d	6	Total 6	Mg 6	0

3 Residue-property plots

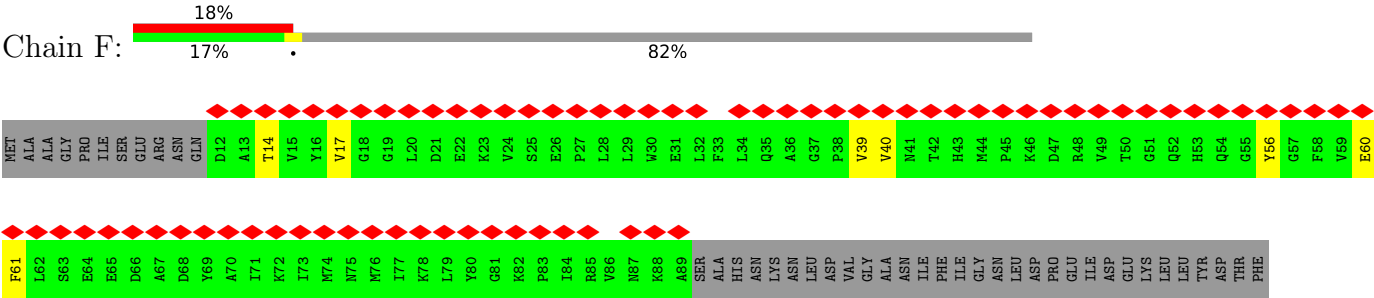
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Splicing factor 3B subunit 3





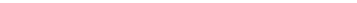
• Molecule 6: Splicing factor 3B subunit 4





[illegible]

- Molecule 9: Splicing factor 3A subunit 3

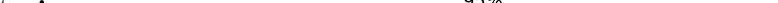
Chain J:  12% 86%

[illegible]

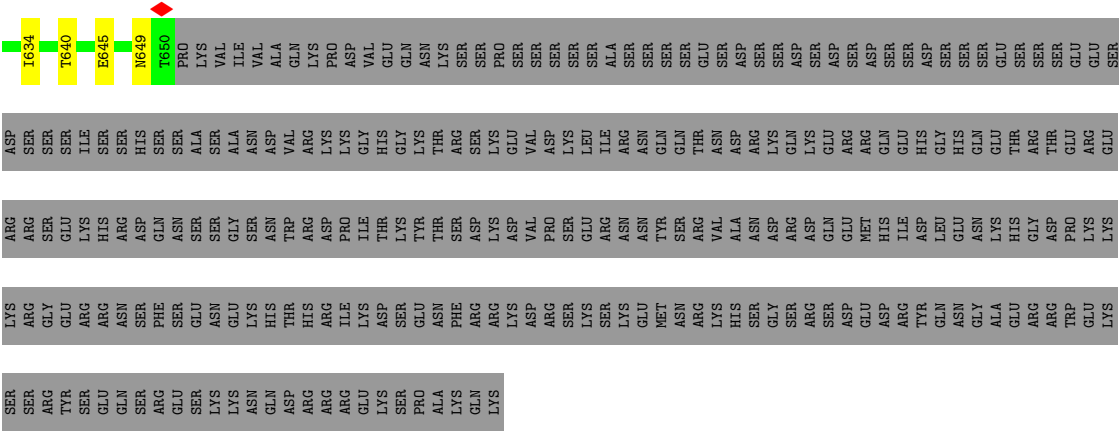
 M442
  T450
  Q451
  K463
  L464

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

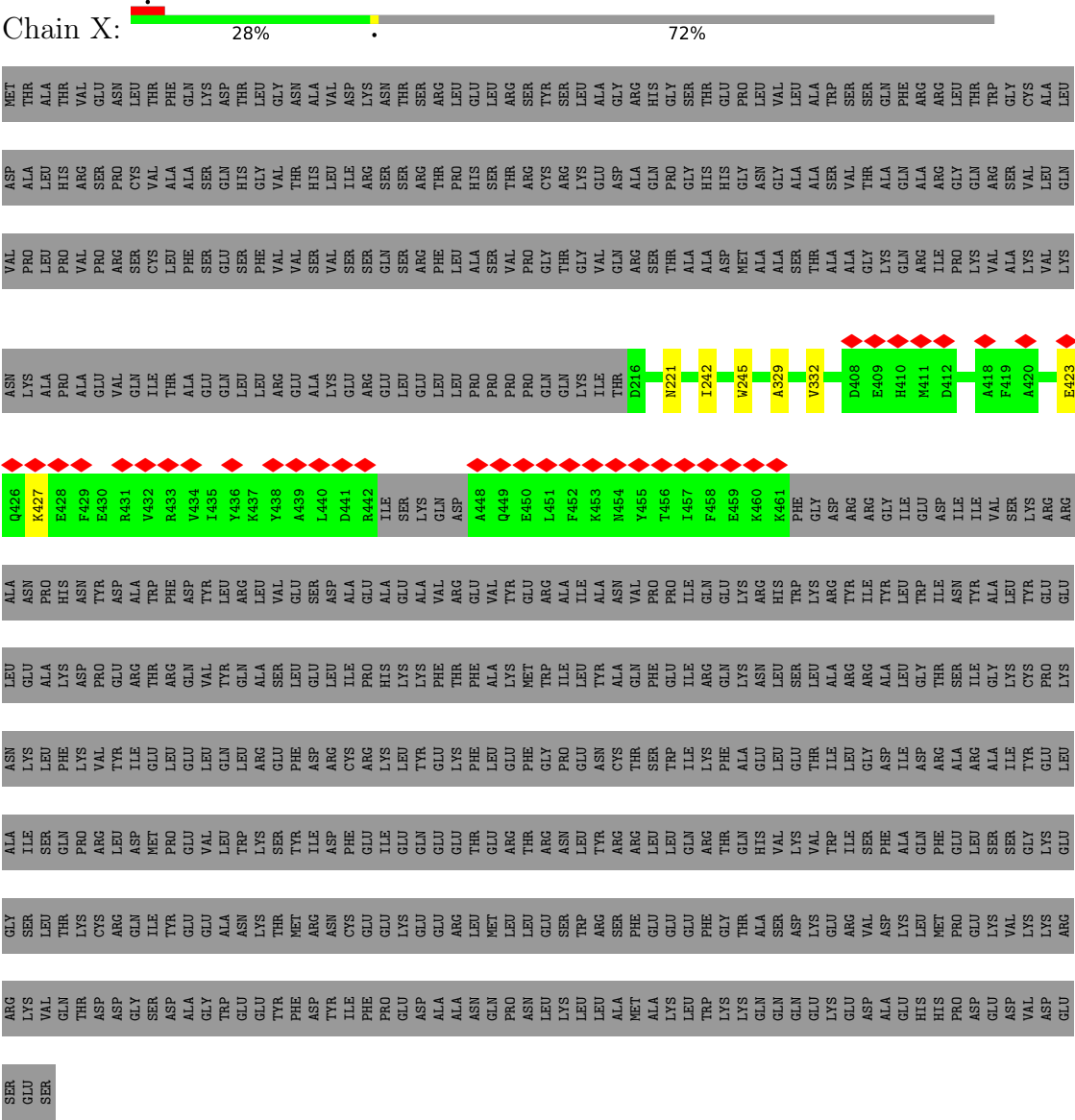
- Molecule 10: BUD13 homolog

Chain L:  95%

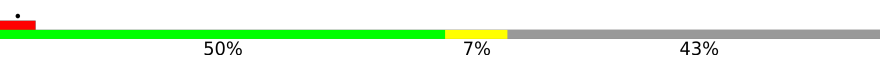
[illegible]

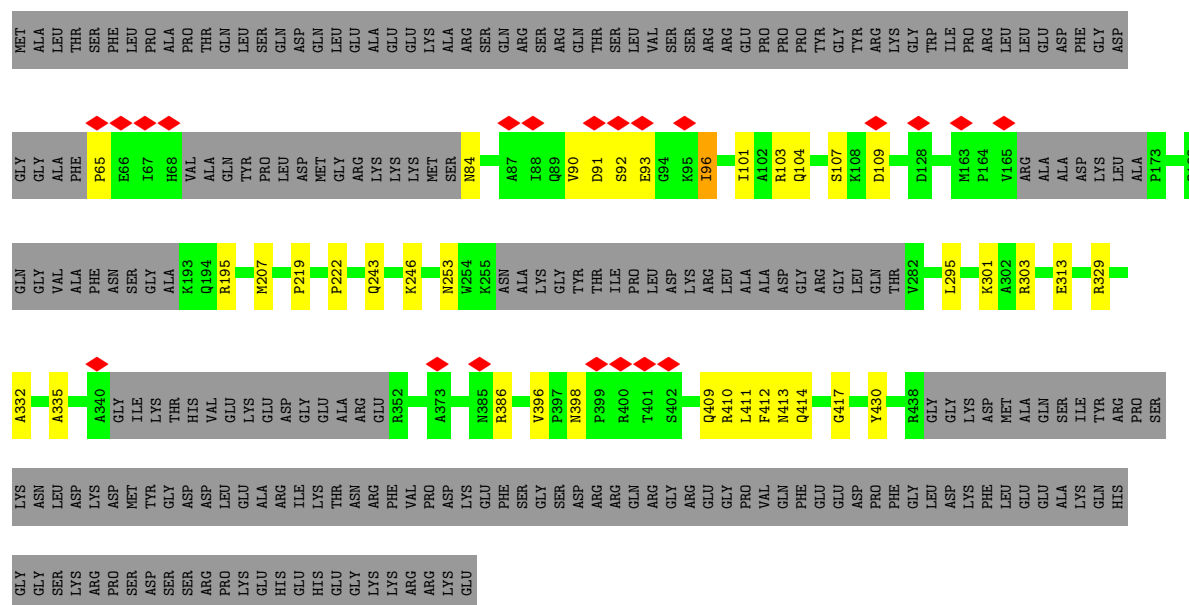


• Molecule 19: Crooked neck-like protein 1



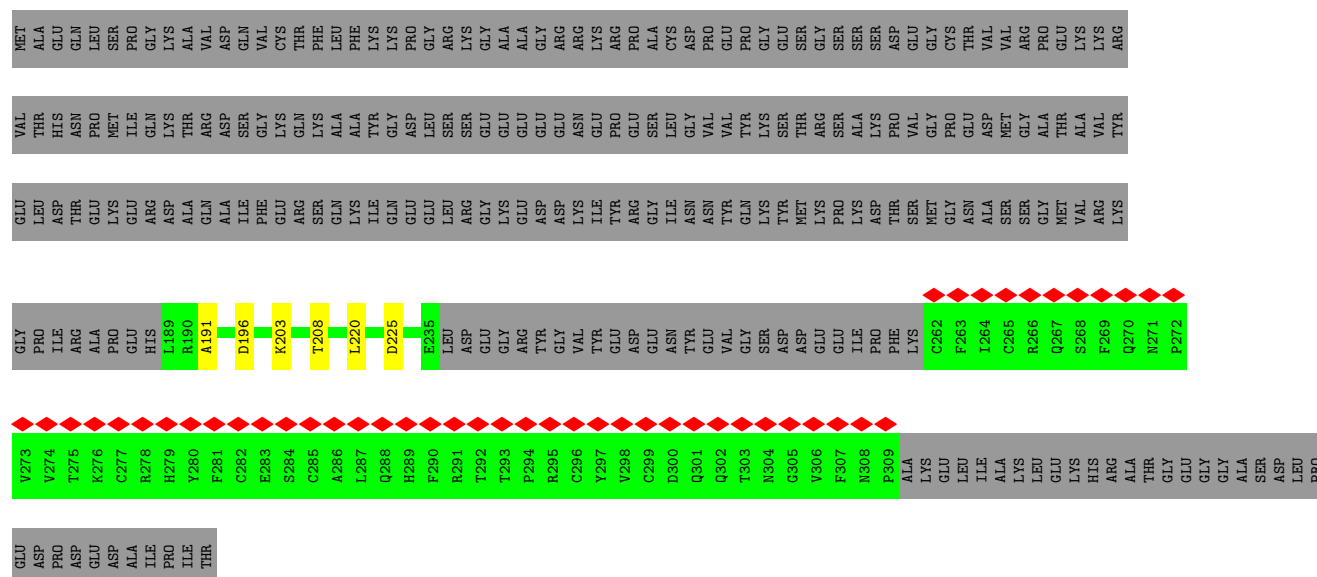
• Molecule 20: SNW domain-containing protein 1

Chain Y: 



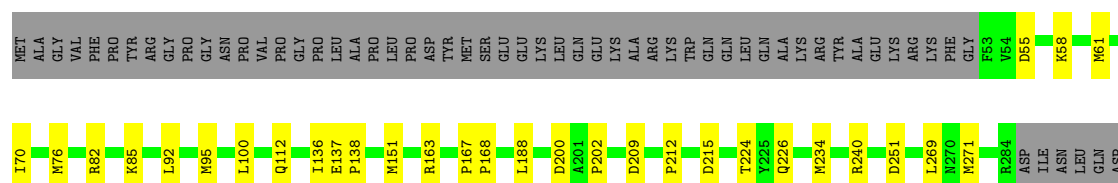
• Molecule 21: RING finger protein 113A

Chain Z: 



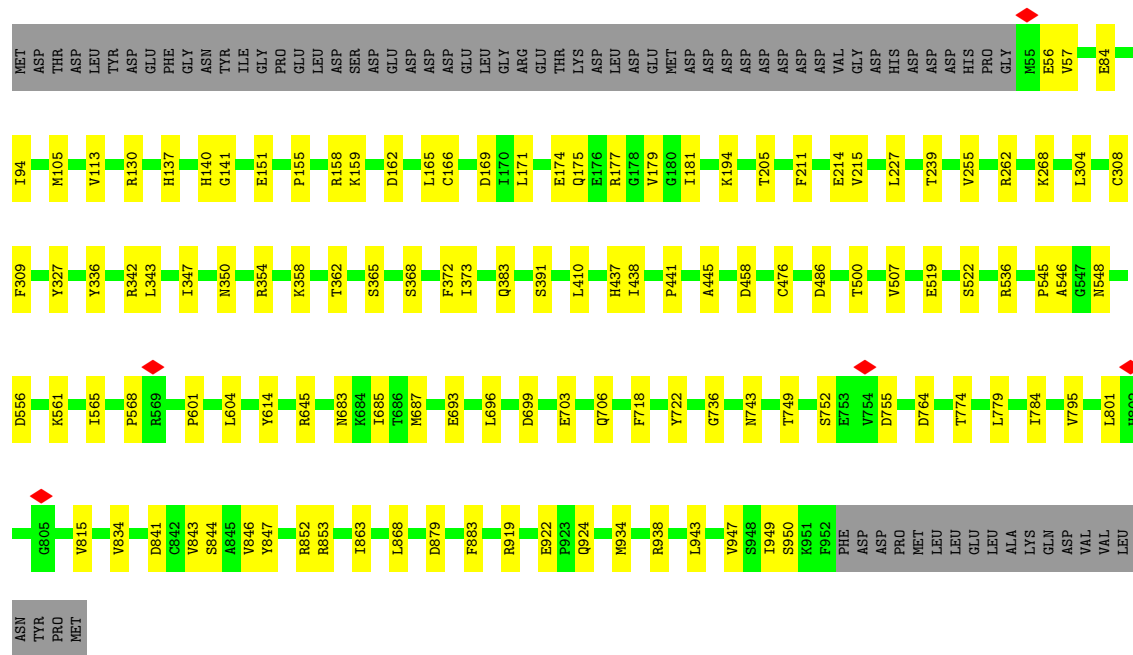
• Molecule 22: Pre-mRNA-processing-splicing factor 8

Chain a: 



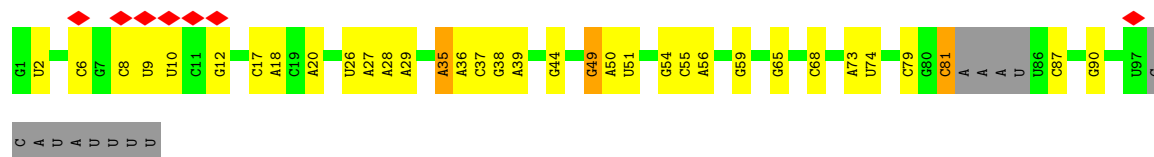
- Molecule 23: 116 kDa U5 small nuclear ribonucleoprotein component

Chain b:



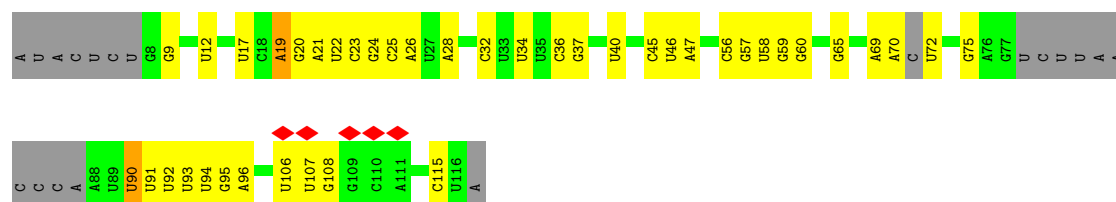
- Molecule 24: U6snRNA

Chain d:



