wwPDB EM Validation Summary Report

Dec 15, 2024 – 06:33 am GMT

PDB ID	:	9ER2
EMDB ID	:	EMD-19909
Title	:	PolII-TCR-STK19 structure.
Authors	:	Kokic, G.
Deposited on	:	2024-03-22
Resolution	:	3.30 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:

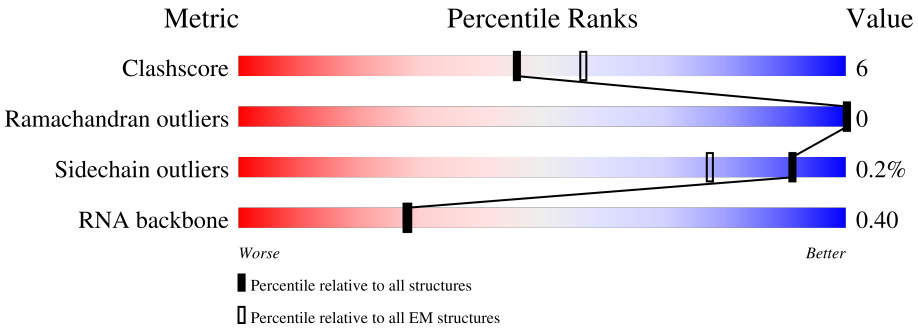
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	P	14	29% 50% 36% 14%
2	Q	258	7% 79% 8% 13%
3	A	1984	60% 11% 29%
4	B	1167	83% 14%
5	C	275	84% 11% 5%
6	D	142	82% 74% 16% 10%
7	E	210	83% 16%

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Mol	Chain	Length	Quality of chain
8	F	127	51% 13% 35%
9	G	172	65% 80% 19%
10	H	150	84% 15%
11	I	125	10% 65% 29% 6%
12	J	67	87% 13%
13	K	117	85% 13%
14	L	58	69% 10% 21%
15	N	52	8% 69% 8% 23%
16	T	52	94% 6%
17	M	709	16% 5% 79%
17	c	709	10% 15% 85%
18	O	64	95% 5%
19	b	1493	35% 65%
20	a	396	91% 8%
21	d	1140	68% 31%

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 100218 atoms, of which 49569 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 RNA chain called RNA (5'-R(P*CP*AP*AP*AP*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
1	P	14	Total	C	H	N	O	P	0	0
			458	137	152	63	92	14		

- Molecule 2 is a protein called Isoform 1 of Inactive serine/threonine-protein kinase 19.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Q	224	Total	C	H	N	O	S	0	0
			3534	1115	1782	312	317	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	1410	Total	C	H	N	O	S	0	0
			22478	7028	11308	2000	2071	71		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	1130	Total	C	H	N	O	S	0	0
			18132	5725	9084	1591	1668	64		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	260	Total	C	H	N	O	S	0	0
			4120	1309	2031	359	415	6		

- Molecule 6 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	128	Total	C	H	N	O	S	0	0
			1985	636	972	172	201	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	E	209	Total	C	H	N	O	S	0	0
			3457	1089	1737	300	323	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	F	82	Total	C	H	N	O	S	0	0
			1341	418	684	113	121	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	G	171	Total	C	H	N	O	S	0	0
			2667	867	1333	216	243	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	117	Total	C	H	N	O	S	0	0
			1828	587	879	169	182	11		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	67	Total	C	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 14 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 15 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	N	40	Total	C	H	N	O	P	0	0
			1278	393	449	162	234	40		

- Molecule 16 is a DNA chain called TS.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	52	Total	C	H	N	O	P	0	0
			1544	476	553	160	303	52		

- Molecule 17 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	c	108	Total	C	H	N	O	S	0	0
			1365	431	634	164	131	5		
17	M	148	Total	C	H	N	O	S	0	0
			2449	771	1234	217	223	4		

- Molecule 18 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O	64	Total	C	H	N	O	S	0	0
			968	312	463	81	105	7		

- Molecule 19 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	b	520	Total	C	H	N	O	S	0	0
			8558	2746	4299	746	746	21		

- Molecule 20 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	a	365	Total	C	H	N	O	S	0	0
			5618	1775	2769	507	548	19		

- Molecule 21 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	d	781	Total	C	H	N	O	S	0	0
			12320	3916	6159	1038	1173	34		

