



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 04:45 PM EST

PDB ID : 6N7P
EMDB ID : EMD-0360
Title : S. cerevisiae spliceosomal E complex (UBC4)
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2018-11-27
Resolution : 3.60 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:

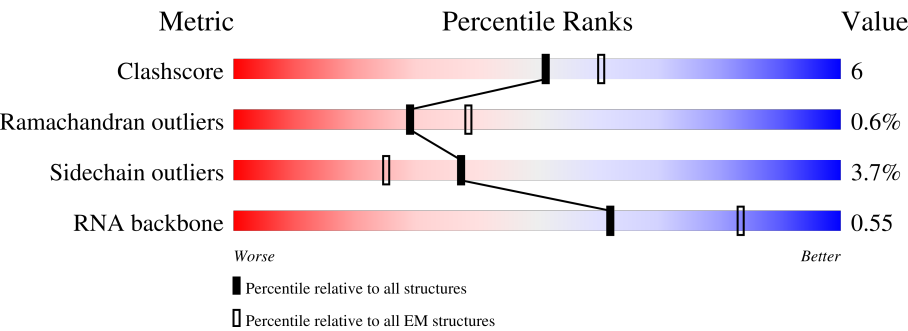
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	300	<div><div>33%</div><div>56%</div><div>38%</div></div>
2	B	231	<div><div>10%</div><div>68%</div><div>14%</div><div>16%</div></div>
3	C	350	<div><div>7%</div><div>29%</div><div>8%</div><div>62%</div></div>
4	D	544	<div><div>83%</div><div>16%</div></div>
5	E	629	<div><div>36%</div><div>84%</div><div>7%</div><div>8%</div></div>
6	F	523	<div><div>17%</div><div>43%</div><div>7%</div><div>49%</div></div>
7	G	492	<div><div>40%</div><div>7%</div><div>51%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	105	
9	I	261	
10	J	583	
11	K	196	
12	L	146	
13	M	110	
14	N	101	
15	O	94	
16	P	86	
17	Q	77	
18	R	568	
19	r	253	
20	X	861	
21	Y	208	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 41488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	186	Total	C	N	O	S	0	0
			1207	745	228	233	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total	C	N	O	S	0	0
			1570	976	301	288	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	132	Total	C	N	O	S	0	0
			1058	674	193	187	4		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLY	-	expression tag	UNP P32605
C	300	ARG	-	expression tag	UNP P32605
C	301	ARG	-	expression tag	UNP P32605
C	302	ILE	-	expression tag	UNP P32605
C	303	PRO	-	expression tag	UNP P32605
C	304	GLY	-	expression tag	UNP P32605
C	305	LEU	-	expression tag	UNP P32605
C	306	ILE	-	expression tag	UNP P32605
C	307	ASN	-	expression tag	UNP P32605
C	308	PRO	-	expression tag	UNP P32605
C	309	TRP	-	expression tag	UNP P32605
C	310	LYS	-	expression tag	UNP P32605
C	311	ARG	-	expression tag	UNP P32605
C	312	ARG	-	expression tag	UNP P32605
C	313	TRP	-	expression tag	UNP P32605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
C	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
C	320	VAL	-	expression tag	UNP P32605
C	321	SER	-	expression tag	UNP P32605
C	322	ALA	-	expression tag	UNP P32605
C	323	ALA	-	expression tag	UNP P32605
C	324	ASN	-	expression tag	UNP P32605
C	325	ARG	-	expression tag	UNP P32605
C	326	PHE	-	expression tag	UNP P32605
C	327	LYS	-	expression tag	UNP P32605
C	328	LYS	-	expression tag	UNP P32605
C	329	ILE	-	expression tag	UNP P32605
C	330	SER	-	expression tag	UNP P32605
C	331	SER	-	expression tag	UNP P32605
C	332	SER	-	expression tag	UNP P32605
C	333	GLY	-	expression tag	UNP P32605
C	334	ALA	-	expression tag	UNP P32605
C	335	LEU	-	expression tag	UNP P32605
C	336	ASP	-	expression tag	UNP P32605
C	337	TYR	-	expression tag	UNP P32605
C	338	ASP	-	expression tag	UNP P32605
C	339	ILE	-	expression tag	UNP P32605
C	340	PRO	-	expression tag	UNP P32605
C	341	THR	-	expression tag	UNP P32605
C	342	THR	-	expression tag	UNP P32605
C	343	ALA	-	expression tag	UNP P32605
C	344	SER	-	expression tag	UNP P32605
C	345	GLU	-	expression tag	UNP P32605
C	346	ASN	-	expression tag	UNP P32605
C	347	LEU	-	expression tag	UNP P32605
C	348	TYR	-	expression tag	UNP P32605
C	349	PHE	-	expression tag	UNP P32605
C	350	GLN	-	expression tag	UNP P32605

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	544	Total	C	N	O	S	0	0
			4561	2990	723	828	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	576	Total	C	N	O	S	0	0
			3981	2527	693	752	9		

- Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	267	Total	C	N	O	S	0	0
			1818	1128	326	353	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1954	1267	321	354	12		

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	105	Total	C	N	O	S	0	0
			685	425	127	132	1		

- Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1409	878	262	258	11		

- Molecule 10 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	198	Total	C	N	O	S	0	0
			984	588	198	198			

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	123	Total	C	N	O	S	0	0
			1008	636	191	178	3		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	107	Total	C	N	O	S	0	0
			858	545	159	150	4		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	93	Total	C	N	O	S	0	0
			710	450	122	134	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	74	Total	C	N	O	S	0	0
			563	375	90	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	74	Total	C	N	O	S	0	0
			584	377	103	103	1		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	71	Total	C	N	O	S	0	0
			543	344	95	103	1		

- Molecule 18 is a RNA chain called U1 snRNA.

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

- Molecule 19 is a RNA chain called UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	22	Total	C	N	O	P	0	0
			471	211	85	153	22		

- Molecule 20 is a protein called Nuclear cap-binding protein complex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	826	Total	C	N	O	0	0
			4101	2449	826	826		

- Molecule 21 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	138	Total	C	N	O	0	0
			677	401	138	138		

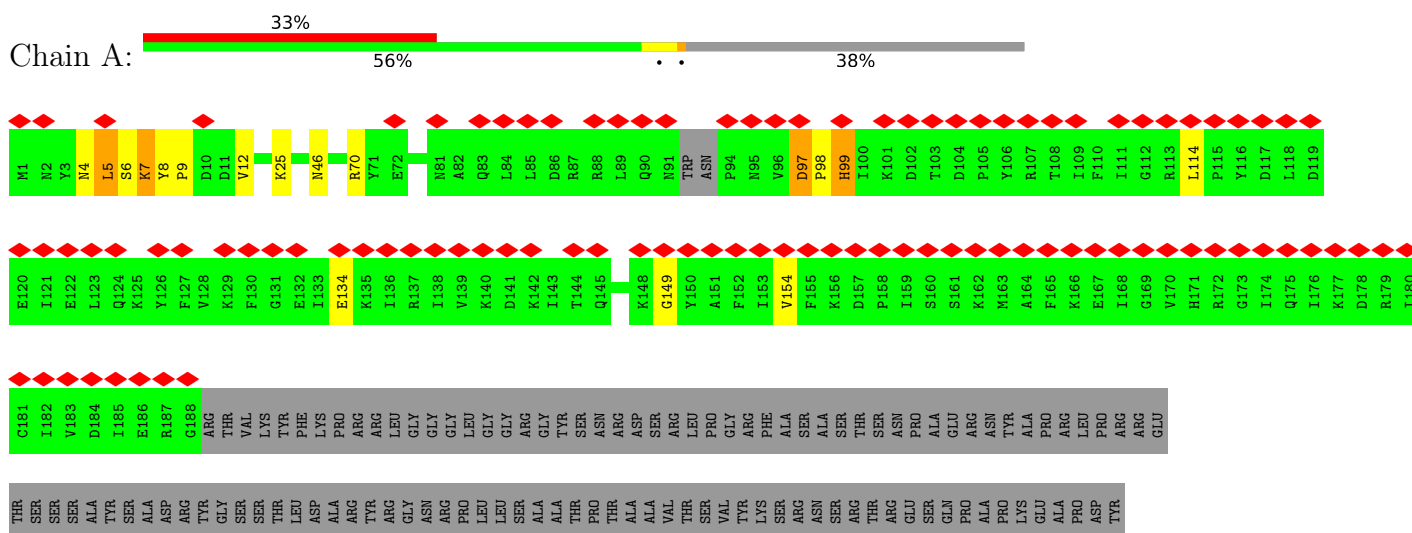
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	

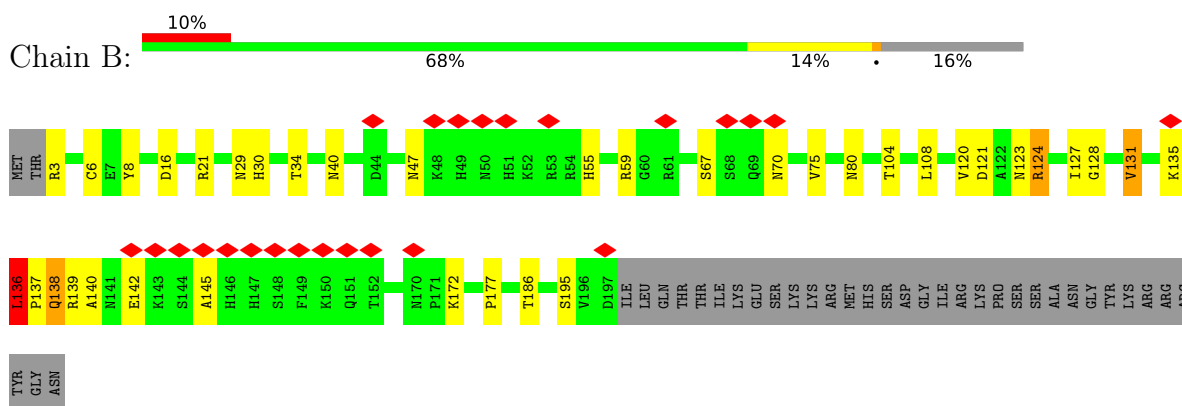
3 Residue-property plots

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.

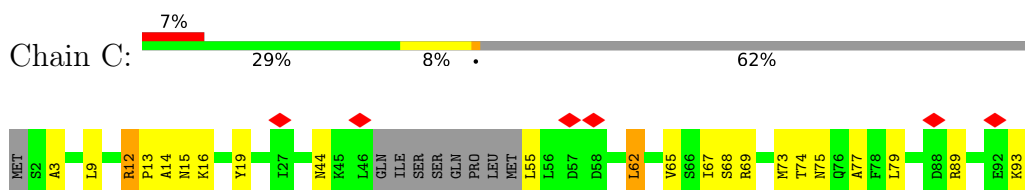
- Molecule 1: U1 small nuclear ribonucleoprotein 70 kDa homolog

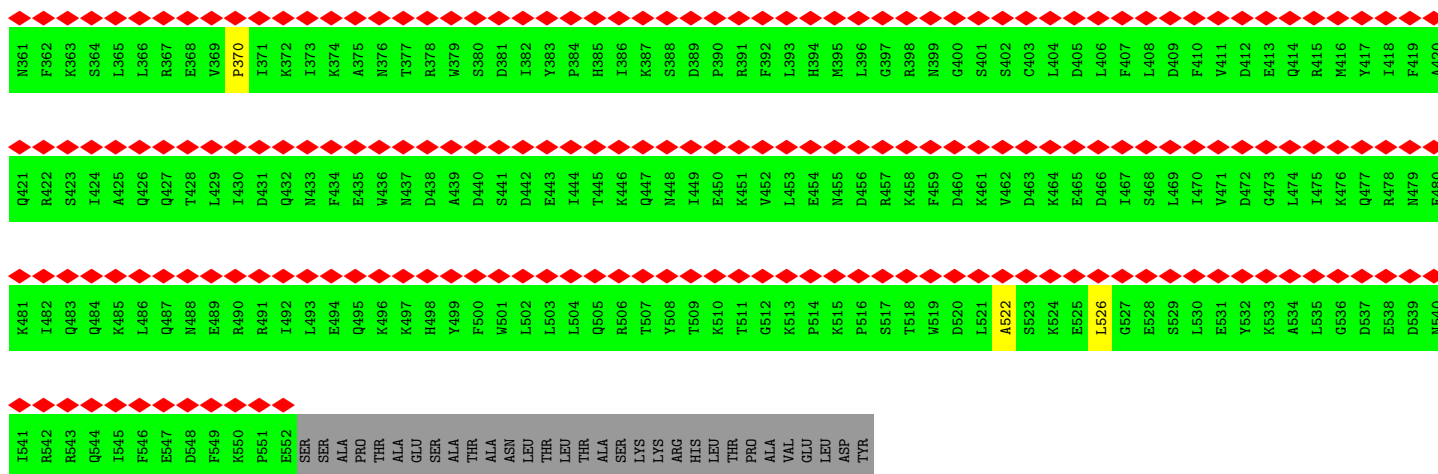


- Molecule 2: U1 small nuclear ribonucleoprotein C

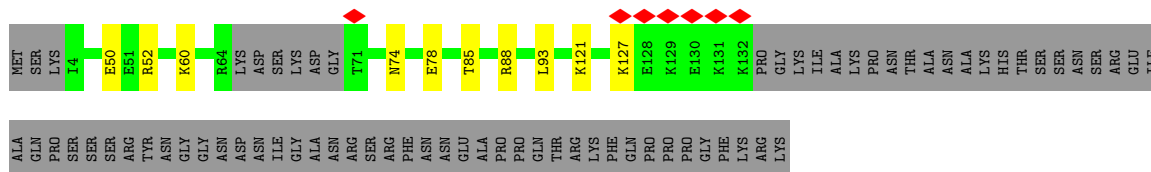


- Molecule 3: U1 small nuclear ribonucleoprotein A

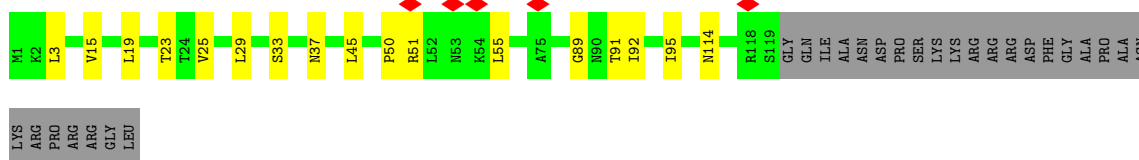




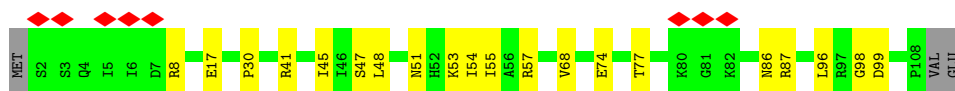
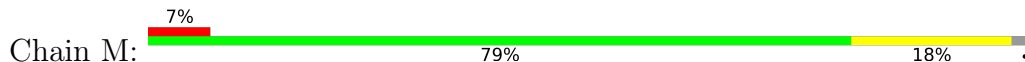
- Molecule 11: Small nuclear ribonucleoprotein-associated protein B