- Molecule 25: U5 snRNA

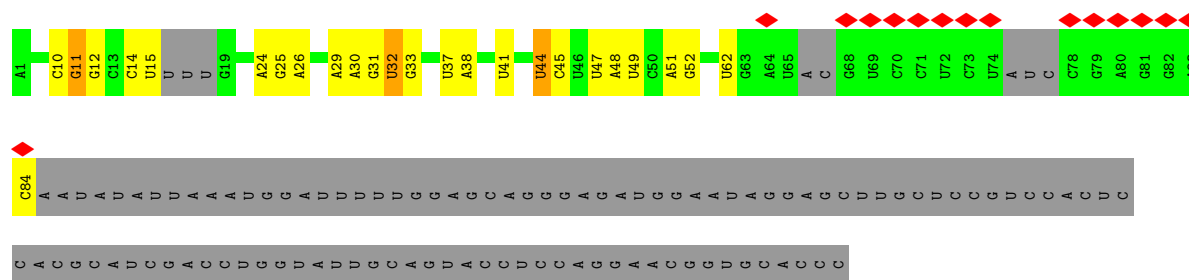
Chain e:



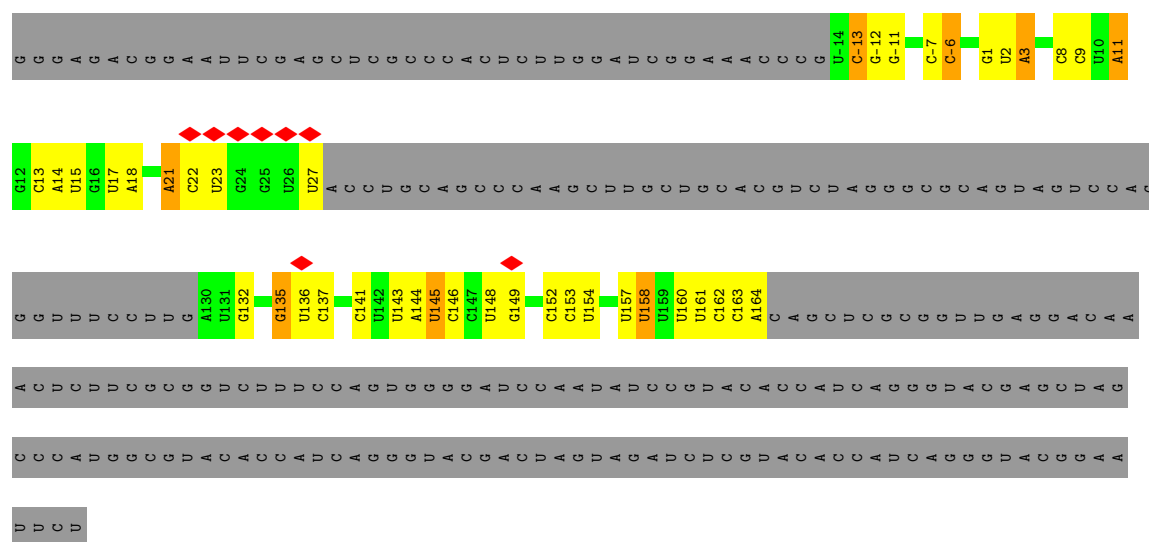
- Molecule 26: U2snRNA

Chain f:

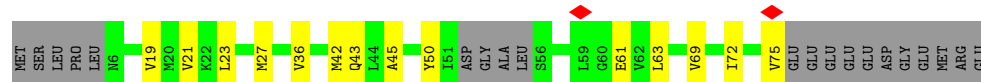




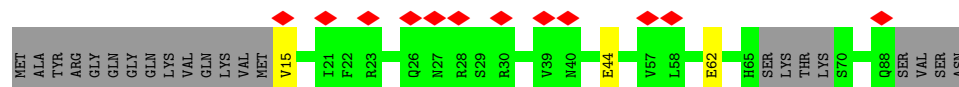
• Molecule 27: MINX



• Molecule 28: Small nuclear ribonucleoprotein F



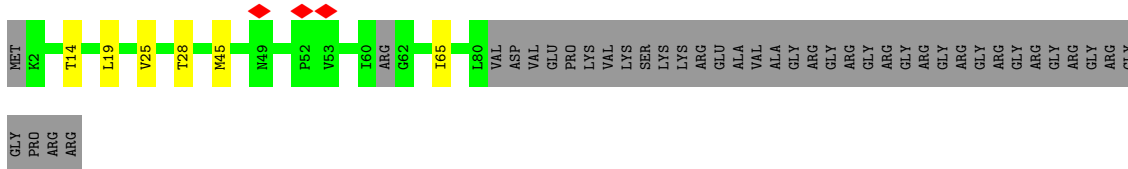
• Molecule 29: Small nuclear ribonucleoprotein E



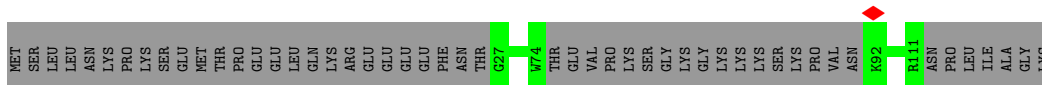
• Molecule 30: Small nuclear ribonucleoprotein Sm D3



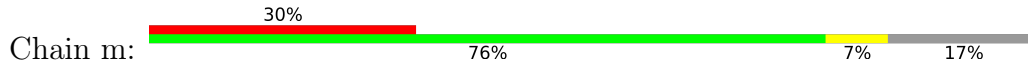
- Molecule 31: Small nuclear ribonucleoprotein Sm D1



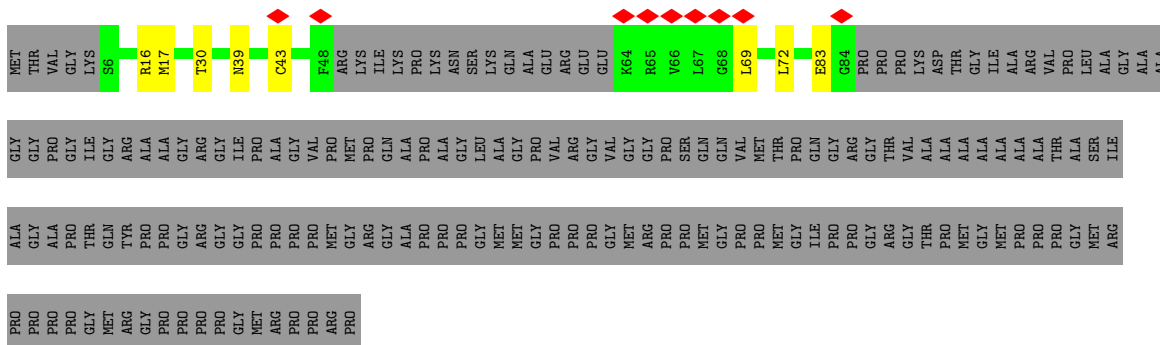
- Molecule 32: Small nuclear ribonucleoprotein Sm D2



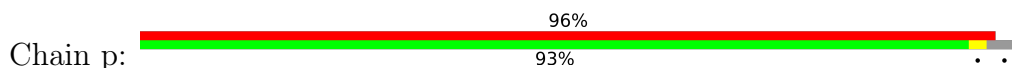
- Molecule 33: Small nuclear ribonucleoprotein G



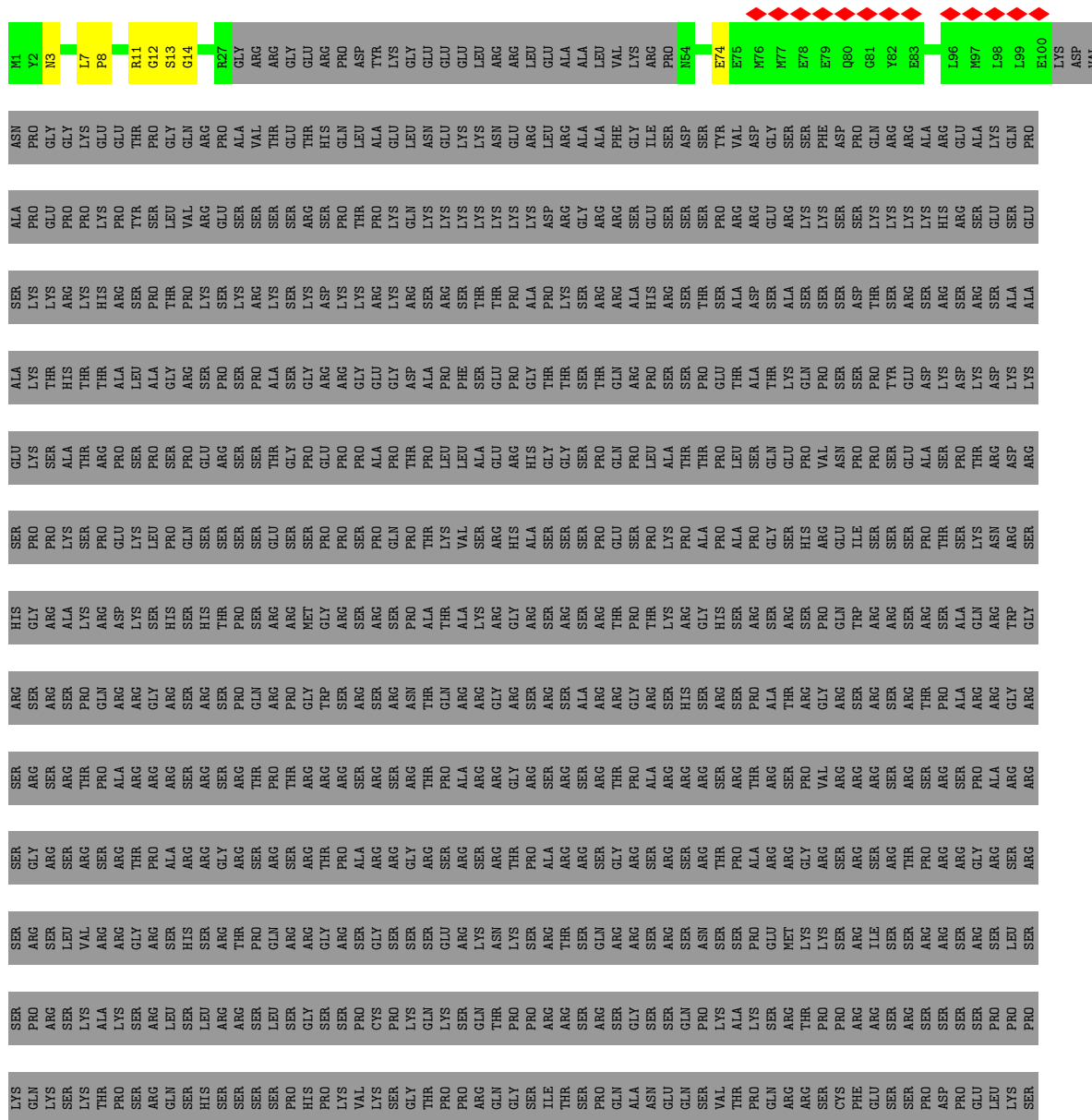
- Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 35: Peptidyl-prolyl cis-trans isomerase-like 1



- Molecule 36: Serine/arginine repetitive matrix protein 2





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146157	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 ($e^-/\text{\AA}^2$)	45.47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/5737	0.35	0/7975
2	B	0.12	0/351	0.36	0/489
3	C	0.23	0/5209	0.53	0/7211
4	D	0.20	0/660	0.67	3/893 (0.3%)
5	E	0.16	0/1383	0.42	0/1887
6	F	0.11	0/382	0.30	0/529
7	G	0.25	0/370	0.59	0/513
8	I	0.15	0/540	0.35	0/733
9	J	0.17	0/525	0.47	0/717
10	L	0.22	0/178	0.67	0/240
11	N	0.22	0/6278	0.59	2/8506 (0.0%)
12	O	0.26	0/2586	0.54	0/3527
13	P	0.19	0/1176	0.49	0/1589
14	Q	0.26	0/836	0.64	1/1117 (0.1%)
15	T	0.27	0/1202	0.62	0/1611
16	U	0.21	0/2118	0.53	1/2881 (0.0%)
17	V	0.17	0/2026	0.48	0/2760
18	W	0.20	0/2954	0.46	0/4033
19	X	0.18	0/1623	0.45	0/2240
20	Y	0.27	0/2290	0.63	3/3103 (0.1%)
21	Z	0.18	0/618	0.49	0/845
22	a	0.25	0/15587	0.51	8/21197 (0.0%)
23	b	0.23	0/7206	0.54	3/9800 (0.0%)
24	d	0.22	0/2225	0.37	1/3464 (0.0%)
25	e	0.24	0/2307	0.41	0/3584
26	f	0.19	0/1780	0.36	0/2760
27	g	0.19	0/1734	0.38	0/2691
28	h	0.12	0/320	0.41	0/440
29	i	0.15	0/344	0.43	0/476
30	j	0.15	0/334	0.44	0/463
31	k	0.12	0/387	0.33	0/537
32	l	0.13	0/335	0.39	0/464

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	m	0.13	0/306	0.40	0/420
34	n	0.11	0/313	0.36	0/432
35	p	0.11	0/775	0.31	0/1070
36	q	0.25	0/466	0.59	0/639
37	u	0.15	0/1969	0.44	0/2722
All	All	0.22	0/75430	0.49	22/104558 (0.0%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	519	ASP	CA-C-N	8.04	136.91	121.54
22	a	519	ASP	C-N-CA	8.04	136.91	121.54
14	Q	65	GLU	N-CA-CB	5.98	120.15	110.40
20	Y	207	MET	CB-CG-SD	5.96	130.58	112.70
23	b	56	GLU	CA-C-N	5.59	132.03	121.97
23	b	56	GLU	C-N-CA	5.59	132.03	121.97
11	N	997	MET	CB-CG-SD	5.46	129.09	112.70
16	U	224	ASP	O-C-N	5.45	124.03	120.27
23	b	105	MET	CB-CG-SD	5.42	128.98	112.70
22	a	95	MET	N-CA-C	5.24	121.40	109.81
11	N	906	ARG	N-CA-C	-5.24	108.65	114.62
20	Y	430	TYR	CA-C-N	5.21	131.49	121.54
20	Y	430	TYR	C-N-CA	5.21	131.49	121.54
24	d	50	A	C2'-C3'-O3'	5.19	121.48	113.70
22	a	1652	MET	CA-CB-CG	5.16	124.41	114.10
22	a	732	PRO	CA-C-N	5.14	126.52	120.09
22	a	732	PRO	C-N-CA	5.14	126.52	120.09
4	D	60	ILE	CA-C-N	5.11	131.29	121.54
4	D	60	ILE	C-N-CA	5.11	131.29	121.54
4	D	60	ILE	N-CA-C	-5.01	98.91	109.34
22	a	1418	ARG	CA-C-N	5.01	130.98	121.97
22	a	1418	ARG	C-N-CA	5.01	130.98	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5744	0	2562	24	0
2	B	350	0	167	0	0
3	C	5115	0	4128	23	0
4	D	649	0	597	9	0
5	E	1350	0	1111	11	0
6	F	383	0	173	4	0
7	G	364	0	226	1	0
8	I	533	0	410	5	0
9	J	510	0	430	7	0
10	L	177	0	140	2	0
11	N	6157	0	5996	73	0
12	O	2517	0	2466	24	0
13	P	1151	0	1096	8	0
14	Q	823	0	779	8	0
15	T	1176	0	1178	9	0
16	U	2080	0	1803	26	0
17	V	1996	0	1727	19	0
18	W	2921	0	2168	11	0
19	X	1587	0	1176	4	0
20	Y	2250	0	2095	29	0
21	Z	607	0	402	5	0
22	a	15194	0	14361	127	0
23	b	7046	0	7031	71	0
24	d	1989	0	1006	11	0
25	e	2070	0	1046	12	0
26	f	1600	0	813	17	0
27	g	1559	0	794	27	0
28	h	322	0	138	7	0
29	i	346	0	144	2	0
30	j	335	0	148	3	0
31	k	388	0	164	3	0
32	l	337	0	139	0	0
33	m	309	0	135	4	0
34	n	315	0	134	4	0
35	p	776	0	358	3	0
36	q	461	0	354	7	0
37	u	1963	0	1065	10	0
38	D	3	0	0	0	0
38	I	1	0	0	0	0
38	J	1	0	0	0	0
38	T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	U	3	0	0	0	0
38	Z	1	0	0	0	0
39	a	36	0	6	0	0
40	b	32	0	12	2	0
41	b	1	0	0	0	0
41	d	6	0	0	0	0
All	All	73537	0	58678	520	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 4.

