



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 07:15 pm BST

PDB ID : 5N5Y / pdb_00005n5y
EMDB ID : EMD-3590
Title : Cryo-EM structure of RNA polymerase I in complex with Rrn3 and Core Factor (Orientation III)
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-02-14
Resolution : 7.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

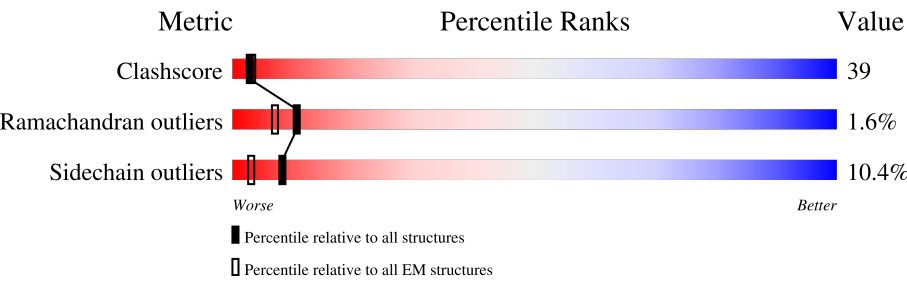
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 7.70 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

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	1664	<div><div>9%</div><div>61%</div><div>24%</div><div>•</div><div>12%</div></div>
2	B	1203	<div><div>12%</div><div>64%</div><div>30%</div><div>•</div><div>•</div></div>
3	C	335	<div><div>5%</div><div>65%</div><div>23%</div><div>••</div><div>9%</div></div>
4	D	137	<div><div>•</div><div>31%</div><div>9%</div><div>••</div><div>58%</div></div>
5	E	215	<div><div>•</div><div>78%</div><div>17%</div><div>••</div></div>
6	F	155	<div><div>5%</div><div>48%</div><div>14%</div><div>•</div><div>35%</div></div>
7	G	326	<div><div>5%</div><div>43%</div><div>15%</div><div>•</div><div>41%</div></div>
8	H	146	<div><div>•</div><div>67%</div><div>21%</div><div>•</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	P	894	
17	Q	514	
18	R	507	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	SO4	R	601	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 48030 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 DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1467	Total	C	N	O	S	0	0
			11598	7327	2017	2193	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9312	5891	1633	1738	50		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	99	Total	C	N	O	S	0	0
			755	472	125	149	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	473	Total	C	N	O	S	0	0
			3907	2533	642	711	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	583	Total	C	N	O	S	0	0
			4729	3010	803	905	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	410	Total	C	N	O	S	0	0
			3421	2219	579	603	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

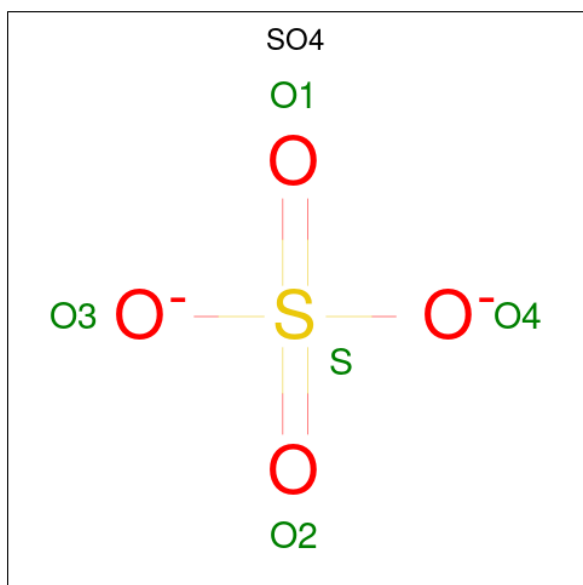
Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	
19	J	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
19	L	1	Total	Zn	0
			1	1	
19	Q	1	Total	Zn	0
			1	1	

- Molecule 20 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
20	P	1	Total	O	S	0
			5	4	1	
20	P	1	Total	O	S	0
			5	4	1	
20	P	1	Total	O	S	0
			5	4	1	
20	Q	1	Total	O	S	0
			5	4	1	
20	R	1	Total	O	S	0
			5	4	1	

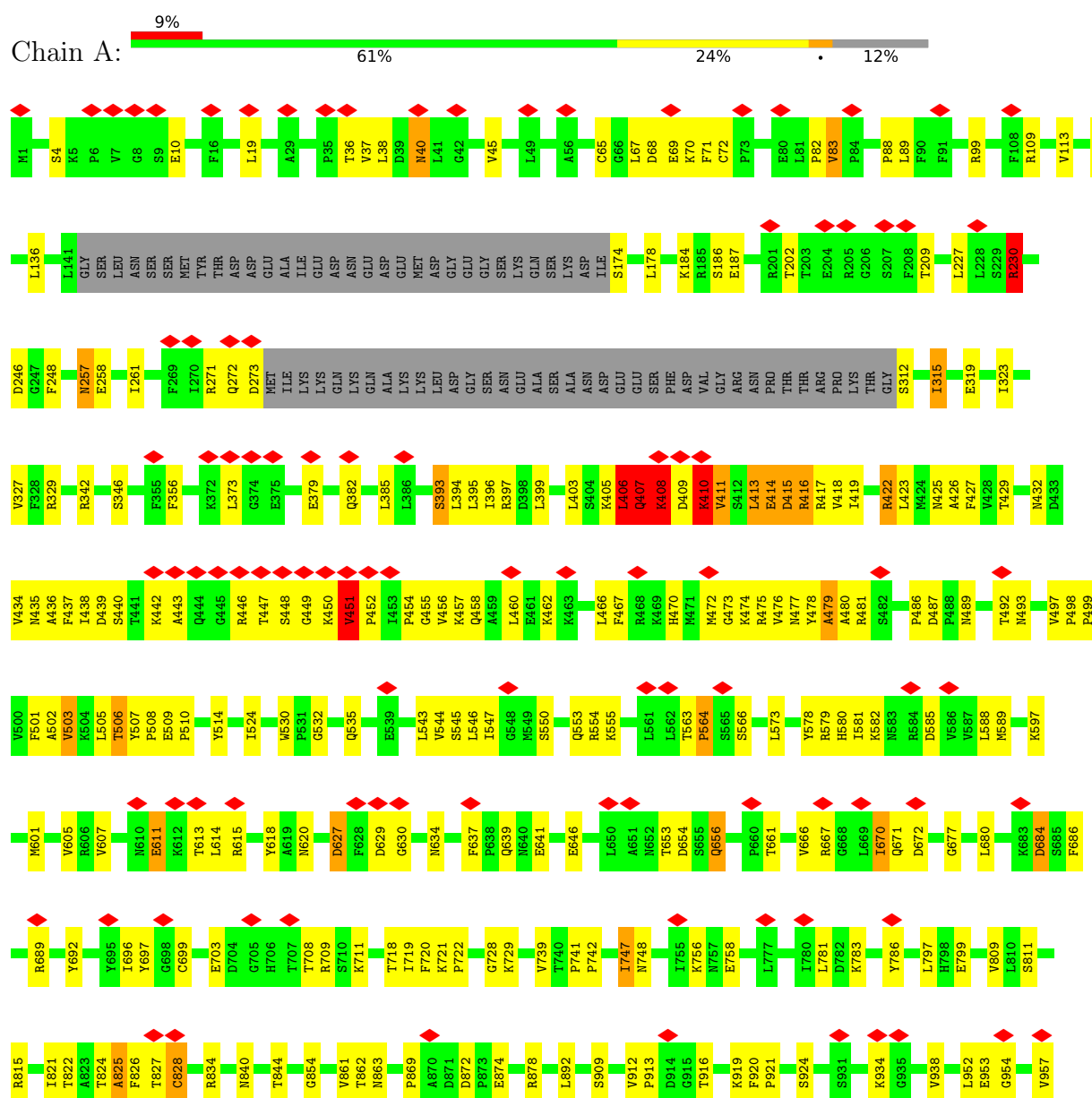
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

