Full wwPDB EM Validation Report

Jan 15, 2025 – 09:44 am GMT

PDB ID	:	8QSZ
EMDB ID	:	EMD-18643
Title	:	Structure of s. pombe RNA polymerase II in complex with DSIF and Rat1/Rai1
Authors	:	Carrique, L.; Kus, K.; Vasiljeva, L.; Grimes, J.M.
Deposited on	:	2023-10-12
Resolution	:	2.67 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

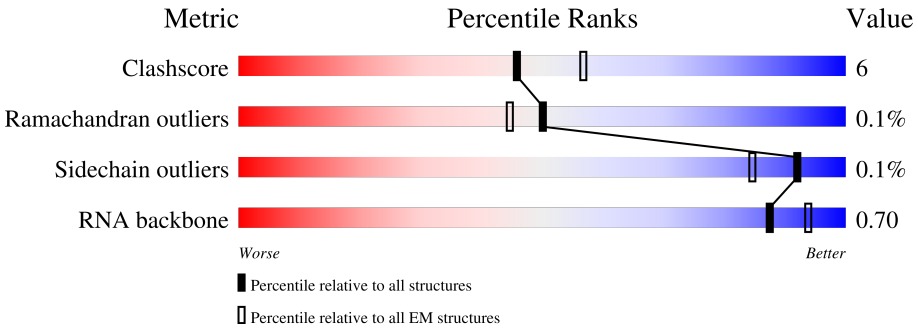
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.67 Å.

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



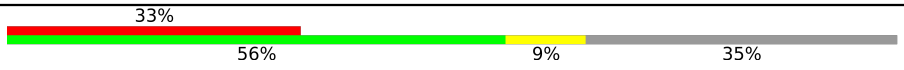
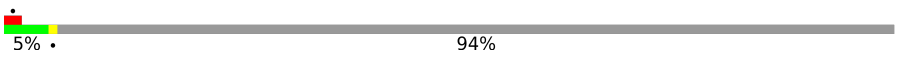
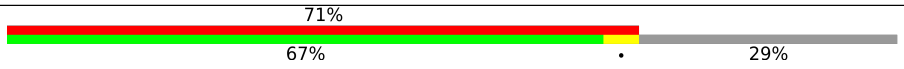
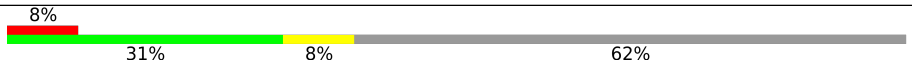
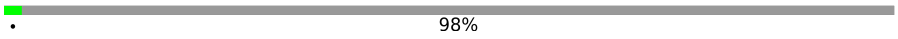
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1752	20% 70% 13% 18%
2	B	1210	15% 83% 16%
3	C	297	76% 11% 12%
4	E	210	30% 91% 8%
5	F	142	52% 6% 42%
6	G	172	16% 27% 71%
7	H	125	14% 87% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	141	
9	J	71	
10	K	123	
11	L	63	
12	Y	1122	
13	N	48	
14	P	26	
15	T	48	
16	X	896	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 62805 atoms, of which 31004 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 DNA-directed RNA polymerase II subunit rpb1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1441	22818	7172	11405	2007	2166	68	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1201	19128	6022	9539	1701	1803	63	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	260	4086	1300	2025	352	397	12	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	207	3348	1050	1684	301	307	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	82	1325	413	674	111	124	3	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit rpb7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	G	50	810	266	408	64	70	2	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	125	Total	C	H	N	O	S	0	0
			2022	636	1017	168	197	4		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9,RBP9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	92	Total	C	H	N	O	S	0	0
			1468	471	711	133	142	11		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	66	Total	C	H	N	O	S	0	0
			1079	339	547	89	97	7		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	116	Total	C	H	N	O	S	0	0
			1885	596	950	156	177	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	45	Total	C	H	N	O	S	0	0
			745	225	377	74	61	8		

- Molecule 12 is a protein called Transcription elongation factor spt5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	72	Total	C	H	N	O	S	0	0
			1165	352	600	107	104	2		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-131	MET	-	initiating methionine	UNP O13936
Y	-130	LYS	-	expression tag	UNP O13936
Y	-129	HIS	-	expression tag	UNP O13936
Y	-128	HIS	-	expression tag	UNP O13936

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-127	HIS	-	expression tag	UNP O13936
Y	-126	HIS	-	expression tag	UNP O13936
Y	-125	HIS	-	expression tag	UNP O13936
Y	-124	HIS	-	expression tag	UNP O13936
Y	-123	PRO	-	expression tag	UNP O13936
Y	-122	MET	-	expression tag	UNP O13936
Y	-121	SER	-	expression tag	UNP O13936
Y	-120	ASP	-	expression tag	UNP O13936
Y	-119	LYS	-	expression tag	UNP O13936
Y	-118	ILE	-	expression tag	UNP O13936
Y	-117	ILE	-	expression tag	UNP O13936
Y	-116	HIS	-	expression tag	UNP O13936
Y	-115	LEU	-	expression tag	UNP O13936
Y	-114	THR	-	expression tag	UNP O13936
Y	-113	ASP	-	expression tag	UNP O13936
Y	-112	ASP	-	expression tag	UNP O13936
Y	-111	SER	-	expression tag	UNP O13936
Y	-110	PHE	-	expression tag	UNP O13936
Y	-109	ASP	-	expression tag	UNP O13936
Y	-108	THR	-	expression tag	UNP O13936
Y	-107	ASP	-	expression tag	UNP O13936
Y	-106	VAL	-	expression tag	UNP O13936
Y	-105	LEU	-	expression tag	UNP O13936
Y	-104	LYS	-	expression tag	UNP O13936
Y	-103	ALA	-	expression tag	UNP O13936
Y	-102	ASP	-	expression tag	UNP O13936
Y	-101	GLY	-	expression tag	UNP O13936
Y	-100	ALA	-	expression tag	UNP O13936
Y	-99	ILE	-	expression tag	UNP O13936
Y	-98	LEU	-	expression tag	UNP O13936
Y	-97	VAL	-	expression tag	UNP O13936
Y	-96	ASP	-	expression tag	UNP O13936
Y	-95	PHE	-	expression tag	UNP O13936
Y	-94	TRP	-	expression tag	UNP O13936
Y	-93	ALA	-	expression tag	UNP O13936
Y	-92	GLU	-	expression tag	UNP O13936
Y	-91	TRP	-	expression tag	UNP O13936
Y	-90	CYS	-	expression tag	UNP O13936
Y	-89	GLY	-	expression tag	UNP O13936
Y	-88	PRO	-	expression tag	UNP O13936
Y	-87	CYS	-	expression tag	UNP O13936
Y	-86	LYS	-	expression tag	UNP O13936

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-85	MET	-	expression tag	UNP O13936
Y	-84	ILE	-	expression tag	UNP O13936
Y	-83	ALA	-	expression tag	UNP O13936
Y	-82	PRO	-	expression tag	UNP O13936
Y	-81	ILE	-	expression tag	UNP O13936
Y	-80	LEU	-	expression tag	UNP O13936
Y	-79	ASP	-	expression tag	UNP O13936
Y	-78	GLU	-	expression tag	UNP O13936
Y	-77	ILE	-	expression tag	UNP O13936
Y	-76	ALA	-	expression tag	UNP O13936
Y	-75	ASP	-	expression tag	UNP O13936
Y	-74	GLU	-	expression tag	UNP O13936
Y	-73	TYR	-	expression tag	UNP O13936
Y	-72	GLN	-	expression tag	UNP O13936
Y	-71	GLY	-	expression tag	UNP O13936
Y	-70	LYS	-	expression tag	UNP O13936
Y	-69	LEU	-	expression tag	UNP O13936
Y	-68	THR	-	expression tag	UNP O13936
Y	-67	VAL	-	expression tag	UNP O13936
Y	-66	ALA	-	expression tag	UNP O13936
Y	-65	LYS	-	expression tag	UNP O13936
Y	-64	LEU	-	expression tag	UNP O13936
Y	-63	ASN	-	expression tag	UNP O13936
Y	-62	ILE	-	expression tag	UNP O13936
Y	-61	ASP	-	expression tag	UNP O13936
Y	-60	GLN	-	expression tag	UNP O13936
Y	-59	ASN	-	expression tag	UNP O13936
Y	-58	PRO	-	expression tag	UNP O13936
Y	-57	GLY	-	expression tag	UNP O13936
Y	-56	THR	-	expression tag	UNP O13936
Y	-55	ALA	-	expression tag	UNP O13936
Y	-54	PRO	-	expression tag	UNP O13936
Y	-53	LYS	-	expression tag	UNP O13936
Y	-52	TYR	-	expression tag	UNP O13936
Y	-51	GLY	-	expression tag	UNP O13936
Y	-50	ILE	-	expression tag	UNP O13936
Y	-49	ARG	-	expression tag	UNP O13936
Y	-48	GLY	-	expression tag	UNP O13936
Y	-47	ILE	-	expression tag	UNP O13936
Y	-46	PRO	-	expression tag	UNP O13936
Y	-45	THR	-	expression tag	UNP O13936
Y	-44	LEU	-	expression tag	UNP O13936

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-43	LEU	-	expression tag	UNP O13936
Y	-42	LEU	-	expression tag	UNP O13936
Y	-41	PHE	-	expression tag	UNP O13936
Y	-40	LYS	-	expression tag	UNP O13936
Y	-39	ASN	-	expression tag	UNP O13936
Y	-38	GLY	-	expression tag	UNP O13936
Y	-37	GLU	-	expression tag	UNP O13936
Y	-36	VAL	-	expression tag	UNP O13936
Y	-35	ALA	-	expression tag	UNP O13936
Y	-34	ALA	-	expression tag	UNP O13936
Y	-33	THR	-	expression tag	UNP O13936
Y	-32	LYS	-	expression tag	UNP O13936
Y	-31	VAL	-	expression tag	UNP O13936
Y	-30	GLY	-	expression tag	UNP O13936
Y	-29	ALA	-	expression tag	UNP O13936
Y	-28	LEU	-	expression tag	UNP O13936
Y	-27	SER	-	expression tag	UNP O13936
Y	-26	LYS	-	expression tag	UNP O13936
Y	-25	GLY	-	expression tag	UNP O13936
Y	-24	GLN	-	expression tag	UNP O13936
Y	-23	LEU	-	expression tag	UNP O13936
Y	-22	LYS	-	expression tag	UNP O13936
Y	-21	GLU	-	expression tag	UNP O13936
Y	-20	PHE	-	expression tag	UNP O13936
Y	-19	LEU	-	expression tag	UNP O13936
Y	-18	ASP	-	expression tag	UNP O13936
Y	-17	ALA	-	expression tag	UNP O13936
Y	-16	ASN	-	expression tag	UNP O13936
Y	-15	LEU	-	expression tag	UNP O13936
Y	-14	ALA	-	expression tag	UNP O13936
Y	-13	GLY	-	expression tag	UNP O13936
Y	-12	SER	-	expression tag	UNP O13936
Y	-11	GLY	-	expression tag	UNP O13936
Y	-10	SER	-	expression tag	UNP O13936
Y	-9	GLY	-	expression tag	UNP O13936
Y	-8	SER	-	expression tag	UNP O13936
Y	-7	GLU	-	expression tag	UNP O13936
Y	-6	ASN	-	expression tag	UNP O13936
Y	-5	LEU	-	expression tag	UNP O13936
Y	-4	TYR	-	expression tag	UNP O13936
Y	-3	PHE	-	expression tag	UNP O13936
Y	-2	GLN	-	expression tag	UNP O13936

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-1	GLY	-	expression tag	UNP O13936
Y	0	ALA	-	expression tag	UNP O13936

- Molecule 13 is a DNA chain called DNA none template (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	34	Total	C	H	N	O	P	0	0
			1091	335	383	136	203	34		

- Molecule 14 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	10	Total	C	H	N	O	P	0	0
			327	97	109	42	69	10		

- Molecule 15 is a DNA chain called DNA template (40-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
15	T	40	Total	C	H	N	O	P	0	0
			1257	385	449	143	240	40		

- Molecule 16 is a protein called 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	16	Total	C	H	N	O	0	0
			250	72	126	29	23		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	237	ALA	ASP	conflict	UNP P40848
X	886	GLY	TYR	conflict	UNP P40848
X	887	SER	ARG	conflict	UNP P40848
X	889	HIS	GLY	conflict	UNP P40848
X	891	HIS	GLN	conflict	UNP P40848
X	892	HIS	SER	conflict	UNP P40848
X	893	HIS	TYR	conflict	UNP P40848
X	894	HIS	-	expression tag	UNP P40848
X	895	HIS	-	expression tag	UNP P40848
X	896	HIS	-	expression tag	UNP P40848

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

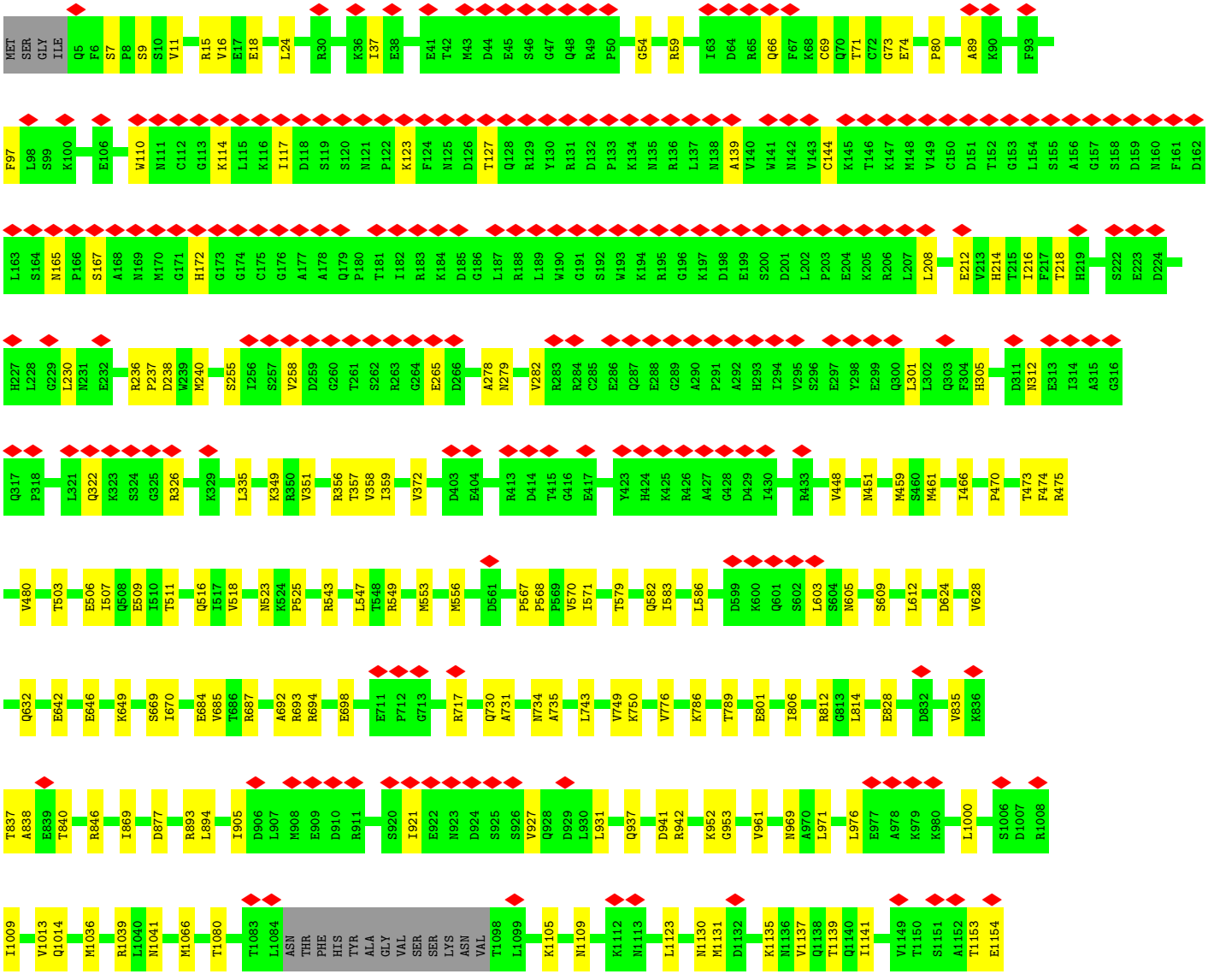
Mol	Chain	Residues	Atoms	AltConf
17	C	1	Total Zn 1 1	0