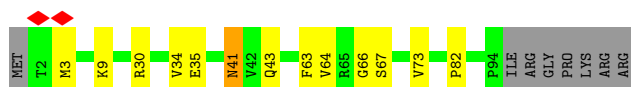
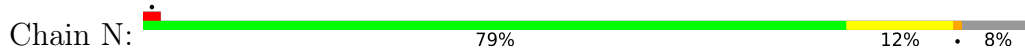
- Molecule 12: Small nuclear ribonucleoprotein Sm D1



- Molecule 13: Small nuclear ribonucleoprotein Sm D2

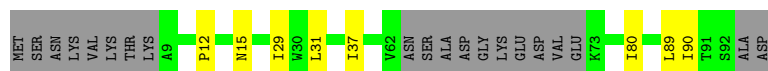


- Molecule 14: Small nuclear ribonucleoprotein Sm D3



- Molecule 15: Small nuclear ribonucleoprotein E

Chain O:  70% 9% 21%




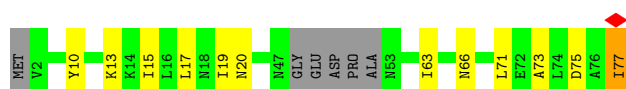
• Molecule 16: Small nuclear ribonucleoprotein F

Chain P:  67% 16% 14%



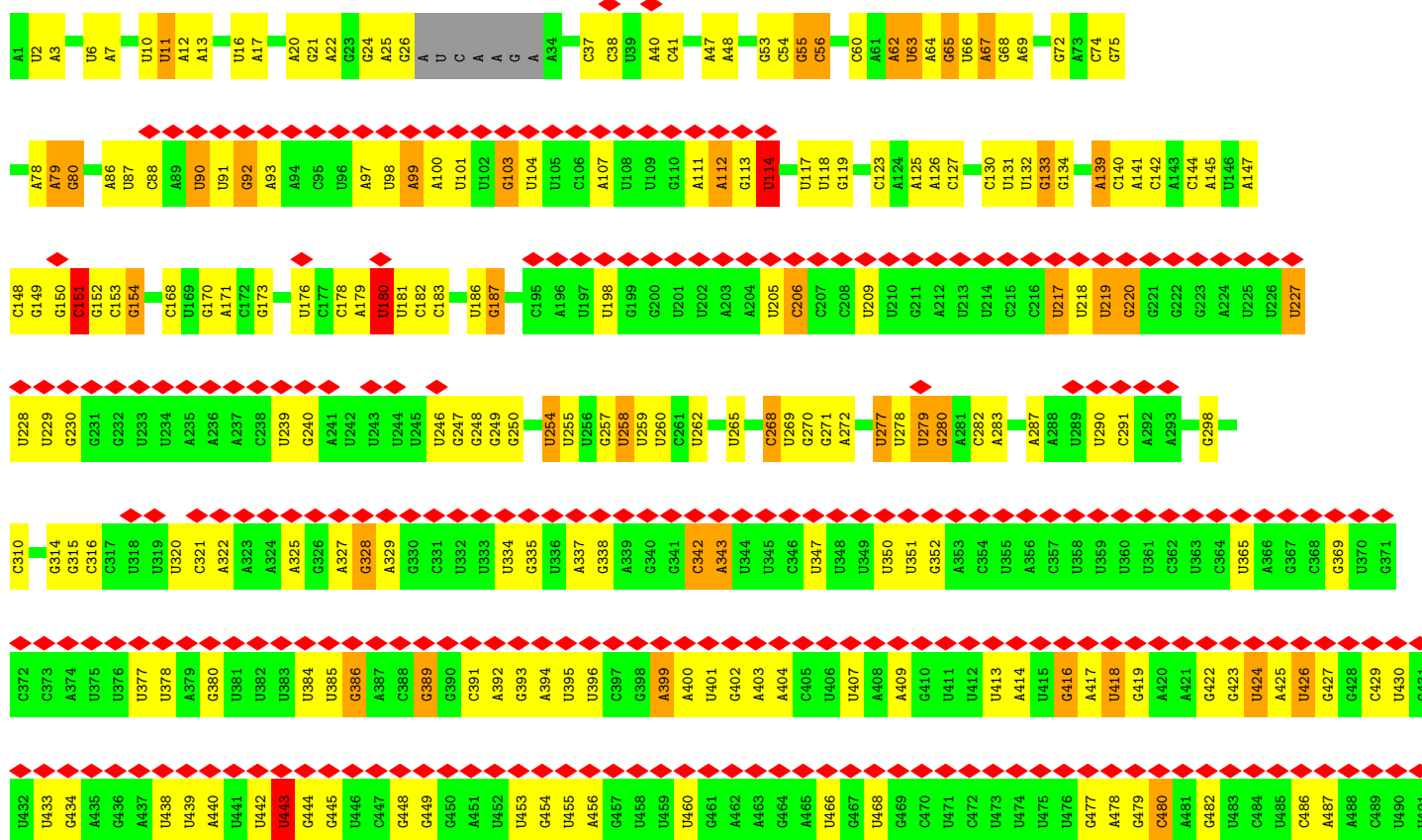
• Molecule 17: Small nuclear ribonucleoprotein G

Chain Q:  77% 14% 8%



• Molecule 18: U1 snRNA

Chain R:  51% 52% 38% 8%



T421	L481	P541	T601	L661	F721	D781	A841
I422	D482	Q542	H602	K662	N722	E782	I842
L423	W483	E543	K603	E663	E723	D783	P843
G424	F484	F544	A604	D664	T724	I784	H844
L425	S485	T545	N605	L665	G725	E785	E845
L426	I486	K546	N606	K666	L726	I786	S846
F427	Q487	Y547	S607	T667	K727	F787	T847
K428	M488	L548	R608	I668	N728	K788	R848
L429	S489	D549	E609	F669	M729	V789	R849
P430	N490	T550	V610	A670	G730	N790	T850
S431	F491	S551	T611	K671	L731	G791	I851
V432	N492	Y552	E612	I672	I732	E792	S852
S433	F493	L553	L613	E673	E733	N793	L853
Q434	S494	P554	E614	L674	A734	D794	V854
P435	W495	R555	S615	D675	T735	I795	I855
F436	K496	D556	I616	I676	A736	D796	Q856
A437	W497	Q557	L617	E677	I737	I797	E857
Y438	N498	L558	G618	T678	E738	I798	T858
F439	E499	I559	E619	K679	A739	E799	K859
Y440	W500	N560	L620	E680	V740	D800	E860
T441	E501	Y561	K621	Y681	F741	D801	V861
L442	D502	L562	N622	I682	R742	K802	L803
L443	D503	Q563	E623	I683	N743	L804	D804
V444	S504	S564	Y624	I684	L744	L805	L806
D445	I505	L565	G625	E685	S745	K806	R807
I446	K506	F566	S626	A686	Q746	W807	K808
C447	F507	T567	I627	V687	Q747	L809	Y809
Q448	G508	G568	I628	L688	I748	Y809	F810
N449	K509	Y569	S629	T689	S749	T811	T612
S450	Y510	T570	D630	F690	E750	V612	I613
P451	F511	V571	F631	W691	E751	I614	G614
K452	Y512	E572	N632	A692	N752	F615	R616
A453	E573	D574	R633	A693	E753	S617	S618
I454	P514	E575	F634	N694	S754	I619	L620
A455	K515	S575	V635	P695	G755	R621	R622
P456	V516	V576	I636	Q696	N756	Y623	S624
V457	N517	R577	I637	T697	N757	H625	E626
F458	F518	K578	L638	G698	F758	Y627	R628
G459	A519	N579	L639	F699	E759	E629	L630
R460	K520	D580	V640	L700	F760	A631	D632
A461	N521	L581	Q641	V701	V761	K633	F634
F462	L522	Y582	A642	A702	F762	I635	A636
R463	I523	F583	V643	D703	E763	N637	I638
F464	Q524	R584	T644	A704	R764	D639	N640
F465	K525	Q585	D645	F705	L765		
F466	K526	E586	S646	K706	G766		
S467	L527	G587	G647	Y707	T767		
H468	R528	V588	S648	A708	I768		
L469	L529	P589	R649	G709	N769		
D470	T530	M590	S650	L710	A770		
S471	S531	E591	L651	L711	S771		
L472	N532	N592	S652	T712	T772		
D473	F533	T593	H653	S713	I773		
F474	S534	Y594	A654	R714	D774		
E475	E535	R595	M655	T715	L775		
L476	V536	K596	K656	I716	L776		
K477	E537	I597	Y657	F717	D777		
L478	D538	L598	T599	T718	V778		
R479	S539	D599	M659	F719	N779		
Y480	L540	Y600	D660	I720	A780		

• Molecule 21: Nuclear cap-binding protein subunit 2



MET	D19	Q61	L121	ASN
SER	T20	I62	D122	TYR
GLU	P21	V63	P123	ILE
GLU	R22	E64	G124	PRO
PHE	S23	L65	F125	PRO
ASP	Y24	F66	E126	ASP
GLU	L25	S67	D127	ALA
VAL	T26	K68	L128	MET
LYS	R27	C69	G129	GLY
ASP	K28	H70	A130	PHE
HIS	A29	G71	Q131	ARG
SER	R30	T72	F132	PRO
THR	N31	I73	G133	GLY
LYS	D32	K74	R134	ASP
ARG	E33	R75	G135	GLU
LEU	L34	I76	K136	GLU
D19	T35	M77	S137	ARG
T20	R36	E78	G138	ASP
P21	K37	G79	A139	ASN
R22	Y38	L79	V140	VAL
S23	L39	D80	S141	PRO
Y24	R40	R81	D142	GLN
L25	C41	F82	E143	
T26	E42	K83	L144	
R27	M43	H84	A145	
K28	K44	T85	F146	
A29	S45	P86	D147	
R30	A46	C87	F148	
N31	L47	G88	D149	
P32	I48	F89	A150	
P33	V49	C90	S151	
N34	T50	F91	R152	
G35	E51	I92	G153	
C36	S42	N93	Y154	
L36	M43	Y94	F155	
Q37	K44	S95	A156	
E38	S45	C96	TLE	
L39	S46	P97	PRO	
R40	A47	D98	PHE	
R41	A48	E99	ALA	
E41	A49	A100	GLU	
E42	A50	L101	ARG	
M43	A51	M102	VAL	
K44	A52	A103	GLY	
S45	A53	V104	VAL	
T47	A54	K105	PRO	
I48	A55	S106	HIS	
Y49	A56	Y107	SER	
V50	A57	L108	ARG	
G51	A58	S109	THR	
S52	A59	D110	ASN	
L53	A60	T111	SER	
S54	A61	K112	GLN	
F55	A62	L113	SER	
Y56	A63	E114	THR	
G57	A64	K115	ASN	
S58	A65	T116		
E59	A66	I117		
E60	A67	T118		
	A68	I119		
	A69	D120		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124825	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.206	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	522.24, 522.24, 522.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/1224	0.59	0/1675
2	B	0.54	0/1601	0.65	0/2154
3	C	0.44	0/1072	0.68	0/1437
4	D	0.76	0/4676	0.72	0/6320
5	E	0.55	0/4046	0.60	0/5539
6	F	0.60	0/1844	0.68	0/2511
7	G	0.61	0/1996	0.68	0/2682
8	H	0.49	0/428	0.55	0/575
9	I	0.38	0/1428	0.60	0/1924
10	J	0.37	0/983	0.49	0/1371
11	K	0.66	0/1014	0.73	0/1350
12	L	0.57	0/930	0.73	0/1261
13	M	0.53	0/872	0.63	0/1174
14	N	0.71	0/722	0.72	0/979
15	O	0.55	0/573	0.68	0/778
16	P	0.65	0/597	0.74	0/809
17	Q	0.64	0/546	0.69	0/735
18	R	0.66	0/13201	1.19	79/20553 (0.4%)
19	r	0.52	0/527	1.05	0/819
20	X	0.26	0/4100	0.59	4/5721 (0.1%)
21	Y	0.26	0/676	0.55	0/937
All	All	0.59	0/43056	0.87	83/61304 (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
3	C	0	2
20	X	0	24