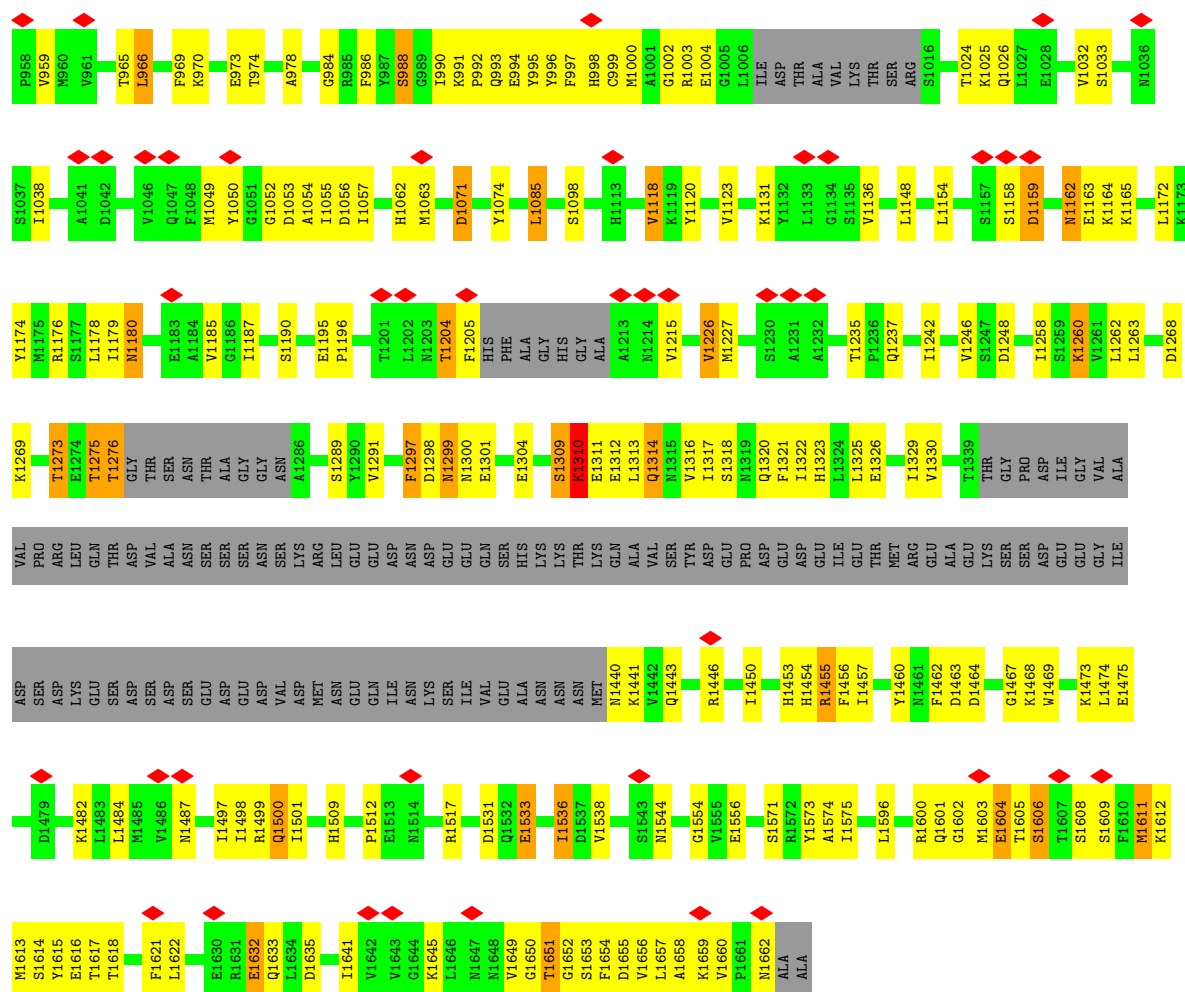
Mol	Chain	Residues	Atoms		AltConf
21	R	1	Total	Mg	0
			1	1	

3 Residue-property plots

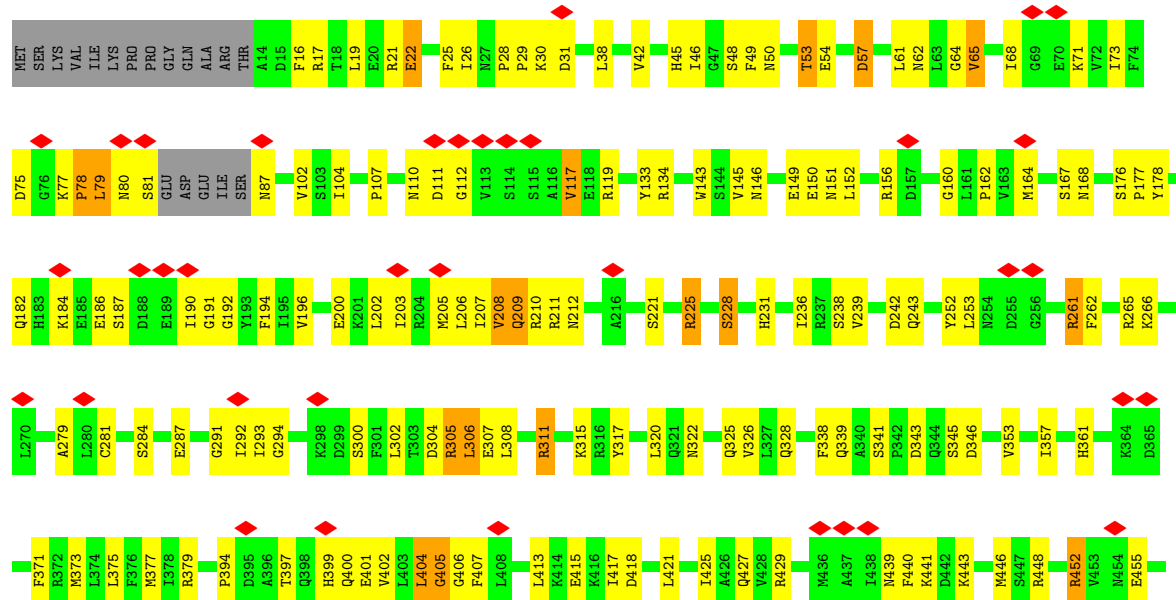
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

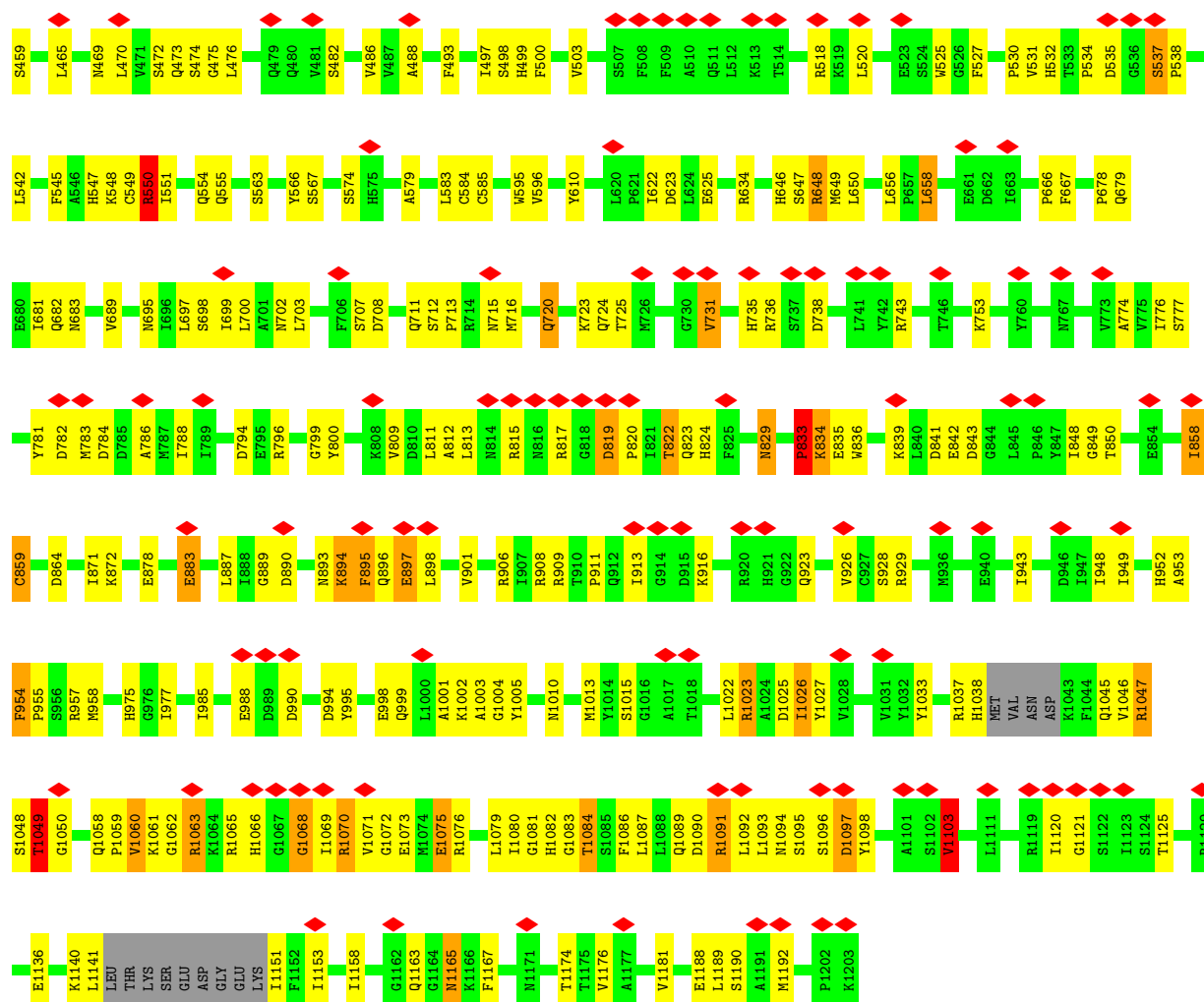
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190