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:41:U:H3	27:g:135:G:H1	1.02	0.99
26:f:33:G:H1	27:g:145:U:H3	1.08	0.99
26:f:44:U:H3	27:g:132:G:H1	1.01	0.90
16:U:24:CYS:SG	16:U:81:CYS:HB2	2.17	0.83
6:F:17:VAL:O	6:F:56:TYR:HA	1.78	0.82
23:b:683:ASN:HA	23:b:795:VAL:O	1.79	0.82
8:I:59:CYS:SG	8:I:72:HIS:CE1	2.79	0.74
23:b:441:PRO:O	23:b:445:ALA:HB2	1.88	0.74
25:e:90:U:HO2'	33:m:4:ALA:N	1.92	0.67
9:J:408:CYS:O	9:J:413:ASN:HA	1.95	0.66
20:Y:396:VAL:HG12	20:Y:398:ASN:H	1.62	0.65
22:a:532:THR:HG21	27:g:3:A:H5'	1.79	0.64
17:V:65:SER:HG	17:V:77:PHE:N	1.97	0.63
18:W:600:ASN:O	18:W:604:LYS:HB2	1.98	0.63
11:N:613:VAL:HB	11:N:672:VAL:HG23	1.81	0.62
16:U:173:CYS:SG	16:U:183:HIS:CE1	2.92	0.62
22:a:1141:ARG:HB3	22:a:1143:MET:HE3	1.81	0.62
20:Y:417:GLY:HA3	22:a:1459:ARG:HH21	1.65	0.61
25:e:12:U:H3	25:e:65:G:H1	1.47	0.61
10:L:545:MET:SD	10:L:545:MET:N	2.74	0.61
22:a:1439:ARG:O	22:a:1443:LYS:HB2	2.01	0.60
9:J:410:ILE:HB	9:J:431:HIS:HE2	1.66	0.60
23:b:171:LEU:HB2	23:b:174:GLU:HG3	1.83	0.60
9:J:408:CYS:HB3	9:J:411:CYS:SG	2.41	0.59
11:N:300:MET:HE3	20:Y:303:ARG:HE	1.67	0.59
17:V:4:LEU:HB3	17:V:160:VAL:HB	1.83	0.59
12:O:270:VAL:HB	12:O:284:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:752:VAL:HG13	11:N:757:ARG:HH11	1.68	0.58
15:T:117:CYS:SG	15:T:118:ILE:N	2.76	0.58
1:A:695:GLY:HA3	1:A:717:SER:H	1.68	0.58
5:E:530:ARG:HH22	5:E:578:TRP:HB3	1.68	0.58
9:J:402:LEU:HD13	9:J:417:ARG:HH21	1.69	0.58
22:a:1640:SER:HB3	22:a:1652:MET:HA	1.85	0.58
4:D:3:LYS:N	27:g:143:U:HO2'	2.01	0.58
12:O:272:CYS:HB3	12:O:282:ARG:HB2	1.86	0.57
22:a:443:VAL:HG12	22:a:610:HIS:HB3	1.85	0.57
22:a:1072:LEU:HD22	22:a:1087:LEU:HD22	1.85	0.57
23:b:601:PRO:O	23:b:604:LEU:HB2	2.05	0.57
22:a:202:PRO:HB2	22:a:234:MET:HB3	1.87	0.57
31:k:19:LEU:HA	31:k:65:ILE:HA	1.88	0.56
11:N:357:LEU:H	18:W:629:ASN:HD21	1.52	0.56
22:a:269:LEU:HB3	22:a:271:MET:HE3	1.88	0.56
1:A:785:PRO:HA	1:A:801:GLU:HA	1.88	0.56
8:I:56:CYS:O	8:I:60:LEU:N	2.39	0.55
9:J:410:ILE:HD13	9:J:438:LEU:HD11	1.88	0.55
12:O:210:ILE:HG12	12:O:221:THR:HG22	1.88	0.55
12:O:455:GLN:HG2	14:Q:212:ASN:HB2	1.88	0.55
34:n:17:MET:HA	34:n:83:GLU:H	1.71	0.55
9:J:396:LEU:O	9:J:400:HIS:HB2	2.07	0.55
23:b:476:CYS:HB2	23:b:565:ILE:HB	1.89	0.55
22:a:1214:TRP:NE1	22:a:1276:GLU:OE1	2.40	0.55
23:b:205:THR:HB	23:b:215:VAL:HG22	1.88	0.55
12:O:294:LEU:HD12	12:O:303:LEU:HD11	1.88	0.55
1:A:336:ALA:HA	1:A:351:SER:HA	1.89	0.54
5:E:531:THR:HG22	5:E:570:LYS:HG2	1.90	0.54
16:U:97:ARG:NH2	16:U:136:MET:SD	2.80	0.54
22:a:671:THR:O	22:a:676:ARG:NH1	2.40	0.54
5:E:549:MET:HA	5:E:552:LYS:HB2	1.89	0.54
12:O:345:ILE:HB	12:O:357:TRP:HB2	1.89	0.54
23:b:151:GLU:O	23:b:158:ARG:NH2	2.41	0.54
22:a:151:MET:HE1	22:a:629:PHE:HB2	1.90	0.54
30:j:22:THR:HA	30:j:68:ILE:HA	1.90	0.54
23:b:774:THR:HA	23:b:784:ILE:HD12	1.90	0.54
16:U:26:THR:OG1	16:U:159:ARG:NH2	2.40	0.54
22:a:1214:TRP:HB2	22:a:1228:CYS:HB3	1.89	0.54
3:C:815:PHE:HA	3:C:819:TRP:HD1	1.71	0.54
6:F:39:VAL:HA	6:F:61:PHE:HA	1.88	0.54
17:V:2:ALA:HA	17:V:14:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:23:LEU:HA	28:h:69:VAL:HA	1.89	0.53
18:W:584:LYS:HG3	18:W:634:ILE:HG12	1.88	0.53
4:D:49:CYS:HB3	4:D:87:LYS:HD3	1.90	0.53
11:N:779:ASP:OD1	11:N:779:ASP:N	2.41	0.53
13:P:33:ARG:NH1	24:d:49:G:OP2	2.42	0.53
22:a:1622:MET:O	22:a:1683:LYS:NZ	2.42	0.53
23:b:166:CYS:O	23:b:536:ARG:NH2	2.42	0.53
25:e:70:A:H4'	25:e:72:U:H1'	1.90	0.53
20:Y:295:LEU:HD13	22:a:995:ARG:HG3	1.90	0.53
12:O:392:PRO:HG3	12:O:415:ILE:HA	1.90	0.53
22:a:1412:TRP:O	22:a:1420:ASN:ND2	2.42	0.53
23:b:852:ARG:NH1	27:g:-13:C:O2	2.41	0.53
16:U:133:PRO:HG2	16:U:137:LEU:HB2	1.90	0.53
22:a:82:ARG:NH2	27:g:15:U:OP2	2.42	0.53
17:V:7:THR:HG22	17:V:156:ILE:HG12	1.91	0.53
22:a:215:ASP:OD1	22:a:215:ASP:N	2.42	0.53
11:N:841:LEU:HD11	11:N:918:LEU:HB3	1.90	0.53
23:b:141:GLY:N	40:b:1500:GTP:O1B	2.42	0.53
23:b:343:LEU:HD13	23:b:373:ILE:HD11	1.91	0.53
23:b:458:ASP:OD1	23:b:458:ASP:N	2.42	0.53
24:d:81:C:HO2'	26:f:15:U:H3	1.56	0.53
20:Y:103:ARG:NH1	20:Y:107:SER:O	2.43	0.52
26:f:32:U:O4	27:g:146:C:N3	2.42	0.52
5:E:574:ALA:HA	5:E:578:TRP:HB2	1.90	0.52
13:P:30:GLN:HG2	13:P:33:ARG:HE	1.74	0.52
24:d:38:G:O6	27:g:8:C:N4	2.41	0.52
1:A:861:GLN:HA	1:A:885:ASN:HA	1.91	0.52
22:a:1020:LYS:NZ	26:f:26:A:OP1	2.42	0.52
22:a:318:TYR:O	23:b:645:ARG:NH1	2.43	0.52
5:E:549:MET:SD	5:E:549:MET:N	2.77	0.52
11:N:763:VAL:HG12	11:N:766:LEU:HD12	1.92	0.52
14:Q:195:LYS:HD3	37:u:198:LYS:HB3	1.91	0.52
3:C:1062:LEU:HD22	3:C:1077:THR:HG23	1.92	0.52
13:P:211:ASN:ND2	19:X:221:ASN:O	2.43	0.52
27:g:13:C:H2'	27:g:14:A:H8	1.74	0.52
14:Q:33:ARG:NH1	25:e:32:C:OP1	2.43	0.52
34:n:39:ASN:HA	34:n:72:LEU:O	2.10	0.52
37:u:239:ALA:HB2	37:u:266:ILE:HB	1.91	0.52
17:V:97:VAL:HG22	17:V:109:LEU:HD23	1.92	0.51
18:W:501:ARG:O	22:a:1414:ARG:NH2	2.43	0.51
28:h:21:VAL:HA	28:h:72:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1017:LEU:HD13	3:C:1050:VAL:HG21	1.92	0.51
15:T:44:GLU:O	15:T:47:TRP:HB2	2.10	0.51
22:a:390:ASP:OD1	22:a:390:ASP:N	2.43	0.51
22:a:1433:ASP:OD1	22:a:1439:ARG:NH1	2.43	0.51
17:V:199:ASP:OD1	17:V:199:ASP:N	2.43	0.51
20:Y:410:ARG:O	20:Y:414:GLN:NE2	2.43	0.51
22:a:1146:ASP:OD2	22:a:1182:ASN:ND2	2.43	0.51
22:a:1359:HIS:HB2	22:a:1363:GLN:HG3	1.92	0.51
1:A:62:ILE:HA	1:A:82:SER:HA	1.93	0.51
16:U:259:ARG:H	16:U:274:PHE:HA	1.75	0.51
17:V:44:ASN:HB3	17:V:52:GLN:HB3	1.92	0.51
11:N:511:LEU:HB3	11:N:514:TYR:HB2	1.93	0.51
11:N:752:VAL:O	11:N:757:ARG:NH1	2.44	0.51
3:C:806:ILE:HG23	3:C:810:ILE:HD12	1.92	0.51
12:O:356:LEU:HB2	12:O:366:VAL:HB	1.91	0.51
3:C:1030:LYS:O	3:C:1034:ASN:ND2	2.44	0.51
15:T:120:ARG:NH2	24:d:20:A:O2'	2.43	0.51
23:b:130:ARG:NH1	23:b:438:ILE:O	2.44	0.51
11:N:654:ASP:N	11:N:654:ASP:OD1	2.41	0.51
11:N:835:SER:OG	11:N:932:CYS:SG	2.69	0.51
16:U:84:CYS:O	16:U:201:ARG:NH2	2.44	0.51
11:N:970:ILE:HD13	11:N:997:MET:HG3	1.92	0.50
22:a:1052:VAL:O	22:a:1160:ARG:NH1	2.44	0.50
22:a:1410:ASP:OD1	22:a:1410:ASP:N	2.41	0.50
8:I:67:GLY:HA3	13:P:14:THR:HG23	1.93	0.50
16:U:27:CYS:HB3	16:U:84:CYS:SG	2.52	0.50
22:a:439:GLN:O	22:a:444:ARG:NH1	2.44	0.50
37:u:364:GLY:N	37:u:383:THR:O	2.44	0.50
16:U:64:ARG:HG3	16:U:162:PRO:HA	1.93	0.50
20:Y:90:VAL:HG22	20:Y:96:ILE:H	1.77	0.50
22:a:974:ASN:OD1	22:a:1100:ARG:NH1	2.42	0.50
23:b:755:ASP:OD1	23:b:755:ASP:N	2.44	0.50
11:N:333:ARG:NH1	22:a:1460:HIS:O	2.45	0.50
12:O:308:ARG:NH1	22:a:684:GLU:OE2	2.45	0.50
16:U:129:ASP:N	16:U:129:ASP:OD1	2.44	0.50
17:V:117:ASP:OD1	17:V:117:ASP:N	2.43	0.50
11:N:251:LEU:HD11	11:N:273:LYS:HB3	1.93	0.50
23:b:174:GLU:HG2	23:b:181:ILE:HD12	1.94	0.50
16:U:123:ARG:NH1	20:Y:222:PRO:O	2.44	0.50
37:u:239:ALA:O	37:u:240:HIS:ND1	2.44	0.49
1:A:41:LEU:HA	1:A:53:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:779:LEU:HB3	23:b:934:MET:HE1	1.94	0.49
11:N:297:ARG:NH1	20:Y:313:GLU:OE1	2.45	0.49
23:b:486:ASP:OD1	23:b:486:ASP:N	2.44	0.49
16:U:29:GLY:O	20:Y:195:ARG:NH2	2.45	0.49
22:a:1632:PHE:HE1	22:a:1659:LYS:HE2	1.78	0.49
4:D:35:SER:OG	4:D:36:TYR:N	2.44	0.49
17:V:21:ARG:NH1	17:V:81:GLU:O	2.45	0.49
22:a:823:SER:OG	22:a:933:ARG:NH1	2.42	0.49
5:E:524:LEU:O	5:E:529:LYS:NZ	2.46	0.49
22:a:857:ASN:ND2	22:a:860:GLN:OE1	2.46	0.49
23:b:844:SER:O	23:b:847:TYR:HB2	2.13	0.49
18:W:573:GLU:OE2	18:W:622:ARG:NH1	2.46	0.49
20:Y:101:ILE:O	20:Y:104:GLN:NE2	2.45	0.49
4:D:21:ARG:HG3	4:D:65:GLY:HA3	1.94	0.49
11:N:630:ASP:OD1	11:N:633:ARG:NH2	2.45	0.49
22:a:336:ASN:O	23:b:262:ARG:NH2	2.46	0.49
23:b:556:ASP:OD1	23:b:556:ASP:N	2.46	0.49
23:b:703:GLU:O	23:b:706:GLN:NE2	2.46	0.49
1:A:928:TYR:HA	1:A:940:LEU:H	1.77	0.49
1:A:956:GLN:O	1:A:958:ARG:N	2.46	0.49
3:C:1078:VAL:HG11	3:C:1114:VAL:HG12	1.94	0.49
22:a:523:ASN:OD1	22:a:552:ARG:NH2	2.43	0.49
22:a:600:ARG:NH1	22:a:601:GLN:OE1	2.44	0.48
22:a:1288:LEU:HD13	22:a:1330:MET:HG2	1.94	0.48
12:O:353:THR:HG22	12:O:369:THR:HG22	1.95	0.48
12:O:493:ASP:OD1	12:O:493:ASP:N	2.46	0.48
25:e:37:G:H4'	36:q:12:GLY:HA2	1.95	0.48
11:N:697:GLN:O	11:N:709:LEU:HA	2.13	0.48
3:C:1026:ASN:O	3:C:1032:GLN:NE2	2.46	0.48
22:a:1418:ARG:HE	22:a:1464:LEU:HD23	1.77	0.48
16:U:25:GLN:OE1	20:Y:195:ARG:NH2	2.44	0.48
16:U:31:ASN:O	20:Y:195:ARG:NH1	2.46	0.48
22:a:758:ARG:HD2	22:a:758:ARG:HA	1.66	0.48
26:f:33:G:O6	27:g:145:U:O4	2.31	0.48
29:i:15:VAL:N	33:m:32:ARG:O	2.46	0.48
11:N:819:PRO:O	27:g:157:U:N3	2.47	0.48
17:V:88:HIS:ND1	17:V:120:ASP:OD1	2.39	0.48
22:a:402:ILE:HG21	23:b:268:LYS:HD3	1.95	0.48
10:L:534:MET:HE1	18:W:541:THR:HG22	1.94	0.48
11:N:716:LYS:NZ	11:N:743:TYR:O	2.45	0.48
15:T:109:ARG:NH2	22:a:55:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:169:ASP:O	23:b:175:GLN:NE2	2.46	0.48
4:D:11:CYS:HB2	4:D:85:CYS:HB3	1.96	0.48
23:b:211:PHE:O	23:b:214:GLU:HB2	2.13	0.48
3:C:1006:MET:HG2	3:C:1046:GLY:HA3	1.96	0.48
11:N:277:ARG:NH1	11:N:278:ASP:OD1	2.47	0.48
12:O:307:SER:OG	12:O:308:ARG:N	2.47	0.48
22:a:1631:LEU:HB2	22:a:1660:TYR:HB3	1.96	0.48
23:b:194:LYS:NZ	23:b:336:TYR:OH	2.47	0.48
17:V:13:VAL:HB	17:V:131:GLU:HB3	1.96	0.48
21:Z:191:ALA:O	22:a:1617:ARG:NH2	2.46	0.48
22:a:678:GLU:OE2	22:a:778:ARG:NH2	2.47	0.48
28:h:45:ALA:HA	28:h:61:GLU:HA	1.95	0.48
11:N:768:LYS:NZ	11:N:806:GLY:O	2.45	0.47
16:U:175:ARG:HB2	16:U:179:CYS:HB2	1.95	0.47
22:a:372:PRO:HG2	23:b:342:ARG:HD2	1.95	0.47
1:A:92:TYR:HA	1:A:99:PHE:HA	1.96	0.47
11:N:981:PRO:HG2	11:N:984:LEU:HD22	1.96	0.47
20:Y:91:ASP:OD1	20:Y:91:ASP:N	2.47	0.47
11:N:451:THR:HA	11:N:496:MET:O	2.14	0.47
11:N:527:LEU:HD21	11:N:763:VAL:HG21	1.96	0.47
22:a:1889:LEU:HA	22:a:2014:MET:HA	1.96	0.47
28:h:43:GLN:HA	28:h:63:LEU:HA	1.95	0.47
17:V:7:THR:HA	17:V:156:ILE:HA	1.97	0.47
1:A:457:ASN:N	1:A:477:SER:O	2.47	0.47
22:a:945:THR:OG1	22:a:946:GLU:OE1	2.32	0.47
22:a:1593:LEU:HD12	22:a:1664:ILE:HD11	1.95	0.47
23:b:350:ASN:O	23:b:354:ARG:N	2.48	0.47
1:A:1028:THR:O	5:E:496:ASN:ND2	2.48	0.47
11:N:633:ARG:NH1	20:Y:413:ASN:O	2.48	0.47
11:N:865:ASP:OD1	11:N:868:ARG:NH2	2.47	0.47
16:U:11:ASN:ND2	20:Y:219:PRO:O	2.44	0.47
1:A:820:ALA:HA	1:A:839:ALA:HB1	1.97	0.47
4:D:48:GLU:HA	4:D:51:TYR:HB3	1.96	0.47
11:N:838:GLU:OE2	11:N:915:ARG:NH2	2.47	0.47
22:a:58:LYS:NZ	22:a:482:PHE:O	2.48	0.47
23:b:308:CYS:SG	23:b:309:PHE:N	2.88	0.47
11:N:460:SER:OG	11:N:464:ARG:NH1	2.48	0.47
22:a:419:ARG:NH2	22:a:423:ASP:O	2.48	0.47
23:b:947:VAL:HB	23:b:950:SER:HB2	1.95	0.47
5:E:514:LYS:HD3	5:E:517:ILE:HD11	1.97	0.47
16:U:288:PHE:HA	16:U:300:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:225:ASP:OD1	21:Z:225:ASP:N	2.48	0.47
22:a:1069:ASN:OD1	22:a:1075:GLN:NE2	2.47	0.47
23:b:327:TYR:OH	23:b:372:PHE:O	2.31	0.47
1:A:14:ILE:HA	1:A:34:ARG:HA	1.97	0.46
20:Y:409:GLN:O	20:Y:412:PHE:HB3	2.14	0.46
1:A:670:GLN:HA	1:A:698:PRO:HA	1.97	0.46
11:N:476:GLU:HA	11:N:492:VAL:H	1.80	0.46
22:a:372:PRO:O	23:b:358:LYS:NZ	2.43	0.46
22:a:1602:ASP:N	22:a:1602:ASP:OD1	2.48	0.46
8:I:54:TYR:HB2	8:I:63:HIS:HB2	1.98	0.46
22:a:310:THR:HG1	36:q:3:ASN:H	1.63	0.46
11:N:161:GLU:HB3	11:N:164:TRP:HB2	1.97	0.46
11:N:909:ARG:NH1	20:Y:386:ARG:O	2.48	0.46
23:b:343:LEU:O	23:b:368:SER:OG	2.32	0.46
11:N:405:ARG:NH1	11:N:406:GLU:OE2	2.49	0.46
20:Y:92:SER:OG	20:Y:93:GLU:N	2.45	0.46
24:d:73:A:OP2	27:g:3:A:O2'	2.30	0.46
28:h:36:VAL:HA	28:h:42:MET:HA	1.97	0.46
3:C:942:ASN:O	3:C:948:ARG:NH1	2.46	0.46
11:N:278:ASP:OD1	11:N:281:ARG:NH2	2.48	0.46
20:Y:65:PRO:HB3	35:p:90:LEU:HA	1.97	0.46
22:a:76:MET:O	22:a:85:LYS:NZ	2.45	0.46
12:O:282:ARG:NH1	14:Q:38:HIS:O	2.48	0.46
18:W:516:MET:HE3	18:W:559:SER:HA	1.97	0.46
23:b:779:LEU:O	23:b:938:ARG:NH1	2.46	0.46
22:a:200:ASP:OD1	22:a:240:ARG:NH2	2.45	0.46
22:a:591:MET:HG2	22:a:598:LEU:HD22	1.97	0.46
22:a:981:PHE:O	22:a:1166:THR:OG1	2.33	0.46
22:a:1134:TRP:O	22:a:1139:ARG:NH1	2.49	0.46
22:a:1610:GLN:HB2	22:a:1630:LEU:HB3	1.98	0.46
23:b:687:MET:HE3	23:b:815:VAL:HG12	1.98	0.46
16:U:182:ARG:NH1	16:U:184:GLU:OE2	2.46	0.46
20:Y:65:PRO:HA	35:p:91:LYS:H	1.81	0.46
11:N:421:GLU:HB3	11:N:557:THR:HG21	1.98	0.46
11:N:520:ASP:N	11:N:520:ASP:OD1	2.48	0.46
19:X:329:ALA:O	19:X:332:VAL:HB	2.16	0.46
20:Y:332:ALA:O	20:Y:335:ALA:HB3	2.16	0.46
22:a:603:ARG:NH2	27:g:-6:C:O2	2.49	0.46
22:a:1589:ILE:HG22	22:a:1664:ILE:HD13	1.98	0.46
22:a:1660:TYR:OH	22:a:1717:ASN:O	2.32	0.46
1:A:895:ARG:HA	1:A:903:TRP:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:425:HIS:HB3	9:J:431:HIS:ND1	2.31	0.45
11:N:677:ALA:O	11:N:725:ARG:NE	2.49	0.45
16:U:68:THR:HA	16:U:83:THR:HG22	1.97	0.45
17:V:143:PHE:HB3	17:V:152:GLN:HE22	1.81	0.45
22:a:76:MET:HG3	22:a:506:LEU:HD11	1.97	0.45
22:a:1198:PRO:O	22:a:1202:THR:OG1	2.32	0.45