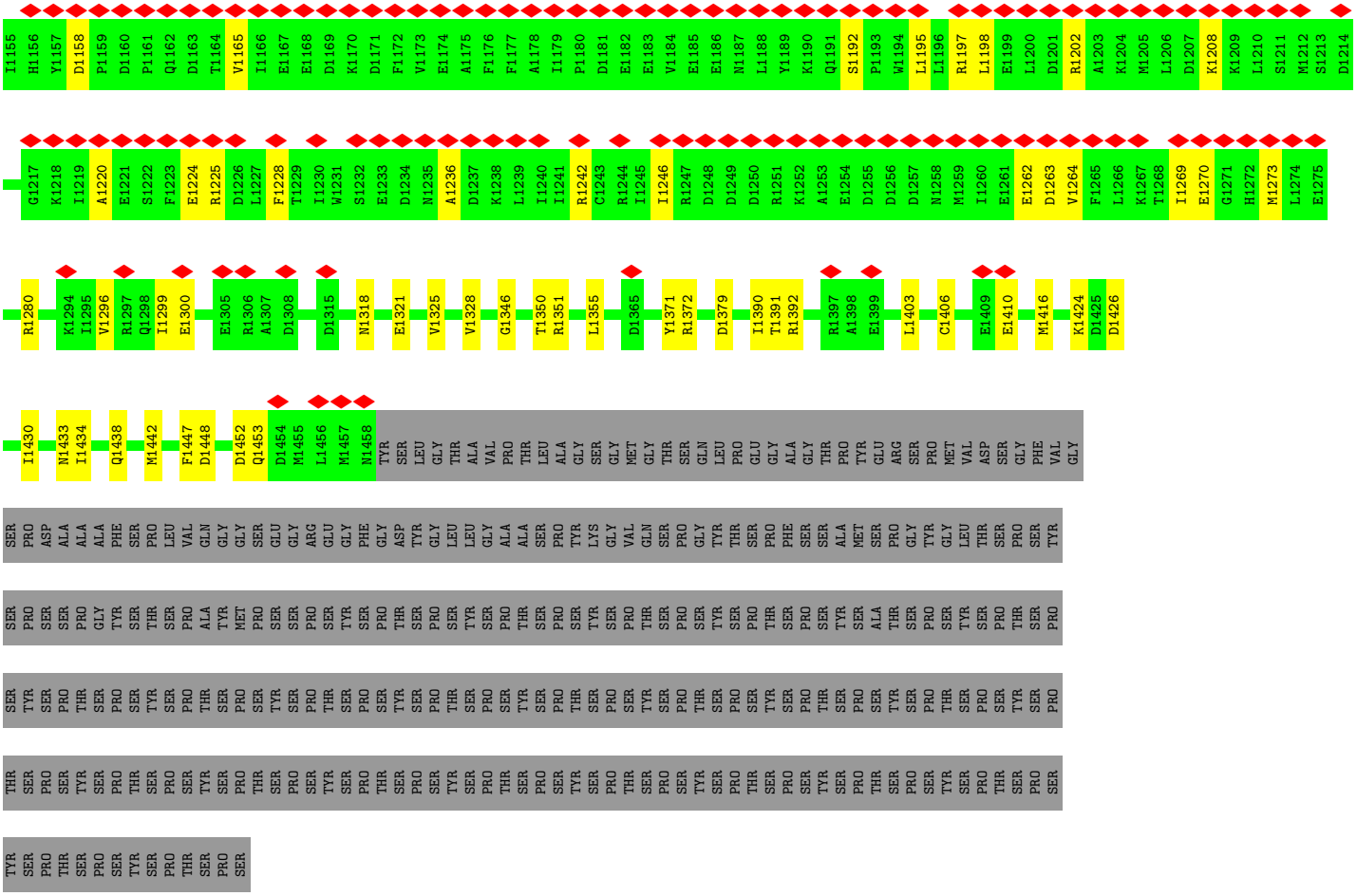
3 Residue-property plots (i)

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

• Molecule 1: DNA-directed RNA polymerase II subunit rpb1

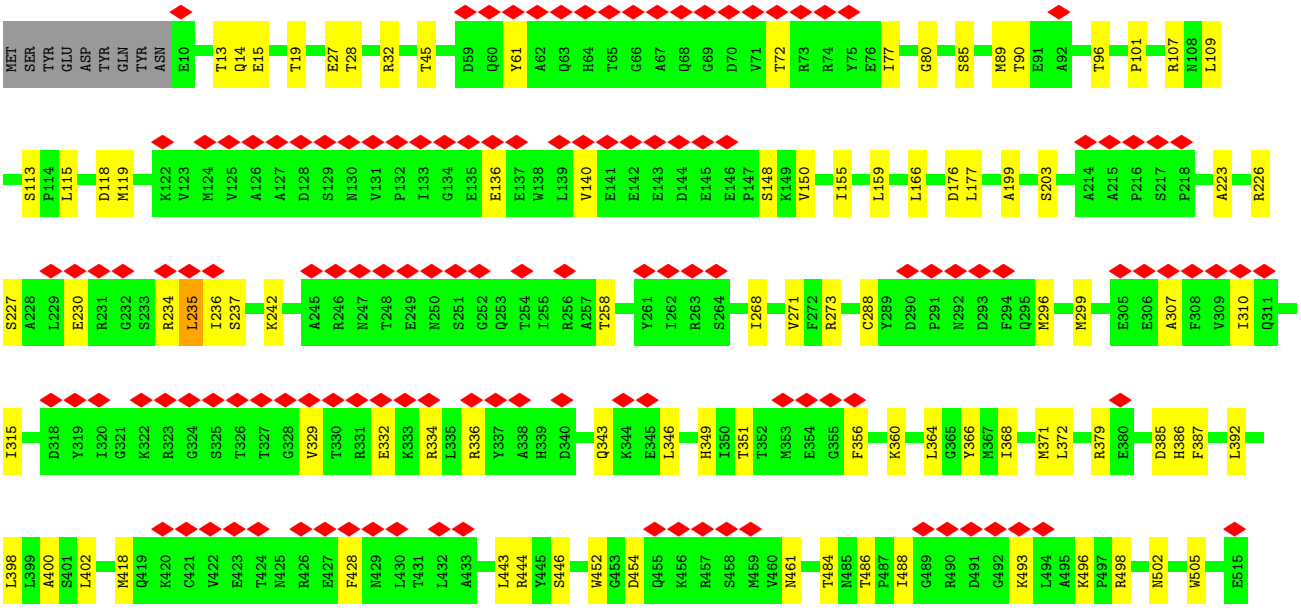
Chain A:

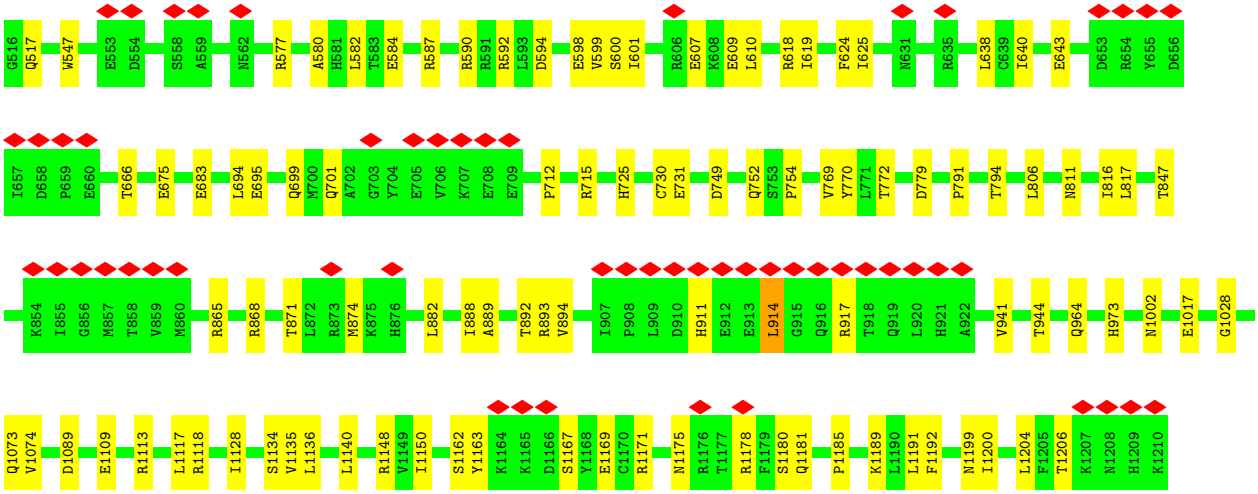




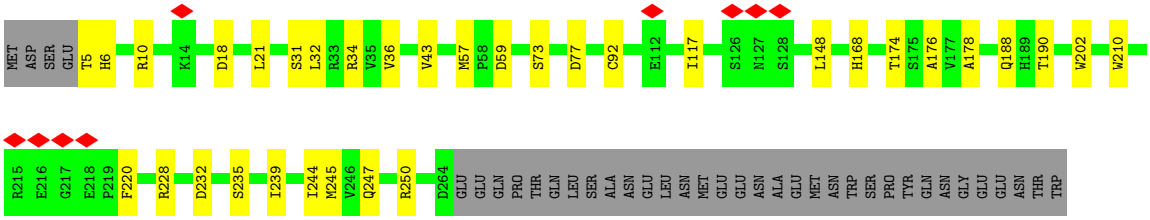
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

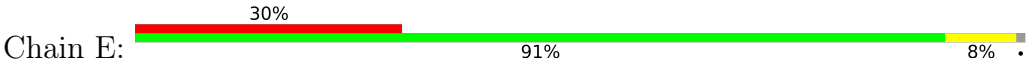


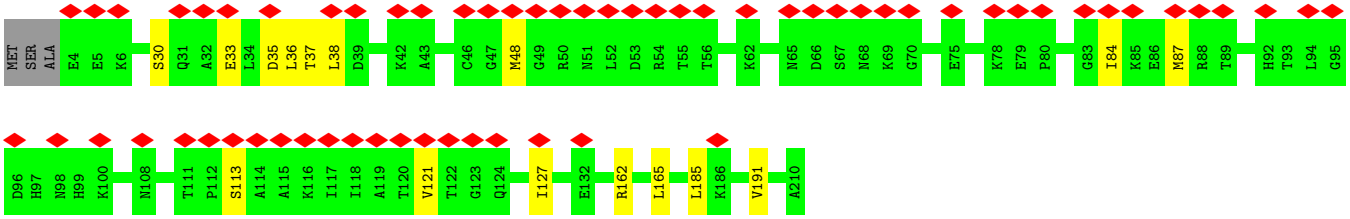


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

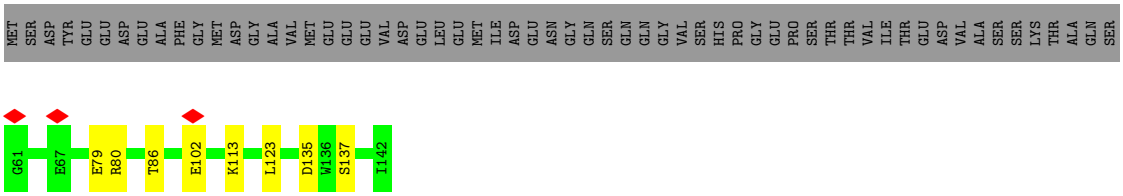


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



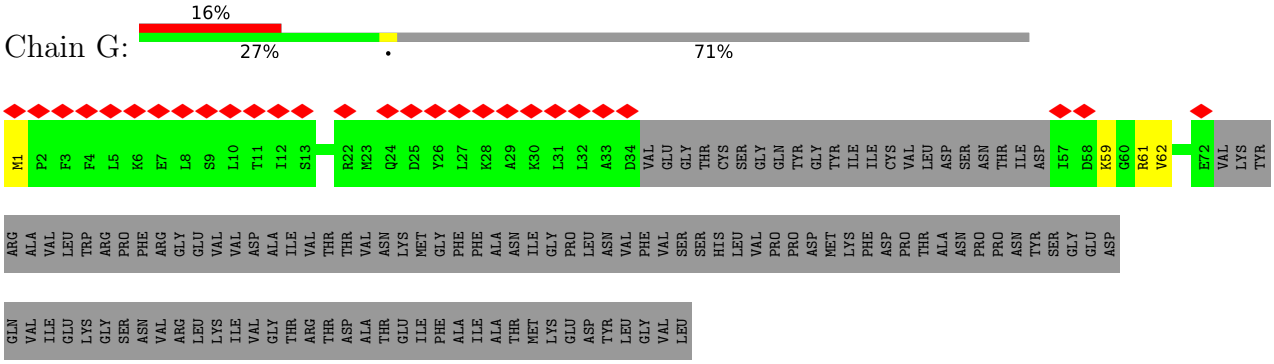


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



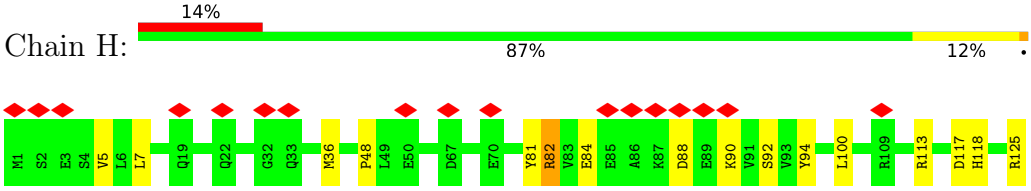
• Molecule 6: DNA-directed RNA polymerase II subunit rpb7

Chain G:



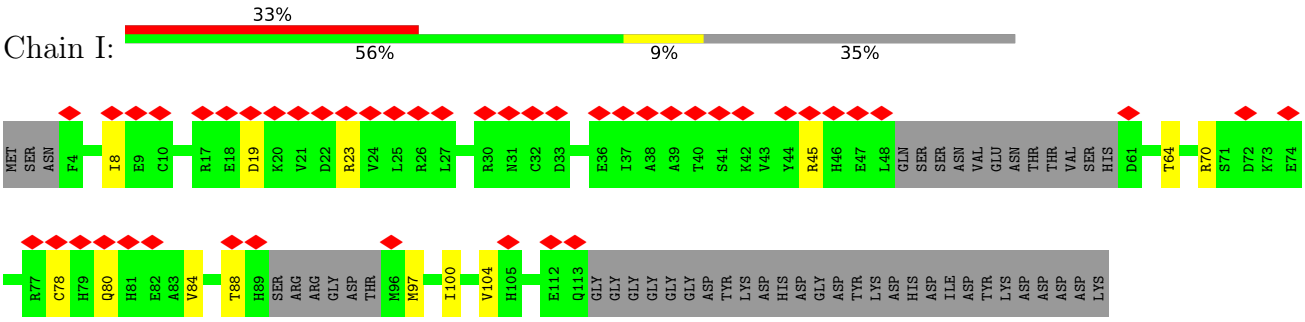
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