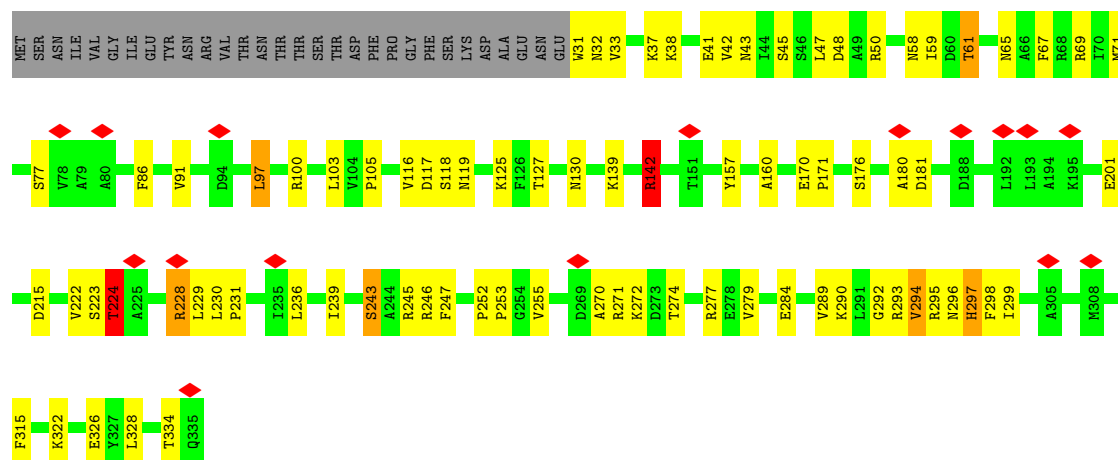


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

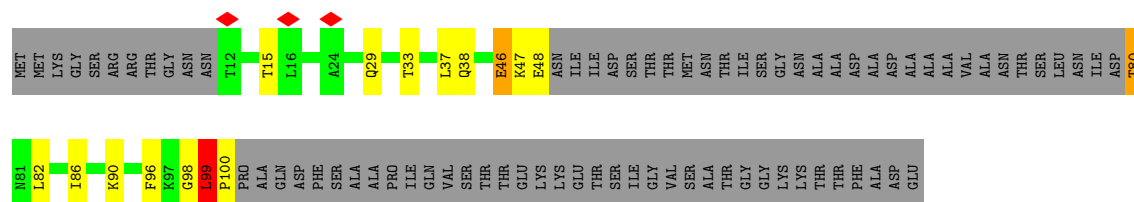




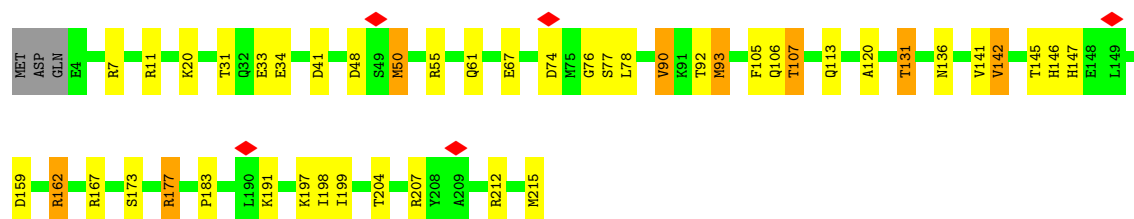
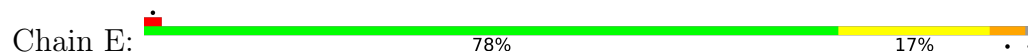
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



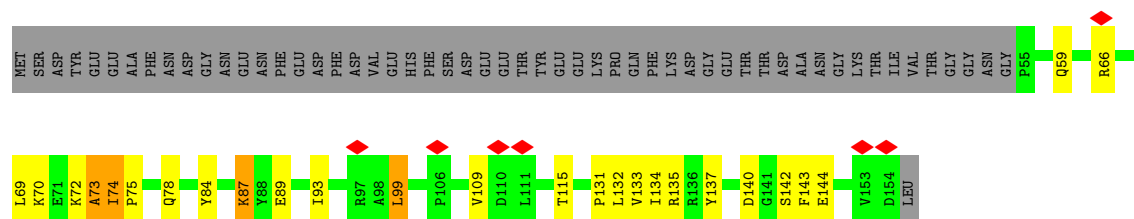
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14



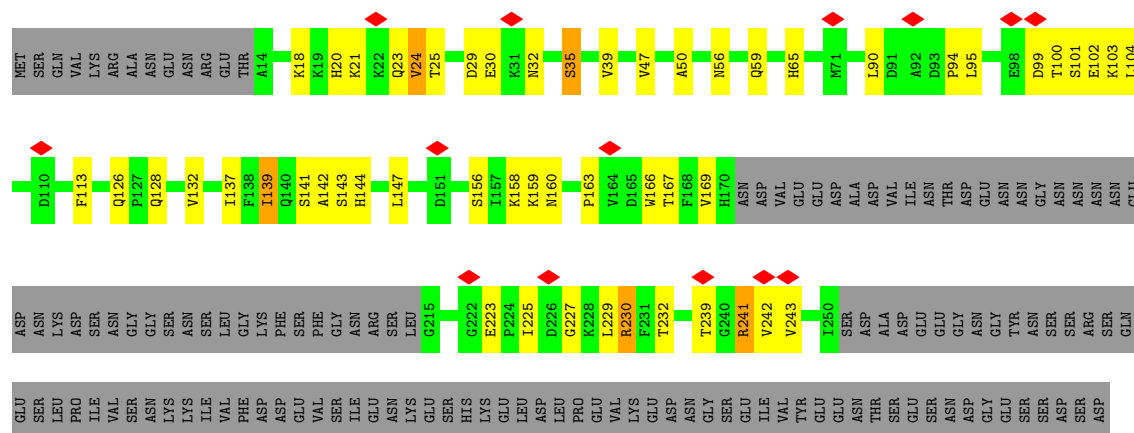
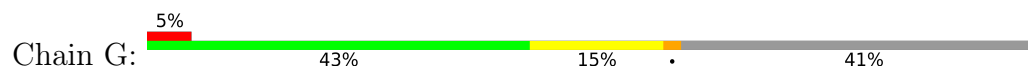
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

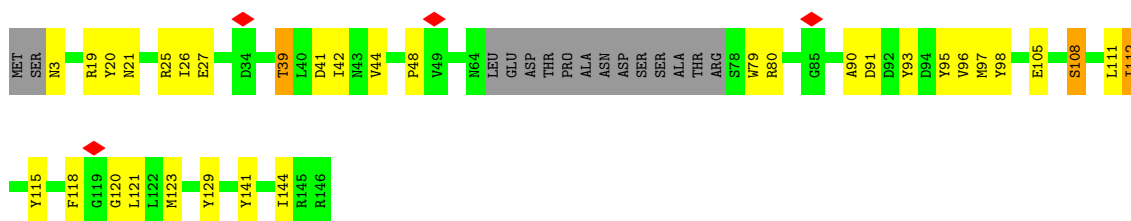


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



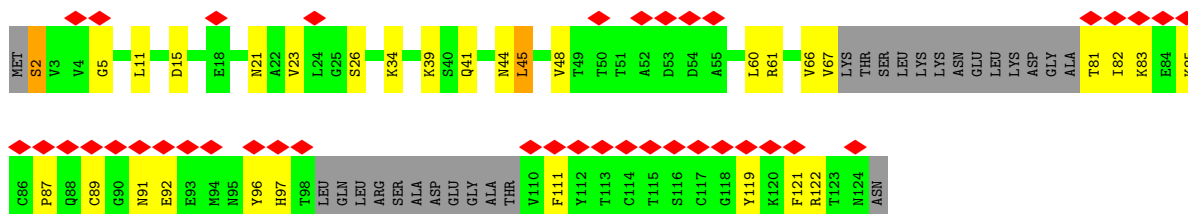
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



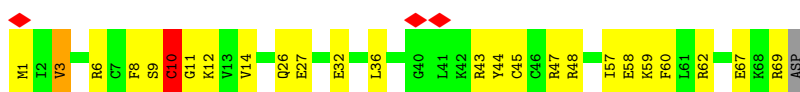
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I: 



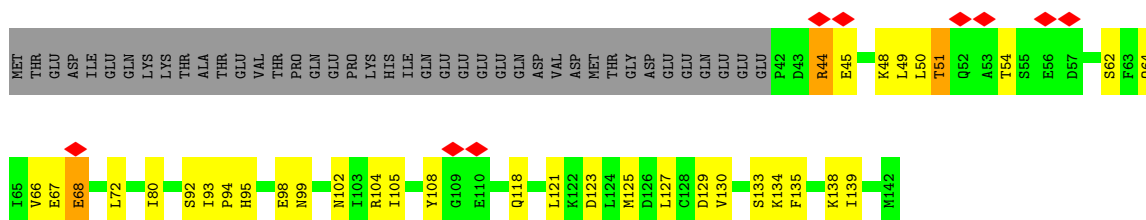
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 