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	26

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	227	U	N1-C2-O2	12.02	131.22	122.80
18	R	227	U	C2-N1-C1'	11.79	131.85	117.70
18	R	227	U	N3-C2-O2	-11.14	114.40	122.20
18	R	442	U	OP2-P-O3'	-10.46	82.18	105.20
18	R	442	U	OP1-P-O3'	-10.46	82.20	105.20
18	R	557	U	N3-C2-O2	-9.34	115.66	122.20
18	R	557	U	N1-C2-O2	9.16	129.21	122.80
18	R	130	C	C6-N1-C2	-8.40	116.94	120.30
18	R	130	C	C2-N1-C1'	8.35	127.99	118.80
18	R	11	U	C2-N1-C1'	8.26	127.62	117.70
18	R	227	U	C6-N1-C1'	-8.21	109.71	121.20
18	R	557	U	C2-N1-C1'	7.94	127.23	117.70
18	R	254	U	N3-C2-O2	-7.45	116.99	122.20
18	R	103	G	C4-N9-C1'	7.40	136.12	126.50
18	R	11	U	N1-C2-O2	7.32	127.92	122.80
18	R	291	C	N1-C2-O2	7.15	123.19	118.90
18	R	11	U	N3-C2-O2	-7.15	117.19	122.20
18	R	80	G	C4-N9-C1'	7.15	135.80	126.50
18	R	443	U	OP1-P-OP2	7.11	130.27	119.60
18	R	139	A	O4'-C1'-N9	6.86	113.69	108.20
18	R	148	C	C2-N1-C1'	6.80	126.28	118.80
18	R	130	C	C5-C6-N1	6.76	124.38	121.00
18	R	103	G	C8-N9-C1'	-6.74	118.24	127.00
18	R	277	U	P-O3'-C3'	6.63	127.66	119.70
18	R	498	U	N3-C2-O2	-6.58	117.59	122.20
20	X	673	GLU	C-N-CA	6.53	138.02	121.70
18	R	291	C	C6-N1-C2	-6.45	117.72	120.30
18	R	144	C	C2-N1-C1'	6.41	125.84	118.80
18	R	258	U	P-O3'-C3'	6.38	127.35	119.70
18	R	63	U	P-O3'-C3'	6.32	127.29	119.70
18	R	180	U	C2-N1-C1'	6.22	125.16	117.70
18	R	500	C	C6-N1-C2	-6.18	117.83	120.30
18	R	265	U	N3-C2-O2	-6.13	117.91	122.20
18	R	80	G	N3-C4-C5	-6.12	125.54	128.60
18	R	63	U	C5-C6-N1	6.11	125.75	122.70
20	X	283	HIS	C-N-CA	6.06	136.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	180	U	N1-C2-O2	6.04	127.03	122.80
18	R	148	C	N1-C2-O2	6.03	122.52	118.90
18	R	80	G	C8-N9-C1'	-6.00	119.20	127.00
18	R	112	A	P-O3'-C3'	5.96	126.85	119.70
18	R	151	C	P-O3'-C3'	5.90	126.78	119.70
18	R	144	C	N1-C2-O2	5.88	122.43	118.90
18	R	148	C	N3-C2-O2	-5.88	117.78	121.90
18	R	80	G	N3-C4-N9	5.81	129.49	126.00
18	R	291	C	N3-C2-O2	-5.80	117.84	121.90
18	R	268	C	P-O3'-C3'	5.70	126.54	119.70
18	R	310	C	C5-C6-N1	5.66	123.83	121.00
18	R	279	U	P-O3'-C3'	5.66	126.49	119.70
18	R	399	A	P-O3'-C3'	5.64	126.47	119.70
18	R	123	C	C6-N1-C2	-5.63	118.05	120.30
20	X	403	TYR	C-N-CA	5.63	135.77	121.70
20	X	391	GLU	C-N-CA	5.62	145.63	122.00
18	R	254	U	N1-C2-N3	5.62	118.27	114.90
18	R	103	G	N3-C4-N9	5.62	129.37	126.00
18	R	127	C	C6-N1-C2	-5.59	118.06	120.30
18	R	99	A	C4-N9-C1'	5.56	136.31	126.30
18	R	342	C	C6-N1-C2	-5.54	118.08	120.30
18	R	206	C	N1-C2-O2	5.50	122.20	118.90
18	R	291	C	C5-C6-N1	5.45	123.72	121.00
18	R	180	U	N3-C2-O2	-5.34	118.46	122.20
18	R	63	U	C2-N1-C1'	5.31	124.07	117.70
18	R	140	C	N1-C2-O2	5.28	122.07	118.90
18	R	154	G	C4-N9-C1'	5.28	133.36	126.50
18	R	11	U	C6-N1-C1'	-5.28	113.81	121.20
18	R	480	C	C6-N1-C2	-5.24	118.20	120.30
18	R	144	C	N3-C2-O2	-5.23	118.24	121.90
18	R	347	U	N3-C2-O2	-5.22	118.55	122.20
18	R	342	C	C5-C6-N1	5.22	123.61	121.00
18	R	310	C	C6-N1-C2	-5.20	118.22	120.30
18	R	557	U	C6-N1-C1'	-5.20	113.92	121.20
18	R	342	C	C2-N1-C1'	5.15	124.46	118.80
18	R	56	C	C6-N1-C2	-5.13	118.25	120.30
18	R	496	C	C6-N1-C2	-5.13	118.25	120.30
18	R	151	C	N1-C2-O2	5.13	121.97	118.90
18	R	118	U	N3-C2-O2	-5.12	118.62	122.20
18	R	11	U	C5-C6-N1	5.12	125.26	122.70
18	R	516	U	C5-C6-N1	5.10	125.25	122.70
18	R	187	G	O5'-P-OP2	5.10	116.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	114	U	O5'-P-OP2	-5.08	101.12	105.70
18	R	277	U	C2'-C3'-O3'	5.06	121.79	113.70
18	R	316	C	C6-N1-C2	-5.05	118.28	120.30
18	R	501	C	C5-C6-N1	5.05	123.53	121.00
18	R	90	U	C5-C6-N1	5.03	125.22	122.70

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	12	ARG	Peptide,Sidechain
20	X	281	TRP	Peptide
20	X	284	LEU	Peptide
20	X	342	GLU	Peptide
20	X	379	THR	Peptide
20	X	380	LEU	Peptide
20	X	381	ASP	Peptide
20	X	383	PHE	Peptide
20	X	388	ILE	Peptide
20	X	389	PHE	Peptide
20	X	405	GLU	Peptide
20	X	408	LEU	Peptide
20	X	410	PRO	Peptide
20	X	550	THR	Peptide
20	X	570	THR	Peptide
20	X	669	PHE	Peptide
20	X	671	LYS	Peptide
20	X	672	ILE	Peptide
20	X	674	LEU	Peptide
20	X	69	GLY	Peptide
20	X	70	HIS	Peptide
20	X	728	ASN	Peptide
20	X	730	GLY	Peptide
20	X	785	GLU	Peptide
20	X	786	ILE	Peptide