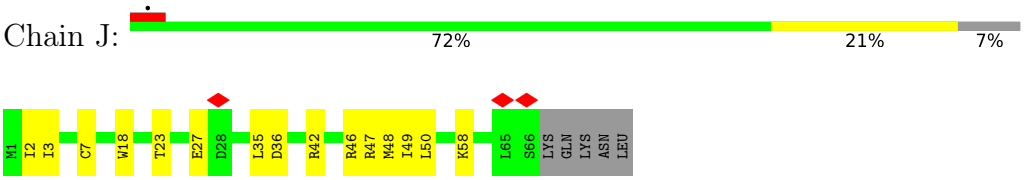
• Molecule 8: DNA-directed RNA polymerase II subunit RPB9,RBP9

Chain I:



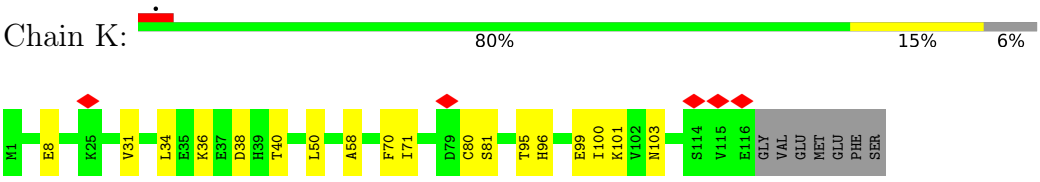
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



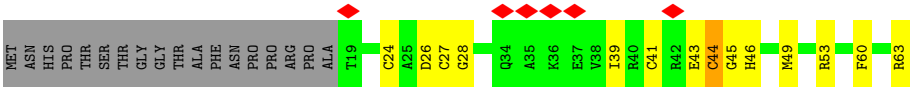
• Molecule 10: DNA-directed RNA polymerase II subunit RPB11

Chain K:



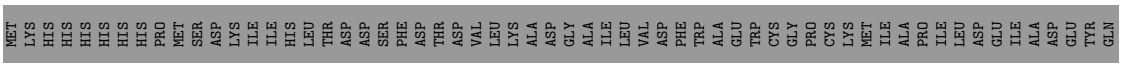
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

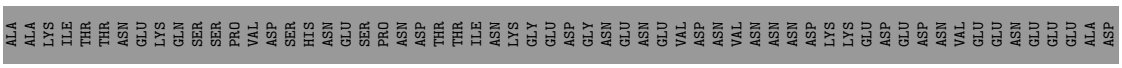
Chain L:

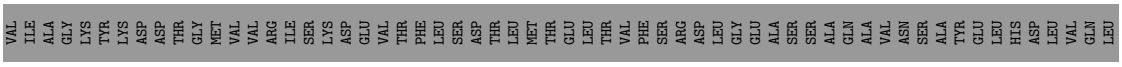


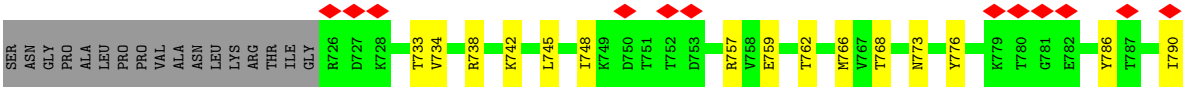
• Molecule 12: Transcription elongation factor spt5

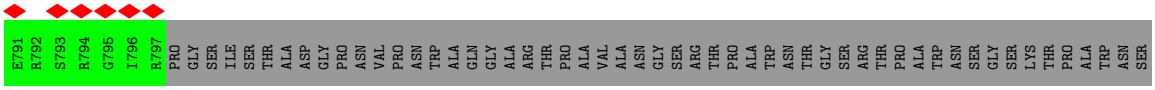
Chain Y: 5% 94%

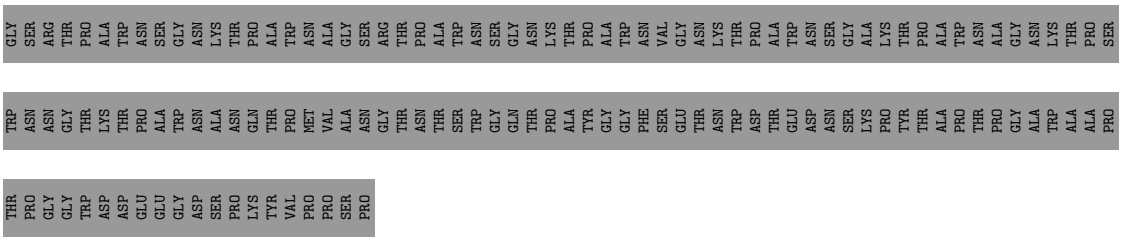




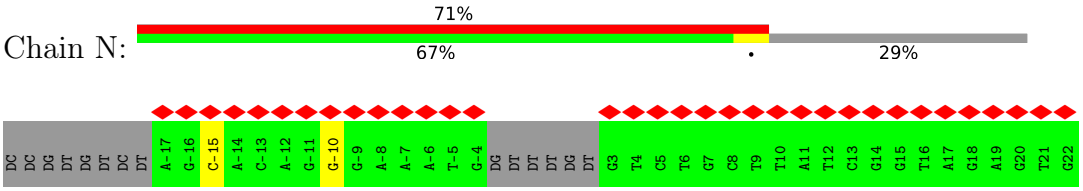




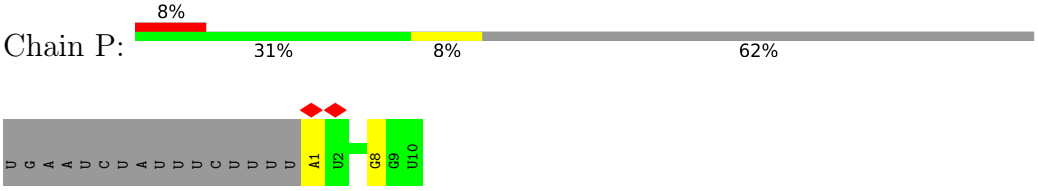




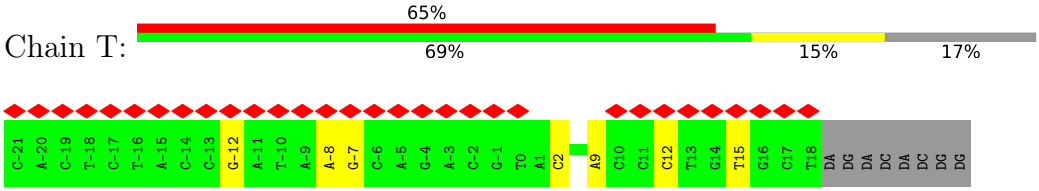
• Molecule 13: DNA none template (34-MER)



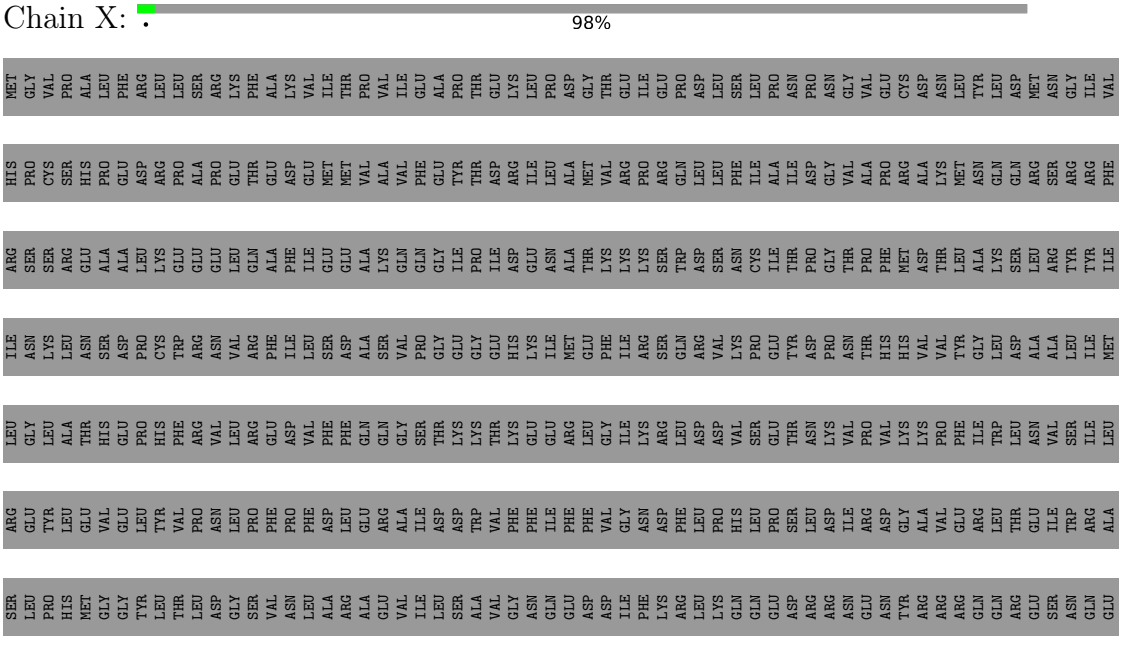
• Molecule 14: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*U)-3')

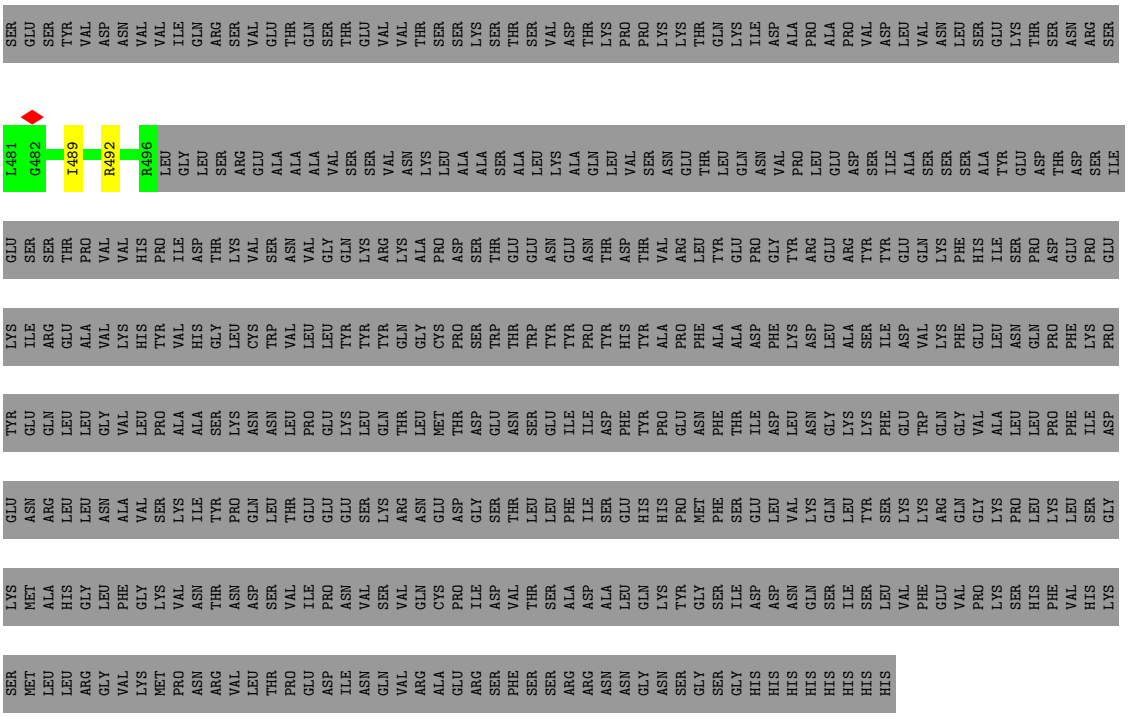


• Molecule 15: DNA template (40-MER)