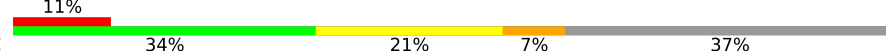


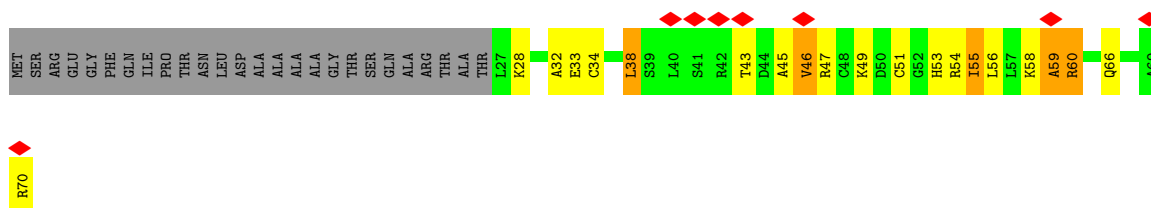
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 

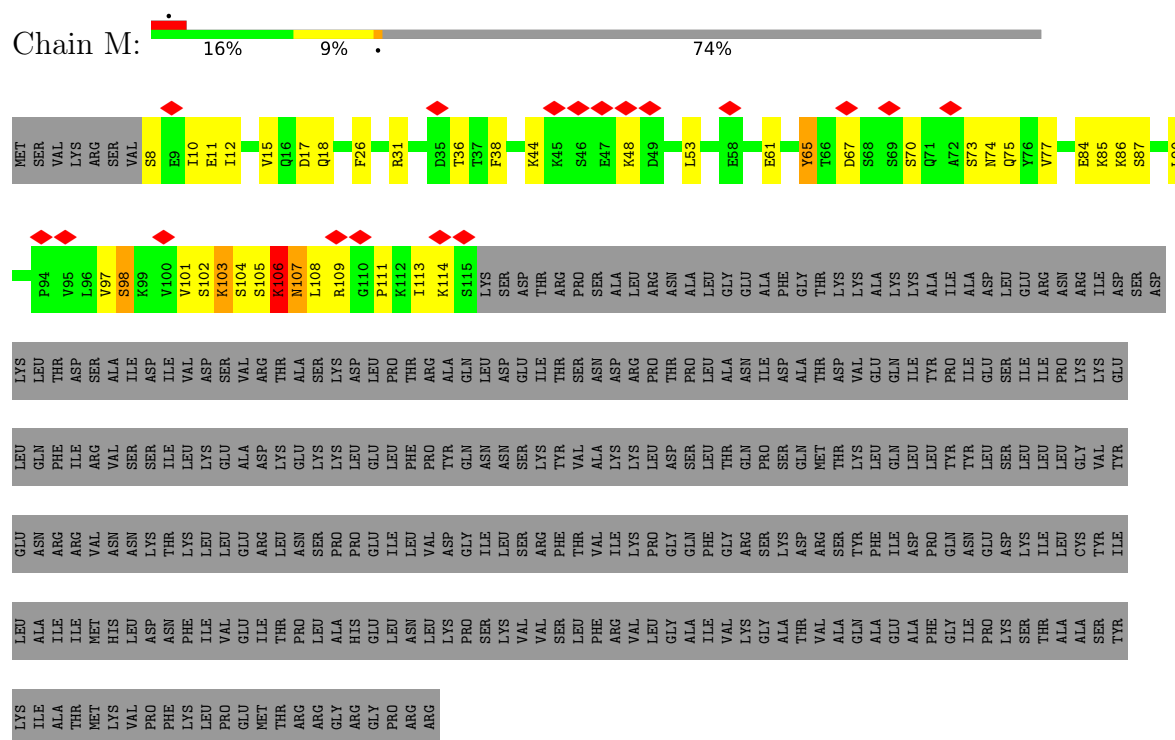


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

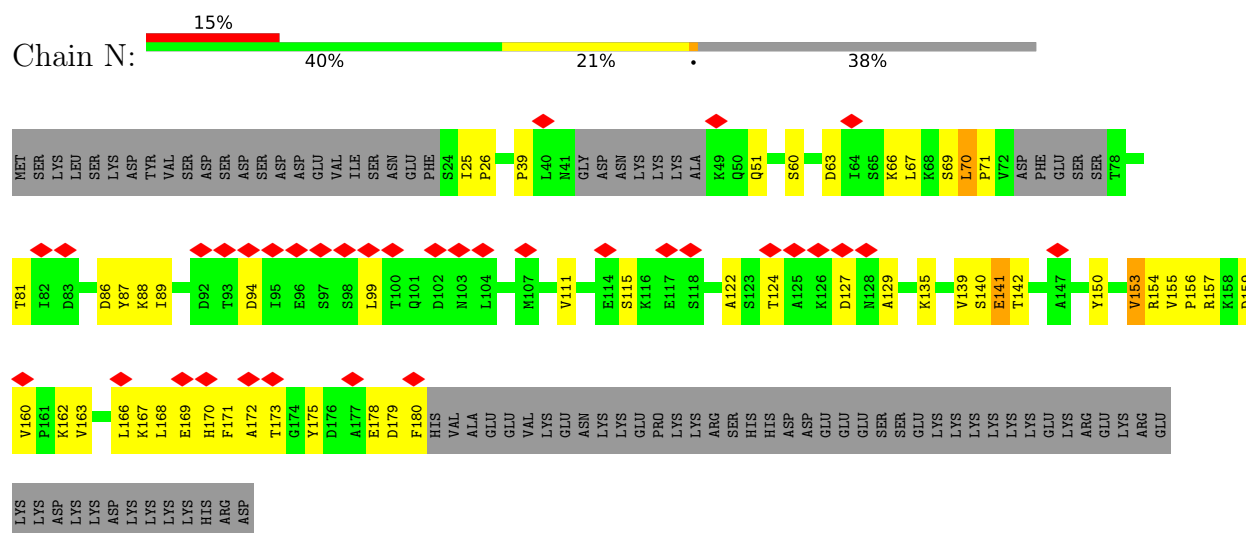
Chain L: 



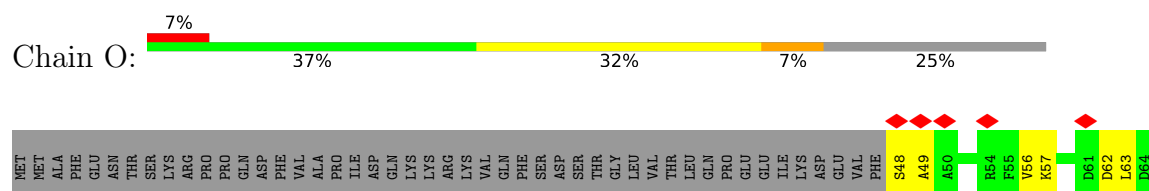
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



- Molecule 14: DNA-directed RNA polymerase I subunit RPA34



- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3



S440	ARG
	LEU
	TYR
	GLY
	GLU
	ALA
	GLN
	ASP
	ILE
	GLN
	GLU
	ARG
	ASP
	VAL
	ALA
	ASN
	VAL
	TYR
	ASP
	SER
	GLU
	ILE
	ASP
	ASN
	SER
	SER
	VAL
	GLU
	ASN
	SER
	SER
	PHE
	GLY
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	TYR
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	ALA
	GLU
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	ASP
	THR
	GLN
	LEU
	MET
	ASP
	LEU
	SER
	PRO
	GLU
	ASN
	GLY
	LEU
	ASP
	GLU
	MET
	HIS

TYR
SER
ASP
GLU
ASP
SER
SER
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8317	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 ($e^-/\text{\AA}^2$)	40	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	0.068	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0205	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SO4

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	0.49	0/11809	0.72	20/15943 (0.1%)
2	B	0.50	2/9518 (0.0%)	0.78	26/12863 (0.2%)
3	C	0.42	0/2475	0.67	3/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.37	0/1563	0.66	3/2124 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.44	0/765	0.58	0/1030
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.79	3/1083 (0.3%)
12	L	0.42	0/354	0.60	0/468
13	M	0.40	0/872	0.55	0/1170
14	N	0.40	0/1172	0.54	0/1580
15	O	0.35	0/3996	0.54	0/5401
16	P	0.41	0/4822	0.68	4/6525 (0.1%)
17	Q	0.38	0/3502	0.64	2/4727 (0.0%)
18	R	0.37	0/2592	0.60	4/3486 (0.1%)
All	All	0.44	3/48966 (0.0%)	0.68	68/66120 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
2	B	0	4
3	C	0	1
6	F	0	1
12	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	3
14	N	0	1
15	O	0	4
16	P	0	26
17	Q	0	8
18	R	0	10
All	All	0	75

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.65	1.95	1.82
2	B	281	CYS	CB-SG	-6.94	1.70	1.82
2	B	859	CYS	CB-SG	-6.12	1.71	1.82