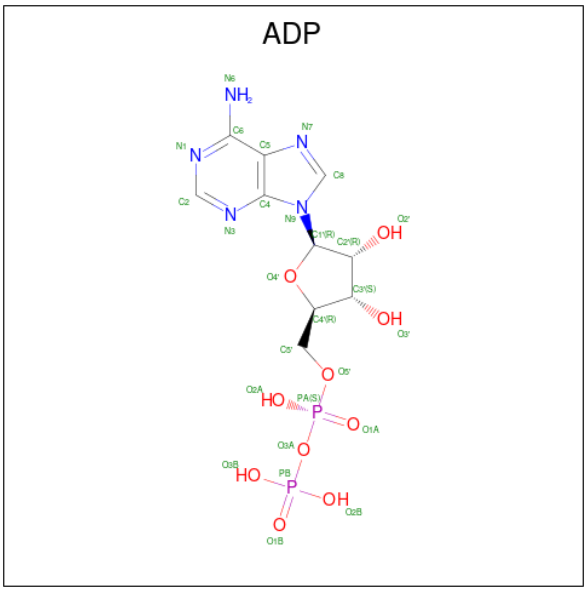
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	C	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	
22	c	2	Total	Zn	0
			2	2	
22	O	1	Total	Zn	0
			1	1	

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

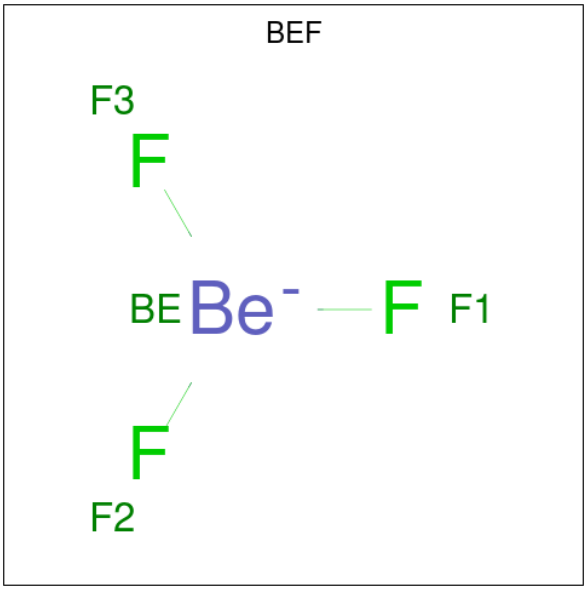
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	
23	b	1	Total	Mg	0
			1	1	

- Molecule 24 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
24	b	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 25 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



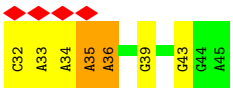
Mol	Chain	Residues	Atoms			AltConf
25	b	1	Total	Be	F	0
			4	1	3	

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.

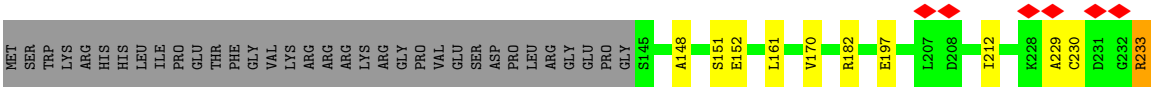
• Molecule 1: RNA (5'-R(P*CP*AP*AP*AP*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3')

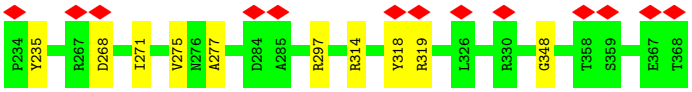
Chain P:



• Molecule 2: Isoform 1 of Inactive serine/threonine-protein kinase 19

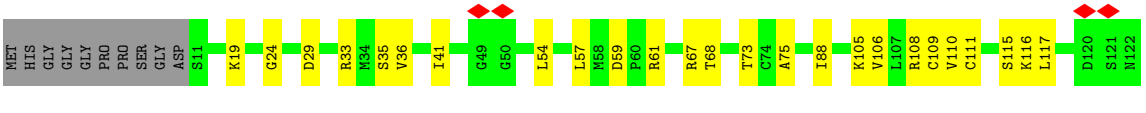
Chain Q:

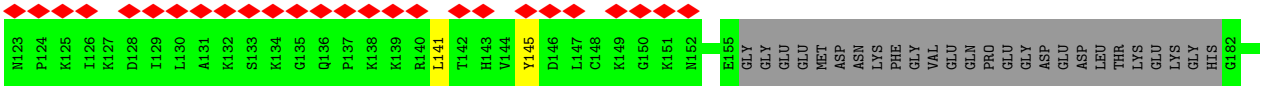


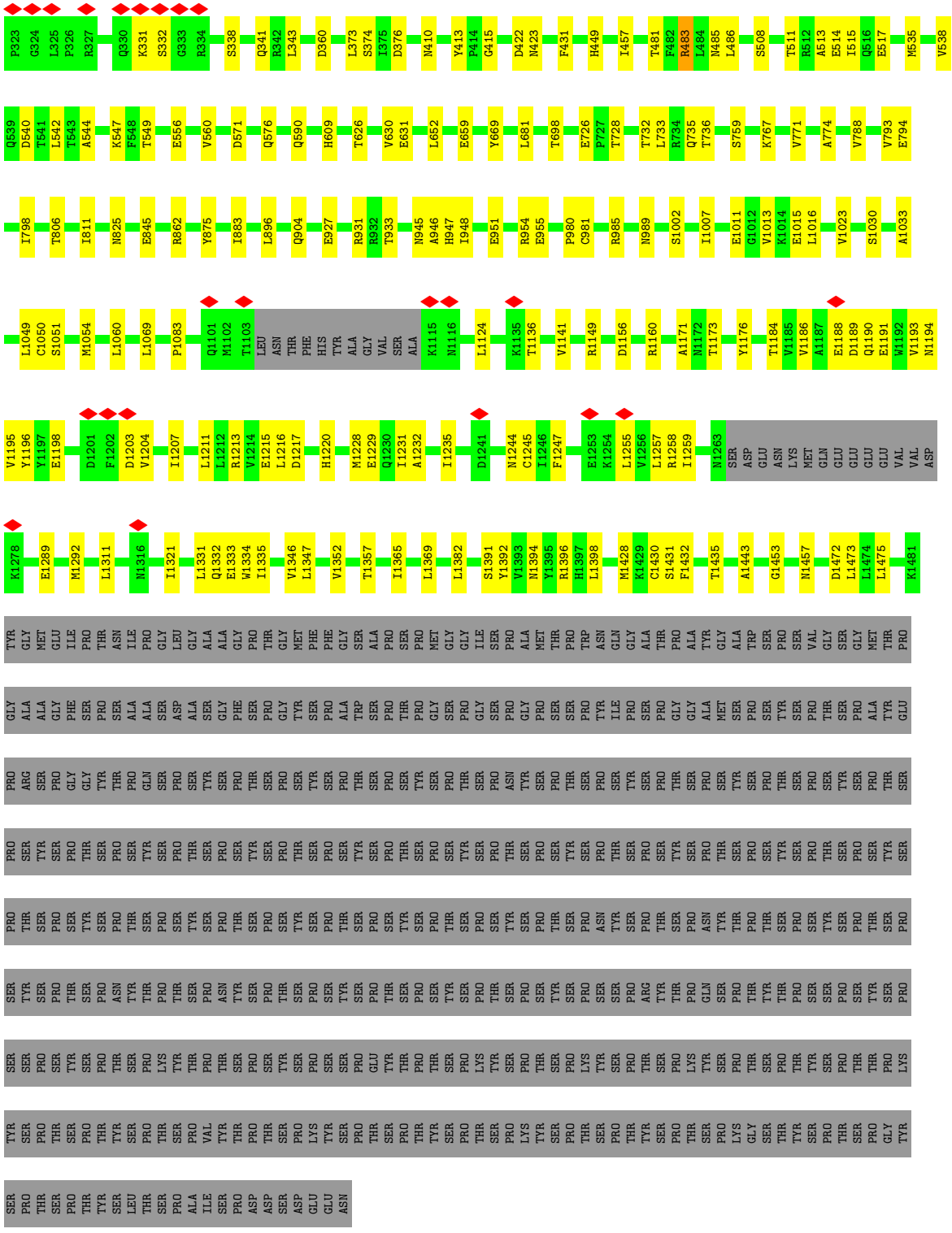


• Molecule 3: DNA-directed RNA polymerase subunit

Chain A:

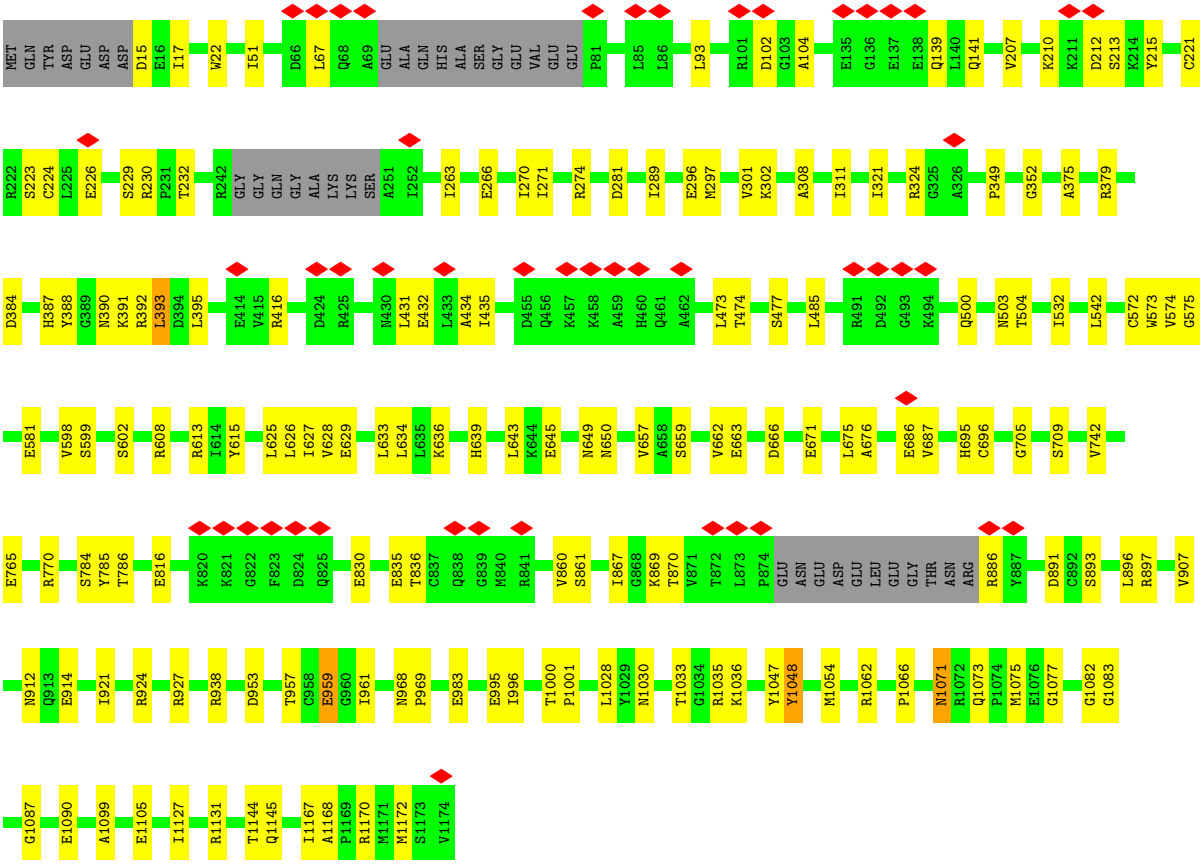






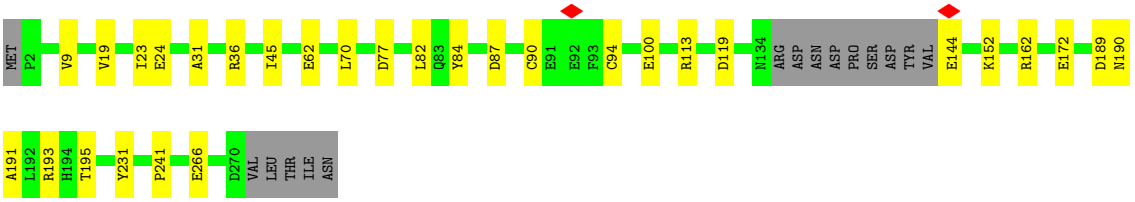
• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain B:



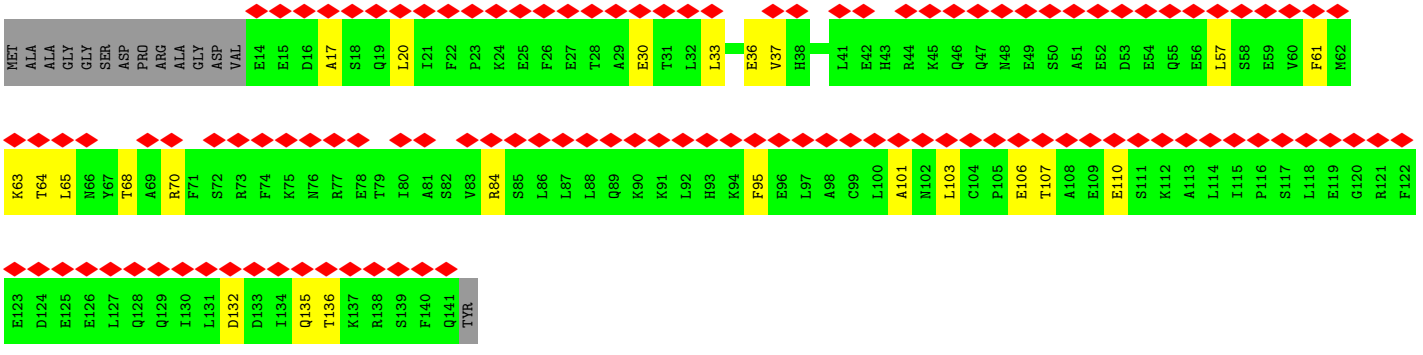
• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C:



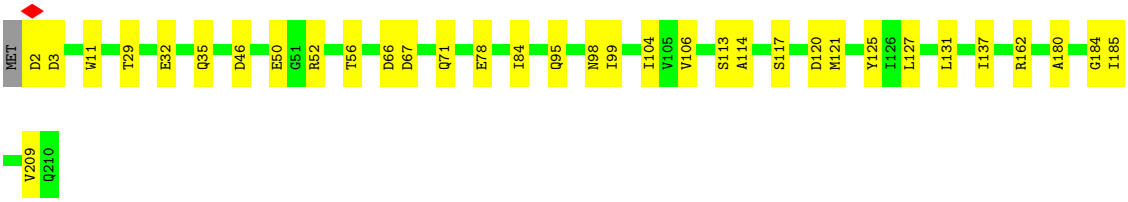
• Molecule 6: RNA polymerase II subunit D

Chain D:



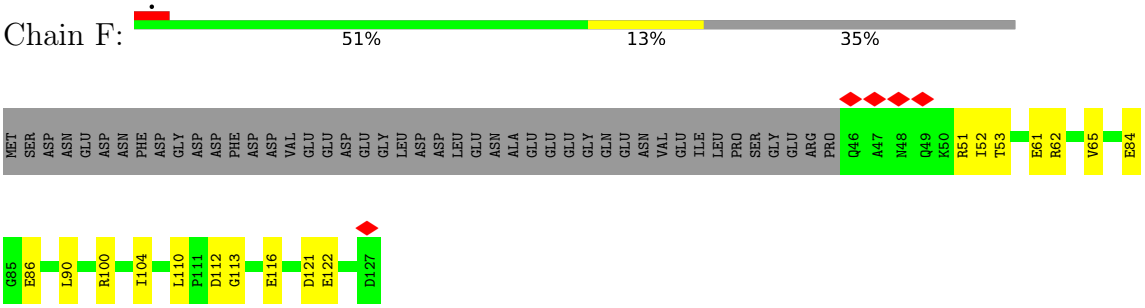
• Molecule 7: DNA-directed RNA polymerase II subunit E

Chain E:



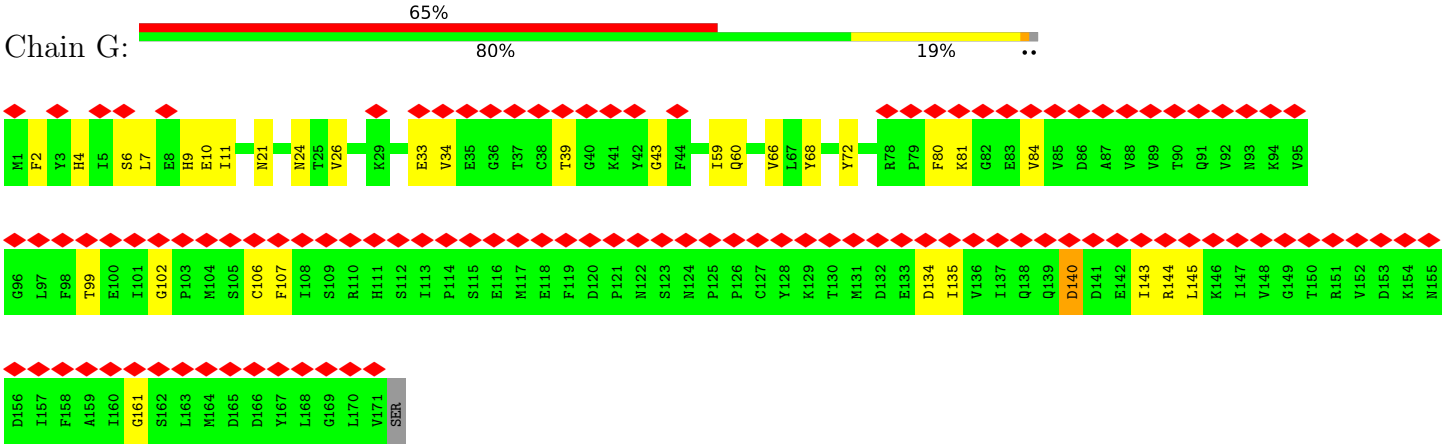
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