• Molecule 16: 5'-3' exoribonuclease 2




SER GLU SER TYR VAL ASP ASN VAL VAL ILE GLN ARG SER VAL GLU THR GLN SER THR GLU VAL VAL THR SER SER LYS SER THR SER VAL ASP THR LYS PRO PRO LYS LYS THR GLN LYS ILE ASP ALA PRO ALA PRO VAL ASP LEU VAL ASN LEU SER GLU LYS THR SER ASN ARG SER
L481 G482 I489 R492 R496
LEU GLY LEU SER ARG GLU ALA ALA ALA VAL SER SER VAL ASN LYS LEU ALA ALA SER ALA LEU LYS ALA GLN LEU GLU ASN GLU ASN THR ASP THR VAL ARG LEU TYR GLU PRO GLY TYR ARG GLU ARG TYR TYR GLU GLN LYS PHE HIS ILE SER PRO ASP GLU PRO GLU
GLU SER SER THR PRO VAL VAL HIS PRO ILE ASP THR LYS VAL SER ASN VAL GLY GLN LYS ARG LYS ALA PRO ASP SER THR GLU GLU ASN GLU ASN THR ASP THR VAL ARG LEU TYR GLU PRO GLY TYR ARG GLU ARG TYR TYR GLU GLN LYS PHE HIS ILE SER PRO ASP GLU PRO GLU
LYS ILE ARG GLU ALA VAL LYS HIS TYR VAL HIS GLY LEU CYS TRP VAL LEU LEU TYR TYR TYR GLN GLY CYS PRO SER TRP THR TRP TYR TYR PRO TYR HIS TYR ALA PRO PHE ALA ALA ASP PHE LYS ASP LEU ALA SER ILE ASP VAL LYS PHE GLU LEU ASN GLN PRO PHE LYS PRO
TYR GLU GLN LEU LEU GLY VAL LEU PRO ALA ALA SER LYS ASN ASN LEU PRO GLU LYS LEU GLN THR LEU MET THR ASP GLU ASN SER GLU ILE GLU ILE ASP PHE TYR PRO GLU ASN PHE THR ILE ASP LEU ASN GLY LYS LYS PHE GLU TRP GLN GLY VAL ALA LEU LEU PRO PHE ILE ASP
GLU ASN ARG LEU LEU ASN ALA VAL SER LYS ILE TYR PRO GLN LEU THR GLU GLU GLU SER LYS ARG ASN GLU ASP GLY SER THR LEU LEU PHE ILE SER GLU HIS HIS PRO MET PHE SER GLU LEU VAL LYS GLN LEU TYR SER LYS LYS ARG GLN GLY LYS PRO LEU LYS LEU SER GLY
LYS MET ALA HIS GLY LEU PHE GLY LYS VAL ASN THR ASN ASP SER VAL ILE PRO ASN VAL SER VAL GLN CYS PRO ILE ASP VAL THR SER ALA ASP ALA ASP ASN GLN SER ILE SER LEU VAL PHE GLU VAL PRO LYS SER HIS PHE VAL HIS LYS
SER MET LEU LEU ARG GLY VAL LYS MET PRO ASN ARG VAL LEU THR PRO GLU ASP ILE ASN GLN VAL ARG ALA GLU ARG SER PHE SER SER ARG ARG ASN ASN GLY ASN SER GLY SER GLY HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	215000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	24000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.573	Depositor
Minimum map value	-1.612	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.336	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	352, 352, 352	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: 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	0.27	0/11626	0.51	0/15713
2	B	0.29	0/9780	0.53	1/13218 (0.0%)
3	C	0.30	0/2108	0.51	0/2868
4	E	0.27	0/1696	0.51	0/2287
5	F	0.29	0/661	0.50	0/893
6	G	0.28	0/412	0.44	0/552
7	H	0.29	0/1019	0.53	0/1373
8	I	0.27	0/773	0.52	0/1042
9	J	0.33	0/540	0.53	0/728
10	K	0.29	0/952	0.48	0/1290
11	L	0.39	0/371	0.71	1/491 (0.2%)
12	Y	0.26	0/570	0.58	0/764
13	N	0.48	0/795	0.86	0/1225
14	P	0.33	0/244	0.63	0/379
15	T	0.53	0/903	0.90	0/1388
16	X	0.21	0/123	0.59	0/164
All	All	0.30	0/32573	0.55	2/44375 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	914	LEU	CB-CG-CD2	6.23	121.59	111.00
11	L	44	CYS	CA-CB-SG	6.08	124.94	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11413	11405	11413	159	0
2	B	9589	9539	9546	145	0
3	C	2061	2025	2025	31	0
4	E	1664	1684	1684	12	0
5	F	651	674	674	6	0
6	G	402	408	407	4	0
7	H	1005	1017	1018	12	0
8	I	757	711	710	12	0
9	J	532	547	546	13	0
10	K	935	950	950	15	0
11	L	368	377	377	11	0
12	Y	565	600	600	12	0
13	N	708	383	384	2	0
14	P	218	109	109	1	0
15	T	808	449	450	7	0
16	X	124	126	126	2	0
17	C	1	0	0	0	0
All	All	31801	31004	31019	374	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 (374) 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)
1:A:1036:MET:O	1:A:1039:ARG:NH1	1.97	0.95
1:A:1153:THR:OG1	1:A:1270:GLU:OE2	1.85	0.93
2:B:366:TYR:OH	2:B:609:GLU:OE2	1.89	0.90
1:A:971:LEU:HD23	1:A:976:LEU:HD12	1.54	0.88
5:F:102:GLU:OE1	5:F:113:LYS:NZ	2.09	0.86
1:A:1424:LYS:NZ	1:A:1426:ASP:OD1	2.09	0.86
1:A:605:ASN:ND2	1:A:609:SER:OG	2.08	0.86
1:A:470:PRO:O	1:A:475:ARG:NH2	2.11	0.83
2:B:444:ARG:NH1	15:T:9:DA:OP1	2.12	0.83
2:B:85:SER:O	2:B:113:SER:OG	1.96	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:OE1	5:F:80:ARG:NH1	2.11	0.82
1:A:894:LEU:O	1:A:942:ARG:NH2	2.13	0.81
3:C:77:ASP:OD2	3:C:247:GLN:NE2	2.14	0.80
2:B:242:LYS:NZ	2:B:258:THR:OG1	2.14	0.80
1:A:893:ARG:NH1	1:A:953:GLY:O	2.15	0.80
2:B:203:SER:OG	2:B:226:ARG:NH1	2.15	0.79
1:A:869:ILE:HD12	4:E:165:LEU:HD11	1.64	0.78
3:C:210:TRP:O	3:C:228:ARG:NH1	2.17	0.77
1:A:1392:ARG:NH1	1:A:1410:GLU:OE2	2.16	0.77
2:B:230:GLU:O	2:B:234:ARG:NH1	2.17	0.77
1:A:349:LYS:NZ	2:B:1140:LEU:O	2.12	0.77
1:A:523:ASN:OD1	1:A:632:GLN:NE2	2.18	0.76
2:B:587:ARG:NH2	2:B:601:ILE:O	2.20	0.75
2:B:893:ARG:NH1	2:B:894:VAL:O	2.20	0.74
1:A:165:ASN:OD1	1:A:167:SER:OG	2.06	0.73
2:B:871:THR:OG1	2:B:874:MET:SD	2.47	0.73
1:A:684:GLU:OE1	1:A:687:ARG:NH2	2.22	0.72
2:B:888:ILE:O	2:B:941:VAL:HG21	1.89	0.72
1:A:921:ILE:HG21	1:A:927:VAL:HG11	1.72	0.71
12:Y:786:TYR:O	12:Y:790:ILE:HD12	1.90	0.71
1:A:89:ALA:N	1:A:279:ASN:OD1	2.23	0.71
1:A:603:LEU:O	7:H:81:TYR:OH	2.07	0.70
2:B:177:LEU:HD21	16:X:489:ILE:HG23	1.73	0.70
2:B:779:ASP:O	2:B:847:THR:OG1	2.04	0.70
3:C:176:ALA:HB3	9:J:42:ARG:NH1	2.07	0.70
3:C:43:VAL:HG12	3:C:73:SER:OG	1.92	0.70
7:H:7:LEU:HD11	7:H:36:MET:HE1	1.72	0.70
1:A:553:MET:HE3	10:K:50:LEU:HD21	1.73	0.69
1:A:236:ARG:NH2	1:A:238:ASP:OD2	2.26	0.69
1:A:66:GLN:HB3	2:B:914:LEU:HD21	1.74	0.69
1:A:1195:LEU:HD11	1:A:1242:ARG:HB3	1.72	0.69
1:A:1105:LYS:O	1:A:1109:ASN:ND2	2.25	0.69
2:B:15:GLU:O	2:B:19:THR:HG23	1.93	0.68
2:B:865:ARG:NH1	2:B:882:LEU:O	2.26	0.68
9:J:3:ILE:HD11	9:J:49:ILE:HD13	1.75	0.67
1:A:7:SER:O	2:B:1148:ARG:NH1	2.26	0.67
2:B:28:THR:HG23	2:B:32:ARG:HD2	1.77	0.67
3:C:5:THR:O	3:C:6:HIS:ND1	2.28	0.67
1:A:1220:ALA:O	1:A:1224:GLU:N	2.28	0.66
1:A:59:ARG:O	1:A:71:THR:OG1	2.14	0.66
2:B:136:GLU:N	2:B:136:GLU:OE1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLN:N	1:A:326:ARG:O	2.27	0.66
1:A:372:VAL:HG21	1:A:466:ILE:HD12	1.78	0.66
3:C:59:ASP:OD2	11:L:53:ARG:NH2	2.28	0.65
1:A:937:GLN:NE2	1:A:941:ASP:OD1	2.30	0.65
1:A:1158:ASP:OD2	1:A:1242:ARG:NH2	2.29	0.65
2:B:811:ASN:O	9:J:47:ARG:NE	2.25	0.64
2:B:176:ASP:OD2	16:X:492:ARG:NH1	2.31	0.64
2:B:1192:PHE:CE1	2:B:1204:LEU:HD21	2.31	0.64
2:B:889:ALA:O	2:B:892:THR:HG22	1.98	0.64
2:B:590:ARG:NH1	2:B:599:VAL:O	2.31	0.64
2:B:752:GLN:HG2	2:B:754:PRO:HD2	1.80	0.64
1:A:669:SER:OG	2:B:816:ILE:O	2.08	0.64
1:A:1318:ASN:ND2	1:A:1321:GLU:OE1	2.32	0.63
2:B:1073:GLN:OE1	3:C:190:THR:OG1	2.14	0.63
8:I:70:ARG:CD	8:I:84:VAL:HG12	2.29	0.63
1:A:97:PHE:HB3	1:A:240:MET:HE2	1.80	0.63
1:A:503:THR:HG23	2:B:1135:VAL:HG22	1.80	0.63
1:A:693:ARG:NH1	1:A:801:GLU:OE1	2.31	0.63
1:A:694:ARG:O	1:A:698:GLU:OE1	2.16	0.62
10:K:95:THR:O	10:K:99:GLU:OE1	2.18	0.62
9:J:36:ASP:OD1	9:J:46:ARG:NH2	2.32	0.62
1:A:567:PRO:HG3	1:A:586:LEU:HD11	1.81	0.62
2:B:1192:PHE:HE1	2:B:1204:LEU:HD21	1.64	0.62
2:B:486:THR:HG22	2:B:488:ILE:HG12	1.81	0.60
2:B:695:GLU:O	2:B:699:GLN:OE1	2.19	0.60
4:E:84:ILE:HD11	4:E:113:SER:OG	2.02	0.59
1:A:18:GLU:HG3	1:A:1424:LYS:HE2	1.84	0.59
2:B:346:LEU:O	2:B:360:LYS:NZ	2.33	0.59
7:H:117:ASP:OD1	7:H:118:HIS:N	2.36	0.59
3:C:31:SER:OG	10:K:40:THR:O	2.18	0.58
1:A:921:ILE:HG22	1:A:921:ILE:O	2.03	0.58
2:B:715:ARG:NH1	2:B:749:ASP:OD2	2.36	0.58
11:L:44:CYS:O	11:L:46:HIS:N	2.36	0.58
1:A:66:GLN:HB3	2:B:914:LEU:HD11	1.85	0.58
2:B:624:PHE:HB3	2:B:638:LEU:HD22	1.85	0.57
2:B:351:THR:HG21	2:B:356:PHE:HB3	1.86	0.57
2:B:351:THR:HG21	2:B:356:PHE:CB	2.35	0.57
2:B:273:ARG:NH1	2:B:307:ALA:O	2.37	0.56
1:A:114:LYS:NZ	1:A:172:HIS:O	2.38	0.56
1:A:258:VAL:HG22	14:P:1:A:C4	2.41	0.56
8:I:70:ARG:HD2	8:I:84:VAL:HG12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ILE:HD11	2:B:1135:VAL:HG21	1.86	0.56
2:B:398:LEU:O	2:B:452:TRP:HZ2	1.89	0.56
12:Y:786:TYR:CE1	12:Y:790:ILE:HD11	2.41	0.56
1:A:37:ILE:HG23	1:A:54:GLY:O	2.06	0.55
1:A:110:TRP:CH2	1:A:208:LEU:HD22	2.42	0.55
1:A:1141:ILE:HD13	1:A:1325:VAL:HG21	1.88	0.55
12:Y:734:VAL:HG11	12:Y:748:ILE:HD11	1.88	0.55
1:A:356:ARG:HB2	2:B:1117:LEU:HD11	1.88	0.55
3:C:178:ALA:HB3	3:C:232:ASP:HB3	1.88	0.55
3:C:36:VAL:CG1	3:C:174:THR:HG21	2.37	0.54
7:H:48:PRO:O	7:H:125:ARG:NH2	2.40	0.54
2:B:402:LEU:HD21	2:B:446:SER:HB2	1.88	0.54
12:Y:738:ARG:O	12:Y:773:ASN:ND2	2.38	0.54
1:A:1154:GLU:OE2	8:I:45:ARG:HD2	2.08	0.54
2:B:402:LEU:HD21	2:B:446:SER:CB	2.37	0.54
13:N:-15:DC:N4	15:T:15:DT:O4	2.41	0.54
2:B:498:ARG:NH1	2:B:517:GLN:O	2.38	0.54
1:A:1192:SER:OG	1:A:1262:GLU:OE1	2.12	0.54
1:A:568:PRO:O	1:A:582:GLN:NE2	2.37	0.54
1:A:1135:LYS:O	1:A:1139:THR:HG23	2.08	0.54
1:A:1403:LEU:HA	1:A:1406:CYS:SG	2.48	0.53
3:C:247:GLN:OE1	3:C:250:ARG:NH1	2.41	0.53
9:J:3:ILE:HD13	9:J:18:TRP:HB2	1.89	0.53
2:B:964:GLN:NE2	2:B:1089:ASP:OD2	2.41	0.53
1:A:1066:MET:CE	1:A:1430:ILE:HD11	2.38	0.53
1:A:694:ARG:NH1	1:A:698:GLU:OE2	2.41	0.53
1:A:1195:LEU:HD21	1:A:1242:ARG:HE	1.73	0.53
1:A:212:GLU:O	1:A:216:ILE:HG13	2.08	0.53
12:Y:733:THR:CG2	12:Y:745:LEU:HD11	2.39	0.53
2:B:1028:GLY:HA2	9:J:50:LEU:HD11	1.89	0.52
2:B:893:ARG:HG3	12:Y:759:GLU:OE1	2.10	0.52
2:B:888:ILE:HG12	2:B:892:THR:HG21	1.91	0.52
1:A:692:ALA:HB2	1:A:731:ALA:HB2	1.90	0.52
2:B:725:HIS:CE1	8:I:70:ARG:HB2	2.45	0.52
1:A:16:VAL:N	1:A:1438:GLN:OE1	2.40	0.52
10:K:34:LEU:HD12	10:K:70:PHE:CZ	2.45	0.52
1:A:214:HIS:O	1:A:218:THR:HG23	2.10	0.52
1:A:1066:MET:SD	1:A:1442:MET:HB3	2.50	0.52
2:B:101:PRO:HG2	2:B:166:LEU:HD11	1.91	0.52
2:B:299:MET:HE2	2:B:372:LEU:HD22	1.92	0.52
1:A:335:LEU:HD22	2:B:1191:LEU:CD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:GLY:O	1:A:1350:THR:OG1	2.22	0.51
3:C:34:ARG:NH2	10:K:38:ASP:OD2	2.37	0.51
2:B:387:PHE:CE1	2:B:619:ILE:HD12	2.45	0.51
9:J:3:ILE:HD11	9:J:49:ILE:CD1	2.41	0.51
1:A:1066:MET:HE1	1:A:1430:ILE:HD11	1.92	0.51
2:B:119:MET:CE	2:B:150:VAL:HG21	2.40	0.51
12:Y:786:TYR:CZ	12:Y:790:ILE:HD11	2.46	0.51
1:A:1325:VAL:O	1:A:1328:VAL:HG22	2.11	0.51
2:B:625:ILE:HD11	2:B:675:GLU:HB2	1.93	0.51
1:A:570:VAL:HG21	1:A:579:THR:HG23	1.93	0.51
2:B:27:GLU:OE2	2:B:666:THR:OG1	2.16	0.51
5:F:86:THR:CG2	6:G:62:VAL:HG11	2.41	0.51
1:A:74:GLU:OE2	2:B:1163:TYR:N	2.44	0.50
2:B:392:LEU:CD1	2:B:619:ILE:HD11	2.40	0.50
2:B:769:VAL:O	2:B:769:VAL:HG13	2.11	0.50
4:E:48:MET:SD	4:E:48:MET:N	2.84	0.50
1:A:11:VAL:HG23	2:B:1181:GLN:HB2	1.93	0.50
2:B:227:SER:OG	2:B:349:HIS:ND1	2.26	0.50
2:B:791:PRO:HG2	2:B:794:THR:HG22	1.93	0.50
3:C:32:LEU:HD21	3:C:245:MET:HE1	1.93	0.50
1:A:11:VAL:HG21	2:B:1150:ILE:HD12	1.92	0.50
1:A:670:ILE:HD11	1:A:749:VAL:HG22	1.94	0.49
1:A:1351:ARG:NE	1:A:1379:ASP:OD1	2.44	0.49
1:A:1208:LYS:O	1:A:1280:ARG:NH2	2.43	0.49
2:B:398:LEU:HB3	2:B:452:TRP:CZ2	2.48	0.49
1:A:624:ASP:O	1:A:628:VAL:HG22	2.12	0.49
2:B:80:GLY:N	2:B:118:ASP:O	2.35	0.49
1:A:66:GLN:CB	2:B:914:LEU:HD11	2.43	0.49
4:E:87:MET:HE1	4:E:127:ILE:HG21	1.95	0.49
2:B:234:ARG:O	2:B:235:LEU:HB3	2.13	0.49
4:E:30:SER:N	4:E:33:GLU:OE1	2.45	0.49
2:B:119:MET:HE3	2:B:150:VAL:HG21	1.94	0.49
2:B:140:VAL:HG23	2:B:140:VAL:O	2.13	0.49