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	7	GLY	C-N-CD	-15.27	87.00	120.60
2	B	1023	ARG	NE-CZ-NH2	-13.77	113.42	120.30
2	B	452	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	397	ARG	NE-CZ-NH1	13.12	126.86	120.30
2	B	448	ARG	NE-CZ-NH2	-13.05	113.77	120.30

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	LYS	Peptide
1	A	406	LEU	Peptide
1	A	407	GLN	Peptide
1	A	410	LYS	Peptide
1	A	411	VAL	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	11598	0	11666	1168	0
2	B	9312	0	9200	980	0
3	C	2423	0	2412	139	0
4	D	459	0	462	8	0
5	E	1735	0	1764	30	0
6	F	823	0	839	96	0
7	G	1526	0	1534	151	0
8	H	1052	0	1021	55	0
9	I	755	0	728	104	0
10	J	569	0	584	55	0
11	K	793	0	790	54	0
12	L	352	0	371	58	0
13	M	856	0	852	59	0
14	N	1151	0	1168	166	0
15	O	3907	0	3902	406	0
16	P	4729	0	4670	579	0
17	Q	3421	0	3463	446	0
18	R	2535	0	2606	599	0
19	A	2	0	0	1	0
19	B	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	Q	1	0	0	0	0
20	P	15	0	0	2	0
20	Q	5	0	0	1	0
20	R	5	0	0	4	0
21	R	1	0	0	0	0
All	All	48030	0	48032	3777	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 39.

The worst 5 of 3777 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)
3:C:272:LYS:HA	14:N:175:TYR:CE1	1.16	1.69
1:A:990:ILE:CB	1:A:994:GLU:HB2	1.19	1.66
1:A:995:TYR:CD2	2:B:708:ASP:HA	1.29	1.65
16:P:473:HIS:CD2	18:R:1:MET:HB2	1.16	1.63
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.62

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	1449/1664 (87%)	1375 (95%)	60 (4%)	14 (1%)	13	49
2	B	1164/1203 (97%)	1095 (94%)	51 (4%)	18 (2%)	8	40
3	C	303/335 (90%)	288 (95%)	12 (4%)	3 (1%)	13	49
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	20
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	13	49
6	F	98/155 (63%)	95 (97%)	2 (2%)	1 (1%)	13	49
7	G	187/326 (57%)	173 (92%)	12 (6%)	2 (1%)	12	47
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	91/125 (73%)	80 (88%)	8 (9%)	3 (3%)	3	21
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2	16
13	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	6	32
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	5	29
15	O	467/627 (74%)	426 (91%)	35 (8%)	6 (1%)	10	43
16	P	569/894 (64%)	474 (83%)	75 (13%)	20 (4%)	3	20
17	Q	398/514 (77%)	347 (87%)	41 (10%)	10 (2%)	4	26
18	R	291/507 (57%)	243 (84%)	42 (14%)	6 (2%)	5	30
All	All	5861/7778 (75%)	5374 (92%)	393 (7%)	94 (2%)	10	38

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	LYS

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Mol	Chain	Res	Type
1	A	479	ALA
1	A	1651	THR
2	B	111	ASP
2	B	895	PHE

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	1297/1465 (88%)	1215 (94%)	82 (6%)	15	36
2	B	1025/1053 (97%)	960 (94%)	65 (6%)	15	36
3	C	269/296 (91%)	253 (94%)	16 (6%)	16	37
4	D	55/116 (47%)	49 (89%)	6 (11%)	5	18
5	E	194/197 (98%)	180 (93%)	14 (7%)	12	32
6	F	90/137 (66%)	86 (96%)	4 (4%)	24	45
7	G	171/291 (59%)	159 (93%)	12 (7%)	12	32
8	H	115/128 (90%)	111 (96%)	4 (4%)	31	51
9	I	89/110 (81%)	85 (96%)	4 (4%)	23	45
10	J	64/65 (98%)	57 (89%)	7 (11%)	5	18
11	K	91/130 (70%)	84 (92%)	7 (8%)	10	30
12	L	39/57 (68%)	36 (92%)	3 (8%)	10	30
13	M	98/371 (26%)	85 (87%)	13 (13%)	3	13
14	N	135/220 (61%)	129 (96%)	6 (4%)	24	45
15	O	439/576 (76%)	387 (88%)	52 (12%)	4	16
16	P	539/828 (65%)	396 (74%)	143 (26%)	0	3
17	Q	383/476 (80%)	318 (83%)	65 (17%)	1	9
18	R	286/474 (60%)	228 (80%)	58 (20%)	1	6
All	All	5379/6990 (77%)	4818 (90%)	561 (10%)	8	19

5 of 561 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	218	SER
17	Q	318	LEU
17	Q	207	LEU
18	R	160	HIS
7	G	169	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	521	ASN
17	Q	406	GLN
15	O	547	ASN
16	P	348	HIS
18	R	212	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	SO4	R	601	18	4,4,4	0.17	0	6,6,6	0.11	0
20	SO4	P	902	-	4,4,4	0.14	0	6,6,6	0.23	0
20	SO4	Q	1002	-	4,4,4	0.14	0	6,6,6	0.26	0
20	SO4	P	903	-	4,4,4	0.14	0	6,6,6	0.10	0
20	SO4	P	901	-	4,4,4	0.11	0	6,6,6	0.24	0

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	601	SO4	4	0
20	P	902	SO4	1	0
20	Q	1002	SO4	1	0
20	P	903	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
7	G	1
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	24:VAL	C	25:THR	N	4.53
1	I	45:LEU	C	46:LYS	N	3.17
1	A	438:ILE	C	439:ASP	N	2.97
1	A	991:LYS	C	992:PRO	N	2.86

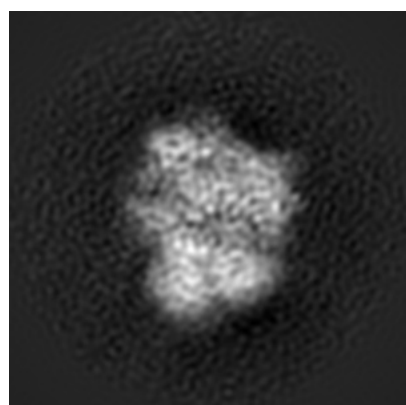
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3590. These allow visual inspection of the internal detail of the map and identification of artifacts.

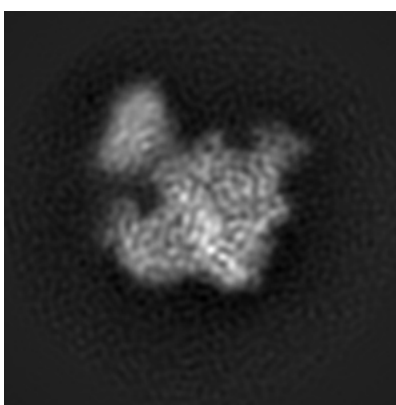
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

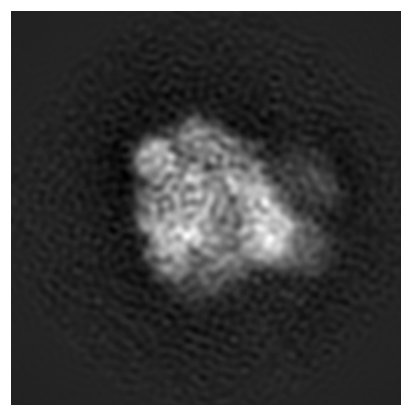
6.1.1 Primary map



X



Y

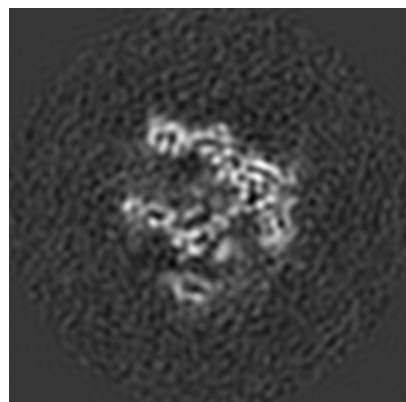


Z

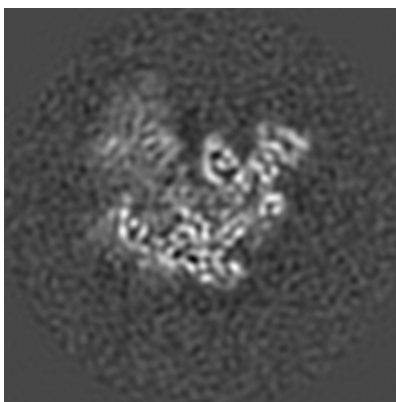
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