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	1207	0	927	14	0
2	B	1570	0	1553	33	0
3	C	1058	0	1118	26	0
4	D	4561	0	4549	72	0
5	E	3981	0	3282	35	0
6	F	1818	0	1567	29	0
7	G	1954	0	1961	44	0
8	H	685	0	477	4	0
9	I	1409	0	1285	24	0
10	J	984	0	416	1	0
11	K	1008	0	1109	9	0
12	L	921	0	972	10	0
13	M	858	0	882	13	0
14	N	710	0	730	16	0
15	O	563	0	594	5	0
16	P	584	0	586	11	0
17	Q	543	0	560	7	0
18	R	11822	0	5939	99	0
19	r	471	0	236	0	0
20	X	4101	0	1779	14	0
21	Y	677	0	298	1	0
22	B	1	0	0	0	0
22	I	2	0	0	0	0
All	All	41488	0	30820	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (413) 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)
4:D:303:LEU:CD1	4:D:312:VAL:HG11	1.70	1.21
2:B:8:TYR:CE1	14:N:82:PRO:HG3	1.80	1.15
3:C:13:PRO:HD2	3:C:19:TYR:CD1	1.82	1.14
2:B:136:LEU:HD23	2:B:137:PRO:HD2	1.11	1.09
2:B:8:TYR:HE1	14:N:82:PRO:CG	1.64	1.09
3:C:13:PRO:HD2	3:C:19:TYR:HD1	0.94	1.06
4:D:303:LEU:CD1	4:D:312:VAL:CG1	2.36	1.03
4:D:303:LEU:HD11	4:D:312:VAL:CG1	1.90	1.01
1:A:7:LYS:HD3	1:A:7:LYS:H	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:303:LEU:HD12	4:D:312:VAL:HG11	1.43	1.00
18:R:380:G:H1	18:R:438:U:H3	1.07	0.99
2:B:8:TYR:CE1	14:N:82:PRO:CG	2.44	0.98
18:R:384:U:H3	18:R:434:G:H1	1.01	0.98
2:B:8:TYR:CD1	14:N:82:PRO:HG3	1.99	0.97
4:D:303:LEU:HD11	4:D:312:VAL:HG12	1.45	0.95
2:B:136:LEU:HD23	2:B:137:PRO:CD	1.95	0.95
16:P:22:LEU:HD22	16:P:27:VAL:HG12	1.48	0.95
3:C:13:PRO:CD	3:C:19:TYR:HD1	1.82	0.93
2:B:8:TYR:HE1	14:N:82:PRO:CD	1.84	0.90
9:I:45:CYS:HB2	9:I:70:GLN:HB2	1.52	0.89
7:G:68:SER:HB2	7:G:224:PHE:CD2	2.07	0.89
7:G:68:SER:HB2	7:G:224:PHE:HD2	1.38	0.89
3:C:62:LEU:HD21	3:C:79:LEU:HD11	1.58	0.85
18:R:55:G:N2	18:R:151:C:C2	2.45	0.85
18:R:389:G:H1	18:R:430:U:H3	0.86	0.84
16:P:22:LEU:HD22	16:P:27:VAL:CG1	2.09	0.83
5:E:321:LEU:HD22	5:E:322:PRO:HD2	1.60	0.83
7:G:68:SER:HA	7:G:224:PHE:CD2	2.14	0.82
2:B:6:CYS:SG	2:B:30:HIS:CE1	2.72	0.81
2:B:8:TYR:CE1	14:N:82:PRO:CD	2.63	0.79
5:E:321:LEU:HD22	5:E:322:PRO:CD	2.13	0.79
4:D:448:TYR:CD2	5:E:480:SER:HA	2.18	0.78
4:D:7:LEU:O	4:D:7:LEU:HD22	1.84	0.77
9:I:201:CYS:SG	9:I:226:HIS:HE1	2.09	0.76
3:C:15:ASN:OD1	3:C:16:LYS:N	2.19	0.76
12:L:51:ARG:HD3	13:M:87:ARG:HH12	1.52	0.75
7:G:68:SER:CB	7:G:224:PHE:CD2	2.70	0.74
18:R:171:A:H61	18:R:540:G:H1	1.35	0.74
9:I:44:ILE:N	9:I:44:ILE:HD12	2.02	0.74
9:I:41:ASP:HB3	9:I:42:PRO:CD	2.18	0.73
6:F:411:GLN:HA	6:F:411:GLN:NE2	2.04	0.73
7:G:68:SER:CB	7:G:224:PHE:HD2	2.01	0.73
2:B:136:LEU:CD2	2:B:137:PRO:HD2	2.05	0.72
4:D:24:PRO:HD2	7:G:260:LEU:CB	2.20	0.72
4:D:33:LEU:O	4:D:33:LEU:HD22	1.90	0.71
1:A:5:LEU:O	1:A:5:LEU:HD23	1.90	0.70
6:F:410:LEU:HD23	6:F:410:LEU:O	1.91	0.70
5:E:582:GLN:HE21	5:E:606:ARG:HD2	1.56	0.69
5:E:317:ALA:O	5:E:321:LEU:HB2	1.92	0.69
1:A:5:LEU:HD23	1:A:5:LEU:C	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ARG:NH2	18:R:60:C:C5	2.60	0.68
4:D:306:LEU:O	4:D:306:LEU:HD12	1.93	0.68
7:G:70:LEU:HD23	7:G:70:LEU:C	2.14	0.68
18:R:425:A:H2'	18:R:426:U:H4'	1.76	0.67
7:G:43:GLN:HE22	7:G:53:ARG:HG3	1.59	0.67
20:X:670:ALA:HB3	20:X:676:ILE:HA	1.77	0.67
1:A:7:LYS:HD3	1:A:7:LYS:N	2.04	0.66
4:D:307:ALA:O	4:D:313:TRP:NE1	2.25	0.66
2:B:138:GLN:O	2:B:140:ALA:N	2.29	0.66
4:D:304:LEU:HB2	4:D:305:PRO:HD3	1.78	0.65
7:G:98:LEU:HD23	7:G:98:LEU:C	2.18	0.64
7:G:68:SER:CA	7:G:224:PHE:CD2	2.81	0.64
4:D:24:PRO:HD2	7:G:260:LEU:HB2	1.80	0.63
4:D:140:HIS:HB3	4:D:143:SER:HB3	1.80	0.63
2:B:75:VAL:HG22	4:D:224:PRO:HB3	1.80	0.63
18:R:55:G:N2	18:R:151:C:O2	2.31	0.63
18:R:386:G:H1	18:R:433:U:H3	1.45	0.63
18:R:171:A:N6	18:R:540:G:H1	1.97	0.62
9:I:42:PRO:O	9:I:70:GLN:NE2	2.32	0.62
4:D:310:ASP:HA	4:D:313:TRP:HD1	1.64	0.62
7:G:226:LYS:NZ	18:R:119:G:N7	2.47	0.62
3:C:12:ARG:NH2	18:R:60:C:C4	2.68	0.62
7:G:72:LEU:O	7:G:72:LEU:HG	1.99	0.62
5:E:405:THR:O	5:E:409:ASN:HB2	2.00	0.61
2:B:6:CYS:SG	2:B:30:HIS:HE1	2.17	0.61
5:E:355:VAL:HG11	5:E:372:TYR:HB2	1.80	0.61
21:Y:48:ILE:HA	21:Y:121:LEU:HA	1.82	0.61
3:C:68:SER:OG	3:C:73:MET:SD	2.59	0.61
6:F:407:GLN:HG3	6:F:408:PRO:HD2	1.83	0.61
18:R:78:A:H4'	18:R:79:A:H5'	1.81	0.61
11:K:85:THR:HG22	14:N:73:VAL:HG22	1.82	0.61
18:R:342:C:H2'	18:R:343:A:H4'	1.82	0.60
7:G:186:SER:HB3	7:G:214:GLU:HG2	1.83	0.60
11:K:88:ARG:NH1	14:N:66:GLY:O	2.35	0.60
3:C:100:LYS:HE3	3:C:100:LYS:O	2.02	0.59
18:R:320:U:H3	18:R:521:G:H1	1.50	0.59
9:I:44:ILE:HD12	9:I:44:ILE:H	1.66	0.59
3:C:14:ALA:O	3:C:69:ARG:NH1	2.36	0.59
6:F:330:ARG:HE	6:F:342:VAL:HG21	1.67	0.59
13:M:30:PRO:HG2	16:P:46:ASP:HB2	1.83	0.59
18:R:217:U:O2	18:R:220:G:O6	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:445:VAL:HG23	4:D:445:VAL:O	2.01	0.59
9:I:193:SER:O	9:I:197:LYS:N	2.36	0.58
11:K:121:LYS:NZ	18:R:280:G:O6	2.35	0.58
7:G:92:TYR:HD1	7:G:92:TYR:N	2.01	0.58
1:A:97:ASP:O	1:A:99:HIS:N	2.36	0.58
4:D:266:SER:O	4:D:269:THR:HG22	2.04	0.58
6:F:377:ARG:O	6:F:379:ARG:NH2	2.34	0.58
18:R:88:C:N3	18:R:111:A:N6	2.52	0.58
4:D:440:LEU:O	4:D:444:LEU:HD12	2.04	0.58
3:C:62:LEU:CD2	3:C:79:LEU:HD21	2.34	0.57
4:D:374:SER:O	8:H:50:ARG:NH2	2.37	0.57
7:G:68:SER:HA	7:G:224:PHE:HD2	1.68	0.57
9:I:45:CYS:HB2	9:I:70:GLN:CB	2.31	0.57
16:P:34:ASN:HB3	16:P:36:THR:HG23	1.86	0.57
20:X:674:LEU:HA	20:X:677:GLU:H	1.67	0.57
18:R:131:U:O2'	18:R:132:U:H5'	2.04	0.57
4:D:411:GLN:HE22	4:D:449:SER:HB2	1.68	0.57
5:E:326:LYS:O	5:E:326:LYS:HG2	2.04	0.57
11:K:127:LYS:NZ	18:R:173:G:OP1	2.37	0.57
14:N:34:VAL:HG12	14:N:35:GLU:HG2	1.85	0.57
15:O:12:PRO:HD2	15:O:15:ASN:HD22	1.68	0.57
18:R:524:G:H2'	18:R:525:G:H8	1.69	0.57
4:D:7:LEU:HD22	4:D:7:LEU:C	2.25	0.57
7:G:92:TYR:N	7:G:92:TYR:CD1	2.73	0.57
12:L:33:SER:HB3	12:L:37:ASN:HB2	1.87	0.57
13:M:47:SER:OG	13:M:53:LYS:NZ	2.38	0.57
7:G:68:SER:CA	7:G:224:PHE:HD2	2.16	0.56
6:F:345:PRO:HD2	6:F:350:CYS:O	2.06	0.56
2:B:138:GLN:C	2:B:140:ALA:H	2.07	0.56
2:B:142:GLU:HA	2:B:145:ALA:HB3	1.88	0.56
6:F:320:LEU:HD22	6:F:324:VAL:HG11	1.87	0.56
9:I:45:CYS:SG	9:I:47:SER:OG	2.63	0.56
18:R:209:U:H3	18:R:229:U:H3	1.54	0.56
6:F:385:SER:OG	6:F:386:ALA:N	2.39	0.56
7:G:58:LYS:HB3	7:G:61:ALA:HB2	1.87	0.56
13:M:41:ARG:O	13:M:57:ARG:NH1	2.39	0.56
17:Q:17:LEU:HB3	17:Q:71:LEU:HD12	1.87	0.55
9:I:198:LEU:HD12	9:I:207:TYR:HB3	1.88	0.55
4:D:372:GLU:OE1	4:D:391:TYR:OH	2.23	0.55
9:I:41:ASP:HB3	9:I:42:PRO:HD2	1.89	0.55
18:R:502:C:H2'	18:R:503:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:339:ILE:HD11	6:F:342:VAL:HG13	1.89	0.55
4:D:448:TYR:CE2	5:E:480:SER:HA	2.41	0.55
2:B:40:ASN:HD21	18:R:298:G:H21	1.53	0.55
4:D:334:LEU:HD22	4:D:347:ILE:HG23	1.88	0.55
18:R:239:U:H2'	18:R:240:G:H8	1.72	0.55
6:F:326:GLU:HG2	6:F:344:ILE:HG23	1.89	0.55
7:G:68:SER:CB	7:G:224:PHE:CE2	2.90	0.55
15:O:89:LEU:HD13	17:Q:63:ILE:HG13	1.89	0.54
18:R:448:G:H2'	18:R:449:G:H8	1.72	0.54
16:P:37:GLU:OE2	16:P:39:ARG:NH2	2.40	0.54
4:D:193:ILE:HG22	4:D:230:LYS:HE2	1.90	0.54
18:R:198:U:H3	18:R:240:G:H1	1.54	0.54
6:F:411:GLN:HA	6:F:411:GLN:HE21	1.73	0.54
18:R:384:U:O4	18:R:434:G:O6	2.25	0.54
20:X:834:PHE:O	20:X:839:ASP:N	2.40	0.54
3:C:13:PRO:HG2	3:C:19:TYR:HB2	1.88	0.54
4:D:24:PRO:HD2	7:G:260:LEU:HB3	1.90	0.54
7:G:187:ILE:HD11	7:G:215:LEU:HD22	1.90	0.53
13:M:98:GLY:O	16:P:74:ARG:NH1	2.41	0.53
9:I:41:ASP:CB	9:I:42:PRO:CD	2.86	0.53
5:E:274:LEU:O	5:E:278:LEU:N	2.38	0.53
11:K:50:GLU:OE2	11:K:52:ARG:NH2	2.37	0.53
3:C:67:ILE:HG22	3:C:77:ALA:HB1	1.90	0.53
4:D:369:GLU:HA	4:D:372:GLU:HG2	1.91	0.53
9:I:73:LEU:HB3	9:I:76:HIS:HD2	1.74	0.53
2:B:186:THR:OG1	4:D:242:MET:SD	2.66	0.53
7:G:228:GLU:OE1	7:G:230:ASN:N	2.42	0.53
9:I:39:LEU:HD13	9:I:79:GLN:OE1	2.09	0.53
15:O:80:ILE:HG22	16:P:82:ARG:HB3	1.91	0.53
6:F:197:HIS:HA	6:F:204:SER:HA	1.90	0.53
7:G:95:LYS:HZ2	7:G:95:LYS:HB2	1.73	0.53
5:E:573:HIS:HD2	5:E:576:ILE:HB	1.73	0.52
18:R:62:A:H8	18:R:65:G:HO2'	1.57	0.52
4:D:437:GLN:NE2	4:D:472:TYR:OH	2.39	0.52
9:I:39:LEU:HG	9:I:39:LEU:O	2.08	0.52
18:R:391:C:N4	18:R:423:G:O2'	2.37	0.52
4:D:489:ASP:OD2	4:D:492:ARG:NH2	2.42	0.52
18:R:131:U:H2'	18:R:132:U:C6	2.45	0.52
7:G:68:SER:HB2	7:G:224:PHE:CE2	2.45	0.52
13:M:45:ILE:HG12	13:M:55:ILE:HG12	1.91	0.52
5:E:383:ASN:OD1	5:E:383:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:72:LEU:HD23	7:G:115:ILE:HB	1.93	0.51
4:D:496:ASP:OD1	4:D:496:ASP:N	2.36	0.51
5:E:619:LEU:HD13	6:F:379:ARG:HB3	1.93	0.51
3:C:44:ASN:ND2	3:C:55:LEU:O	2.44	0.51
20:X:815:PHE:O	20:X:819:ILE:N	2.43	0.51
13:M:8:ARG:NH1	13:M:17:GLU:OE1	2.43	0.51
5:E:321:LEU:CD2	5:E:322:PRO:CD	2.88	0.51
12:L:19:LEU:HD12	12:L:23:THR:HG23	1.92	0.51
16:P:76:ASN:ND2	18:R:559:G:OP2	2.43	0.51
1:A:4:ASN:HD22	1:A:6:SER:HB3	1.76	0.50
1:A:8:TYR:HB3	1:A:12:VAL:HB	1.93	0.50
3:C:89:ARG:O	3:C:93:LYS:HB2	2.12	0.50
4:D:428:LEU:HA	4:D:437:GLN:HE22	1.75	0.50
7:G:98:LEU:HD23	7:G:99:ARG:N	2.25	0.50
18:R:439:U:H2'	18:R:440:A:C8	2.46	0.50
13:M:54:ILE:HG22	13:M:74:GLU:HG2	1.93	0.50
1:A:25:LYS:HD3	11:K:78:GLU:HB3	1.93	0.50
6:F:358:ARG:NH2	6:F:362:GLU:OE2	2.44	0.50
5:E:326:LYS:HG3	5:E:330:TYR:HE2	1.76	0.50
7:G:117:LEU:HD11	7:G:128:VAL:HG11	1.94	0.50
4:D:506:TRP:HE1	4:D:521:LEU:HD11	1.76	0.50
6:F:341:TYR:C	6:F:341:TYR:CD2	2.85	0.50
4:D:88:SER:HB2	18:R:114:U:H4'	1.94	0.50
5:E:321:LEU:CD2	5:E:322:PRO:HD3	2.42	0.50
20:X:830:LEU:O	20:X:834:PHE:N	2.40	0.50
18:R:21:G:H2'	18:R:22:A:H8	1.75	0.50
2:B:8:TYR:CD1	2:B:8:TYR:N	2.79	0.49
3:C:135:LEU:HD12	18:R:426:U:H2'	1.94	0.49
18:R:249:G:H2'	18:R:250:G:H8	1.77	0.49
14:N:63:PHE:HB3	17:Q:71:LEU:HB3	1.94	0.49
11:K:88:ARG:HH12	14:N:67:SER:HA	1.77	0.49
6:F:407:GLN:HG3	6:F:408:PRO:CD	2.41	0.49
6:F:417:TYR:HB2	7:G:281:MET:HE2	1.94	0.49
10:J:522:ALA:O	10:J:526:LEU:N	2.45	0.49
20:X:811:THR:O	20:X:815:PHE:N	2.40	0.49
20:X:379:THR:O	20:X:381:ASP:N	2.44	0.49
18:R:392:A:N6	18:R:424:U:O3'	2.46	0.49
5:E:322:PRO:HD2	5:E:325:PHE:CE2	2.48	0.49