23:b:601:PRO:HA	23:b:604:LEU:HD12	1.98	0.45
13:P:226:ASP:O	20:Y:84:ASN:N	2.49	0.45
22:a:100:LEU:HD21	25:e:56:C:H4'	1.98	0.45
22:a:658:ARG:NH2	24:d:65:G:OP2	2.49	0.45
34:n:43:CYS:HA	34:n:69:LEU:HA	1.97	0.45
36:q:13:SER:OG	36:q:14:GLY:N	2.47	0.45
3:C:1142:ASN:ND2	27:g:141:C:OP1	2.42	0.45
22:a:61:MET:HB2	22:a:61:MET:HE3	1.73	0.45
22:a:913:PRO:HA	22:a:916:LYS:HB2	1.97	0.45
1:A:904:TYR:HA	1:A:928:TYR:O	2.17	0.45
11:N:683:ILE:HB	11:N:686:ILE:HD11	1.97	0.45
23:b:922:GLU:O	23:b:924:GLN:NE2	2.47	0.45
11:N:696:LYS:HD2	11:N:709:LEU:HG	1.98	0.45
23:b:507:VAL:HA	23:b:568:PRO:HD3	1.98	0.45
6:F:40:VAL:N	6:F:60:GLU:O	2.49	0.45
11:N:817:GLU:HG2	11:N:924:ARG:HH21	1.81	0.45
22:a:485:THR:OG1	22:a:486:LYS:N	2.50	0.45
22:a:641:MET:HA	22:a:644:ILE:HG22	1.98	0.45
11:N:649:ALA:O	11:N:906:ARG:NH2	2.50	0.45
11:N:953:ARG:HH11	11:N:958:GLY:H	1.63	0.45
11:N:706:MET:HE1	11:N:708:SER:HB3	1.98	0.45
16:U:92:LEU:HA	27:g:21:A:H61	1.81	0.45
17:V:143:PHE:O	17:V:152:GLN:NE2	2.50	0.45
22:a:92:LEU:HB3	22:a:652:LEU:HB3	1.99	0.45
22:a:1090:ARG:NH1	22:a:1092:ILE:O	2.45	0.45
25:e:58:U:H2'	25:e:59:G:H8	1.81	0.45
1:A:339:MET:HA	1:A:349:VAL:HA	1.99	0.45
1:A:924:PHE:HA	1:A:944:PRO:HA	1.99	0.45
18:W:645:GLU:OE2	18:W:649:ASN:ND2	2.46	0.45
23:b:227:LEU:HB3	23:b:255:VAL:HG22	1.99	0.45
22:a:796:LYS:HE2	22:a:796:LYS:HB3	1.86	0.44
18:W:525:PHE:HA	18:W:528:ILE:HG22	1.98	0.44
22:a:1093:ASP:OD1	22:a:1093:ASP:N	2.47	0.44
24:d:38:G:H2'	24:d:39:A:H8	1.83	0.44
25:e:19:A:H62	25:e:58:U:H3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:640:ARG:HH12	11:N:668:ARG:HH21	1.66	0.44
22:a:919:ASP:OD2	22:a:1012:LYS:NZ	2.48	0.44
22:a:1737:ASN:HB3	22:a:1740:LEU:HB2	1.99	0.44
23:b:685:ILE:HB	23:b:815:VAL:HG21	1.98	0.44
3:C:813:PRO:O	3:C:817:HIS:ND1	2.49	0.44
22:a:209:ASP:HB2	22:a:212:PRO:HA	1.99	0.44
22:a:901:LEU:O	22:a:1242:ASN:ND2	2.46	0.44
23:b:834:VAL:HG11	23:b:883:PHE:HE2	1.82	0.44
1:A:457:ASN:H	1:A:478:PHE:HA	1.81	0.44
3:C:901:GLN:HA	3:C:939:ARG:HH12	1.83	0.44
16:U:24:CYS:SG	16:U:81:CYS:CB	2.93	0.44
23:b:561:LYS:NZ	23:b:614:TYR:O	2.43	0.44
25:e:46:U:O4	25:e:47:A:N6	2.50	0.44
26:f:41:U:O4	27:g:135:G:O6	2.36	0.44
3:C:941:ASN:OD1	3:C:981:TYR:OH	2.35	0.44
11:N:695:CYS:SG	11:N:722:ARG:NH2	2.88	0.44
11:N:700:TYR:HA	11:N:707:GLU:HA	1.98	0.44
11:N:943:ILE:HG21	11:N:1001:LEU:HD13	1.98	0.44
12:O:336:VAL:O	12:O:337:ARG:NH1	2.45	0.44
22:a:137:GLU:OE2	22:a:419:ARG:NH1	2.50	0.44
23:b:155:PRO:O	23:b:158:ARG:NH1	2.50	0.44
11:N:756:GLN:NE2	11:N:783:PRO:O	2.51	0.44
22:a:371:LEU:HD22	23:b:347:ILE:HD11	1.99	0.44
36:q:7:LEU:HD12	36:q:8:PRO:HD2	2.00	0.44
19:X:242:ILE:HA	19:X:245:TRP:HD1	1.81	0.44
22:a:112:GLN:NE2	22:a:188:LEU:O	2.43	0.44
22:a:820:ARG:NH1	22:a:1063:GLY:O	2.43	0.44
3:C:730:PRO:O	3:C:734:GLY:N	2.48	0.44
11:N:268:GLN:NE2	11:N:269:GLU:OE2	2.49	0.44
11:N:674:THR:HG23	11:N:676:ILE:HG12	1.99	0.44
12:O:436:MET:HE1	12:O:479:THR:HG21	2.00	0.44
16:U:81:CYS:SG	16:U:82:GLN:N	2.91	0.44
22:a:1681:ARG:HE	22:a:1681:ARG:HB2	1.66	0.44
24:d:81:C:O2'	26:f:15:U:N3	2.50	0.44
3:C:640:GLY:O	3:C:643:SER:OG	2.36	0.43
22:a:1437:ARG:NH1	22:a:1455:TRP:O	2.51	0.43
29:i:44:GLU:O	29:i:62:GLU:CB	2.66	0.43
31:k:25:VAL:HA	31:k:45:MET:HA	1.99	0.43
1:A:428:GLY:HA3	1:A:433:SER:HA	2.00	0.43
3:C:1213:ASN:ND2	5:E:586:ILE:O	2.51	0.43
12:O:337:ARG:HA	12:O:337:ARG:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:455:GLN:N	12:O:483:ASP:OD2	2.50	0.43
20:Y:411:LEU:HB3	22:a:1405:LEU:HD13	1.99	0.43
22:a:70:ILE:HG21	22:a:495:GLN:HG2	1.99	0.43
22:a:293:TRP:HB2	22:a:1136:ARG:HH22	1.83	0.43
37:u:292:ASN:O	37:u:402:GLY:N	2.51	0.43
4:D:24:GLU:HA	4:D:27:ASP:HB2	2.00	0.43
22:a:251:ASP:OD1	22:a:251:ASP:N	2.51	0.43
22:a:825:ILE:HB	22:a:1001:VAL:HG12	2.00	0.43
22:a:1354:ARG:HH12	36:q:7:LEU:HD13	1.83	0.43
22:a:1543:ASN:HB2	22:a:1569:LEU:HD21	1.99	0.43
11:N:876:GLY:HA3	11:N:1001:LEU:HA	2.00	0.43
12:O:227:THR:HG22	12:O:243:THR:HG22	2.00	0.43
19:X:423:GLU:O	19:X:427:LYS:N	2.41	0.43
22:a:163:ARG:NH1	22:a:576:ASP:OD1	2.51	0.43
22:a:1517:LYS:HD2	22:a:1517:LYS:HA	1.84	0.43
23:b:749:THR:HB	23:b:752:SER:HB2	1.99	0.43
25:e:36:C:O2	36:q:11:ARG:NH2	2.52	0.43
11:N:943:ILE:O	11:N:947:TYR:N	2.49	0.43
22:a:1820:LYS:HA	22:a:1914:MET:HA	2.00	0.43
11:N:696:LYS:NZ	27:g:153:C:OP1	2.52	0.43
12:O:288:LEU:HD23	22:a:669:ALA:HB2	2.01	0.43
12:O:318:ARG:HB3	14:Q:41:ILE:HG13	2.01	0.43
12:O:349:SER:OG	12:O:350:HIS:N	2.50	0.43
14:Q:45:GLN:H	14:Q:48:GLN:HB2	1.84	0.43
22:a:1661:TRP:HD1	22:a:1697:SER:HB3	1.84	0.43
25:e:47:A:O4'	36:q:11:ARG:NH1	2.51	0.43
3:C:978:LEU:HD22	3:C:993:ILE:HG23	2.00	0.43
22:a:61:MET:HE1	22:a:483:GLN:HB3	2.00	0.43
23:b:519:GLU:O	23:b:522:SER:OG	2.36	0.43
26:f:44:U:O4	27:g:132:G:O6	2.37	0.43
3:C:1110:VAL:O	3:C:1113:THR:OG1	2.35	0.43
13:P:20:LYS:HG3	13:P:54:LEU:HD23	1.99	0.43
20:Y:301:LYS:HB3	37:u:203:GLU:HB2	2.01	0.43
22:a:82:ARG:O	22:a:85:LYS:HB2	2.18	0.43
22:a:853:LYS:HA	22:a:853:LYS:HD3	1.77	0.43
11:N:846:MET:HG3	11:N:881:LEU:HB3	2.01	0.43
25:e:17:U:H3	25:e:60:G:H1	1.66	0.43
37:u:331:GLN:HA	37:u:381:PHE:HA	2.00	0.43
11:N:556:ASP:OD1	11:N:556:ASP:N	2.49	0.43
22:a:1413:ASP:O	22:a:1418:ARG:NH1	2.52	0.43
23:b:500:THR:HG22	23:b:545:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:525:ARG:HD2	11:N:525:ARG:HA	1.77	0.42
23:b:177:ARG:HB3	23:b:179:VAL:HG12	2.01	0.42
31:k:14:THR:HA	31:k:28:THR:HA	2.00	0.42
16:U:136:MET:HE3	16:U:136:MET:HB3	1.92	0.42
22:a:1638:ASN:ND2	22:a:1653:ASP:OD1	2.49	0.42
1:A:86:ARG:HA	1:A:106:THR:HA	2.02	0.42
3:C:900:PHE:HA	3:C:910:MET:HE1	2.02	0.42
22:a:787:GLU:OE2	22:a:790:ARG:NH2	2.46	0.42
3:C:1223:SER:HB2	26:f:37:U:H4'	2.01	0.42
4:D:30:CYS:HB3	4:D:35:SER:H	1.83	0.42
18:W:628:ILE:HA	18:W:640:THR:HG21	2.00	0.42
22:a:1021:ASP:OD1	22:a:1021:ASP:N	2.51	0.42
23:b:764:ASP:OD1	23:b:764:ASP:N	2.50	0.42
26:f:41:U:O2	27:g:135:G:N2	2.40	0.42
34:n:16:ARG:HA	34:n:30:THR:HA	2.02	0.42
7:G:169:LEU:HD13	11:N:790:LEU:HD11	2.00	0.42
11:N:606:GLN:HA	11:N:607:PRO:HD3	1.77	0.42
11:N:648:TYR:HB2	11:N:651:LEU:HB2	2.01	0.42
11:N:651:LEU:HD12	11:N:652:PRO:HD2	2.01	0.42
16:U:162:PRO:O	16:U:182:ARG:NE	2.45	0.42
17:V:14:ILE:HG12	17:V:129:VAL:HG22	2.01	0.42
21:Z:203:LYS:NZ	27:g:3:A:OP2	2.49	0.42
21:Z:220:LEU:HB3	22:a:1571:ILE:HG23	2.01	0.42
22:a:1234:ASP:OD1	22:a:1234:ASP:N	2.53	0.42
23:b:546:ALA:O	23:b:548:ASN:ND2	2.53	0.42
23:b:938:ARG:NE	23:b:943:LEU:O	2.41	0.42
30:j:43:MET:O	30:j:61:VAL:N	2.52	0.42
30:j:61:VAL:HA	33:m:71:GLU:HA	2.02	0.42
23:b:362:THR:OG1	23:b:365:SER:OG	2.38	0.42
26:f:51:A:H2'	26:f:52:G:H8	1.85	0.42
1:A:637:PRO:HA	1:A:669:LEU:HA	2.02	0.42
5:E:549:MET:HA	5:E:552:LYS:HD2	2.01	0.42
11:N:945:ALA:HA	11:N:1011:VAL:HG21	2.02	0.42
16:U:134:VAL:HB	16:U:135:GLY:H	1.68	0.42
20:Y:243:GLN:HA	20:Y:246:LYS:HG3	2.02	0.42
23:b:841:ASP:OD1	23:b:841:ASP:N	2.42	0.42
1:A:1083:VAL:HA	1:A:1103:THR:HA	2.02	0.42
21:Z:196:ASP:OD1	22:a:1570:LYS:NZ	2.45	0.42
22:a:1362:ASP:OD1	22:a:1362:ASP:N	2.44	0.42
11:N:507:SER:HB3	27:g:158:U:H3	1.85	0.42
22:a:224:THR:O	22:a:226:GLN:NE2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:383:GLN:OE1	23:b:391:SER:OG	2.36	0.42
23:b:693:GLU:HB2	23:b:696:LEU:HD12	2.01	0.42
4:D:3:LYS:N	27:g:143:U:O3'	2.53	0.42
14:Q:52:GLU:O	14:Q:56:ASN:ND2	2.53	0.42
23:b:843:VAL:O	23:b:846:VAL:HB	2.20	0.42
26:f:44:U:O2	27:g:132:G:N2	2.38	0.42
28:h:27:MET:HA	28:h:50:TYR:O	2.19	0.42
23:b:162:ASP:OD1	23:b:162:ASP:N	2.43	0.41
26:f:10:C:H2'	26:f:11:G:C8	2.55	0.41
26:f:37:U:H2'	26:f:38:A:H8	1.85	0.41
11:N:541:ARG:HD3	11:N:541:ARG:HA	1.84	0.41
12:O:223:SER:OG	12:O:224:ALA:N	2.52	0.41
18:W:570:LEU:HD23	18:W:570:LEU:HA	1.96	0.41
23:b:159:LYS:HG3	23:b:165:LEU:H	1.85	0.41
23:b:699:ASP:OD2	23:b:722:TYR:OH	2.38	0.41
6:F:14:THR:HA	6:F:60:GLU:HA	2.01	0.41
22:a:975:VAL:HG11	22:a:1153:VAL:HG11	2.01	0.41
33:m:19:LEU:HA	33:m:70:LEU:HA	2.02	0.41
37:u:324:SER:HA	37:u:330:ILE:HA	2.02	0.41
11:N:273:LYS:HD3	11:N:273:LYS:HA	1.89	0.41
11:N:960:ARG:NH1	11:N:961:THR:O	2.53	0.41
13:P:48:ALA:O	13:P:52:GLU:HB2	2.20	0.41
22:a:167:PRO:HA	22:a:168:PRO:HD3	1.97	0.41
3:C:1062:LEU:HA	3:C:1065:LEU:HB2	2.02	0.41
11:N:970:ILE:HA	11:N:997:MET:HB2	2.02	0.41
17:V:199:ASP:HB2	17:V:201:LYS:HG2	2.02	0.41
22:a:976:MET:HG2	22:a:1187:PHE:HB3	2.03	0.41
23:b:137:HIS:HB2	23:b:239:THR:HG23	2.02	0.41
11:N:929:LEU:HD23	11:N:929:LEU:HA	1.94	0.41
12:O:419:LEU:HD22	12:O:427:LEU:HD11	2.03	0.41
22:a:414:ARG:NH1	23:b:410:LEU:O	2.46	0.41
23:b:919:ARG:HB2	23:b:924:GLN:HE22	1.86	0.41
35:p:99:ALA:HA	35:p:128:ILE:HA	2.03	0.41
13:P:29:ASN:ND2	20:Y:253:ASN:O	2.46	0.41
22:a:615:ARG:HD3	22:a:615:ARG:HA	1.79	0.41
5:E:528:ILE:O	5:E:531:THR:OG1	2.34	0.41
12:O:485:THR:OG1	12:O:487:LYS:NZ	2.53	0.41
14:Q:190:ASP:O	37:u:199:ASN:ND2	2.42	0.41
16:U:289:ASN:H	16:U:299:ASN:HA	1.85	0.41
24:d:17:C:H2'	24:d:18:A:H8	1.85	0.41
1:A:926:TYR:HA	1:A:942:LYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:473:LEU:HD13	11:N:479:TYR:HE2	1.86	0.41
11:N:826:LYS:HG3	11:N:946:GLY:HA2	2.02	0.41
15:T:95:GLN:NE2	24:d:2:U:O2	2.54	0.41
17:V:197:ILE:H	17:V:197:ILE:HG13	1.72	0.41
20:Y:109:ASP:OD1	20:Y:109:ASP:N	2.54	0.41
22:a:863:GLU:OE2	22:a:916:LYS:NZ	2.48	0.41
22:a:1158:LYS:NZ	22:a:1168:VAL:O	2.48	0.41
22:a:1645:LEU:HB2	22:a:1714:ALA:HB3	2.03	0.41
23:b:368:SER:O	23:b:372:PHE:HB2	2.20	0.41
24:d:35:A:H2'	27:g:11:A:H62	1.86	0.41
28:h:19:VAL:HA	28:h:75:VAL:H	1.86	0.41
3:C:998:LYS:HA	3:C:1038:LEU:HD13	2.02	0.41
15:T:101:CYS:HB3	15:T:139:CYS:SG	2.60	0.41
22:a:1659:LYS:HG3	22:a:1697:SER:HB2	2.03	0.41
8:I:56:CYS:O	8:I:60:LEU:CA	2.69	0.40
11:N:229:LYS:HD3	11:N:229:LYS:HA	1.95	0.40
11:N:875:GLY:HA2	11:N:1002:GLU:HB3	2.03	0.40
17:V:226:MET:HE1	20:Y:329:ARG:HG3	2.03	0.40
23:b:853:ARG:NH1	23:b:879:ASP:O	2.44	0.40
23:b:947:VAL:HG12	23:b:949:ILE:H	1.86	0.40
26:f:33:G:N2	27:g:145:U:O2	2.41	0.40
11:N:482:ARG:HD2	27:g:157:U:H5''	2.03	0.40
15:T:41:ARG:HB2	15:T:44:GLU:HB2	2.04	0.40
15:T:134:CYS:HB3	15:T:139:CYS:H	1.87	0.40
22:a:909:TYR:HB2	22:a:1033:GLY:HA3	2.03	0.40
22:a:1700:GLY:O	22:a:1717:ASN:N	2.49	0.40
23:b:140:HIS:N	40:b:1500:GTP:O1B	2.55	0.40
23:b:304:LEU:O	23:b:437:HIS:NE2	2.44	0.40
23:b:736:GLY:HA2	23:b:743:ASN:HB2	2.03	0.40
3:C:981:TYR:HB3	3:C:993:ILE:HD13	2.04	0.40
15:T:120:ARG:NH1	15:T:142:CYS:SG	2.89	0.40
22:a:1086:ARG:HA	22:a:1086:ARG:HD3	1.83	0.40
22:a:1088:PHE:HD1	22:a:1097:ILE:HG12	1.86	0.40
22:a:1318:THR:HB	22:a:1324:GLY:HA3	2.04	0.40
11:N:681:LEU:HD23	11:N:681:LEU:HA	1.93	0.40
17:V:80:ALA:H	17:V:102:ASP:HB3	1.86	0.40
22:a:789:GLU:HB2	37:u:253:THR:HB	2.04	0.40
11:N:238:LYS:HE3	11:N:241:ARG:HH21	1.87	0.40
22:a:136:ILE:HG22	22:a:138:PRO:HD2	2.04	0.40
22:a:799:PRO:HB2	22:a:801:ILE:HG22	2.04	0.40
23:b:718:PHE:O	23:b:722:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:863:ILE:HD12	23:b:868:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1150/1217 (94%)	1099 (96%)	51 (4%)	0	100	100
2	B	68/86 (79%)	66 (97%)	1 (2%)	1 (2%)	8	32
3	C	813/1304 (62%)	788 (97%)	25 (3%)	0	100	100
4	D	87/110 (79%)	72 (83%)	14 (16%)	1 (1%)	11	39
5	E	190/895 (21%)	179 (94%)	11 (6%)	0	100	100
6	F	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
7	G	63/476 (13%)	62 (98%)	1 (2%)	0	100	100
8	I	80/464 (17%)	80 (100%)	0	0	100	100
9	J	70/501 (14%)	64 (91%)	6 (9%)	0	100	100
10	L	26/619 (4%)	24 (92%)	2 (8%)	0	100	100
11	N	782/1041 (75%)	734 (94%)	46 (6%)	2 (0%)	36	67
12	O	318/514 (62%)	303 (95%)	15 (5%)	0	100	100
13	P	142/802 (18%)	132 (93%)	10 (7%)	0	100	100
14	Q	96/229 (42%)	92 (96%)	4 (4%)	0	100	100
15	T	140/144 (97%)	130 (93%)	10 (7%)	0	100	100
16	U	293/420 (70%)	274 (94%)	16 (6%)	3 (1%)	12	41
17	V	279/492 (57%)	263 (94%)	15 (5%)	1 (0%)	30	61
18	W	455/908 (50%)	446 (98%)	9 (2%)	0	100	100
19	X	237/848 (28%)	232 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	294/536 (55%)	271 (92%)	22 (8%)	1 (0%)	36	67
21	Z	91/343 (26%)	86 (94%)	4 (4%)	1 (1%)	11	39
22	a	1926/2335 (82%)	1834 (95%)	86 (4%)	6 (0%)	36	67
23	b	896/972 (92%)	861 (96%)	30 (3%)	5 (1%)	21	52
28	h	62/86 (72%)	62 (100%)	0	0	100	100
29	i	66/92 (72%)	65 (98%)	1 (2%)	0	100	100
30	j	66/126 (52%)	64 (97%)	2 (3%)	0	100	100
31	k	74/119 (62%)	70 (95%)	4 (5%)	0	100	100
32	l	64/118 (54%)	62 (97%)	2 (3%)	0	100	100
33	m	57/76 (75%)	56 (98%)	1 (2%)	0	100	100
34	n	60/240 (25%)	59 (98%)	1 (2%)	0	100	100
35	p	157/166 (95%)	152 (97%)	5 (3%)	0	100	100
36	q	70/2752 (2%)	64 (91%)	5 (7%)	1 (1%)	9	34
37	u	359/520 (69%)	332 (92%)	26 (7%)	1 (0%)	36	67
All	All	9607/19975 (48%)	9149 (95%)	435 (4%)	23 (0%)	44	73