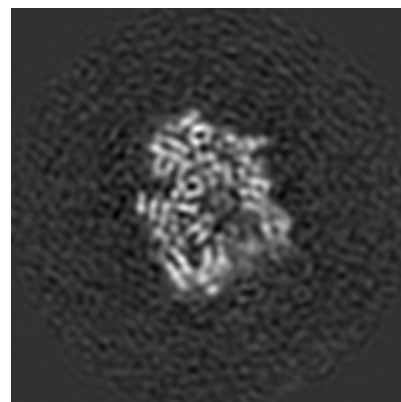
6.2.1 Primary map



X Index: 120



Y Index: 120

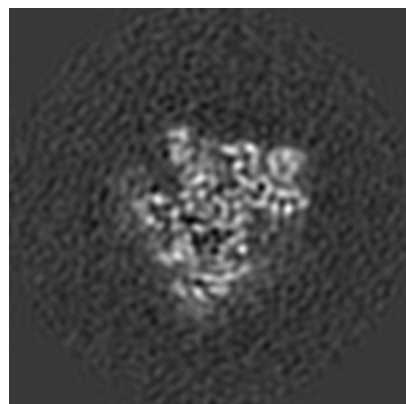


Z Index: 120

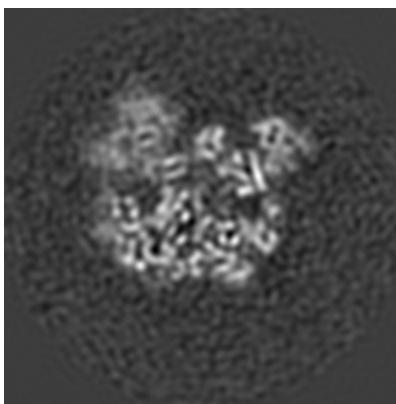
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

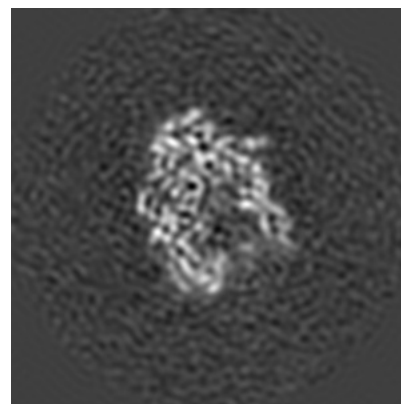
6.3.1 Primary map



X Index: 111



Y Index: 109

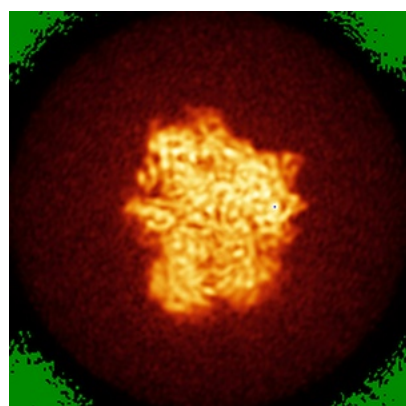


Z Index: 122

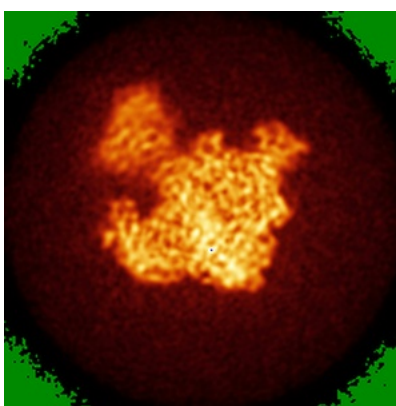
The images above show the largest variance slices of the map in three orthogonal directions.

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

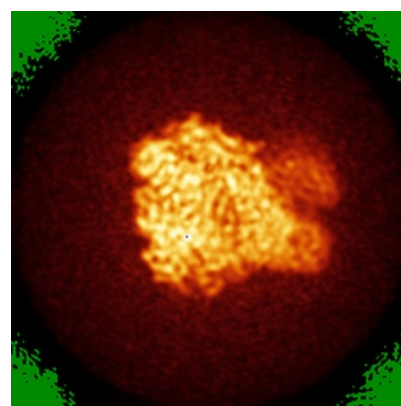
6.4.1 Primary map



X



Y

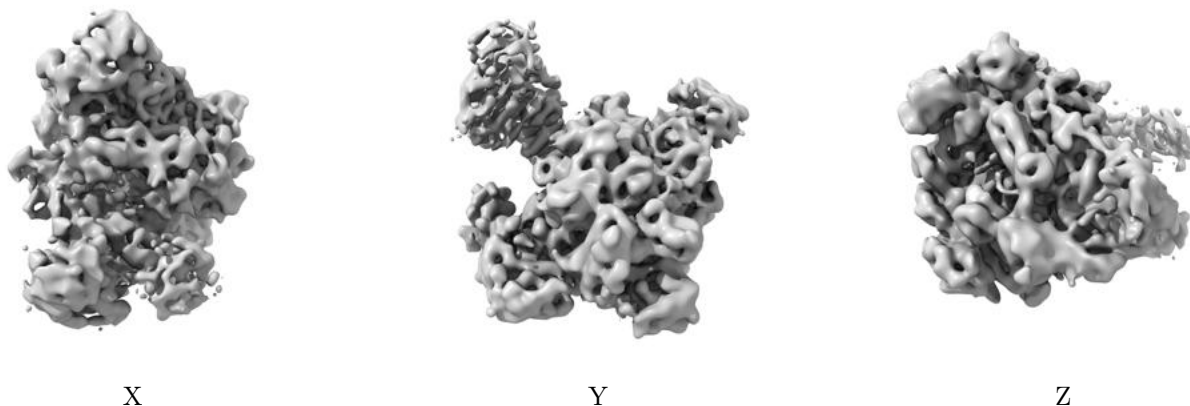


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0205. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

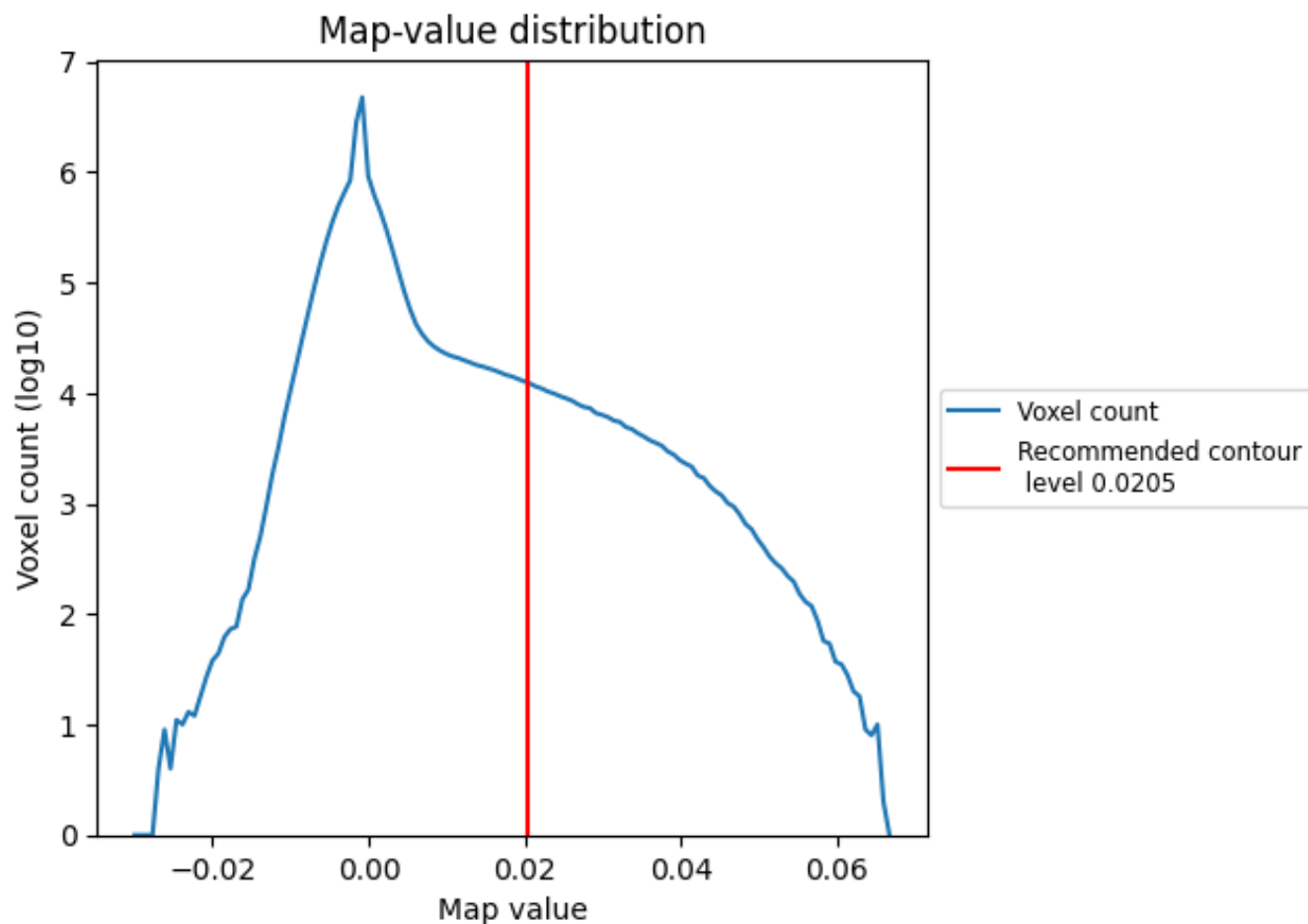
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