18:R:401:U:H2'	18:R:402:G:H8	1.78	0.49
4:D:33:LEU:HD22	4:D:33:LEU:C	2.32	0.49
4:D:195:ASP:OD1	4:D:195:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:503:ARG:NH2	5:E:386:ASP:OD1	2.46	0.49
9:I:213:THR:HG23	9:I:215:ARG:H	1.78	0.49
20:X:64:ILE:O	20:X:68:TYR:N	2.45	0.49
5:E:581:PRO:HG3	5:E:611:ILE:HG22	1.95	0.48
18:R:389:G:O6	18:R:430:U:O4	2.30	0.48
5:E:383:ASN:HD22	5:E:392:ILE:HA	1.78	0.48
5:E:409:ASN:ND2	5:E:414:GLN:O	2.46	0.48
11:K:93:LEU:HD12	12:L:91:THR:HG21	1.96	0.48
2:B:138:GLN:C	2:B:140:ALA:N	2.67	0.48
6:F:381:SER:OG	6:F:382:TRP:N	2.46	0.48
7:G:61:ALA:HB1	7:G:123:LEU:CD1	2.44	0.48
4:D:442:ASN:OD1	4:D:484:ARG:NH1	2.47	0.48
18:R:20:A:H2'	18:R:21:G:H8	1.78	0.48
2:B:195:SER:H	6:F:301:GLN:HE22	1.62	0.47
7:G:71:ILE:HG23	7:G:116:VAL:HG22	1.95	0.47
4:D:424:VAL:HG11	4:D:444:LEU:HD11	1.97	0.47
16:P:36:THR:HG22	16:P:60:VAL:HG22	1.97	0.47
18:R:16:U:O2'	18:R:168:C:OP2	2.23	0.47
18:R:521:G:H2'	18:R:522:A:H8	1.80	0.47
2:B:124:ARG:O	2:B:128:GLY:HA3	2.14	0.47
20:X:776:LEU:O	20:X:780:ALA:N	2.47	0.47
7:G:71:ILE:HD12	7:G:198:PHE:CE2	2.50	0.47
13:M:48:LEU:HD11	13:M:96:LEU:HD11	1.96	0.47
7:G:68:SER:OG	7:G:224:PHE:HE2	1.97	0.47
8:H:22:ASP:OD1	8:H:22:ASP:N	2.47	0.47
9:I:203:VAL:HG12	9:I:229:TYR:HD2	1.80	0.47
18:R:497:G:N2	18:R:498:U:O4	2.46	0.47
18:R:342:C:N4	18:R:480:C:OP2	2.48	0.47
1:A:9:PRO:O	1:A:12:VAL:N	2.45	0.47
4:D:276:ILE:HG23	4:D:311:LEU:HD12	1.97	0.47
18:R:21:G:H2'	18:R:22:A:C8	2.50	0.47
3:C:9:LEU:CD2	3:C:101:VAL:HG21	2.45	0.47
7:G:45:PHE:HB3	7:G:153:LYS:HD3	1.97	0.47
18:R:239:U:H2'	18:R:240:G:C8	2.49	0.47
6:F:195:ILE:HA	6:F:208:GLY:HA3	1.97	0.46
14:N:41:ASN:ND2	14:N:64:VAL:O	2.48	0.46
6:F:323:LEU:HD23	6:F:323:LEU:O	2.14	0.46
9:I:41:ASP:CB	9:I:42:PRO:HD3	2.46	0.46
18:R:24:G:H2'	18:R:25:A:C8	2.50	0.46
3:C:74:THR:OG1	3:C:75:ASN:N	2.48	0.46
13:M:77:THR:HG22	13:M:86:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:TYR:HD1	14:N:82:PRO:HG3	1.71	0.46
4:D:345:THR:HG22	4:D:387:ILE:HD11	1.97	0.46
2:B:104:THR:O	2:B:108:LEU:HB2	2.16	0.46
18:R:429:C:H2'	18:R:430:U:H6	1.81	0.46
9:I:48:TYR:HB2	9:I:53:CYS:HB2	1.98	0.46
15:O:31:LEU:HD12	15:O:37:ILE:HG13	1.97	0.46
18:R:125:A:H2'	18:R:126:A:H8	1.80	0.46
5:E:624:PHE:HE2	6:F:389:THR:HG21	1.79	0.46
7:G:129:LEU:O	7:G:133:LEU:HB2	2.16	0.46
18:R:424:U:H2'	18:R:425:A:C8	2.49	0.46
2:B:59:ARG:HH12	2:B:67:SER:HB3	1.81	0.46
4:D:306:LEU:HB2	4:D:309:TYR:HB2	1.97	0.46
18:R:47:A:H2'	18:R:48:A:C8	2.51	0.46
4:D:208:LEU:HB3	4:D:214:ILE:HG23	1.97	0.45
11:K:60:LYS:NZ	11:K:74:ASN:O	2.37	0.45
7:G:69:LEU:HD23	7:G:164:PRO:CG	2.46	0.45
18:R:180:U:O5'	18:R:533:A:N6	2.48	0.45
4:D:451:ASP:N	4:D:451:ASP:OD1	2.48	0.45
18:R:170:G:H2'	18:R:171:A:H8	1.81	0.45
5:E:321:LEU:HD22	5:E:322:PRO:HD3	1.95	0.45
18:R:486:C:H2'	18:R:487:A:C8	2.52	0.45
4:D:400:ASN:ND2	4:D:413:ASN:O	2.50	0.45
4:D:438:GLU:OE2	4:D:475:ASN:ND2	2.49	0.45
4:D:303:LEU:HD12	4:D:312:VAL:CG1	2.23	0.45
6:F:313:THR:O	6:F:313:THR:OG1	2.35	0.45
18:R:20:A:H2'	18:R:21:G:C8	2.52	0.45
18:R:47:A:H2'	18:R:48:A:H8	1.81	0.45
4:D:57:ARG:NE	4:D:81:GLU:OE2	2.50	0.45
7:G:98:LEU:C	7:G:98:LEU:CD2	2.85	0.45
18:R:334:U:H2'	18:R:335:G:C8	2.52	0.45
18:R:478:A:H2'	18:R:479:G:H8	1.81	0.45
12:L:3:LEU:HD21	13:M:68:VAL:HG23	1.98	0.44
3:C:9:LEU:HD23	3:C:101:VAL:HG21	1.99	0.44
7:G:261:PHE:O	7:G:262:ASP:C	2.53	0.44
18:R:314:G:H2'	18:R:315:G:H8	1.82	0.44
18:R:455:U:H2'	18:R:456:A:H8	1.82	0.44
20:X:369:ASN:O	20:X:373:VAL:N	2.50	0.44
4:D:178:SER:O	4:D:178:SER:OG	2.29	0.44
6:F:306:HIS:HB3	6:F:384:ARG:HG2	1.99	0.44
18:R:55:G:C2	18:R:151:C:O2	2.70	0.44
18:R:403:A:H2'	18:R:404:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASP:O	2:B:131:VAL:HG21	2.17	0.44
14:N:43:GLN:HG2	14:N:63:PHE:HD1	1.82	0.44
18:R:2:U:H2'	18:R:3:A:H8	1.98	0.44
4:D:303:LEU:O	4:D:307:ALA:HB2	2.18	0.44
5:E:323:LEU:H	5:E:323:LEU:HG	1.39	0.44
2:B:8:TYR:CE1	14:N:82:PRO:HD3	2.49	0.44
4:D:501:ILE:HA	4:D:505:ILE:HD13	2.00	0.44
4:D:473:LEU:HD13	4:D:479:TRP:HZ2	1.82	0.44
18:R:321:C:H2'	18:R:322:A:C8	2.52	0.44
18:R:380:G:O6	18:R:438:U:O4	2.36	0.44
4:D:243:VAL:HG11	5:E:583:ILE:HG13	2.00	0.44
4:D:310:ASP:HB3	4:D:341:SER:HB2	2.00	0.44
7:G:105:GLU:HG2	7:G:108:ASP:HA	1.99	0.44
1:A:5:LEU:C	1:A:5:LEU:CD2	2.85	0.44
18:R:6:U:H2'	18:R:7:A:H8	1.83	0.44
4:D:17:THR:HG21	8:H:31:ILE:HA	2.00	0.43
2:B:177:PRO:HB3	4:D:177:HIS:O	2.18	0.43
4:D:303:LEU:CD2	4:D:313:TRP:CH2	3.01	0.43
12:L:92:ILE:HD12	12:L:95:ILE:HD11	2.00	0.43
9:I:58:PHE:HE1	9:I:225:ILE:HA	1.83	0.43
18:R:321:C:H2'	18:R:322:A:H8	1.83	0.43
3:C:13:PRO:HG3	3:C:19:TYR:HA	1.99	0.43
12:L:50:PRO:HB2	12:L:55:LEU:HD23	1.99	0.43
18:R:396:U:H5	18:R:416:G:H1	1.65	0.43
2:B:55:HIS:CE1	18:R:133:G:H2'	2.53	0.43
2:B:124:ARG:O	2:B:128:GLY:CA	2.67	0.43
5:E:621:THR:HA	5:E:625:LEU:HB2	1.99	0.43
18:R:389:G:N2	18:R:430:U:O2	2.33	0.43
1:A:114:LEU:N	1:A:149:GLY:O	2.45	0.43
4:D:460:ILE:O	4:D:464:ILE:HG12	2.18	0.43
9:I:41:ASP:HB3	9:I:42:PRO:HD3	2.00	0.43
18:R:328:G:H2'	18:R:329:A:H8	1.82	0.43
3:C:16:LYS:HG2	3:C:67:ILE:HD11	2.00	0.43
2:B:120:VAL:HG13	2:B:123:ASN:H	1.83	0.43
7:G:97:ILE:HD12	7:G:97:ILE:HA	1.77	0.43
18:R:125:A:H2'	18:R:126:A:C8	2.53	0.43
18:R:219:U:H3'	18:R:220:G:H8	1.83	0.43
18:R:350:U:H1'	18:R:351:U:H5	1.84	0.43
18:R:448:G:H2'	18:R:449:G:C8	2.54	0.43
20:X:414:ILE:O	20:X:418:ALA:N	2.46	0.43
7:G:61:ALA:O	7:G:122:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:70:LEU:C	7:G:70:LEU:CD2	2.85	0.42
4:D:60:TYR:OH	4:D:76:ASP:OD2	2.27	0.42
6:F:168:GLY:HA2	6:F:207:TYR:HA	2.02	0.42
6:F:438:LEU:HD23	6:F:438:LEU:HA	1.85	0.42
9:I:43:LYS:HD3	9:I:43:LYS:HA	1.79	0.42
5:E:126:LEU:O	5:E:130:LYS:N	2.47	0.42
18:R:328:G:H2'	18:R:329:A:C8	2.55	0.42
4:D:18:LEU:HD21	8:H:35:ASP:HB3	2.01	0.42
4:D:447:PHE:HD2	4:D:456:VAL:HG21	1.85	0.42
5:E:605:PHE:HB3	5:E:608:LEU:HD23	2.02	0.42
9:I:213:THR:OG1	9:I:214:ASP:N	2.52	0.42
13:M:99:ASP:HB3	18:R:558:U:H1'	2.01	0.42
16:P:57:GLU:HG2	16:P:67:THR:HG22	2.02	0.42
18:R:418:U:H2'	18:R:419:G:C8	2.55	0.42
3:C:13:PRO:CD	3:C:19:TYR:CD1	2.72	0.42
3:C:65:VAL:HA	3:C:79:LEU:HA	2.02	0.42
6:F:341:TYR:CD2	6:F:341:TYR:O	2.72	0.42
18:R:443:U:H2'	18:R:444:G:H8	1.84	0.42
3:C:103:GLY:HA3	18:R:67:A:N3	2.35	0.42
4:D:169:ARG:NH2	4:D:173:GLU:OE2	2.53	0.42
18:R:68:G:H2'	18:R:69:A:H8	1.85	0.42
12:L:25:VAL:HG22	12:L:45:LEU:HD23	2.01	0.42
12:L:37:ASN:OD1	12:L:89:GLY:N	2.53	0.42
18:R:79:A:H5''	18:R:79:A:H8	1.85	0.42
18:R:91:U:H2'	18:R:92:G:C8	2.55	0.42
18:R:444:G:H2'	18:R:445:G:C8	2.55	0.42
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.88	0.42
5:E:366:ILE:HG21	6:F:522:PHE:HB2	2.02	0.42
14:N:9:LYS:HE3	14:N:9:LYS:HB2	1.89	0.42
18:R:337:A:H2'	18:R:338:G:H8	1.84	0.42
17:Q:13:LYS:HE2	17:Q:77:ILE:HA	2.00	0.42
3:C:3:ALA:HB2	3:C:115:SER:HB2	2.02	0.41
18:R:246:U:H2'	18:R:247:G:C8	2.56	0.41
4:D:289:LEU:HA	5:E:568:TRP:HZ3	1.85	0.41
4:D:447:PHE:CD2	4:D:456:VAL:HG21	2.56	0.41
4:D:310:ASP:HA	4:D:313:TRP:CD1	2.50	0.41
5:E:427:ASP:HB2	5:E:463:LEU:HD22	2.02	0.41
18:R:37:C:H2'	18:R:38:C:C6	2.55	0.41
18:R:403:A:H2'	18:R:404:A:C8	2.55	0.41
2:B:127:ILE:O	2:B:131:VAL:CG2	2.68	0.41
4:D:273:SER:N	6:F:414:ASN:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:73:ALA:HB3	17:Q:77:ILE:HD11	2.02	0.41
18:R:282:C:H2'	18:R:283:A:H8	1.85	0.41
18:R:443:U:H2'	18:R:444:G:C8	2.55	0.41
18:R:510:G:H2'	18:R:511:A:C8	2.55	0.41
4:D:441:LEU:O	4:D:445:VAL:HG13	2.20	0.41
7:G:70:LEU:HD23	7:G:71:ILE:N	2.35	0.41
18:R:438:U:H2'	18:R:439:U:C6	2.56	0.41
1:A:8:TYR:OH	2:B:34:THR:HG21	2.19	0.41
4:D:424:VAL:HG13	4:D:440:LEU:HD12	2.02	0.41
5:E:321:LEU:HD23	5:E:321:LEU:HA	1.68	0.41
17:Q:19:ILE:HD13	17:Q:19:ILE:HA	1.89	0.41
18:R:248:G:H2'	18:R:249:G:H8	1.85	0.41
18:R:413:U:H2'	18:R:414:A:C8	2.56	0.41
5:E:536:ASP:HA	5:E:537:PRO:HD3	1.97	0.41
4:D:417:ASN:HD22	4:D:418:LYS:H	1.69	0.41
9:I:203:VAL:HB	9:I:226:HIS:CE1	2.56	0.41
12:L:15:VAL:HG21	12:L:29:LEU:HD12	2.03	0.41
18:R:444:G:H2'	18:R:445:G:H8	1.85	0.41
18:R:453:U:H2'	18:R:454:G:C8	2.56	0.41
20:X:283:HIS:CB	20:X:292:GLU:H	2.34	0.41
20:X:275:ASN:HA	20:X:409:ALA:HB3	2.03	0.41
2:B:16:ASP:OD2	2:B:21:ARG:NH2	2.54	0.40
5:E:137:ALA:C	5:E:139:SER:H	2.24	0.40
5:E:455:PHE:HD1	5:E:455:PHE:HA	1.76	0.40
1:A:7:LYS:H	1:A:7:LYS:CD	1.97	0.40
3:C:13:PRO:CG	3:C:19:TYR:HA	2.51	0.40
15:O:29:ILE:HG12	15:O:90:ILE:HG12	2.04	0.40
17:Q:10:TYR:HB3	17:Q:15:ILE:HD11	2.02	0.40
1:A:134:GLU:N	1:A:154:VAL:O	2.44	0.40
4:D:365:ARG:HH22	4:D:402:LEU:HD21	1.86	0.40
13:M:99:ASP:HA	16:P:74:ARG:HH12	1.87	0.40
18:R:416:G:H4'	18:R:417:A:H5'	2.03	0.40
18:R:454:G:H2'	18:R:455:U:H6	1.86	0.40
20:X:679:LYS:O	20:X:683:ILE:N	2.48	0.40
7:G:111:MET:SD	7:G:111:MET:N	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/300 (61%)	162 (89%)	17 (9%)	3 (2%)	9	46
2	B	193/231 (84%)	180 (93%)	10 (5%)	3 (2%)	9	46
3	C	126/350 (36%)	120 (95%)	6 (5%)	0	100	100
4	D	542/544 (100%)	515 (95%)	27 (5%)	0	100	100
5	E	570/629 (91%)	532 (93%)	38 (7%)	0	100	100
6	F	259/523 (50%)	240 (93%)	19 (7%)	0	100	100
7	G	235/492 (48%)	218 (93%)	17 (7%)	0	100	100
8	H	50/105 (48%)	47 (94%)	3 (6%)	0	100	100
9	I	186/261 (71%)	174 (94%)	11 (6%)	1 (0%)	29	68
10	J	196/583 (34%)	185 (94%)	10 (5%)	1 (0%)	29	68
11	K	119/196 (61%)	111 (93%)	8 (7%)	0	100	100
12	L	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
13	M	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
14	N	91/101 (90%)	84 (92%)	7 (8%)	0	100	100
15	O	70/94 (74%)	68 (97%)	2 (3%)	0	100	100
16	P	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
17	Q	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
20	X	824/861 (96%)	727 (88%)	80 (10%)	17 (2%)	7	40
21	Y	136/208 (65%)	120 (88%)	15 (11%)	1 (1%)	22	61
All	All	4140/5897 (70%)	3827 (92%)	287 (7%)	26 (1%)	29	64