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	U	225	PRO
16	U	226	PRO
23	b	57	VAL
11	N	860	LYS
16	U	134	VAL
21	Z	208	THR
22	a	520	TYR
22	a	1092	ILE
22	a	1363	GLN
23	b	801	LEU
36	q	74	GLU
37	u	235	LYS
23	b	84	GLU
2	B	78	PRO
4	D	61	CYS
11	N	639	ILE
20	Y	96	ILE
22	a	701	ILE

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Mol	Chain	Res	Type
22	a	1275	ARG
23	b	94	ILE
17	V	235	ILE
23	b	113	VAL
22	a	1419	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	2/77 (3%)	2 (100%)	0	100	100
3	C	342/1104 (31%)	342 (100%)	0	100	100
4	D	69/95 (73%)	69 (100%)	0	100	100
5	E	102/776 (13%)	102 (100%)	0	100	100
7	G	10/397 (2%)	10 (100%)	0	100	100
8	I	33/382 (9%)	33 (100%)	0	100	100
9	J	42/446 (9%)	42 (100%)	0	100	100
10	L	11/545 (2%)	11 (100%)	0	100	100
11	N	625/897 (70%)	625 (100%)	0	100	100
12	O	274/441 (62%)	274 (100%)	0	100	100
13	P	108/709 (15%)	108 (100%)	0	100	100
14	Q	83/203 (41%)	83 (100%)	0	100	100
15	T	129/130 (99%)	129 (100%)	0	100	100
16	U	181/361 (50%)	181 (100%)	0	100	100
17	V	180/451 (40%)	180 (100%)	0	100	100
18	W	180/838 (22%)	178 (99%)	2 (1%)	65	78
19	X	85/751 (11%)	85 (100%)	0	100	100
20	Y	209/459 (46%)	209 (100%)	0	100	100
21	Z	35/294 (12%)	35 (100%)	0	100	100
22	a	1496/2108 (71%)	1496 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	b	784/866 (90%)	784 (100%)	0	100	100
31	k	1/101 (1%)	1 (100%)	0	100	100
36	q	30/2432 (1%)	30 (100%)	0	100	100
37	u	45/456 (10%)	45 (100%)	0	100	100
All	All	5056/15319 (33%)	5054 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	W	458	THR
18	W	575	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	550	HIS
3	C	572	HIS
3	C	1145	ASN
3	C	1184	HIS
5	E	490	HIS
11	N	443	ASN
11	N	629	GLN
11	N	744	GLN
11	N	803	ASN
11	N	933	GLN
12	O	324	HIS
12	O	350	HIS
12	O	407	GLN
12	O	451	HIS
13	P	73	HIS
13	P	81	GLN
14	Q	56	ASN
14	Q	75	ASN
14	Q	196	ASN
15	T	54	HIS
16	U	206	ASN
17	V	44	ASN
17	V	152	GLN
18	W	620	ASN
18	W	629	ASN

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Mol	Chain	Res	Type
19	X	340	GLN
20	Y	84	ASN
20	Y	133	GLN
20	Y	231	HIS
22	a	160	HIS
22	a	294	ASN
22	a	412	ASN
22	a	579	GLN
22	a	775	ASN
22	a	793	ASN
22	a	834	HIS
22	a	1014	ASN
22	a	1023	ASN
22	a	1056	HIS
22	a	1188	ASN
22	a	1218	ASN
22	a	1367	ASN
22	a	1487	HIS
22	a	1586	HIS
23	b	60	HIS
23	b	82	GLN
23	b	542	ASN
23	b	771	GLN
23	b	798	GLN
23	b	924	GLN
36	q	3	ASN
37	u	201	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	d	91/106 (85%)	25 (27%)	0
25	e	95/117 (81%)	27 (28%)	0
26	f	72/188 (38%)	16 (22%)	0
27	g	74/319 (23%)	31 (41%)	0
All	All	332/730 (45%)	99 (29%)	0

All (99) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	d	6	C

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Mol	Chain	Res	Type
24	d	8	C
24	d	9	U
24	d	10	U
24	d	12	G
24	d	26	U
24	d	27	A
24	d	28	A
24	d	29	A
24	d	35	A
24	d	36	A
24	d	37	C
24	d	44	G
24	d	49	G
24	d	51	U
24	d	54	G
24	d	55	C
24	d	56	A
24	d	59	G
24	d	68	C
24	d	74	U
24	d	79	C
24	d	81	C
24	d	87	C
24	d	90	G
25	e	9	G
25	e	19	A
25	e	20	G
25	e	21	A
25	e	22	U
25	e	23	C
25	e	24	G
25	e	25	C
25	e	26	A
25	e	28	A
25	e	34	U
25	e	40	U
25	e	45	C
25	e	57	G
25	e	69	A
25	e	75	G
25	e	90	U
25	e	91	U

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Mol	Chain	Res	Type
25	e	92	U
25	e	93	U
25	e	94	U
25	e	95	G
25	e	96	A
25	e	106	U
25	e	107	U
25	e	108	G
25	e	115	C
26	f	11	G
26	f	12	G
26	f	14	C
26	f	24	A
26	f	25	G
26	f	29	A
26	f	30	A
26	f	31	G
26	f	32	U
26	f	44	U
26	f	45	C
26	f	47	U
26	f	48	A
26	f	49	U
26	f	62	U
26	f	84	C
27	g	-13	C
27	g	-12	G
27	g	-11	G
27	g	-7	C
27	g	-6	C
27	g	1	G
27	g	2	U
27	g	3	A
27	g	9	C
27	g	11	A
27	g	17	U
27	g	18	A
27	g	21	A
27	g	22	C
27	g	23	U
27	g	27	U
27	g	135	G