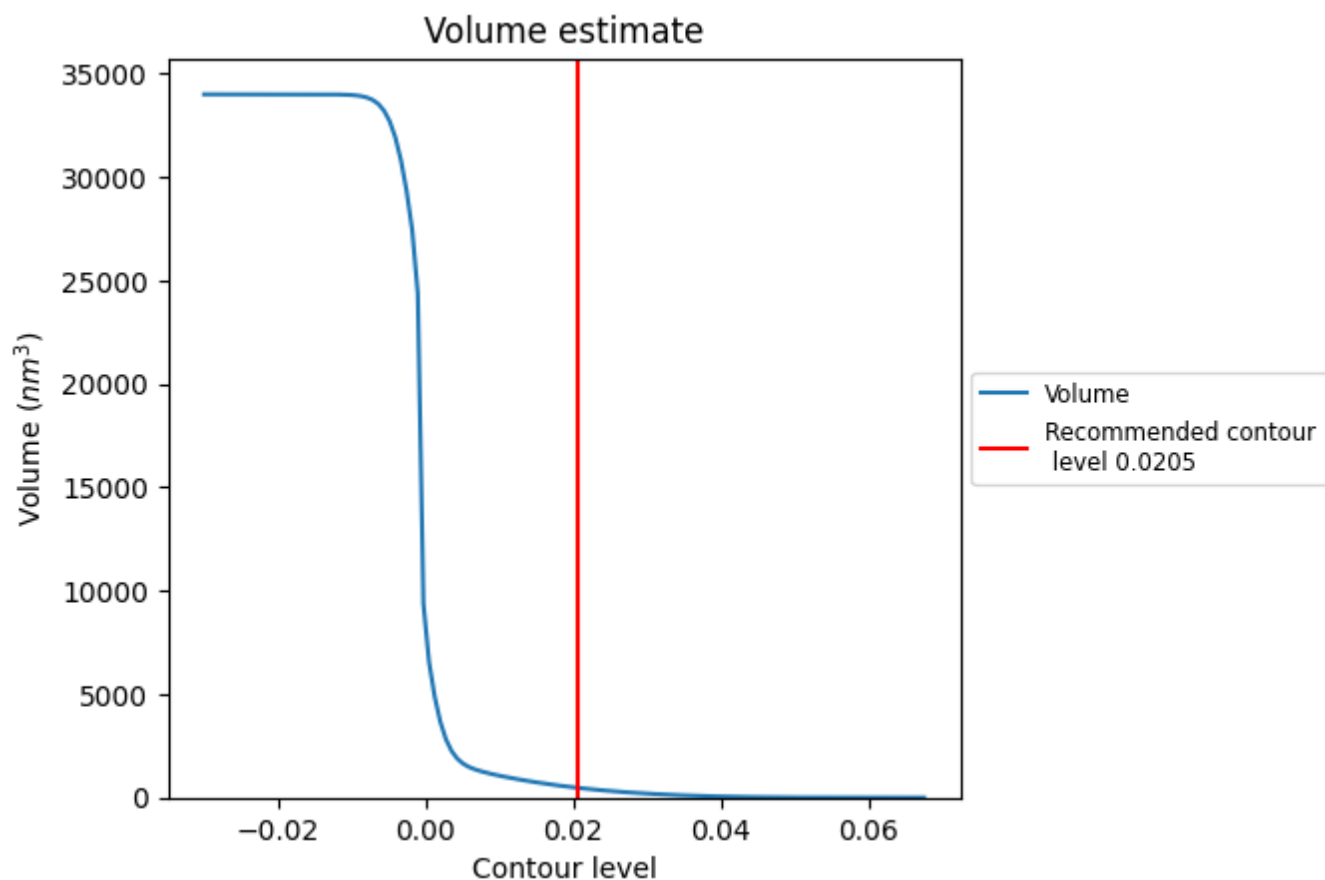
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

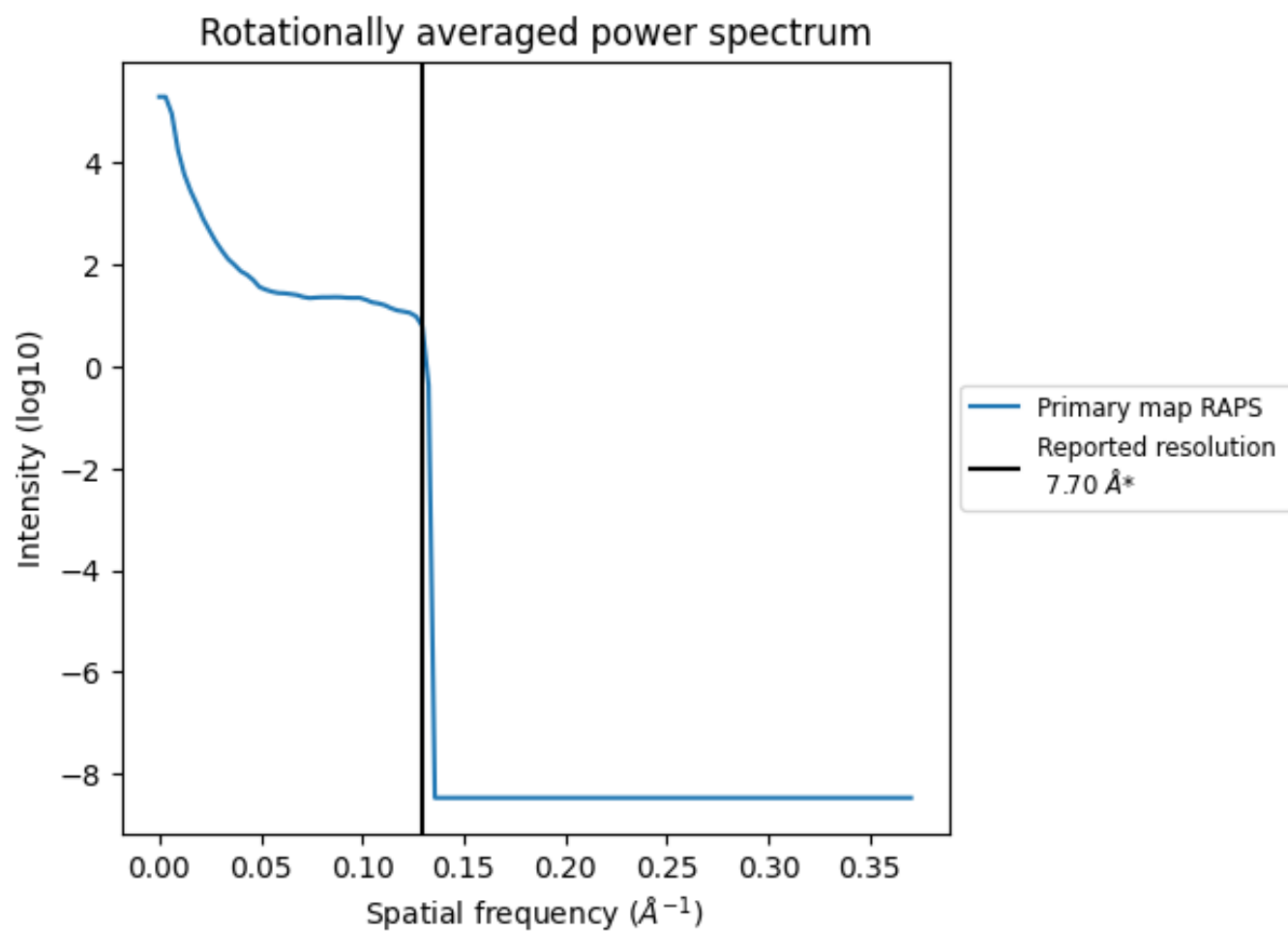
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 475 nm³; this corresponds to an approximate mass of 429 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 0.130 Å⁻¹

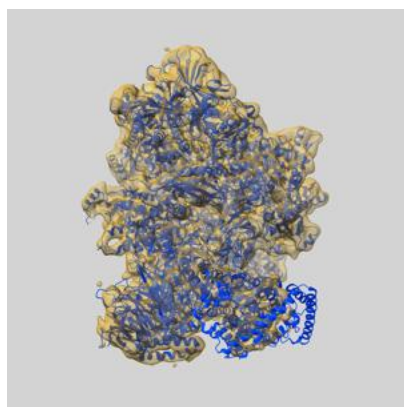
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

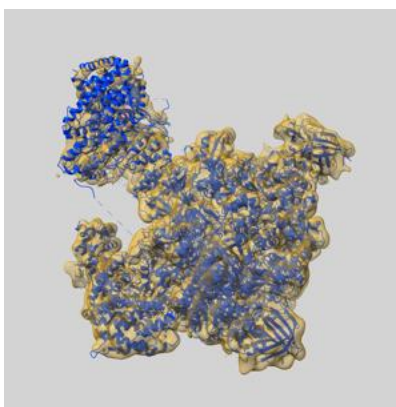
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3590 and PDB model 5N5Y. Per-residue inclusion information can be found in section [3](#) on page [8](#).