2:B:387:PHE:CZ	2:B:619:ILE:HD12	2.48	0.49
2:B:770:TYR:OH	2:B:779:ASP:OD2	2.15	0.49
1:A:459:MET:SD	1:A:516:GLN:HB3	2.52	0.49
1:A:1355:LEU:HD21	1:A:1371:TYR:HE1	1.77	0.49
2:B:234:ARG:O	2:B:235:LEU:CB	2.60	0.49
1:A:451:ASN:HB3	1:A:461:MET:HG2	1.95	0.48
2:B:199:ALA:HB3	2:B:484:THR:HG22	1.95	0.48
4:E:37:THR:HG22	4:E:38:LEU:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:88:ASP:OD2	7:H:90:LYS:NZ	2.46	0.48
3:C:5:THR:HG21	10:K:100:ILE:HD11	1.95	0.48
7:H:5:VAL:O	7:H:113:ARG:NH2	2.46	0.48
13:N:-10:DG:N2	15:T:12:DC:O2	2.47	0.48
1:A:1153:THR:HG22	1:A:1198:LEU:HD22	1.94	0.48
1:A:1202:ARG:NH2	1:A:1236:ALA:O	2.44	0.48
2:B:385:ASP:OD2	2:B:496:LYS:HG3	2.13	0.48
4:E:185:LEU:HD11	4:E:191:VAL:HG11	1.96	0.48
1:A:511:THR:HG22	1:A:511:THR:O	2.12	0.48
2:B:223:ALA:HB2	2:B:371:MET:HB2	1.95	0.48
2:B:547:TRP:CD1	2:B:582:LEU:HD13	2.49	0.48
1:A:1416:MET:SD	2:B:1200:ILE:HD11	2.54	0.48
2:B:640:ILE:HG23	2:B:640:ILE:O	2.14	0.48
1:A:480:VAL:HG12	1:A:480:VAL:O	2.14	0.47
1:A:1000:LEU:O	1:A:1014:GLN:NE2	2.47	0.47
4:E:35:ASP:CG	4:E:35:ASP:O	2.53	0.47
1:A:835:VAL:HG13	2:B:493:LYS:HG2	1.96	0.47
1:A:877:ASP:OD2	1:A:1372:ARG:NH2	2.47	0.47
2:B:772:THR:HG21	9:J:58:LYS:HB3	1.95	0.47
9:J:35:LEU:HD11	9:J:50:LEU:HG	1.94	0.47
1:A:547:LEU:HD12	1:A:583:ILE:HG13	1.97	0.47
2:B:1162:SER:OG	2:B:1167:SER:OG	2.29	0.47
1:A:837:THR:HG23	1:A:838:ALA:N	2.29	0.47
2:B:115:LEU:HD22	2:B:155:ILE:HD11	1.97	0.47
2:B:547:TRP:HD1	2:B:582:LEU:HD13	1.80	0.47
9:J:23:THR:HG22	9:J:27:GLU:OE2	2.14	0.47
1:A:840:THR:HG21	1:A:1080:THR:CG2	2.45	0.47
1:A:1299:ILE:HG22	1:A:1300:GLU:N	2.30	0.47
2:B:817:LEU:HD13	2:B:1074:VAL:HG22	1.97	0.47
3:C:36:VAL:HG13	3:C:174:THR:HG21	1.95	0.47
11:L:24:CYS:HB3	11:L:27:CYS:HB2	1.96	0.47
1:A:80:PRO:O	2:B:1189:LYS:NZ	2.37	0.47
2:B:973:HIS:NE2	2:B:1017:GLU:OE1	2.33	0.47
8:I:19:ASP:O	8:I:23:ARG:N	2.48	0.47
11:L:41:CYS:HB3	11:L:45:GLY:N	2.30	0.47
11:L:60:PHE:HA	12:Y:762:THR:HG22	1.95	0.47
2:B:580:ALA:O	2:B:584:GLU:OE1	2.32	0.47
1:A:846:ARG:NH1	1:A:1109:ASN:OD1	2.48	0.47
2:B:868:ARG:HG2	2:B:868:ARG:HH11	1.80	0.47
1:A:349:LYS:HZ3	2:B:1185:PRO:HB3	1.79	0.47
1:A:646:GLU:OE1	1:A:649:LYS:NZ	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:1:MET:O	6:G:1:MET:HG3	2.14	0.46
2:B:454:ASP:O	2:B:461:ASN:ND2	2.47	0.46
3:C:10:ARG:NH2	3:C:18:ASP:OD1	2.48	0.46
3:C:176:ALA:HB3	9:J:42:ARG:HH11	1.78	0.46
1:A:806:ILE:HG21	1:A:814:LEU:HD22	1.96	0.46
1:A:1263:ASP:OD1	1:A:1264:VAL:N	2.49	0.46
2:B:101:PRO:HB3	2:B:159:LEU:HD11	1.96	0.46
2:B:268:ILE:HG12	2:B:368:ILE:HD11	1.97	0.46
5:F:135:ASP:OD2	6:G:59:LYS:NZ	2.47	0.46
1:A:506:GLU:OE2	2:B:1134:SER:OG	2.30	0.46
2:B:379:ARG:NH1	2:B:607:GLU:OE1	2.49	0.46
1:A:603:LEU:HD23	1:A:612:LEU:HD22	1.97	0.46
2:B:694:LEU:HD11	2:B:730:CYS:HB2	1.97	0.46
2:B:911:HIS:O	2:B:917:ARG:NH1	2.48	0.46
10:K:50:LEU:HD21	10:K:58:ALA:HB3	1.98	0.46
2:B:45:THR:HG21	2:B:400:ALA:CB	2.46	0.46
12:Y:757:ARG:NH1	12:Y:768:THR:OG1	2.49	0.46
1:A:123:LYS:O	1:A:127:THR:HG23	2.16	0.45
1:A:359:ILE:HA	1:A:474:PHE:O	2.16	0.45
8:I:104:VAL:HG12	8:I:104:VAL:O	2.15	0.45
1:A:1208:LYS:O	1:A:1280:ARG:NH1	2.48	0.45
2:B:107:ARG:HG2	2:B:944:THR:HG21	1.98	0.45
10:K:8:GLU:O	10:K:36:LYS:NZ	2.41	0.45
1:A:24:LEU:HD12	2:B:1199:ASN:HA	1.98	0.45
1:A:69:CYS:O	1:A:73:GLY:N	2.46	0.45
1:A:1447:PHE:CZ	5:F:79:GLU:HA	2.52	0.45
3:C:92:CYS:O	12:Y:742:LYS:NZ	2.33	0.45
3:C:117:ILE:HD11	3:C:148:LEU:HD12	1.99	0.45
1:A:255:SER:OG	1:A:265:GLU:OE1	2.35	0.45
1:A:1009:ILE:O	1:A:1013:VAL:HG13	2.17	0.45
1:A:518:VAL:HA	1:A:525:PRO:HA	1.98	0.45
3:C:5:THR:CG2	10:K:96:HIS:NE2	2.80	0.45
12:Y:734:VAL:HG12	12:Y:776:TYR:CD1	2.52	0.45
2:B:310:ILE:HG23	2:B:315:ILE:HG22	2.00	0.44
2:B:77:ILE:HD11	2:B:428:PHE:CZ	2.52	0.44
3:C:6:HIS:HA	10:K:103:ASN:ND2	2.31	0.44
3:C:32:LEU:HD21	3:C:245:MET:CE	2.47	0.44
7:H:82:ARG:NH2	7:H:84:GLU:HG2	2.33	0.44
9:J:7:CYS:HA	9:J:48:MET:SD	2.57	0.44
1:A:553:MET:HE3	10:K:50:LEU:CD2	2.44	0.44
1:A:1165:VAL:HG12	1:A:1165:VAL:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:ILE:HG22	1:A:1434:ILE:HD12	1.99	0.44
2:B:148:SER:O	2:B:150:VAL:HG23	2.16	0.44
11:L:39:ILE:HG23	11:L:49:MET:CE	2.47	0.44
1:A:1269:ILE:O	1:A:1273:MET:HG2	2.17	0.44
2:B:90:THR:HG22	2:B:96:THR:OG1	2.18	0.44
2:B:643:GLU:OE1	2:B:643:GLU:N	2.47	0.44
11:L:43:GLU:N	11:L:43:GLU:OE2	2.51	0.44
2:B:769:VAL:HG13	2:B:806:LEU:HD22	1.99	0.44
4:E:121:VAL:O	4:E:121:VAL:HG22	2.17	0.44
1:A:869:ILE:CD1	4:E:165:LEU:HD11	2.42	0.44
7:H:82:ARG:NH2	7:H:94:TYR:CE2	2.86	0.44
1:A:507:ILE:HD11	2:B:1135:VAL:CG2	2.48	0.44
2:B:236:ILE:HG13	2:B:237:SER:N	2.33	0.44
1:A:730:GLN:NE2	1:A:734:ASN:OD1	2.50	0.43
1:A:1154:GLU:HB2	1:A:1197:ARG:HB3	2.00	0.43
2:B:498:ARG:NH2	2:B:517:GLN:O	2.51	0.43
1:A:503:THR:O	1:A:507:ILE:HG12	2.17	0.43
1:A:743:LEU:HB2	1:A:750:LYS:HD2	2.00	0.43
1:A:1225:ARG:O	1:A:1246:ILE:HD12	2.17	0.43
2:B:61:TYR:HA	2:B:72:THR:HG22	2.00	0.43
2:B:89:MET:SD	2:B:109:LEU:HD13	2.58	0.43
2:B:343:GLN:O	2:B:360:LYS:NZ	2.51	0.43
2:B:505:TRP:NE1	2:B:731:GLU:OE2	2.44	0.43
3:C:57:MET:CE	9:J:2:ILE:HG21	2.48	0.43
1:A:127:THR:HG22	1:A:139:ALA:HB1	1.99	0.43
1:A:685:VAL:HG13	1:A:735:ALA:HB1	1.99	0.43
1:A:812:ARG:NH2	2:B:712:PRO:O	2.51	0.43
1:A:1197:ARG:O	1:A:1198:LEU:HD23	2.18	0.43
1:A:123:LYS:NZ	15:T:-12:DG:OP2	2.47	0.43
1:A:278:ALA:O	1:A:282:VAL:HG23	2.19	0.43
1:A:556:MET:CE	1:A:586:LEU:HD13	2.48	0.43
3:C:174:THR:HG22	3:C:244:ILE:HD13	1.99	0.43
1:A:473:THR:OG1	1:A:475:ARG:HD2	2.19	0.43
2:B:332:GLU:OE2	2:B:336:ARG:NH2	2.46	0.43
2:B:582:LEU:HD23	2:B:610:LEU:CD2	2.49	0.43
1:A:952:LYS:O	1:A:1296:VAL:HG11	2.19	0.43
2:B:1118:ARG:NE	15:T:2:DC:OP1	2.48	0.43
8:I:64:THR:O	8:I:64:THR:HG22	2.18	0.43
1:A:301:LEU:HD23	1:A:305:HIS:CD2	2.53	0.43
1:A:507:ILE:CD1	2:B:1135:VAL:HG21	2.48	0.43
2:B:598:GLU:O	2:B:618:ARG:NH1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:82:ARG:NH2	7:H:94:TYR:HE2	2.16	0.43
10:K:31:VAL:CG1	10:K:71:ILE:HG23	2.49	0.43
11:L:41:CYS:HB3	11:L:46:HIS:H	1.83	0.43
1:A:1390:ILE:O	1:A:1391:THR:HG23	2.19	0.43
2:B:598:GLU:O	2:B:618:ARG:NH2	2.50	0.43
11:L:24:CYS:O	11:L:28:GLY:N	2.40	0.43
1:A:1228:PHE:HB2	1:A:1246:ILE:HD11	2.00	0.42
1:A:312:ASN:O	1:A:312:ASN:ND2	2.52	0.42
2:B:268:ILE:O	2:B:271:VAL:HG12	2.19	0.42
1:A:230:LEU:HD13	1:A:237:PRO:HG3	2.02	0.42
1:A:448:VAL:HG21	1:A:466:ILE:HD11	2.02	0.42
1:A:786:LYS:HG2	2:B:683:GLU:OE2	2.19	0.42
2:B:13:THR:HG22	2:B:14:GLN:N	2.34	0.42
2:B:577:ARG:HG3	2:B:577:ARG:HH11	1.83	0.42
2:B:592:ARG:NH2	2:B:594:ASP:OD2	2.52	0.42
4:E:33:GLU:O	4:E:36:LEU:HD22	2.19	0.42
1:A:9:SER:OG	2:B:1148:ARG:NH1	2.53	0.42
1:A:543:ARG:HG2	7:H:100:LEU:HD23	2.00	0.42
1:A:549:ARG:O	1:A:553:MET:HB2	2.20	0.42
2:B:386:HIS:NE2	2:B:683:GLU:OE1	2.47	0.42
1:A:905:ILE:CG2	1:A:931:LEU:HD13	2.50	0.42
2:B:392:LEU:HD11	2:B:484:THR:HG21	2.02	0.42
3:C:21:LEU:HD11	10:K:100:ILE:HD12	2.01	0.42
7:H:82:ARG:HH22	7:H:94:TYR:HE2	1.67	0.42
1:A:357:THR:OG1	1:A:358:VAL:N	2.53	0.42
1:A:570:VAL:HG23	1:A:571:ILE:HG13	2.01	0.42
1:A:1041:ASN:OD1	1:A:1041:ASN:N	2.52	0.42
1:A:1372:ARG:HG3	1:A:1372:ARG:HH11	1.84	0.42
2:B:600:SER:OG	2:B:618:ARG:NH1	2.53	0.42
3:C:188:GLN:OE1	3:C:220:PHE:CE1	2.73	0.42
7:H:84:GLU:HG2	7:H:92:SER:OG	2.19	0.42
8:I:8:ILE:HG22	8:I:8:ILE:O	2.19	0.42
1:A:237:PRO:O	1:A:240:MET:HB2	2.20	0.42
2:B:1169:GLU:OE2	2:B:1171:ARG:NE	2.52	0.42
3:C:168:HIS:CD2	11:L:63:ARG:HB2	2.55	0.42
3:C:250:ARG:HG2	10:K:101:LYS:HZ1	1.85	0.42
5:F:123:LEU:HD23	5:F:137:SER:HA	2.02	0.42
1:A:117:ILE:HD12	1:A:144:CYS:SG	2.60	0.42
2:B:364:LEU:O	2:B:368:ILE:HD12	2.19	0.42
2:B:701:GLN:NE2	2:B:725:HIS:HD2	2.17	0.42
2:B:1113:ARG:HG2	2:B:1113:ARG:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1175:ASN:ND2	2:B:1178:ARG:O	2.49	0.42
2:B:77:ILE:HD12	2:B:418:MET:SD	2.60	0.41
15:T:-8:DA:H2"	15:T:-7:DG:O5'	2.20	0.41
1:A:789:THR:O	2:B:502:ASN:ND2	2.48	0.41
10:K:80:CYS:SG	10:K:81:SER:N	2.94	0.41
1:A:1123:LEU:HD22	1:A:1137:VAL:HG11	2.03	0.41
2:B:1073:GLN:HG2	3:C:202:TRP:CH2	2.55	0.41
2:B:1109:GLU:O	2:B:1113:ARG:NH2	2.54	0.41
2:B:1128:ILE:HG13	2:B:1136:LEU:HD11	2.01	0.41
8:I:88:THR:HG22	8:I:100:ILE:HD11	2.03	0.41
1:A:1130:ASN:OD1	1:A:1131:MET:N	2.53	0.41
1:A:776:VAL:HA	1:A:828:GLU:OE1	2.20	0.41
3:C:235:SER:OG	3:C:239:ILE:O	2.30	0.41
8:I:78:CYS:SG	8:I:80:GLN:HG2	2.61	0.41
1:A:301:LEU:HD23	1:A:305:HIS:HD2	1.85	0.41
1:A:717:ARG:NH1	8:I:97:MET:SD	2.85	0.41
1:A:642:GLU:OE2	1:A:969:ASN:ND2	2.53	0.41
1:A:1154:GLU:OE2	8:I:45:ARG:CD	2.69	0.41
1:A:1372:ARG:HG3	1:A:1372:ARG:NH1	2.35	0.41
1:A:1452:ASP:OD1	1:A:1452:ASP:O	2.38	0.41
2:B:329:VAL:O	2:B:334:ARG:NH1	2.53	0.41
2:B:1180:SER:OG	2:B:1206:THR:HG21	2.20	0.40
11:L:26:ASP:OD2	11:L:46:HIS:ND1	2.54	0.40
15:T:-8:DA:H4'	15:T:-7:DG:OP1	2.21	0.40
1:A:15:ARG:NH2	1:A:1433:ASN:OD1	2.54	0.40
1:A:506:GLU:CD	2:B:1134:SER:HG	2.24	0.40
2:B:288:CYS:SG	2:B:296:MET:HB3	2.62	0.40
1:A:351:VAL:HG22	2:B:1117:LEU:O	2.21	0.40
1:A:448:VAL:CG2	1:A:466:ILE:HD11	2.52	0.40
2:B:299:MET:CE	2:B:372:LEU:HD22	2.51	0.40
3:C:117:ILE:HD11	3:C:148:LEU:CD1	2.51	0.40
4:E:35:ASP:O	4:E:35:ASP:OD1	2.38	0.40
1:A:1448:ASP:OD1	6:G:61:ARG:NH2	2.54	0.40
1:A:1453:GLN:OE1	1:A:1453:GLN:N	2.51	0.40
2:B:402:LEU:HD23	2:B:443:LEU:HD23	2.02	0.40
12:Y:757:ARG:HG2	12:Y:766:MET:HE2	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	1437/1752 (82%)	1408 (98%)	28 (2%)	1 (0%)	48	71
2	B	1199/1210 (99%)	1157 (96%)	41 (3%)	1 (0%)	48	71
3	C	258/297 (87%)	252 (98%)	6 (2%)	0	100	100
4	E	205/210 (98%)	203 (99%)	2 (1%)	0	100	100
5	F	80/142 (56%)	76 (95%)	4 (5%)	0	100	100
6	G	46/172 (27%)	46 (100%)	0	0	100	100
7	H	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
8	I	86/141 (61%)	80 (93%)	6 (7%)	0	100	100
9	J	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
10	K	114/123 (93%)	110 (96%)	4 (4%)	0	100	100
11	L	43/63 (68%)	40 (93%)	3 (7%)	0	100	100
12	Y	70/1122 (6%)	70 (100%)	0	0	100	100
16	X	14/896 (2%)	14 (100%)	0	0	100	100
All	All	3739/6324 (59%)	3636 (97%)	101 (3%)	2 (0%)	50	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	235	LEU
1	A	961	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1259/1536 (82%)	1259 (100%)	0	100 100
2	B	1055/1064 (99%)	1054 (100%)	1 (0%)	92 98
3	C	233/267 (87%)	233 (100%)	0	100 100
4	E	182/184 (99%)	181 (100%)	1 (0%)	86 95
5	F	70/121 (58%)	70 (100%)	0	100 100
6	G	43/148 (29%)	43 (100%)	0	100 100
7	H	114/114 (100%)	113 (99%)	1 (1%)	75 89
8	I	85/126 (68%)	85 (100%)	0	100 100
9	J	61/66 (92%)	61 (100%)	0	100 100
10	K	107/113 (95%)	107 (100%)	0	100 100
11	L	39/53 (74%)	39 (100%)	0	100 100
12	Y	61/940 (6%)	61 (100%)	0	100 100
16	X	12/805 (2%)	12 (100%)	0	100 100
All	All	3321/5537 (60%)	3318 (100%)	3 (0%)	92 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1002	ASN
4	E	162	ARG
7	H	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	ASN
1	A	605	ASN
1	A	632	GLN
2	B	725	HIS
2	B	750	HIS
3	C	64	HIS
4	E	142	HIS
8	I	89	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/26 (34%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G