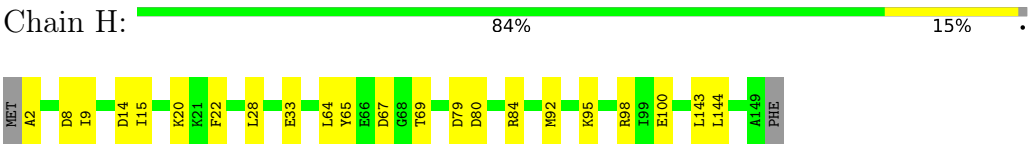
• Molecule 9: DNA-directed RNA polymerase subunit

Chain G:



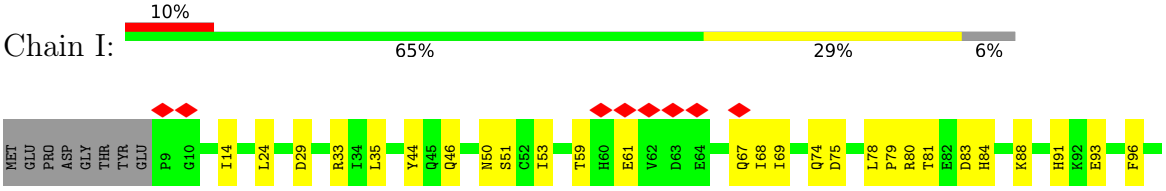
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

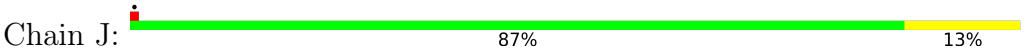


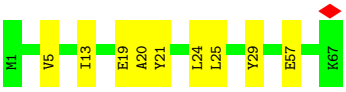
• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I:

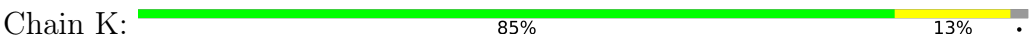


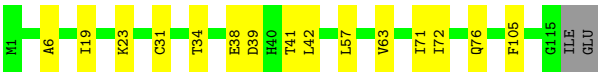
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



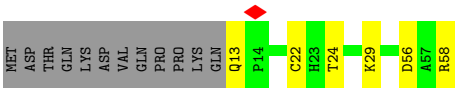


• Molecule 13: DNA-directed RNA polymerase II subunit RPB11-a

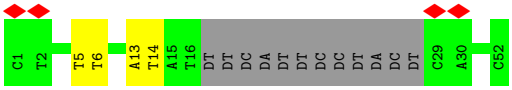




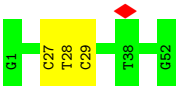
• Molecule 14: RNA polymerase II subunit K