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
2	B	139	ARG

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Mol	Chain	Res	Type
10	J	370	PRO
20	X	71	GLU
20	X	284	LEU
20	X	380	LEU
20	X	672	ILE
20	X	673	GLU
20	X	674	LEU
21	Y	24	TYR
1	A	99	HIS
20	X	70	HIS
20	X	289	THR
20	X	343	THR
20	X	571	VAL
20	X	390	THR
20	X	670	ALA
2	B	70	ASN
20	X	290	GLY
20	X	449	ASN
9	I	41	ASP
2	B	136	LEU
20	X	278	PHE
20	X	389	PHE
20	X	410	PRO
1	A	97	ASP

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	82/265 (31%)	78 (95%)	4 (5%)	25	59
2	B	171/214 (80%)	161 (94%)	10 (6%)	20	55
3	C	117/317 (37%)	112 (96%)	5 (4%)	29	63
4	D	508/519 (98%)	491 (97%)	17 (3%)	38	69
5	E	316/603 (52%)	307 (97%)	9 (3%)	43	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	157/451 (35%)	149 (95%)	8 (5%)	24	58
7	G	218/448 (49%)	207 (95%)	11 (5%)	24	59
8	H	48/48 (100%)	46 (96%)	2 (4%)	30	63
9	I	130/234 (56%)	124 (95%)	6 (5%)	27	61
11	K	114/176 (65%)	114 (100%)	0	100	100
12	L	107/129 (83%)	106 (99%)	1 (1%)	78	90
13	M	95/103 (92%)	94 (99%)	1 (1%)	73	88
14	N	81/89 (91%)	78 (96%)	3 (4%)	34	66
15	O	62/83 (75%)	62 (100%)	0	100	100
16	P	64/77 (83%)	59 (92%)	5 (8%)	12	44
17	Q	59/66 (89%)	55 (93%)	4 (7%)	16	50
All	All	2329/3822 (61%)	2243 (96%)	86 (4%)	37	66

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LYS
1	A	46	ASN
1	A	70	ARG
2	B	3	ARG
2	B	29	ASN
2	B	47	ASN
2	B	80	ASN
2	B	124	ARG
2	B	131	VAL
2	B	135	LYS
2	B	136	LEU
2	B	138	GLN
2	B	172	LYS
3	C	62	LEU
3	C	101	VAL
3	C	107	ARG
3	C	108	MET
3	C	117	LEU
4	D	5	THR
4	D	7	LEU
4	D	8	ILE

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Mol	Chain	Res	Type
4	D	33	LEU
4	D	102	ASN
4	D	263	TYR
4	D	265	THR
4	D	306	LEU
4	D	310	ASP
4	D	366	ASN
4	D	381	ASN
4	D	416	LEU
4	D	417	ASN
4	D	444	LEU
4	D	445	VAL
4	D	446	GLN
4	D	515	GLN
5	E	314	TYR
5	E	321	LEU
5	E	323	LEU
5	E	324	ASP
5	E	349	ASN
5	E	352	ASN
5	E	409	ASN
5	E	472	LEU
5	E	617	ASN
6	F	312	ASN
6	F	314	THR
6	F	322	SER
6	F	341	TYR
6	F	342	VAL
6	F	343	LYS
6	F	344	ILE
6	F	410	LEU
7	G	69	LEU
7	G	72	LEU
7	G	90	HIS
7	G	92	TYR
7	G	95	LYS
7	G	97	ILE
7	G	122	ILE
7	G	123	LEU
7	G	200	GLN
7	G	260	LEU
7	G	261	PHE

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Mol	Chain	Res	Type
8	H	2	ARG
8	H	51	ASN
9	I	39	LEU
9	I	43	LYS
9	I	44	ILE
9	I	73	LEU
9	I	88	LYS
9	I	118	ASN
12	L	114	ASN
13	M	51	ASN
14	N	3	MET
14	N	30	ARG
14	N	41	ASN
16	P	19	LEU
16	P	39	ARG
16	P	47	ASN
16	P	51	LEU
16	P	82	ARG
17	Q	20	ASN
17	Q	66	ASN
17	Q	75	ASP
17	Q	77	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
2	B	29	ASN
2	B	40	ASN
2	B	47	ASN
2	B	80	ASN
3	C	18	ASN
4	D	102	ASN
4	D	153	GLN
4	D	298	ASN
4	D	366	ASN
4	D	381	ASN
4	D	400	ASN
4	D	411	GLN
4	D	417	ASN
4	D	437	GLN
4	D	443	ASN

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Mol	Chain	Res	Type
4	D	474	GLN
5	E	349	ASN
5	E	352	ASN
5	E	409	ASN
5	E	488	ASN
5	E	582	GLN
5	E	617	ASN
6	F	301	GLN
6	F	306	HIS
6	F	311	ASN
6	F	312	ASN
6	F	334	GLN
6	F	407	GLN
6	F	411	GLN
6	F	497	GLN
7	G	43	GLN
7	G	90	HIS
7	G	200	GLN
8	H	51	ASN
9	I	40	HIS
9	I	76	HIS
9	I	118	ASN
9	I	226	HIS
12	L	114	ASN
13	M	51	ASN
13	M	86	ASN
14	N	41	ASN
15	O	15	ASN
16	P	24	ASN
16	P	47	ASN
16	P	50	ASN
17	Q	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	556/568 (97%)	134 (24%)	18 (3%)
19	r	21/253 (8%)	6 (28%)	0
All	All	577/821 (70%)	140 (24%)	18 (3%)

All (140) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	10	U
18	R	11	U
18	R	12	A
18	R	13	A
18	R	17	A
18	R	26	G
18	R	40	A
18	R	41	C
18	R	53	G
18	R	54	C
18	R	55	G
18	R	56	C
18	R	62	A
18	R	63	U
18	R	64	A
18	R	65	G
18	R	66	U
18	R	67	A
18	R	72	G
18	R	74	C
18	R	75	G
18	R	79	A
18	R	80	G
18	R	87	U
18	R	90	U
18	R	92	G
18	R	93	A
18	R	97	A
18	R	98	U
18	R	99	A
18	R	100	A
18	R	101	U
18	R	103	G
18	R	104	U
18	R	107	A
18	R	113	G
18	R	114	U
18	R	117	U
18	R	134	G
18	R	139	A
18	R	141	A
18	R	142	C
18	R	145	A

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Mol	Chain	Res	Type
18	R	147	A
18	R	149	G
18	R	150	G
18	R	151	C
18	R	152	G
18	R	153	C
18	R	154	G
18	R	176	U
18	R	178	C
18	R	179	A
18	R	180	U
18	R	181	U
18	R	182	C
18	R	183	C
18	R	186	U
18	R	187	G
18	R	205	U
18	R	206	C
18	R	217	U
18	R	218	U
18	R	219	U
18	R	220	G
18	R	227	U
18	R	228	U
18	R	230	G
18	R	254	U
18	R	255	U
18	R	257	G
18	R	258	U
18	R	259	U
18	R	260	U
18	R	262	U
18	R	269	U
18	R	270	G
18	R	271	G
18	R	272	A
18	R	278	U
18	R	279	U
18	R	280	G
18	R	287	A
18	R	290	U
18	R	325	A

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Mol	Chain	Res	Type
18	R	327	A
18	R	328	G
18	R	343	A
18	R	352	G
18	R	365	U
18	R	369	G
18	R	377	U
18	R	378	U
18	R	385	U
18	R	386	G
18	R	389	G
18	R	393	G
18	R	394	A
18	R	395	U
18	R	399	A
18	R	400	A
18	R	407	U
18	R	409	A
18	R	416	G
18	R	418	U
18	R	422	G
18	R	424	U
18	R	426	U
18	R	427	G
18	R	443	U
18	R	460	U
18	R	466	U
18	R	468	U
18	R	477	G
18	R	482	G
18	R	493	G
18	R	504	U
18	R	505	U
18	R	506	A
18	R	508	G
18	R	513	A
18	R	540	G
18	R	542	U
18	R	545	A
18	R	551	U
18	R	553	A
18	R	555	U

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Mol	Chain	Res	Type
18	R	559	G
18	R	560	A
18	R	561	U
18	R	562	U
18	R	563	U
18	R	564	A
18	R	565	U
19	r	-8	C
19	r	-6	A
19	r	-5	G
19	r	-4	A
19	r	-2	A
19	r	-1	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	63	U
18	R	64	A
18	R	66	U
18	R	79	A
18	R	86	A
18	R	100	A
18	R	112	A
18	R	113	G
18	R	133	G
18	R	151	C
18	R	152	G
18	R	186	U
18	R	258	U
18	R	268	C
18	R	277	U
18	R	279	U
18	R	399	A
18	R	505	U

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	52:SER	C	1262:UNK	N	64.87

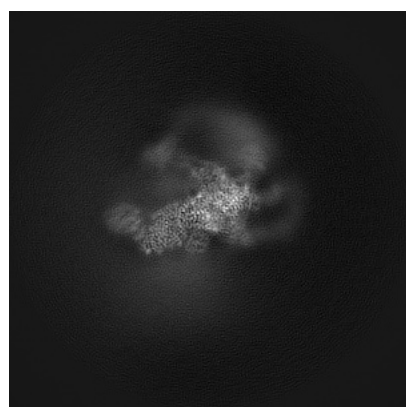
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0360. These allow visual inspection of the internal detail of the map and identification of artifacts.

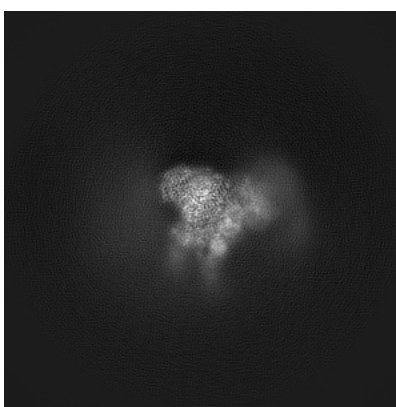
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

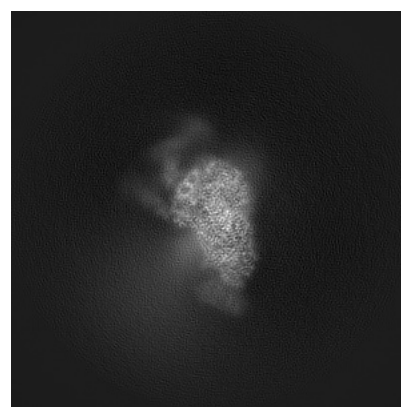
6.1.1 Primary map



X



Y

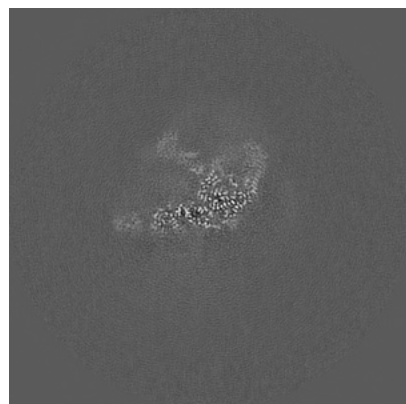


Z

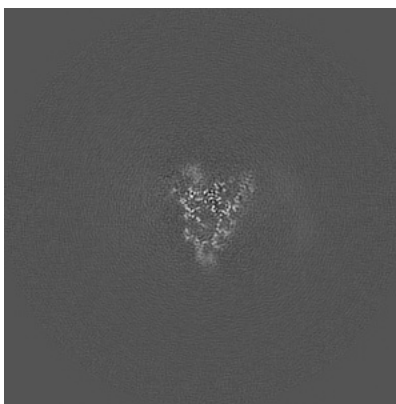
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