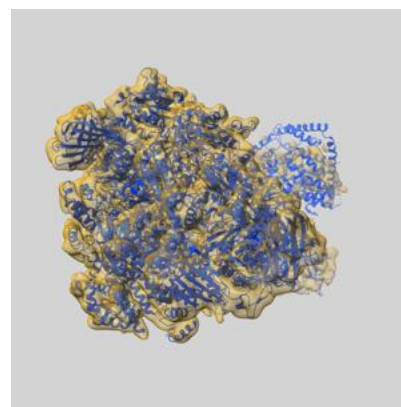
9.1 Map-model overlay [i](#)



X



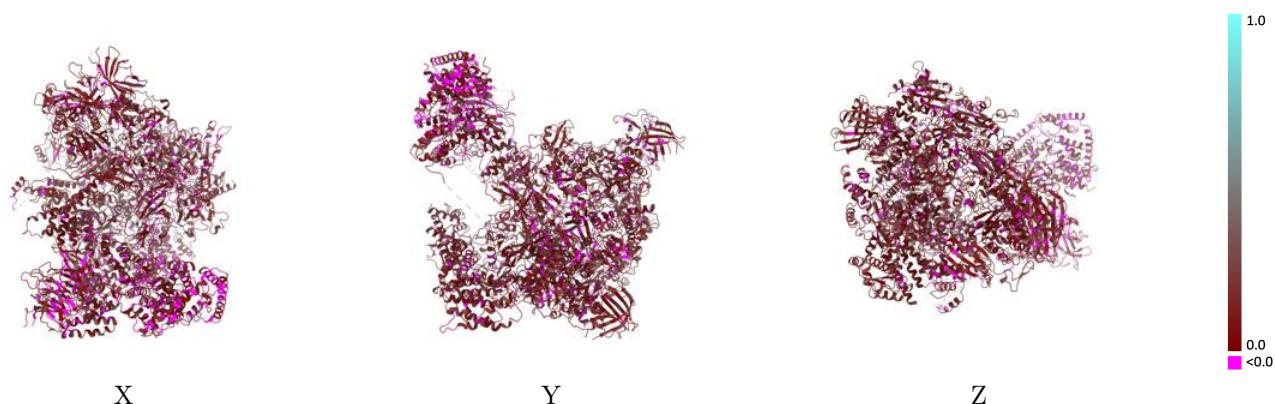
Y



Z

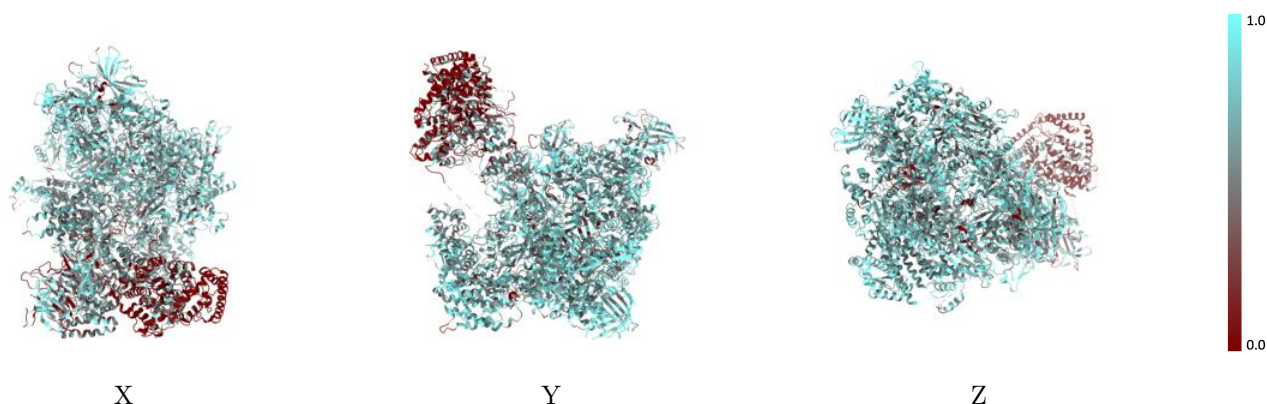
The images above show the 3D surface view of the map at the recommended contour level 0.0205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



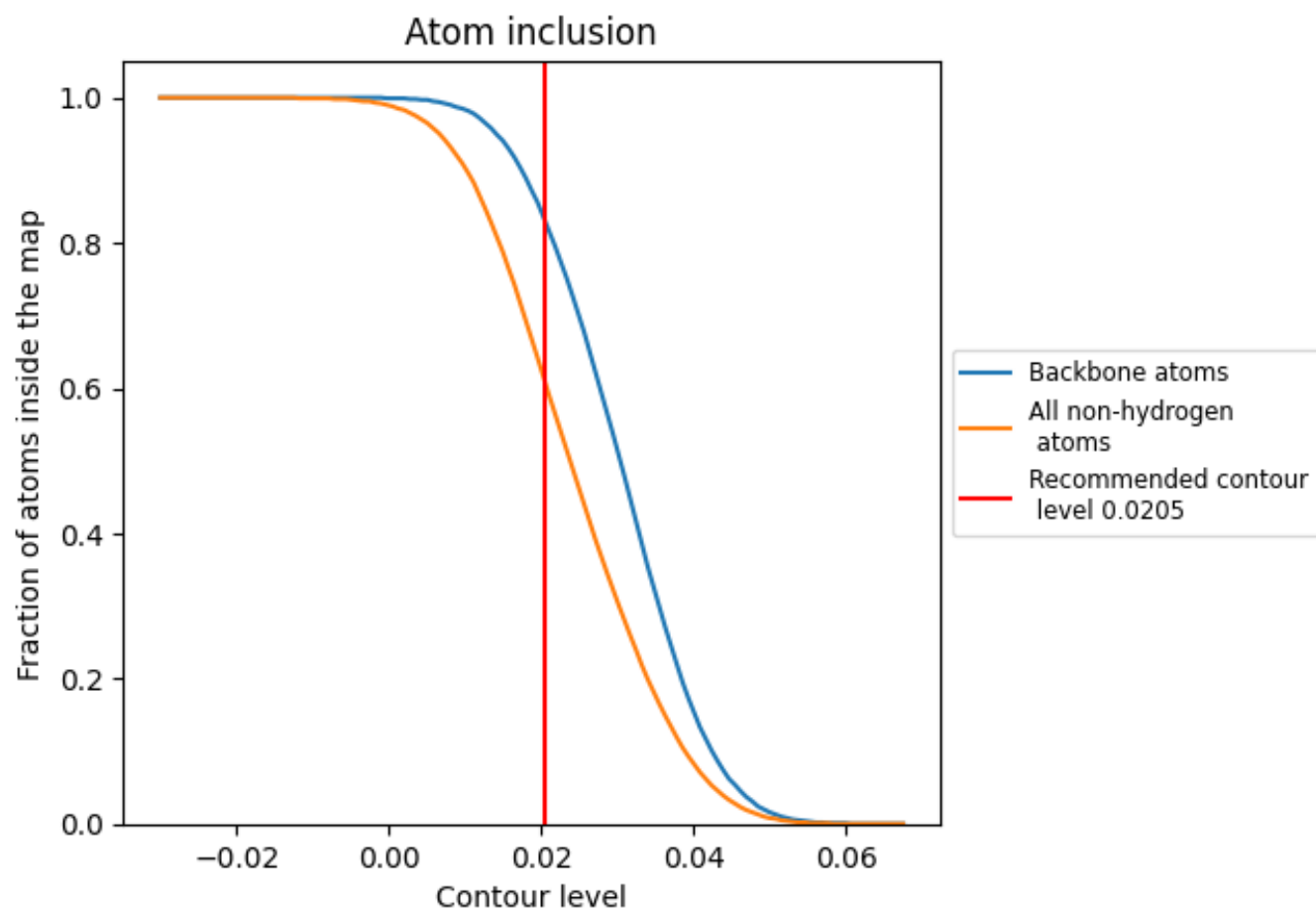
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0205).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 61% 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 (0.0205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.1360
A	 0.6710	 0.1450
B	 0.6630	 0.1390
C	 0.7390	 0.1510
D	 0.7010	 0.1650
E	 0.7490	 0.1640
F	 0.6800	 0.1590
G	 0.7360	 0.1430
H	 0.7800	 0.1650
I	 0.4990	 0.1470
J	 0.7050	 0.1390
K	 0.7080	 0.1590
L	 0.6560	 0.1360
M	 0.6540	 0.1420
N	 0.6120	 0.1470
O	 0.6660	 0.1450
P	 0.3550	 0.0870
Q	 0.2790	 0.0930
R	 0.5080	 0.1370