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 1 ligands modelled in this entry, 1 is 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)

There are no chain breaks in this entry.

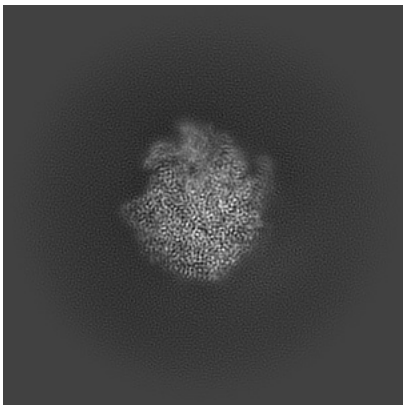
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18643. These allow visual inspection of the internal detail of the map and identification of artifacts.

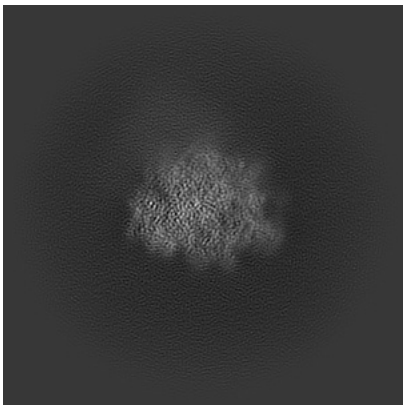
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

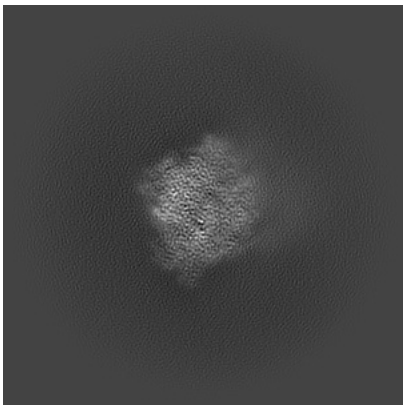
6.1.1 Primary map



X

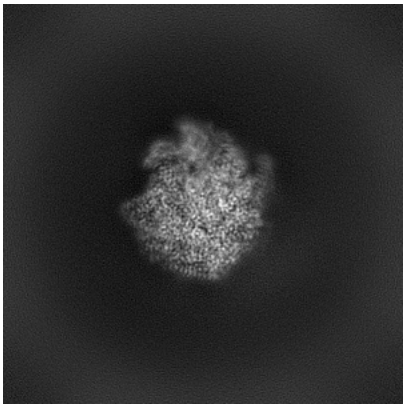


Y

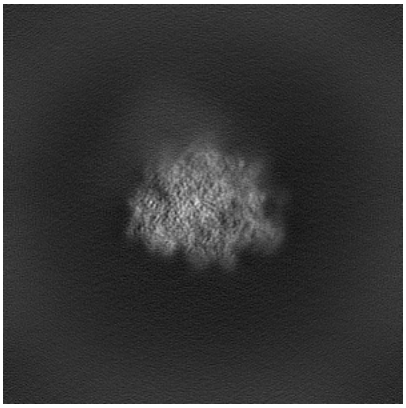


Z

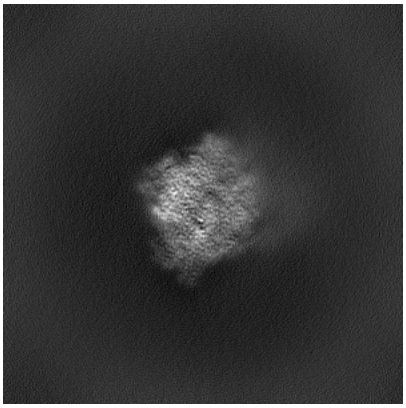
6.1.2 Raw map



X



Y

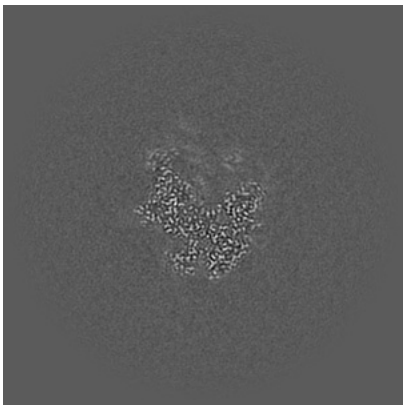


Z

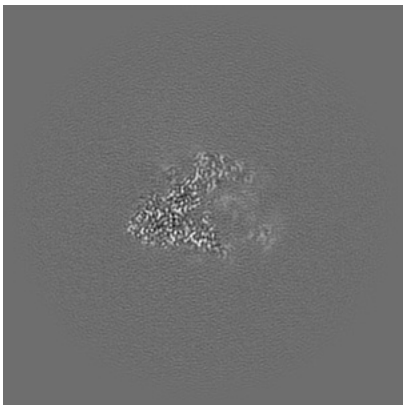
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

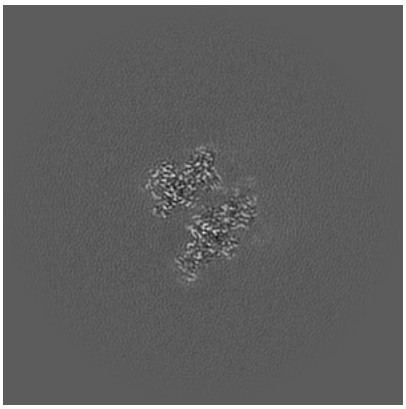
6.2.1 Primary map



X Index: 176

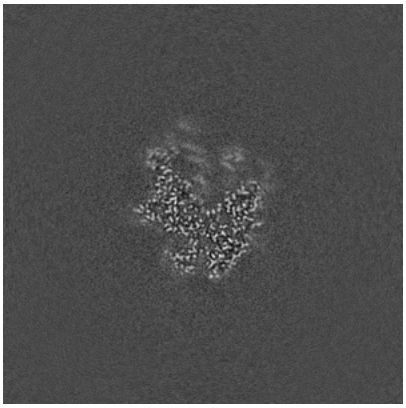


Y Index: 176

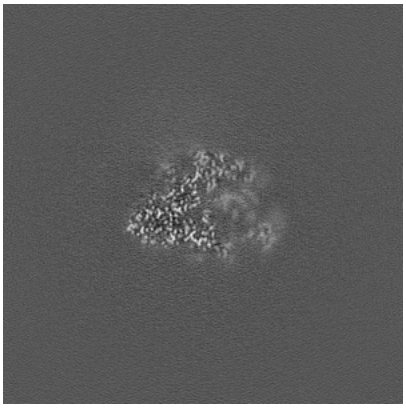


Z Index: 176

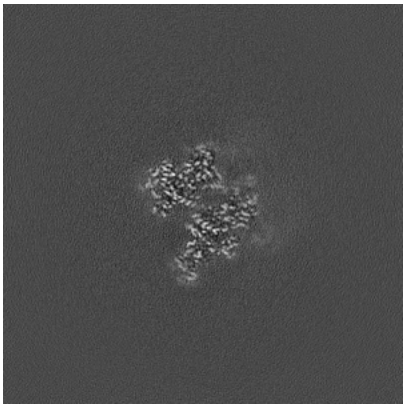
6.2.2 Raw map



X Index: 176



Y Index: 176

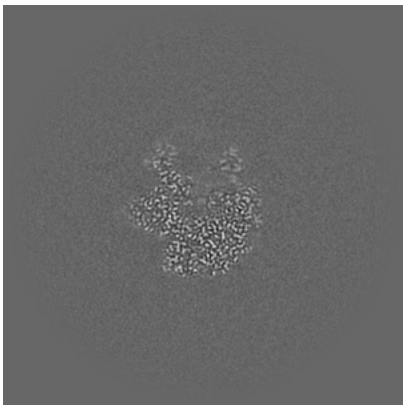


Z Index: 176

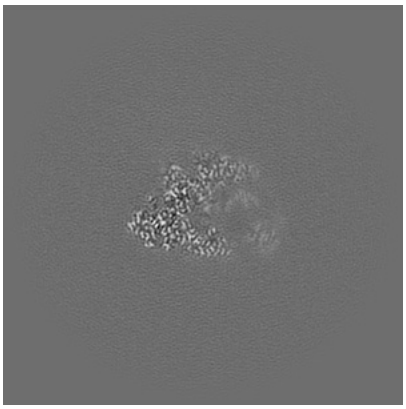
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

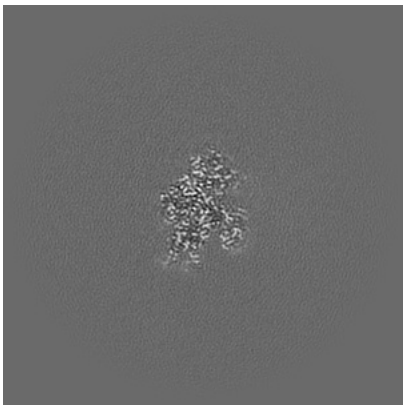
6.3.1 Primary map



X Index: 170

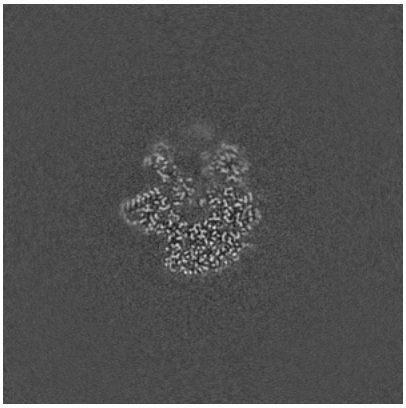


Y Index: 172

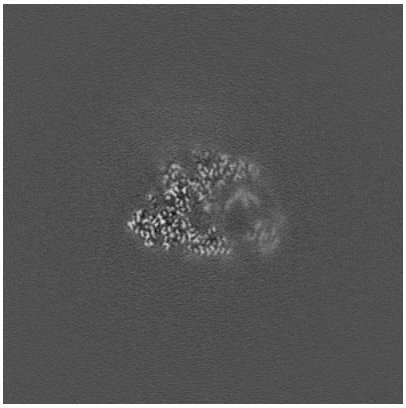


Z Index: 154

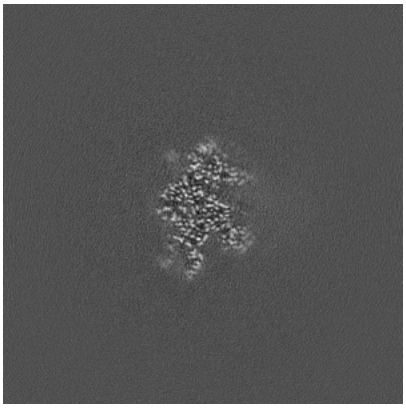
6.3.2 Raw map



X Index: 166



Y Index: 172

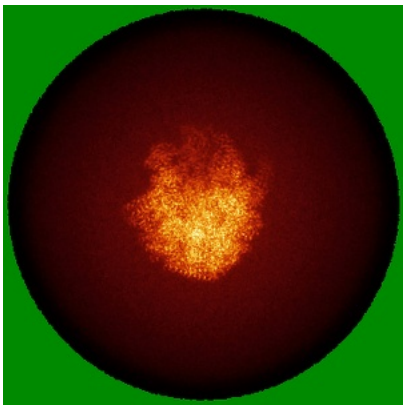


Z Index: 158

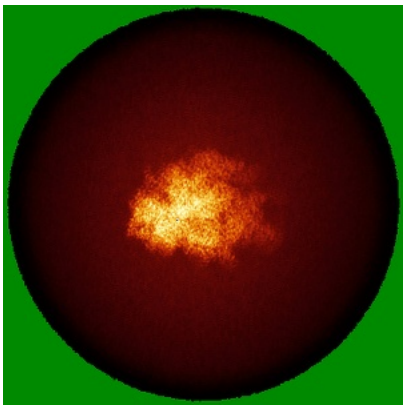
The images above show the largest variance slices of the map in three orthogonal directions.