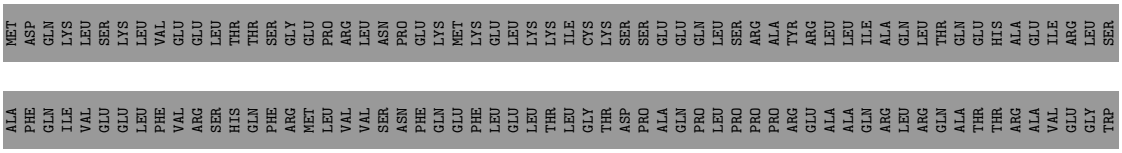
• Molecule 15: NTS

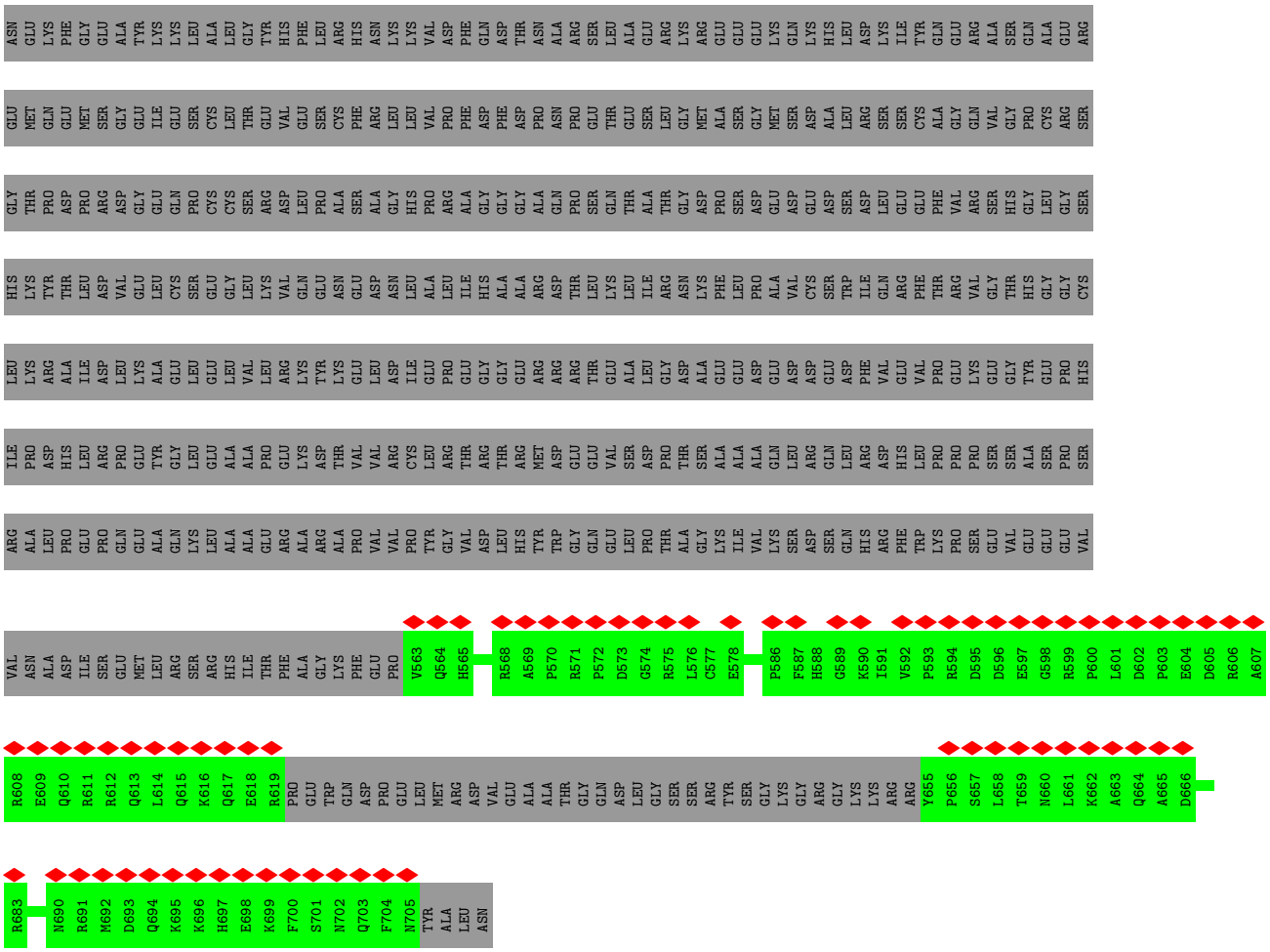


• Molecule 16: TS



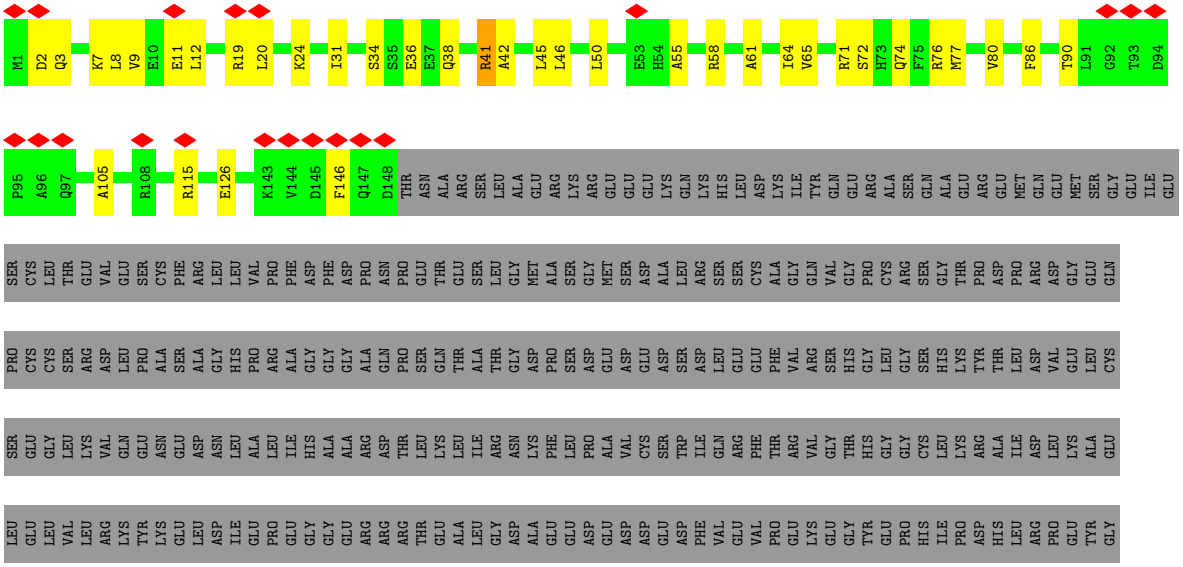
• Molecule 17: UV-stimulated scaffold protein A





• Molecule 17: UV-stimulated scaffold protein A

Chain M:



LEU GLU ALA ALA PRO GLU LYS ASP THR VAL VAL ARG CYS LEU ARG THR ARG THR ARG MET ASP GLU GLU VAL SER ASP PRO THR SER ALA ALA ALA GLN LEU ARG GLN LEU ARG ASP HIS LEU PRO PRO SER SER ALA SER PRO SER ARG ALA LEU PRO GLU PRO GLN GLU ALA GLN

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

SER ARG HIS ILE THR PHE ALA GLY LYS PHE GLU PRO VAL GLN HIS TRP CYS ARG ALA PRO ARG PRO ASP GLY ARG LEU CYS GLU ARG GLN ASP ARG LEU LYS CYS PRO PHE HIS GLY LYS ILE VAL PRO ARG ASP ASP GLU GLY ARG PRO LEU ASP PRO GLU ASP ARG ALA ARG GLU GLN

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

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

- Molecule 18: Transcription elongation factor 1 homolog

Chain O: 95% 5%

L20 T45 Q58 D69 N82 Q83

- Molecule 19: DNA excision repair protein ERCC-6