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Mol	Chain	Res	Type
27	g	136	U
27	g	137	C
27	g	144	A
27	g	145	U
27	g	148	U
27	g	149	G
27	g	152	C
27	g	154	U
27	g	158	U
27	g	160	U
27	g	161	U
27	g	162	C
27	g	163	C
27	g	164	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	IHP	a	3001	-	36,36,36	1.47	6 (16%)	60,60,60	1.51	15 (25%)
40	GTP	b	1500	41	33,34,34	0.92	2 (6%)	50,54,54	1.58	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	IHP	a	3001	-	-	4/30/54/54	0/1/1/1
40	GTP	b	1500	41	-	6/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	a	3001	IHP	P5-O15	3.20	1.65	1.59
39	a	3001	IHP	P3-O13	3.06	1.64	1.59
39	a	3001	IHP	P6-O16	3.03	1.64	1.59
39	a	3001	IHP	P1-O11	3.00	1.64	1.59
39	a	3001	IHP	P2-O12	2.89	1.64	1.59
39	a	3001	IHP	P4-O14	2.88	1.64	1.59
40	b	1500	GTP	C2-N3	2.02	1.38	1.33
40	b	1500	GTP	C5-N7	-2.02	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	b	1500	GTP	C5-C4-N3	-4.95	120.51	128.39
40	b	1500	GTP	C2-N3-C4	4.49	120.04	112.30
39	a	3001	IHP	C6-C1-C2	3.63	118.39	110.43
39	a	3001	IHP	C5-C6-C1	3.29	117.64	110.43
40	b	1500	GTP	N9-C4-N3	3.27	132.50	125.95
40	b	1500	GTP	C2-N1-C6	-3.02	119.64	125.11
40	b	1500	GTP	N9-C8-N7	-2.76	108.28	113.40
39	a	3001	IHP	C3-C2-C1	2.73	116.42	110.43
40	b	1500	GTP	C5-C6-N1	2.53	119.70	113.25
39	a	3001	IHP	P1-O11-C1	-2.53	116.68	123.43
40	b	1500	GTP	O6-C6-C5	-2.52	119.87	126.53
39	a	3001	IHP	O35-P5-O25	-2.52	101.00	110.83
39	a	3001	IHP	O34-P4-O24	-2.51	101.07	110.83
39	a	3001	IHP	O33-P3-O23	-2.48	101.18	110.83
40	b	1500	GTP	C8-N7-C5	2.48	108.67	104.26
39	a	3001	IHP	O32-P2-O22	-2.42	101.39	110.83
39	a	3001	IHP	P3-O13-C3	-2.41	117.00	123.43
39	a	3001	IHP	O36-P6-O26	-2.40	101.47	110.83
39	a	3001	IHP	P4-O14-C4	-2.33	117.22	123.43
39	a	3001	IHP	O31-P1-O21	-2.29	101.92	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	3001	IHP	P6-O16-C6	-2.22	117.52	123.43
39	a	3001	IHP	P5-O15-C5	-2.20	117.55	123.43
39	a	3001	IHP	P2-O12-C2	-2.15	117.68	123.43
40	b	1500	GTP	C3'-C2'-C1'	2.05	105.35	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	b	1500	GTP	C5'-O5'-PA-O3A
40	b	1500	GTP	C5'-O5'-PA-O2A
40	b	1500	GTP	PG-O3B-PB-O2B
39	a	3001	IHP	C2-O12-P2-O22
40	b	1500	GTP	C5'-O5'-PA-O1A
39	a	3001	IHP	C6-O16-P6-O36
40	b	1500	GTP	C4'-C5'-O5'-PA
40	b	1500	GTP	PG-O3B-PB-O1B
39	a	3001	IHP	C1-O11-P1-O41
39	a	3001	IHP	C6-O16-P6-O46

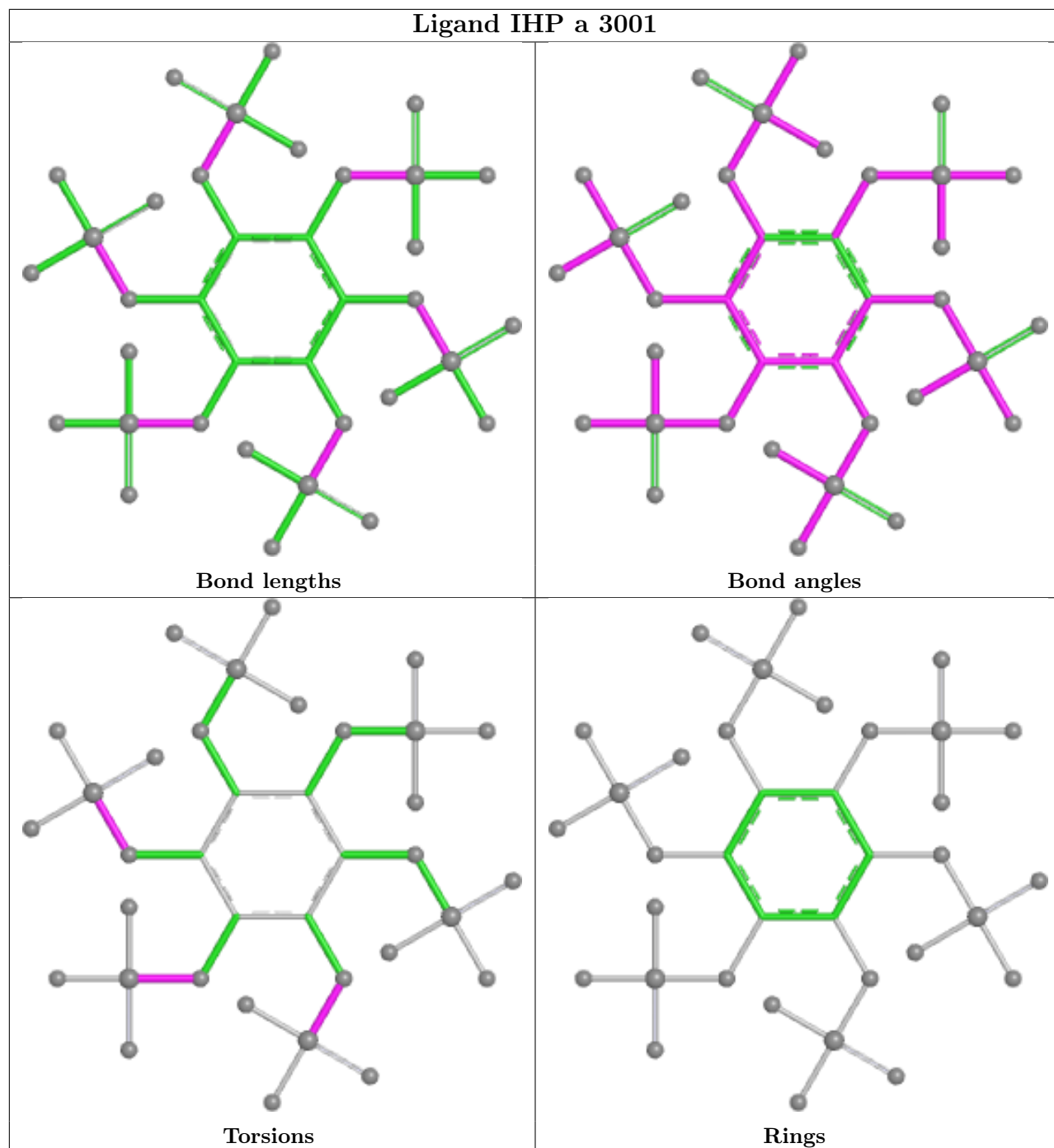
There are no ring outliers.

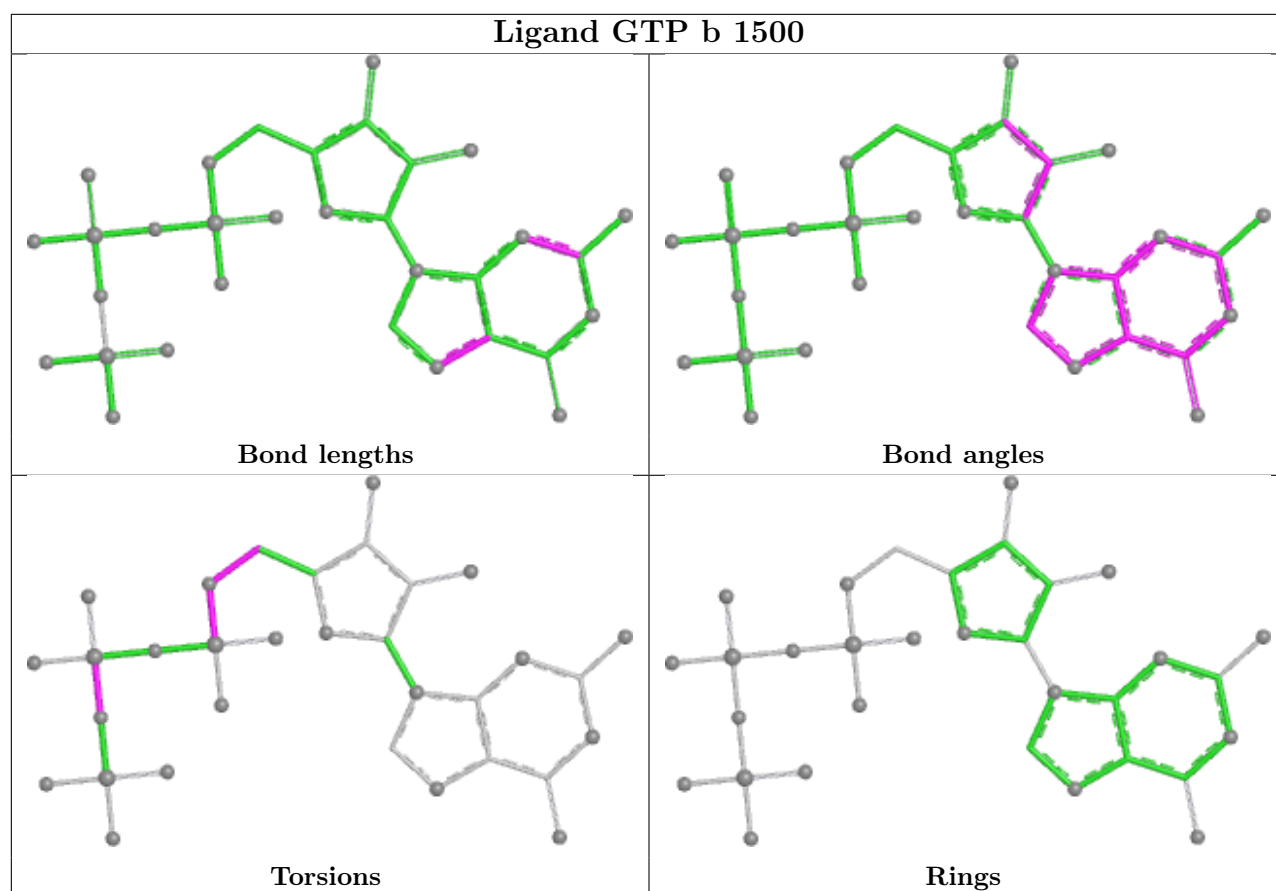
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	b	1500	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IHP a 3001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

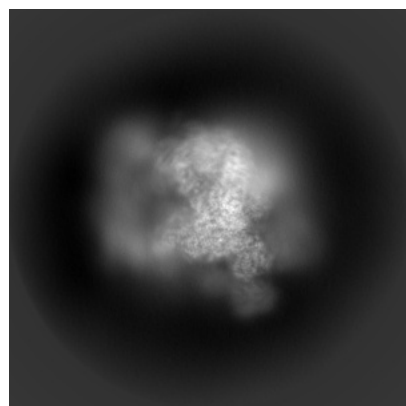
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14146. These allow visual inspection of the internal detail of the map and identification of artifacts.

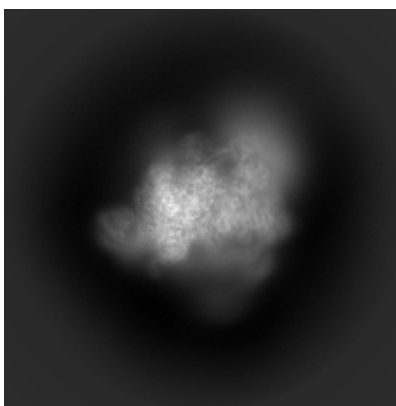
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

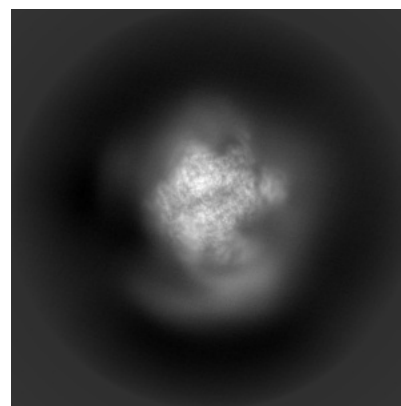
6.1.1 Primary map



X

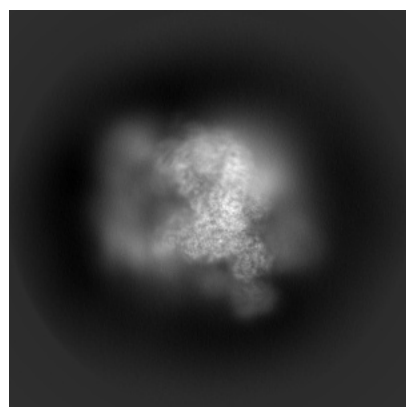


Y

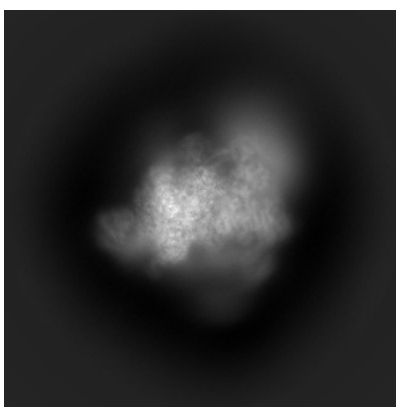


Z

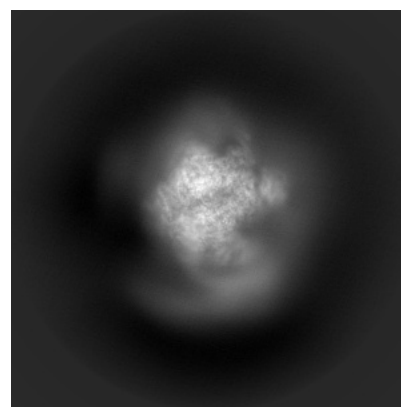
6.1.2 Raw map



X



Y

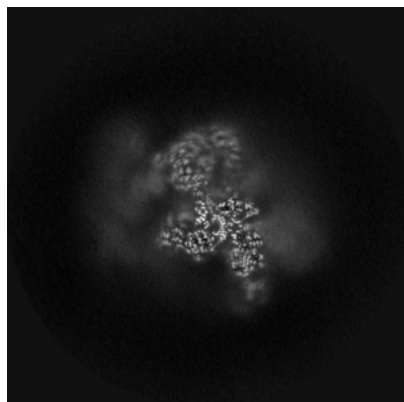


Z

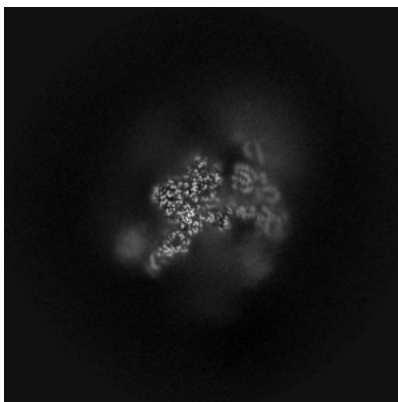
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

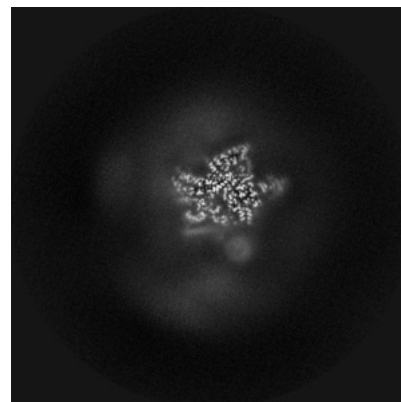
6.2.1 Primary map



X Index: 260

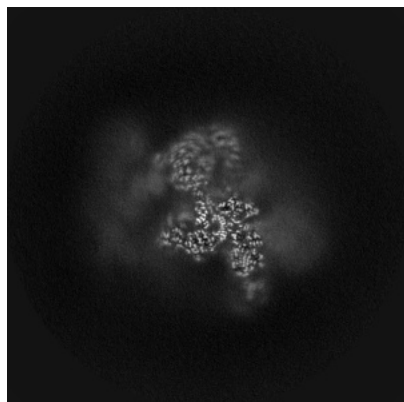


Y Index: 260

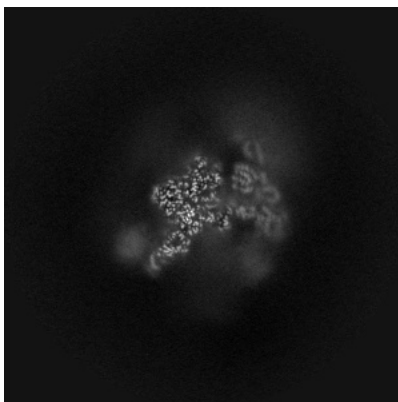


Z Index: 260

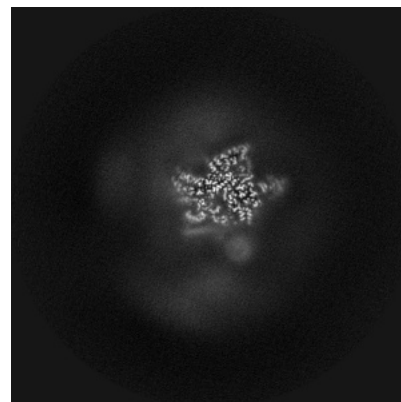
6.2.2 Raw map



X Index: 260



Y Index: 260

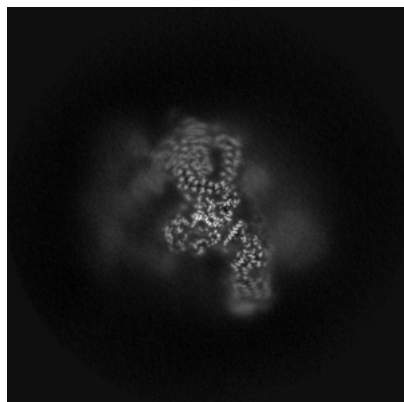


Z Index: 260

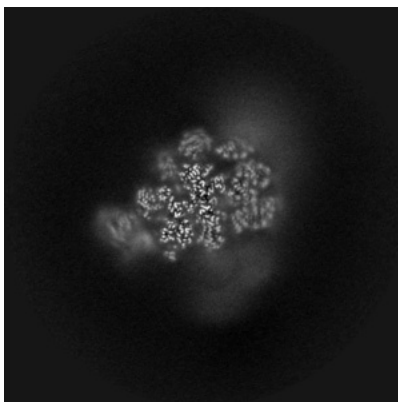
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