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

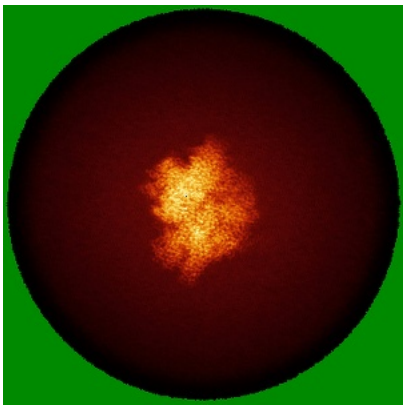
6.4.1 Primary map



X

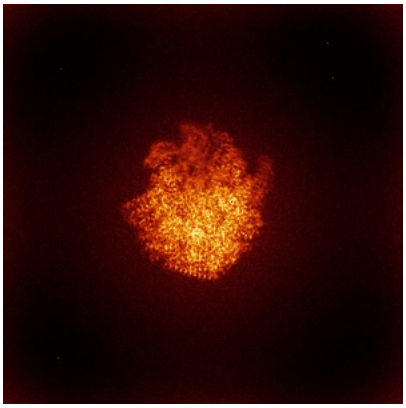


Y

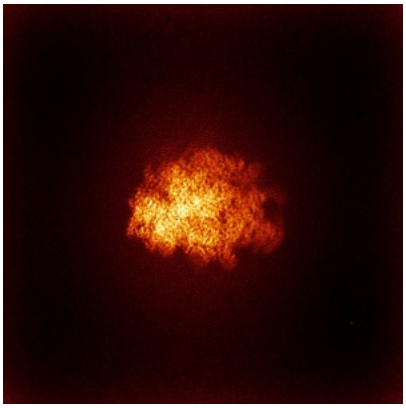


Z

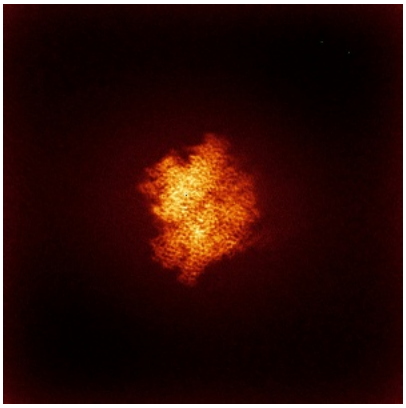
6.4.2 Raw map



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 0.336. 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.

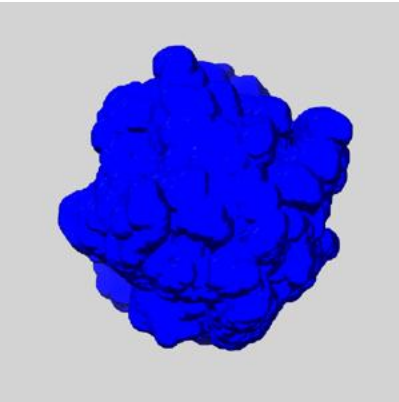
6.6 Mask visualisation (i)

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

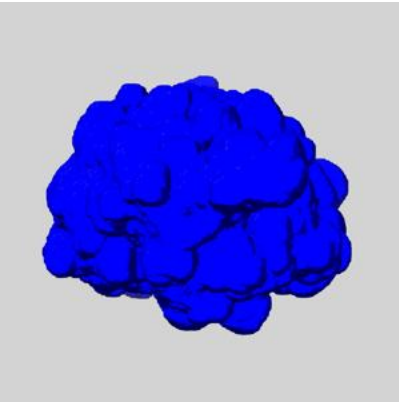
A mask typically either:

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

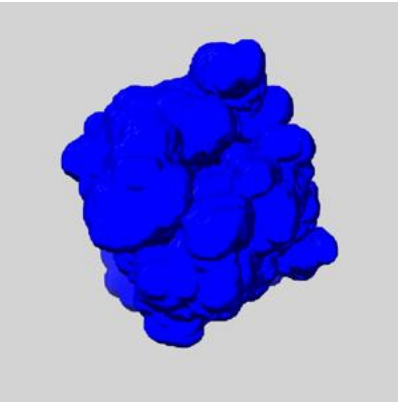
6.6.1 emd_18643_msk_1.map (i)



X



Y

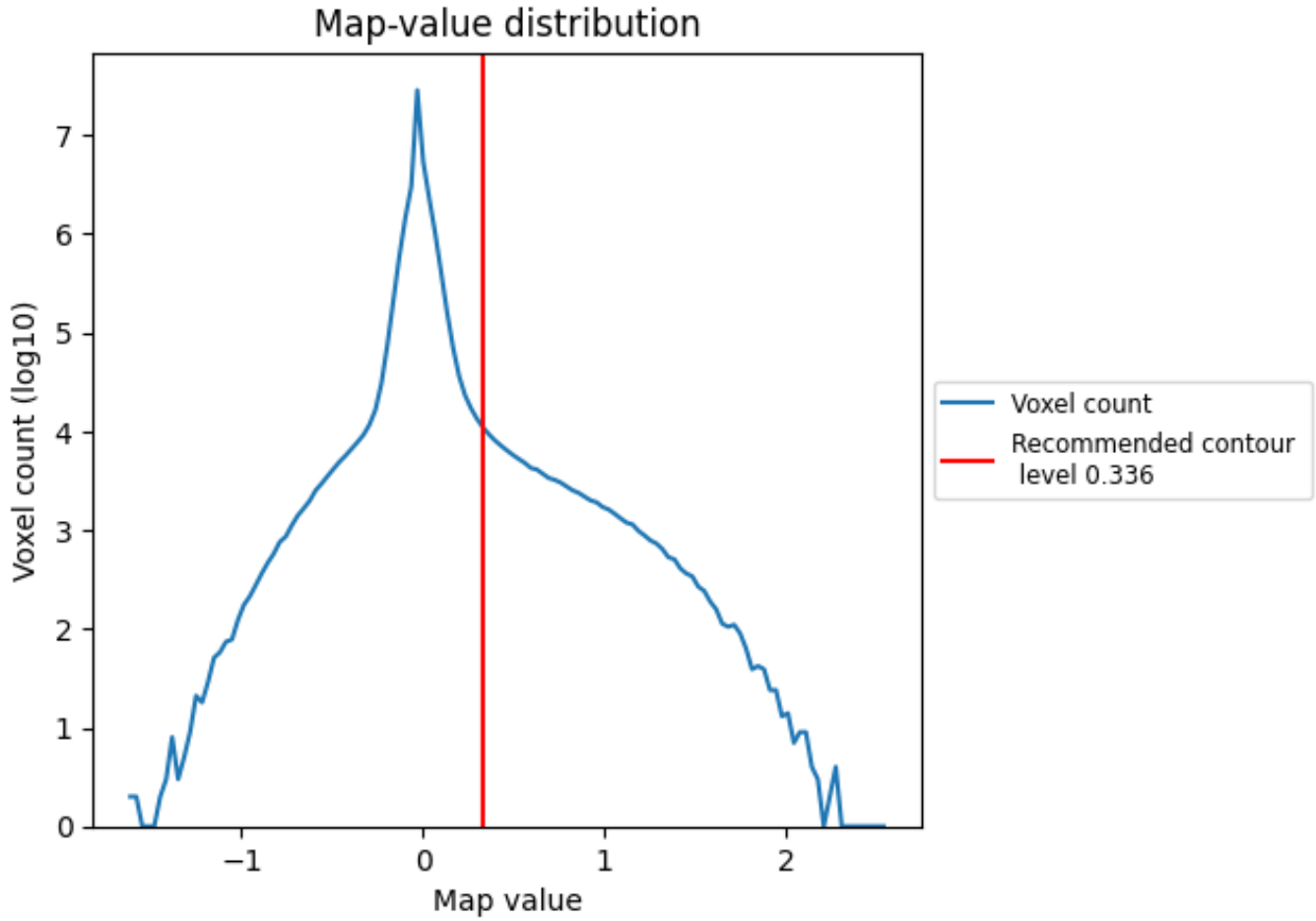


Z

7 Map analysis

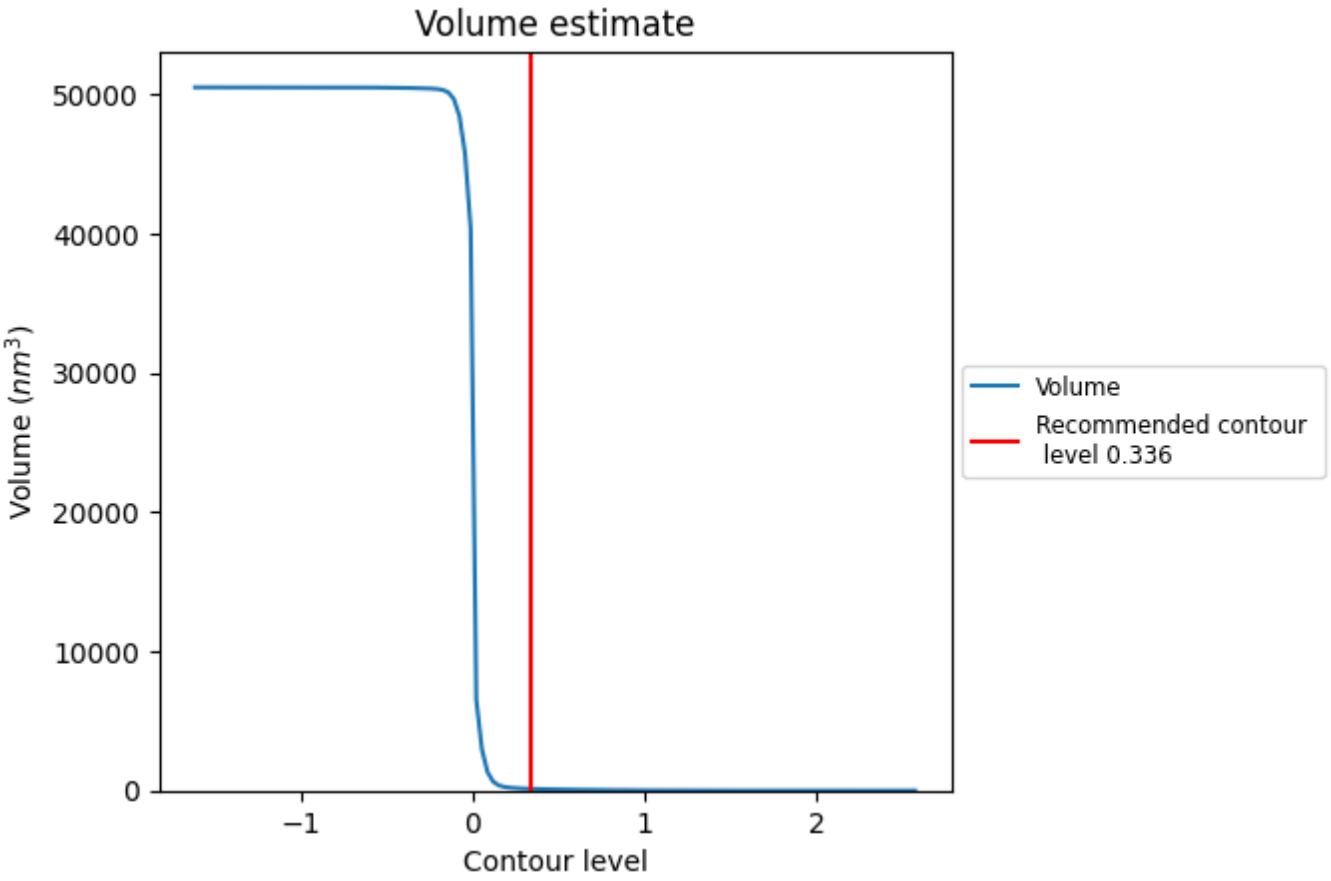
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