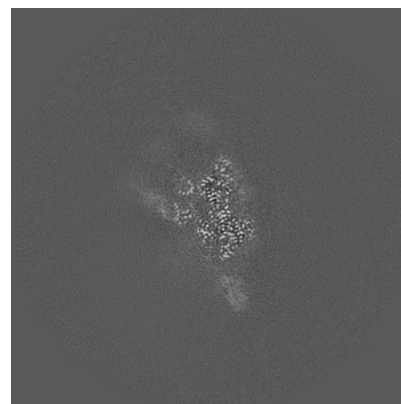
6.2.1 Primary map



X Index: 192



Y Index: 192

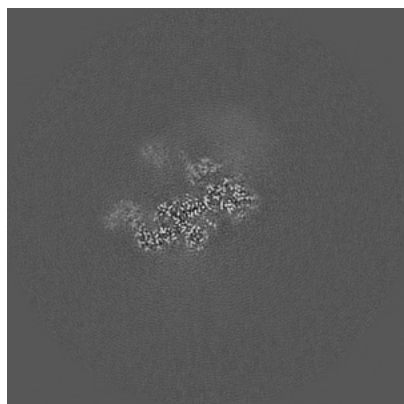


Z Index: 192

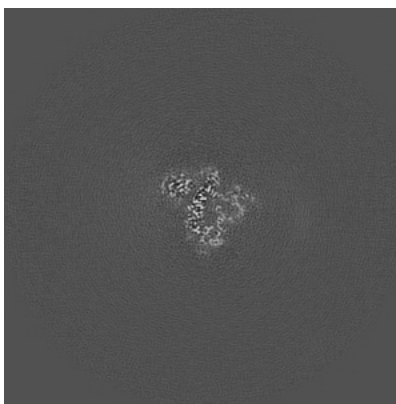
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

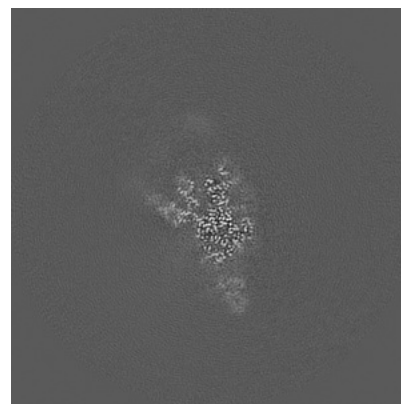
6.3.1 Primary map



X Index: 208



Y Index: 182

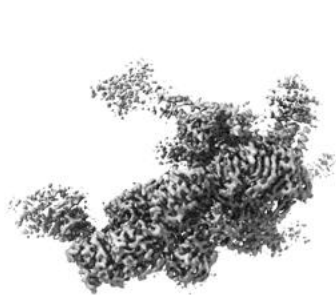


Z Index: 189

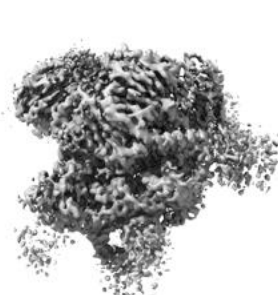
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

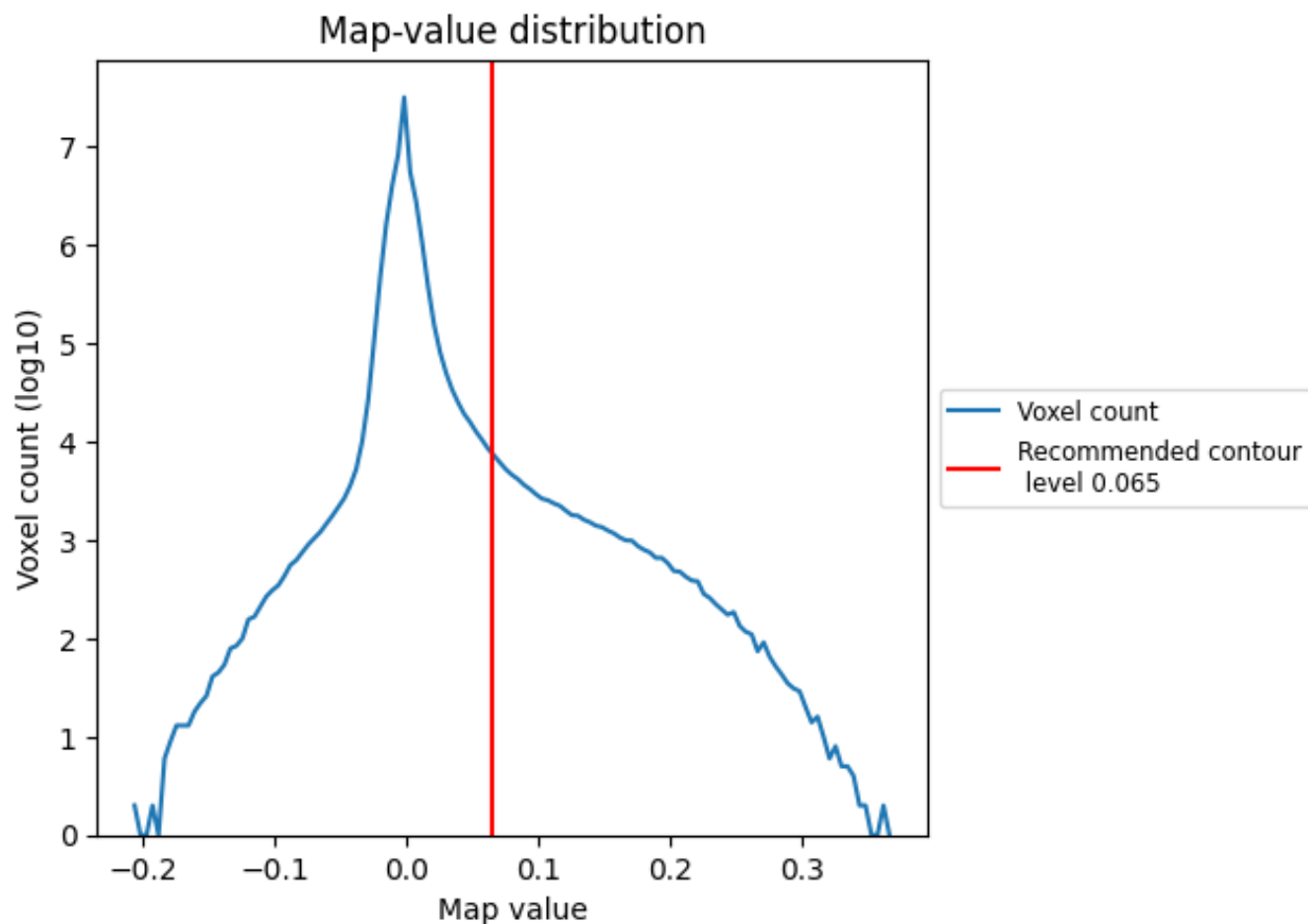
6.5 Mask visualisation

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

7 Map analysis [i](#)

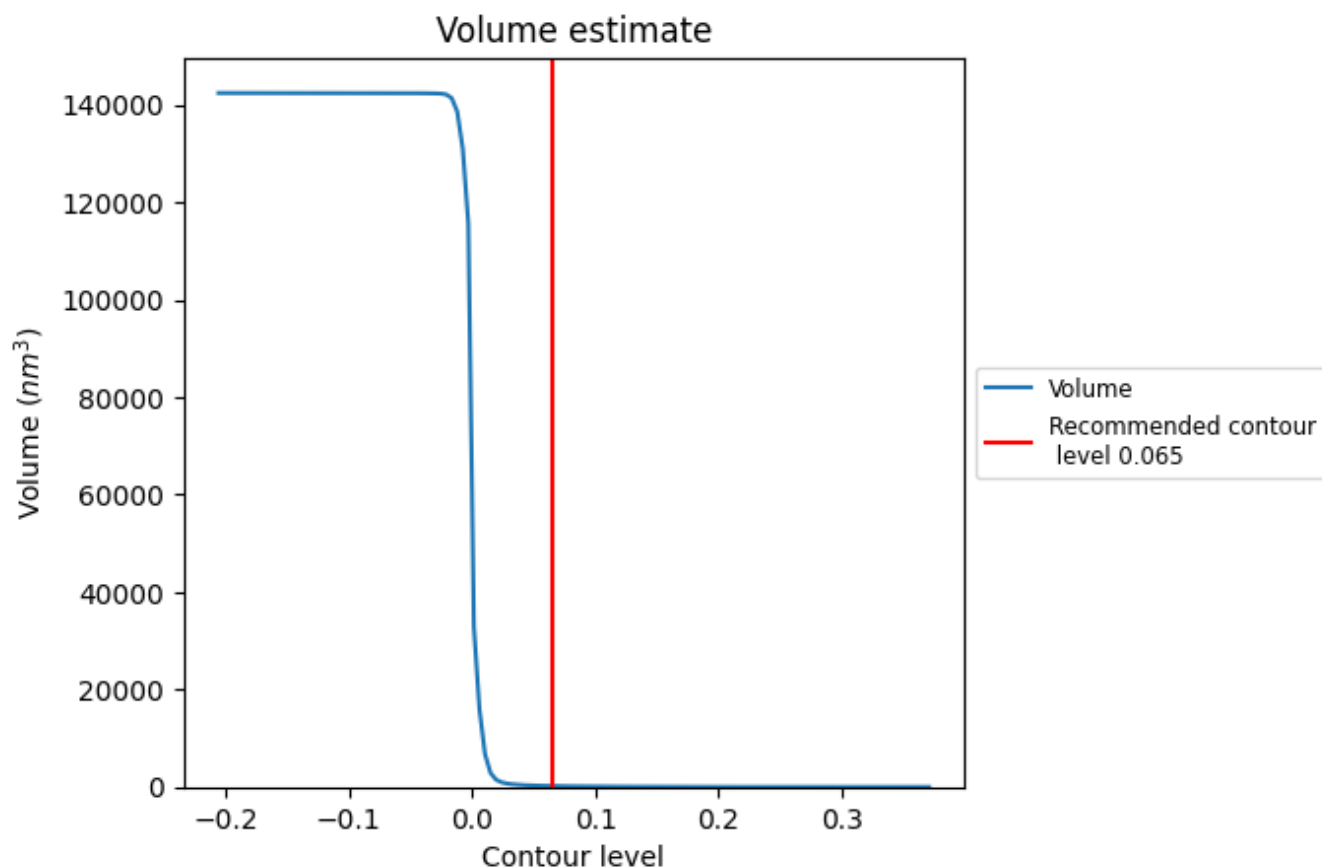
This section contains the results of statistical analysis of the map.

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.

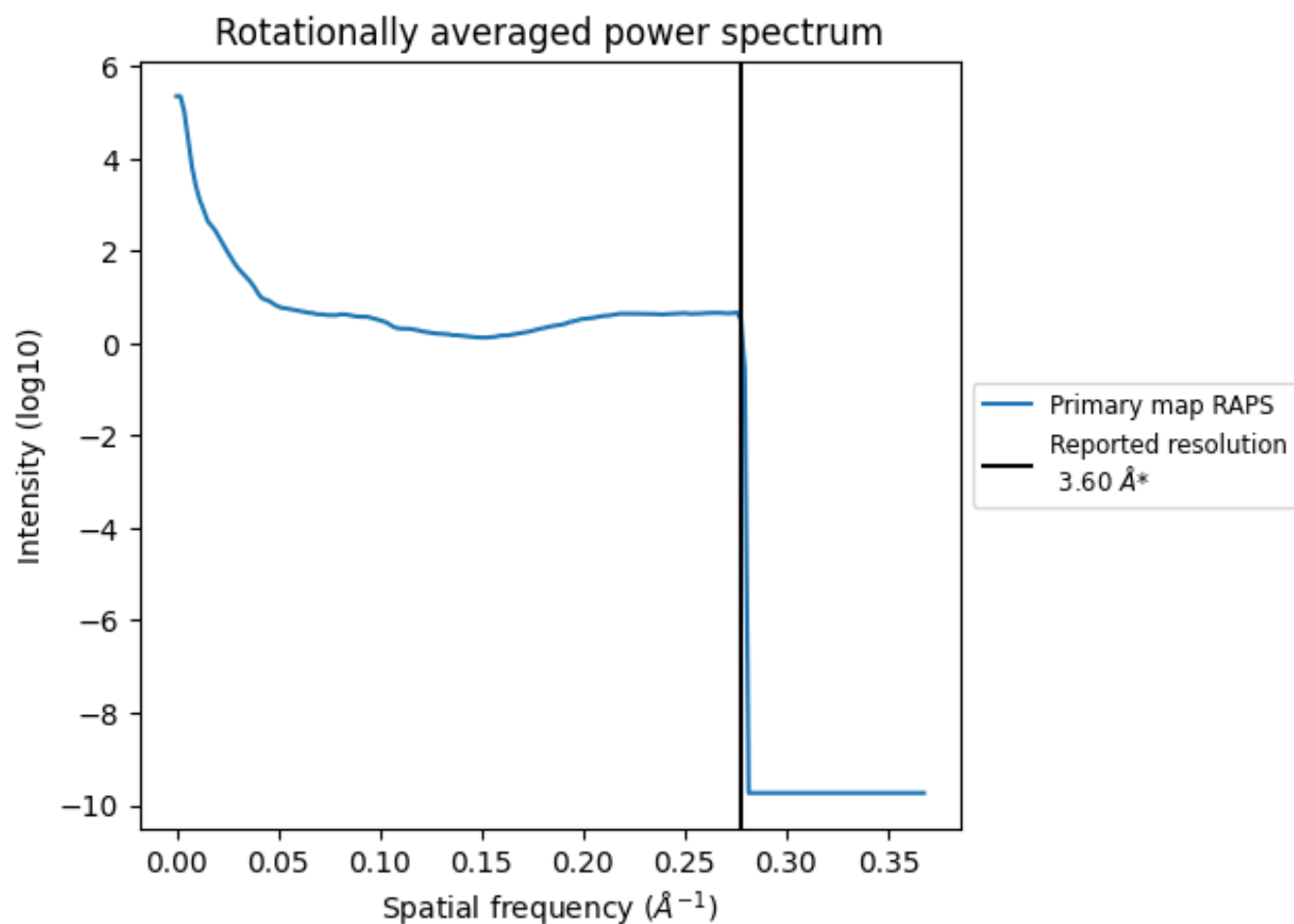
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 171 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 ⓘ