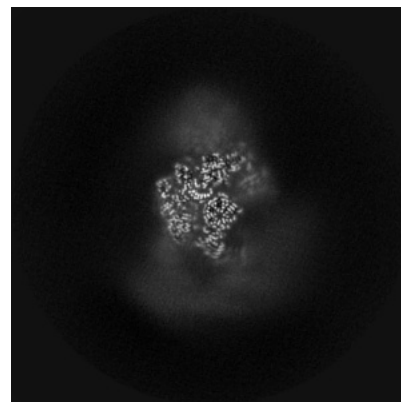
6.3.1 Primary map



X Index: 249

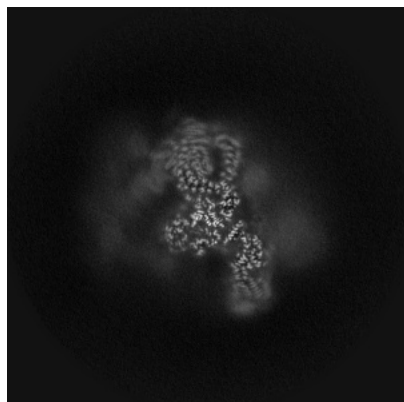


Y Index: 293

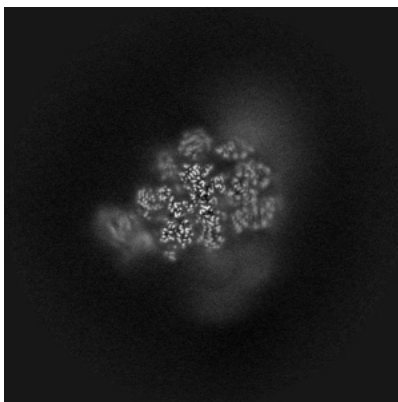


Z Index: 218

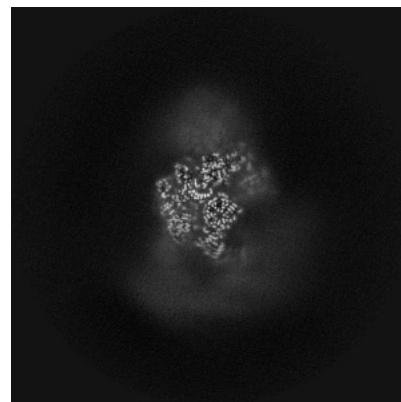
6.3.2 Raw map



X Index: 250



Y Index: 293

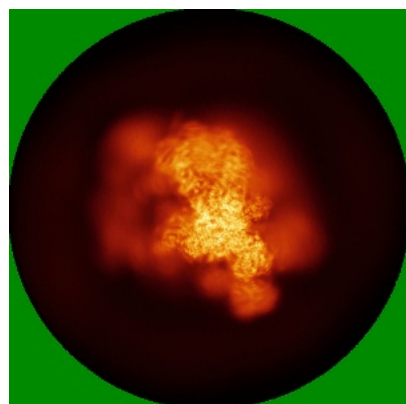


Z Index: 218

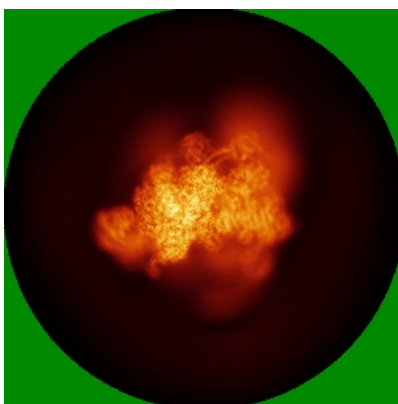
The images above show the largest variance slices of the map in three orthogonal directions.

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

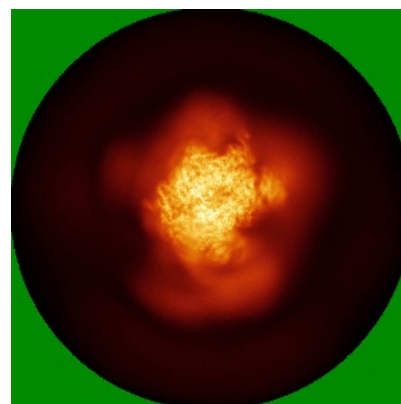
6.4.1 Primary map



X

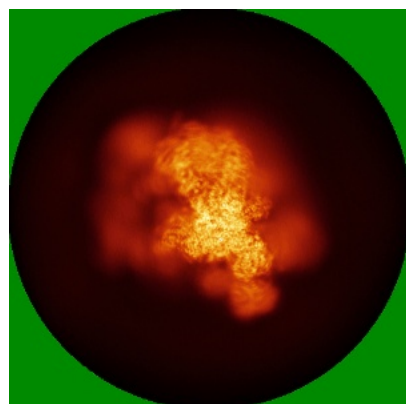


Y

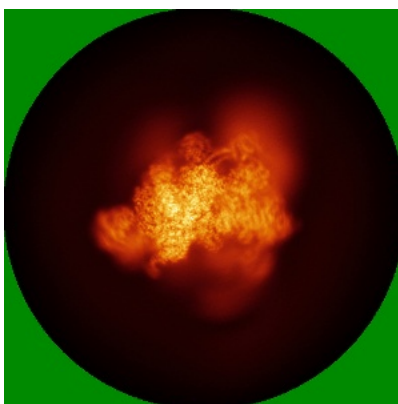


Z

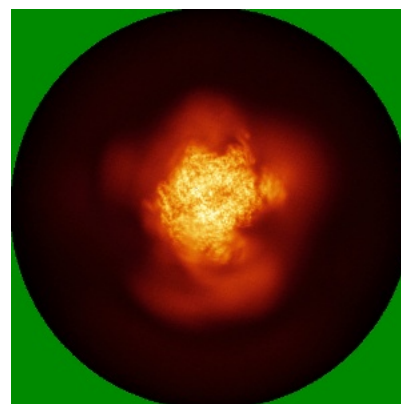
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

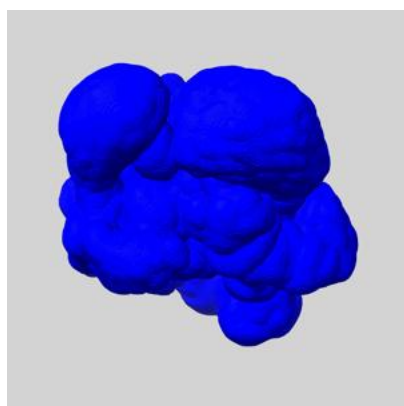
6.6 Mask visualisation [i](#)

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

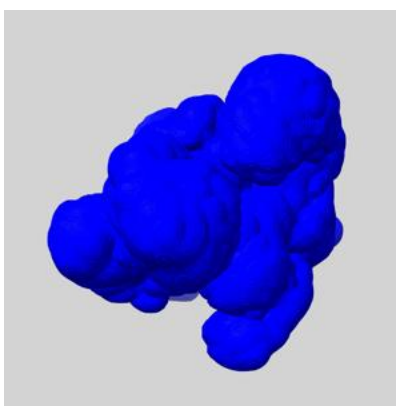
A mask typically either:

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

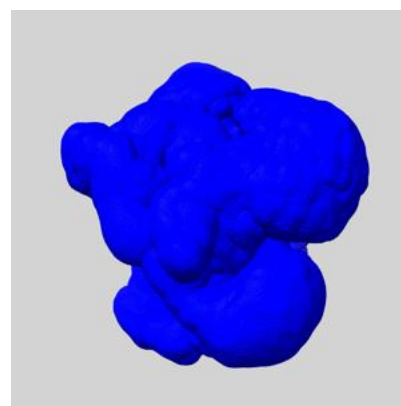
6.6.1 emd_14146_msk_1.map [i](#)



X



Y

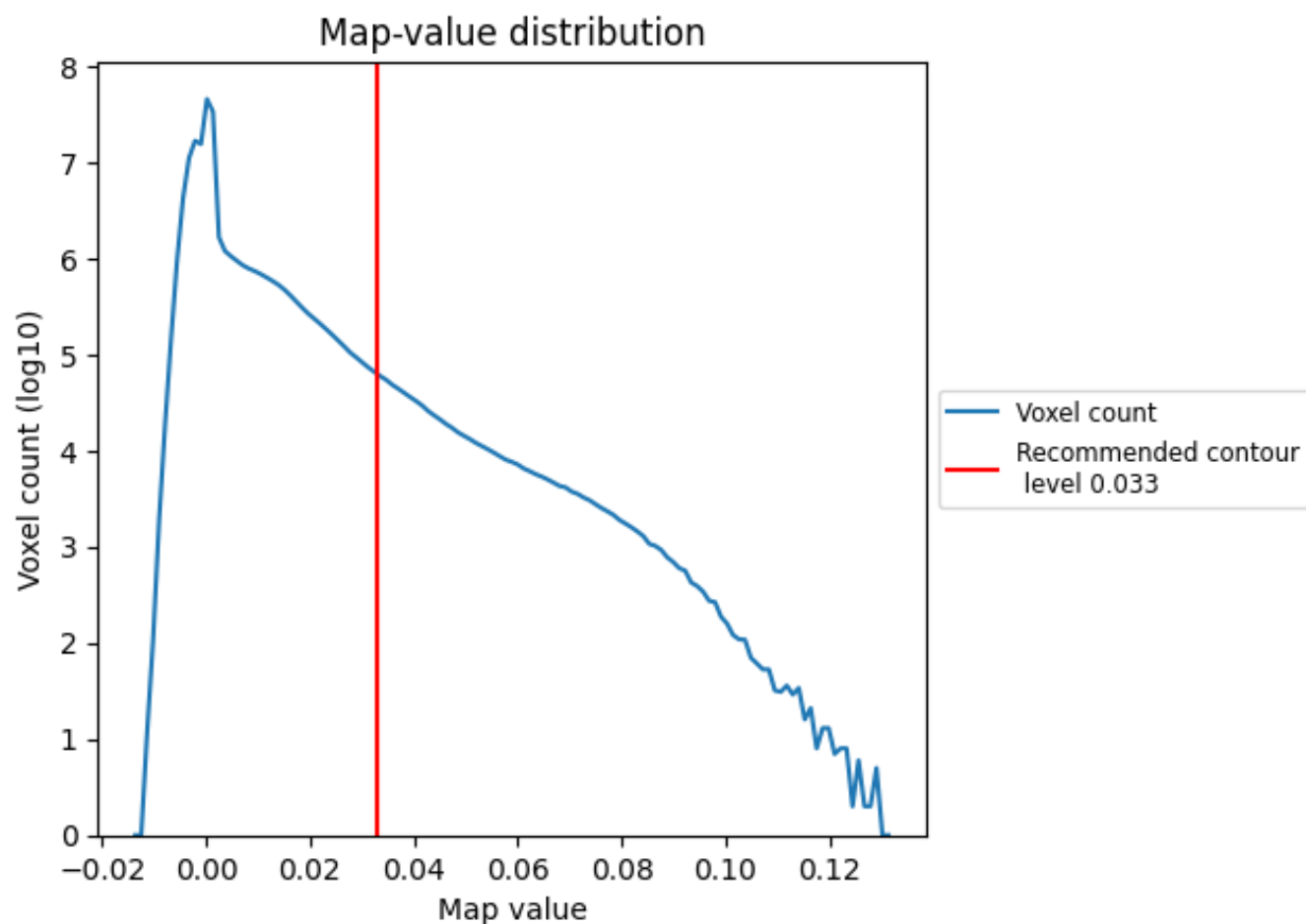


Z

7 Map analysis [i](#)

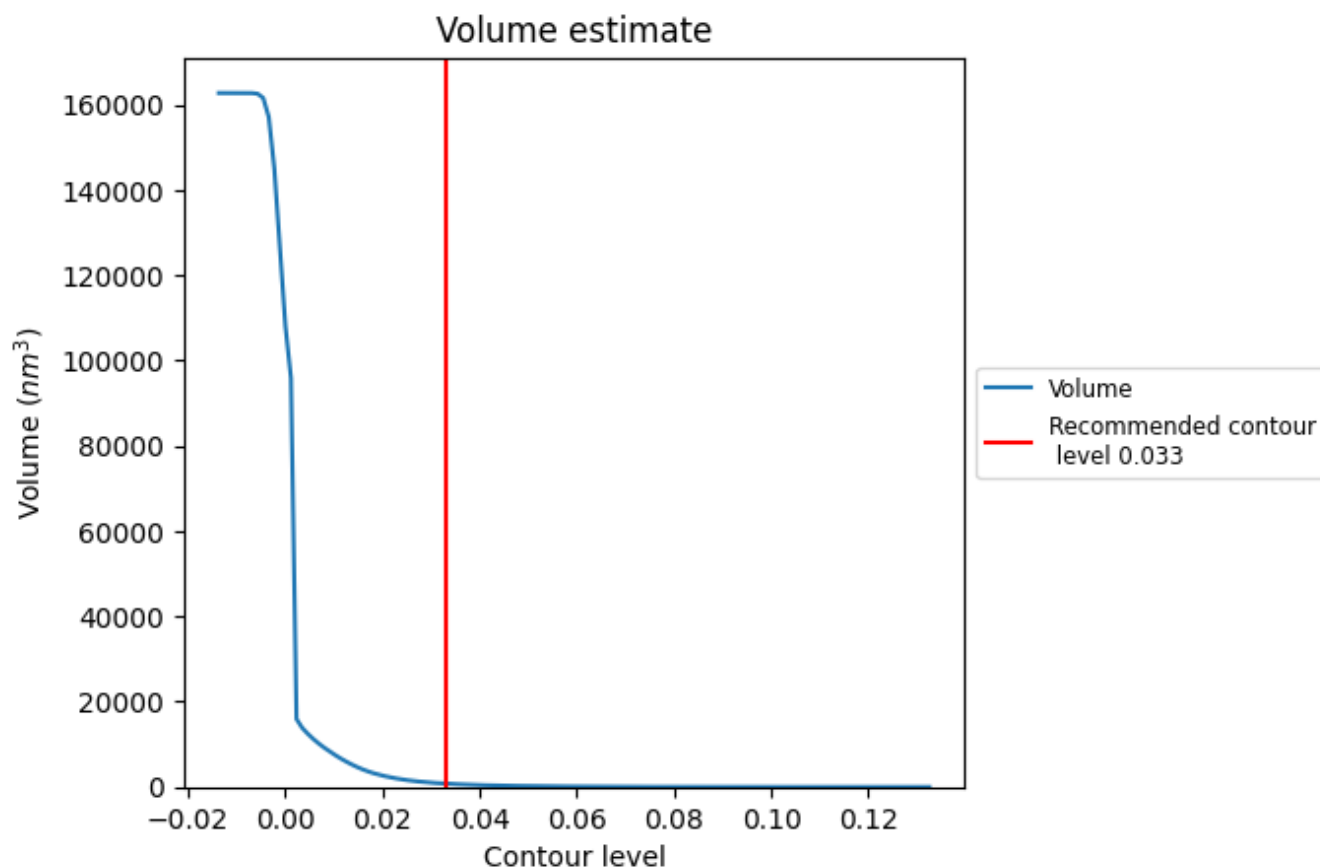
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