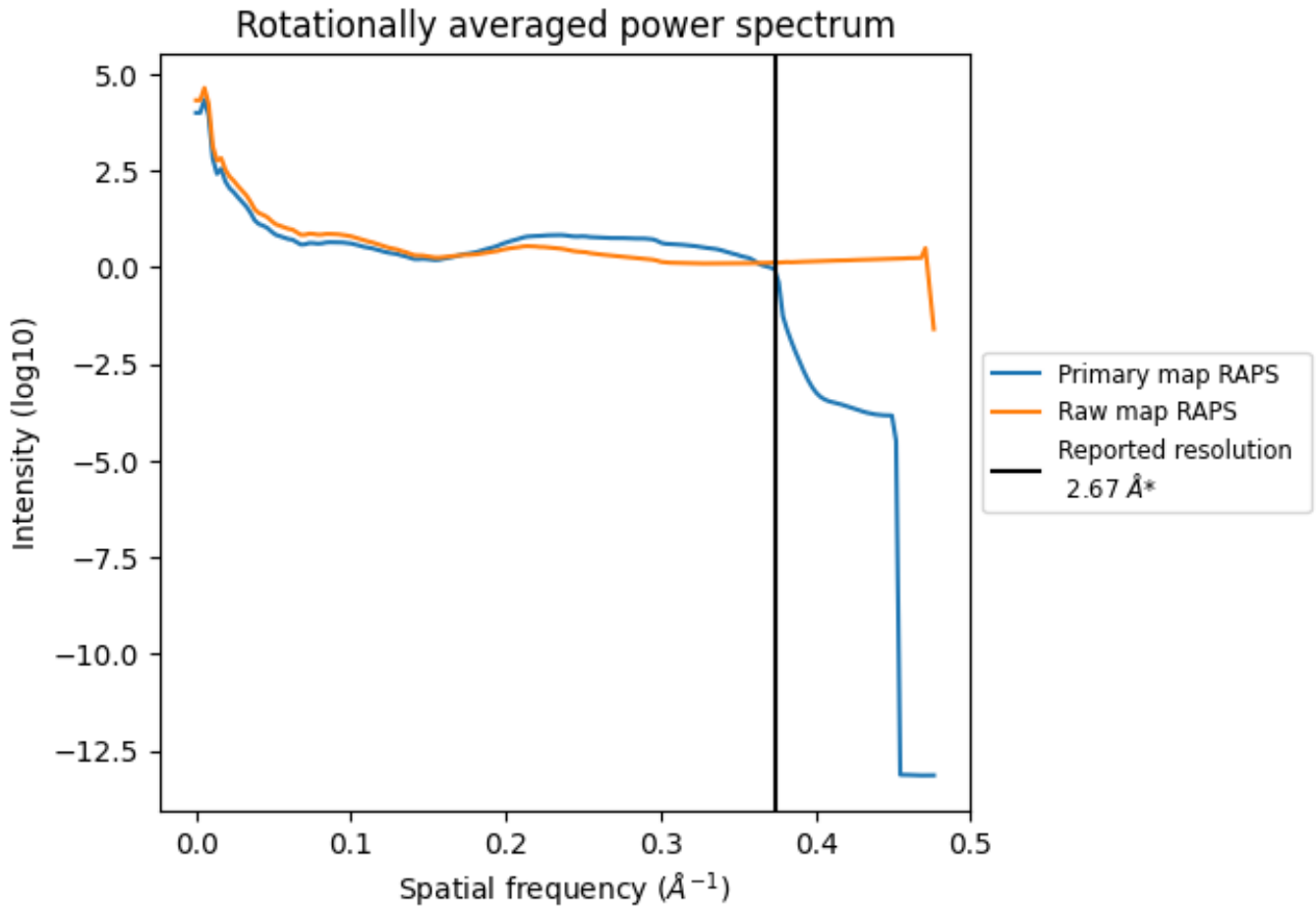
7.2 Volume estimate



The volume at the recommended contour level is 125 nm^3; this corresponds to an approximate mass of 113 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

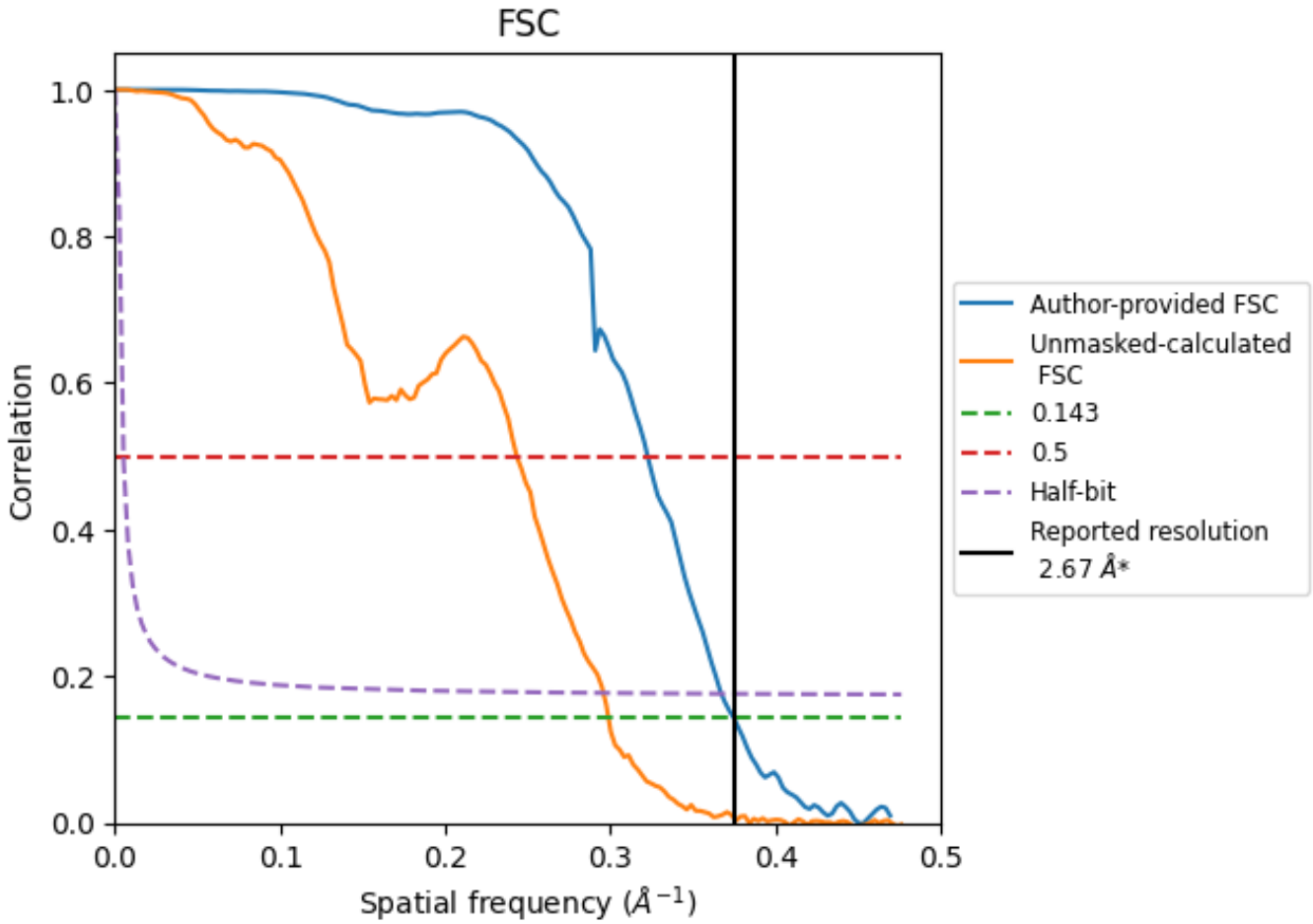


*Reported resolution corresponds to spatial frequency of 0.375 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.375 Å^{-1}

8.2 Resolution estimates (i)

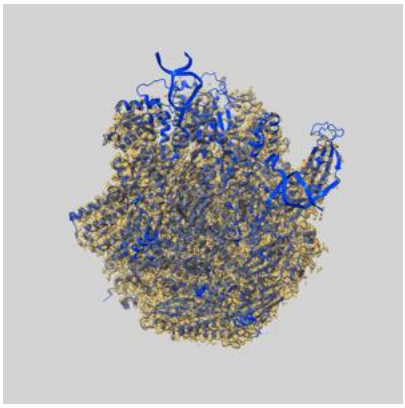
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.10	2.72
Unmasked-calculated*	3.35	4.11	3.38

*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 3.35 differs from the reported value 2.67 by more than 10 %

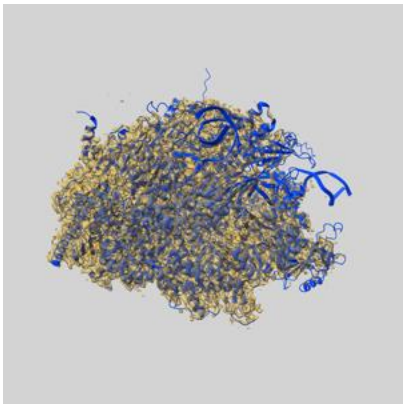
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18643 and PDB model 8QSZ. Per-residue inclusion information can be found in section 3 on page 11.

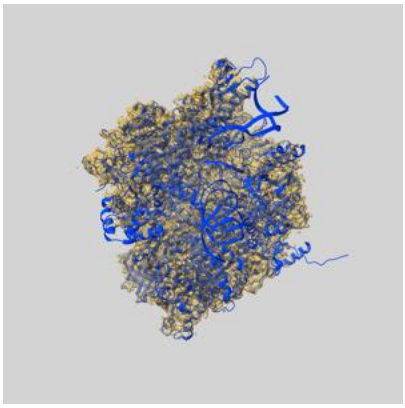
9.1 Map-model overlay



X



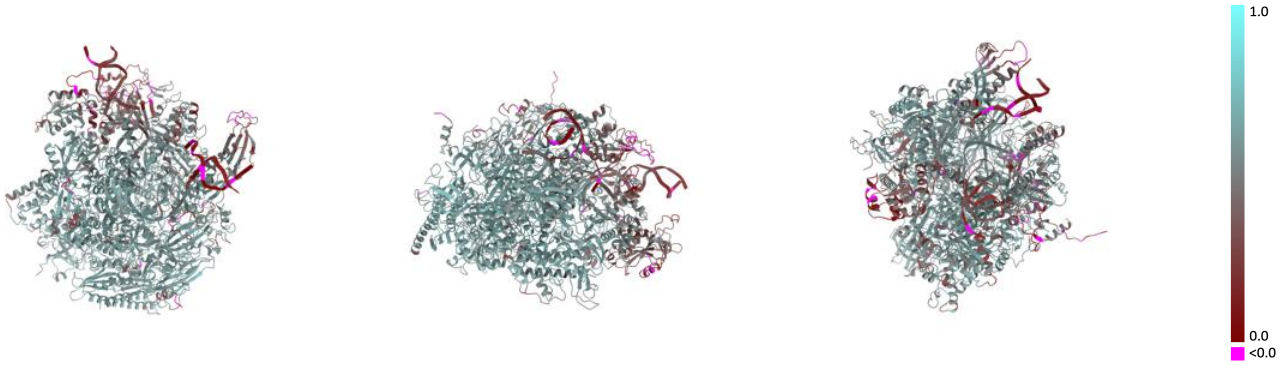
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

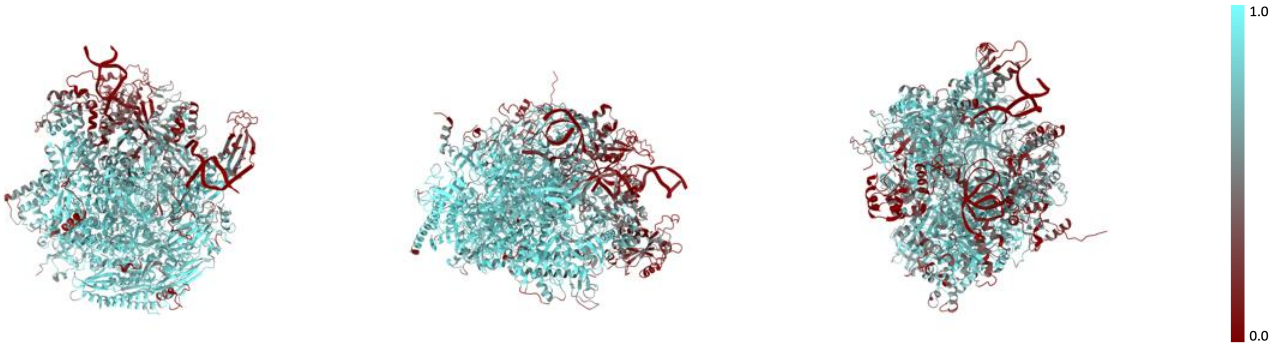
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

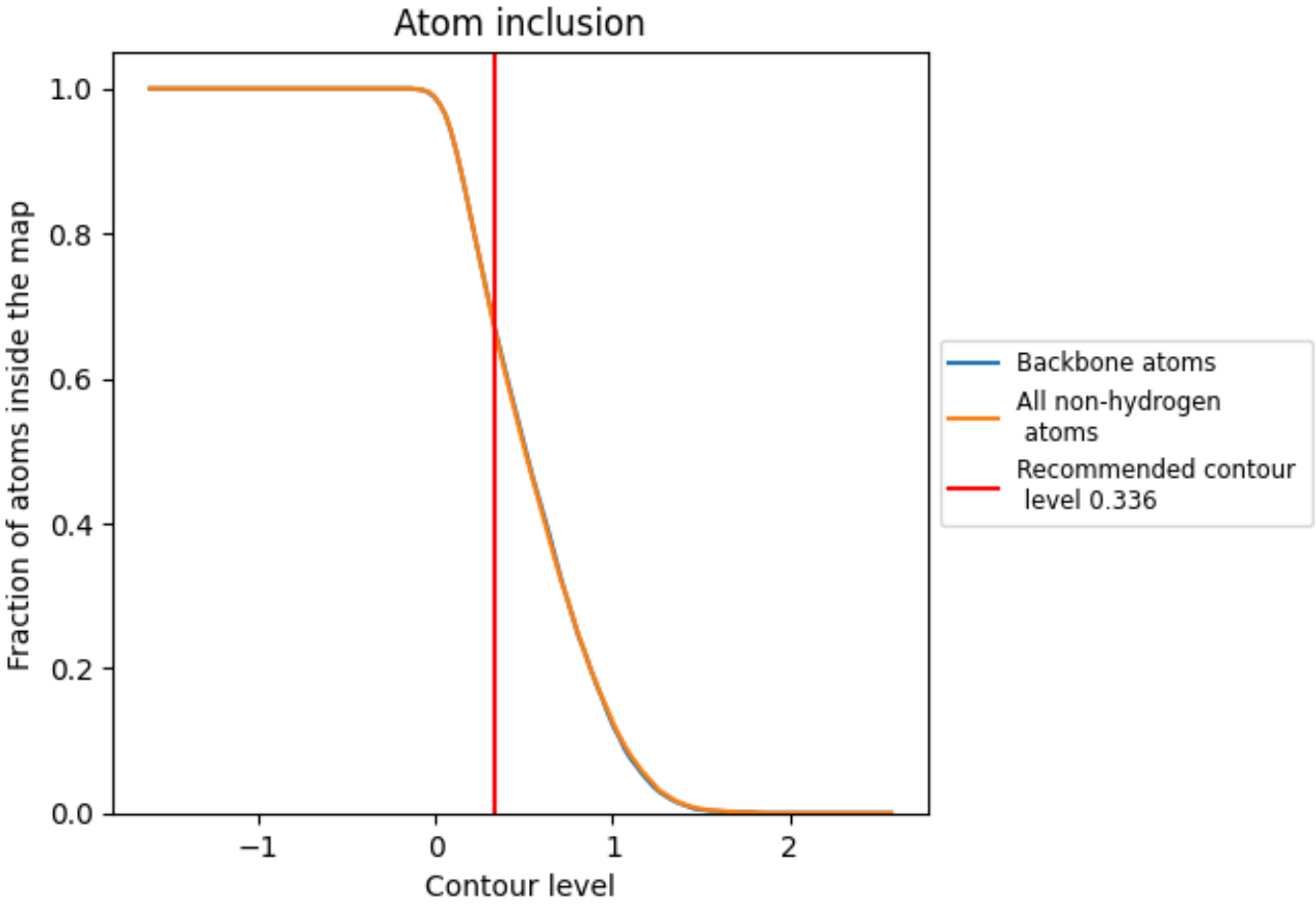
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.336).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (0.336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.5390
A	0.6450	0.5290
B	0.7400	0.5670
C	0.8890	0.6190
E	0.6060	0.5310
F	0.8280	0.6180
G	0.3530	0.4310
H	0.7190	0.5590
I	0.4400	0.4710
J	0.8500	0.6150
K	0.8610	0.6100
L	0.7560	0.5620
N	0.0690	0.2200
P	0.7480	0.5660
T	0.2600	0.3390
X	0.6690	0.5520
Y	0.5980	0.5260