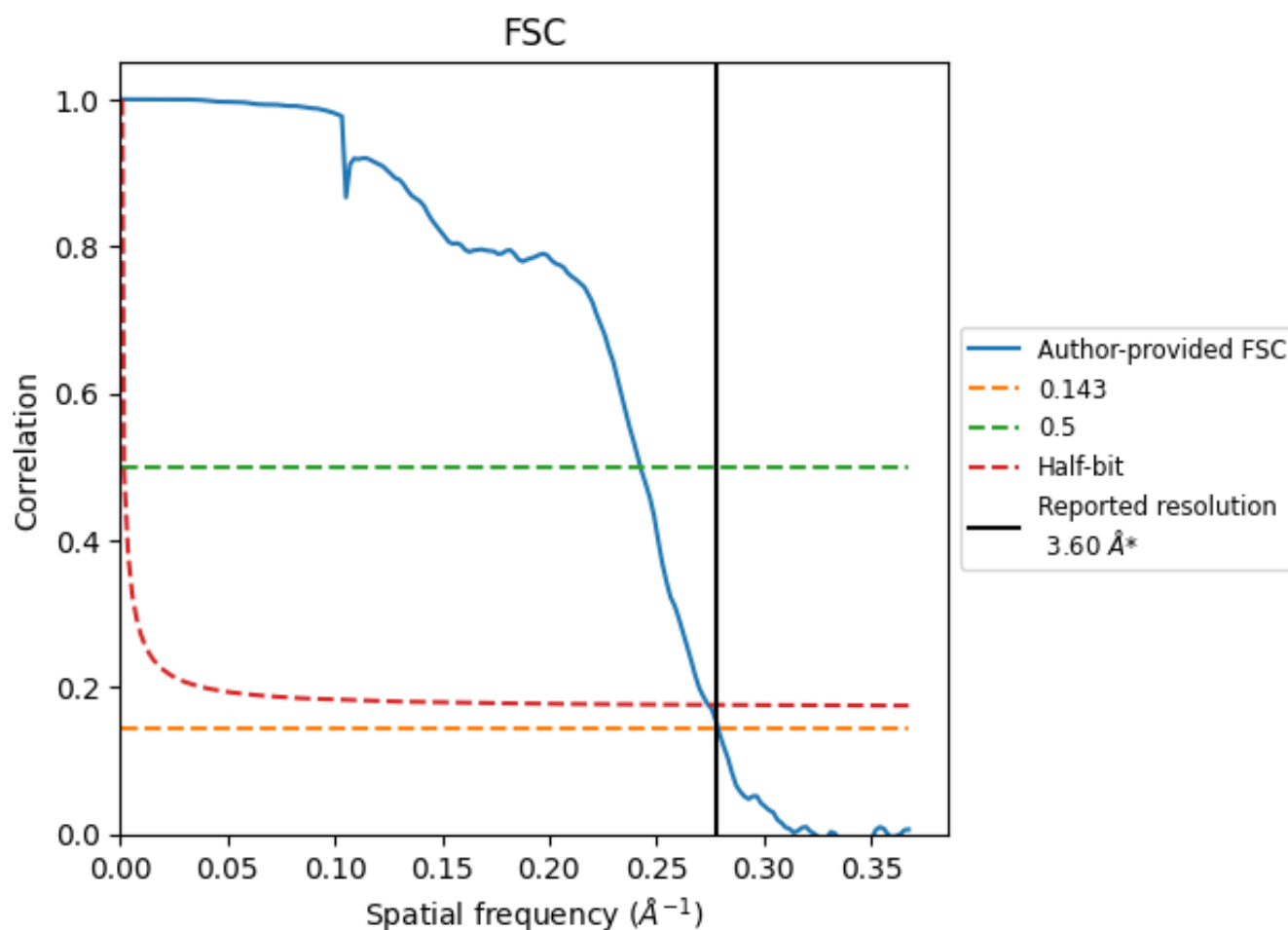


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

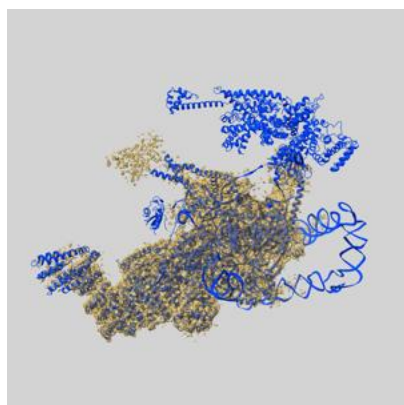
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.12	3.65
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

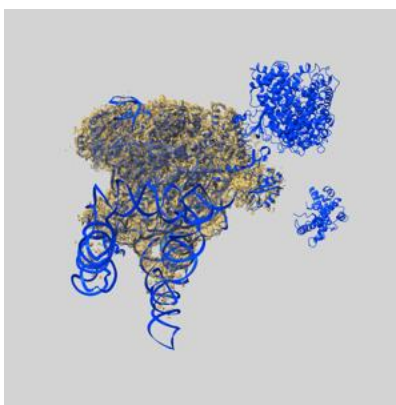
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0360 and PDB model 6N7P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

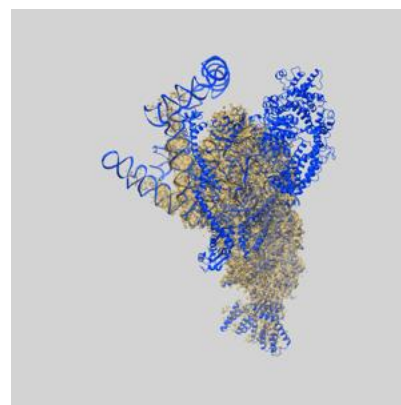
9.1 Map-model overlay [i](#)



X



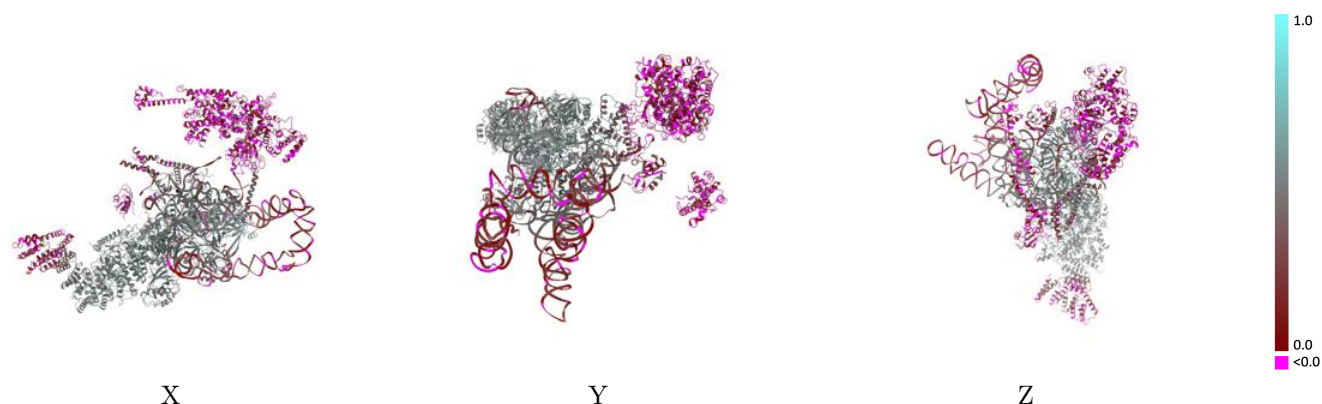
Y



Z

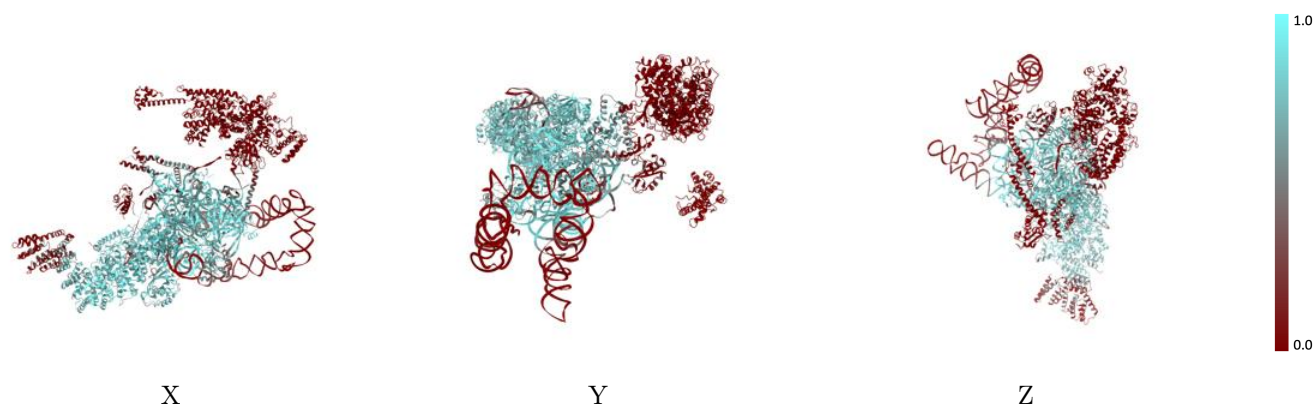
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



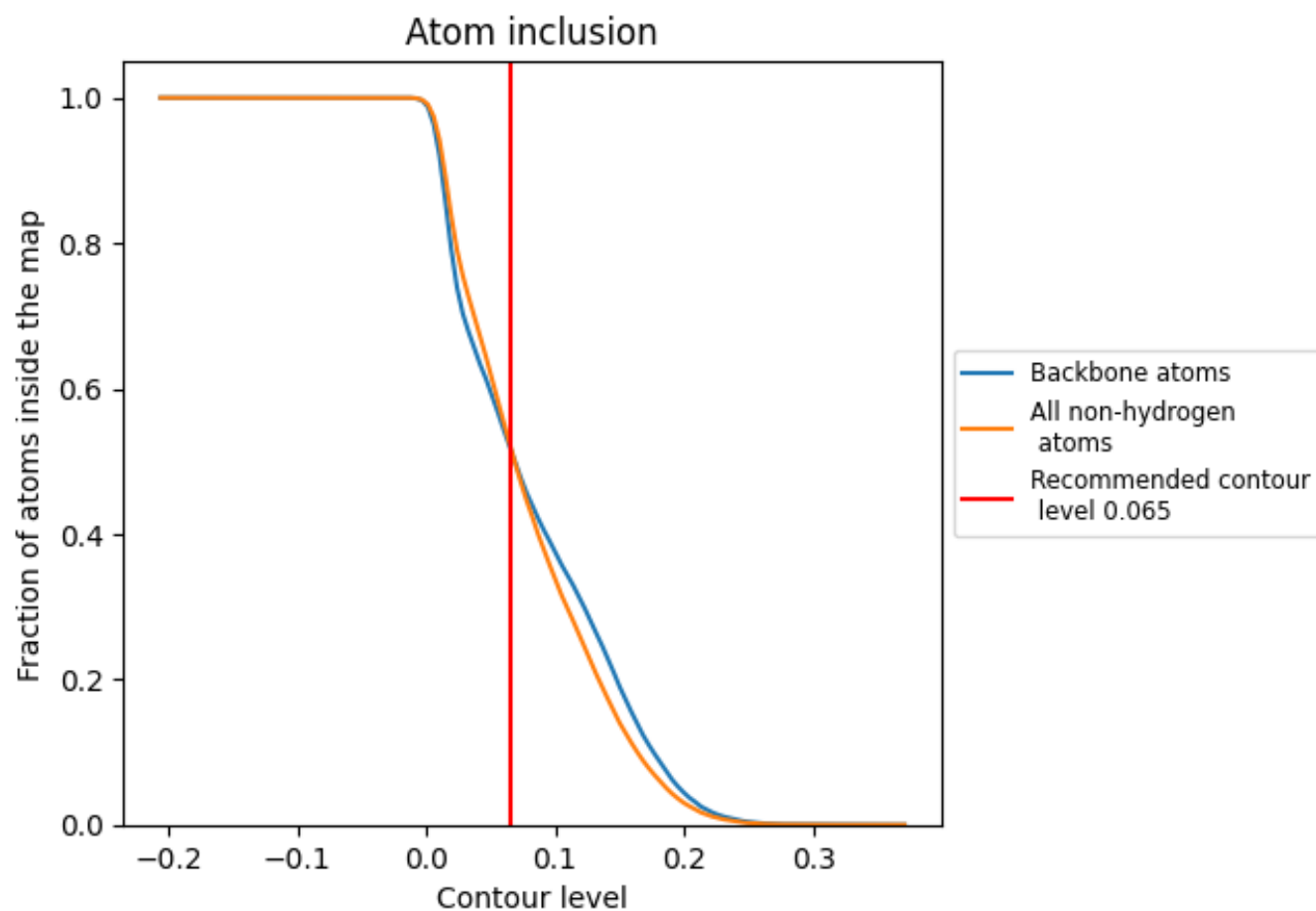
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5232	 0.3520
A	 0.4786	 0.3590
B	 0.7207	 0.4940
C	 0.6145	 0.4190
D	 0.8349	 0.5290
E	 0.5893	 0.3960
F	 0.6129	 0.4260
G	 0.7566	 0.5030
H	 0.6721	 0.4630
I	 0.5690	 0.4080
J	 0.0000	 0.0480
K	 0.7591	 0.5120
L	 0.7974	 0.5130
M	 0.7628	 0.5140
N	 0.7881	 0.5370
O	 0.8071	 0.5180
P	 0.8307	 0.5250
Q	 0.8019	 0.5270
R	 0.4331	 0.2710
X	 0.0000	 0.0480
Y	 0.0000	 0.0440
r	 0.4310	 0.2910