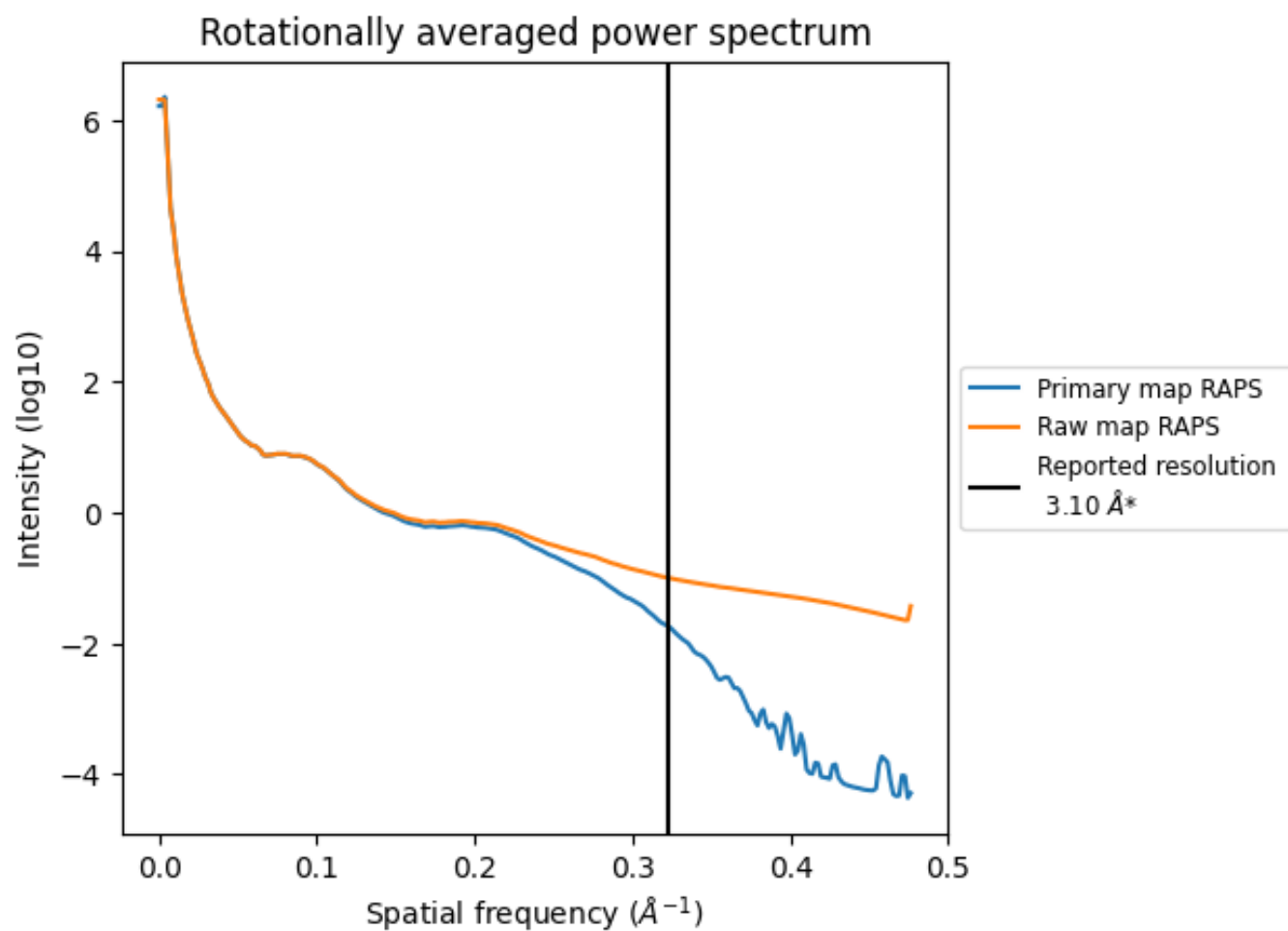
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786 nm^3 ; this corresponds to an approximate mass of 710 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 ⓘ

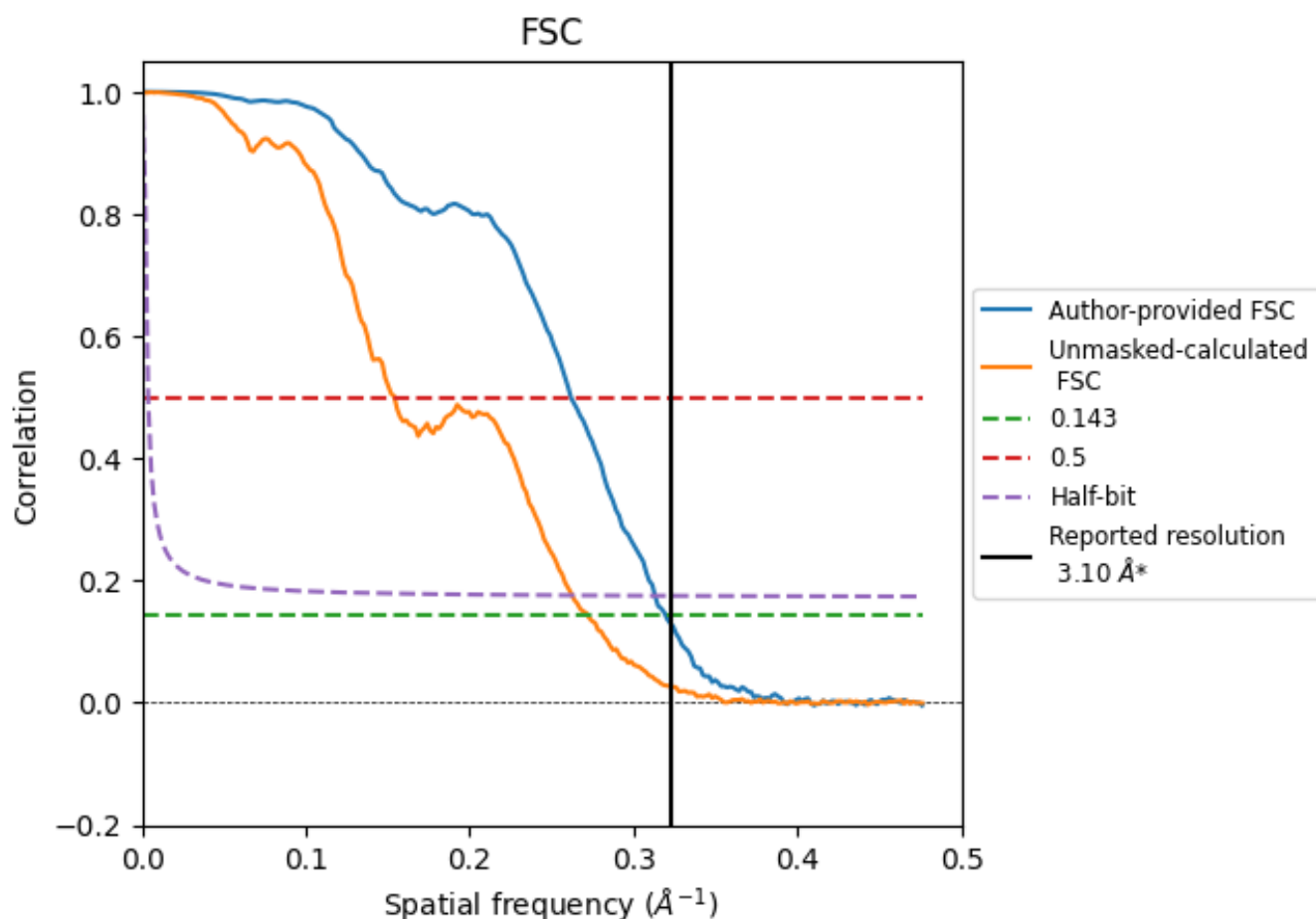


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

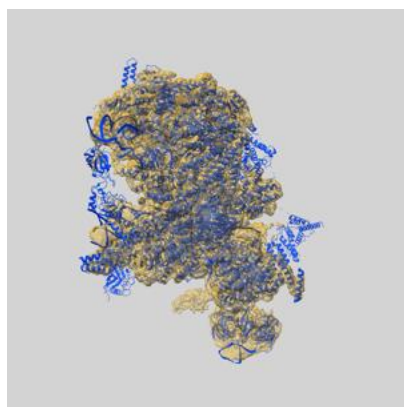
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.82	3.19
Unmasked-calculated*	3.68	6.49	3.81

*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 3.68 differs from the reported value 3.1 by more than 10 %

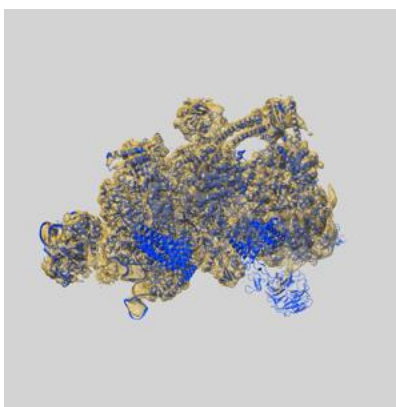
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14146 and PDB model 7QTT. Per-residue inclusion information can be found in section [3](#) on page [13](#).

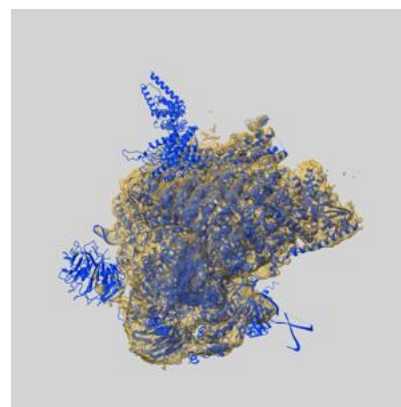
9.1 Map-model overlay [i](#)



X



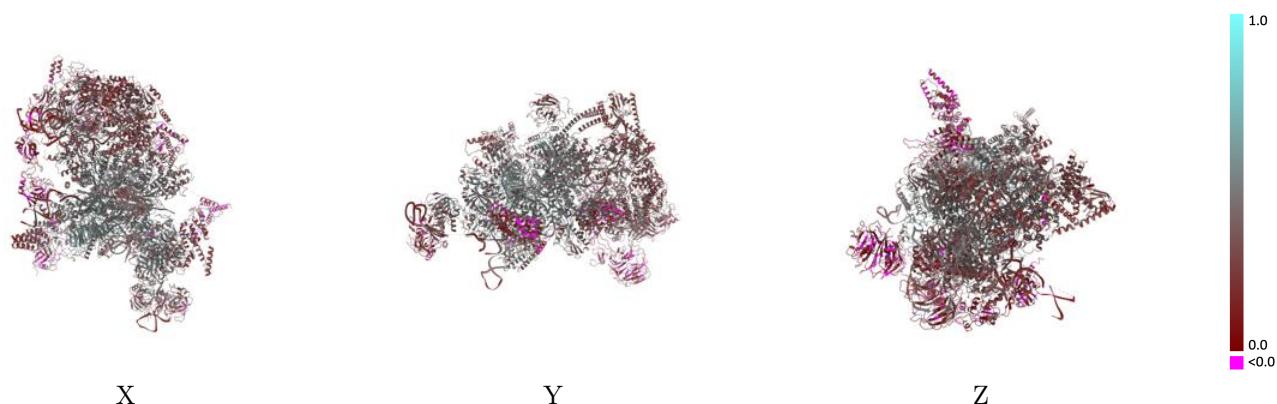
Y



Z

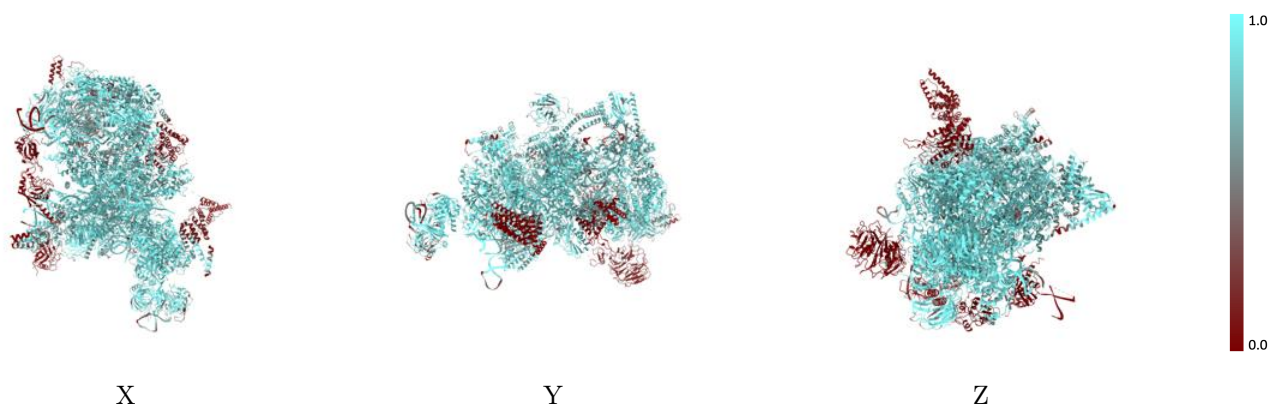
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



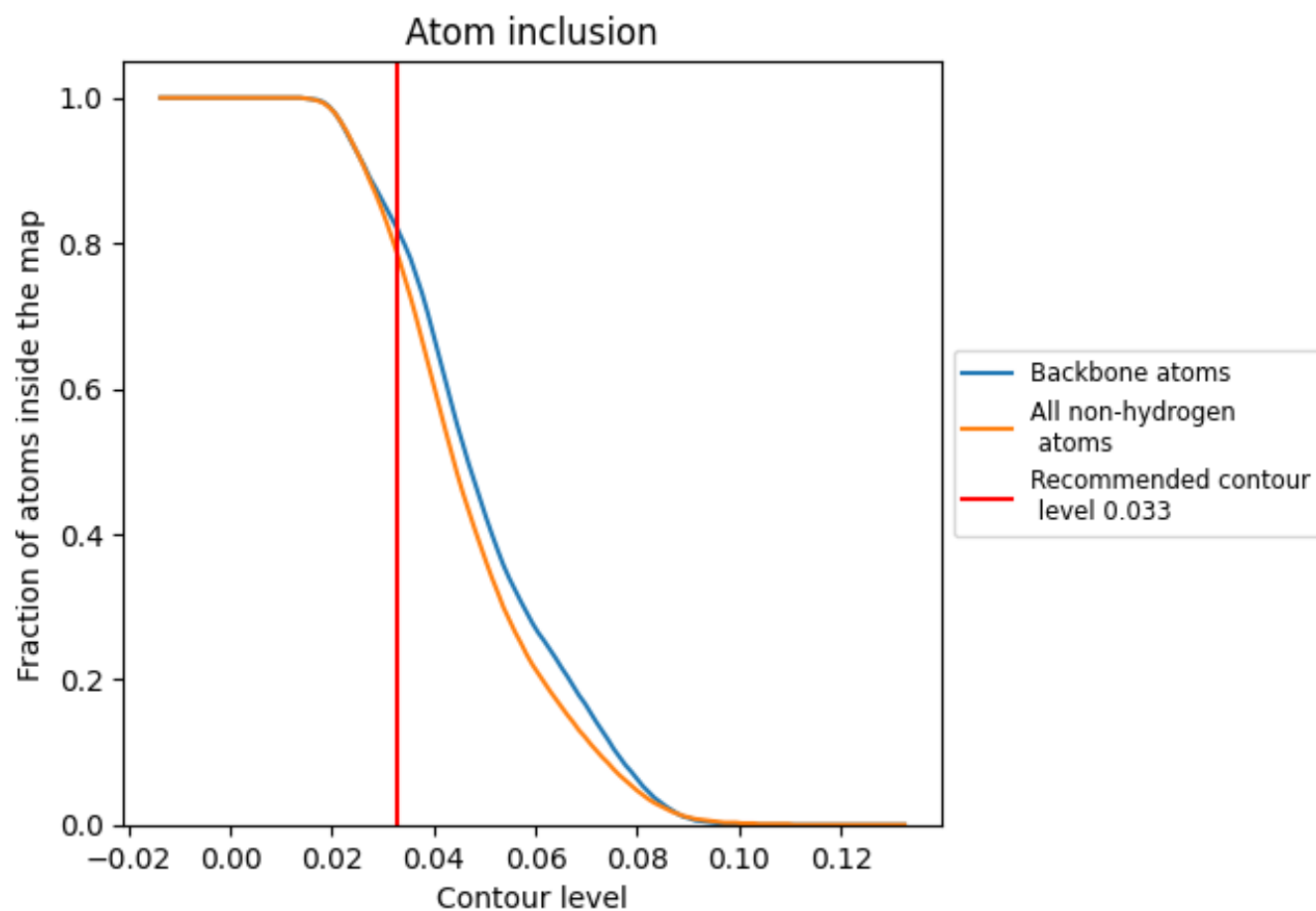
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.3840
A	 0.6410	 0.2660
B	 0.9770	 0.3070
C	 0.9050	 0.3520
D	 0.8210	 0.3490
E	 0.7010	 0.3060
F	 0.0500	 0.1530
G	 0.5660	 0.2900
I	 0.9560	 0.4400
J	 0.8020	 0.2030
L	 0.5250	 0.3130
N	 0.7800	 0.3420
O	 0.9470	 0.5230
P	 0.8580	 0.4280
Q	 0.8410	 0.4580
T	 0.9030	 0.4560
U	 0.6200	 0.3610
V	 0.7750	 0.3290
W	 0.4820	 0.3160
X	 0.8310	 0.3970
Y	 0.8010	 0.4170
Z	 0.5490	 0.3570
a	 0.8460	 0.4650
b	 0.8810	 0.4510
d	 0.9200	 0.4180
e	 0.9020	 0.3930
f	 0.7480	 0.2710
g	 0.8880	 0.3920
h	 0.9470	 0.3220
i	 0.7600	 0.2200
j	 0.7640	 0.2800
k	 0.9330	 0.4370
l	 0.9590	 0.3520
m	 0.6150	 0.2130
n	 0.8220	 0.3960



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Chain	Atom inclusion	Q-score
p	 0.0000	 0.2080
q	 0.7730	 0.3890
u	 0.4500	 0.2900