Chain b: 35% 65%

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

CYS ALA SER ALA ALA PRO ARG ARG GLY PRO ALA LEU LEU HIS ILE ASP ARG HIS GLN ILE GLN ALA VAL GLU PRO SER ALA GLN ALA LEU GLU LEU GLN GLY LEU GLY VAL ASP VAL TYR ASP GLN ASP VAL LEU GLU GLN GLY VAL LEU GLN GLN VAL ASP ASN ALA ILE HIS GLU ALA

SER ARG ALA SER GLN LEU VAL ASP VAL GLU LYS GLU TYR ARG SER VAL LEU ASP ASP LEU THR SER CYS THR THR SER LEU ARG GLN ILE ASN LYS ILE ILE GLU GLN LEU SER PRO GLN ALA ALA THR SER ARG ASP ILE ASN ARG LYS LEU ASP SER VAL LYS ARG GLN LYS TYR ASN

LYS GLU GLN GLN LEU LYS LYS ILE THR ALA LYS GLN LYS HIS LEU GLN ALA ILE LEU GLY GLY ALA GLU VAL LYS ILE GLU LEU ASP HIS ALA SER LEU GLU GLU ASP ALA GLU PRO GLY PRO SER SER LEU GLY SER MET LEU MET PRO VAL GLN GLU THR ALA TRP GLU GLU LEU ILE

ARG THR GLY GLN MET THR PRO PHE GLY THR GLN ILE PRO GLN LYS GLN GLU LYS LYS PRO ARG LYS ILE MET LEU ASN GLU ALA SER GLY PHE GLU LYS TYR LEU ALA ASP GLN ALA LYS LEU SER PHE GLU ARG LYS LYS GLN GLY CYS ASN LYS ARG ALA ALA ARG LYS ALA PRO ALA

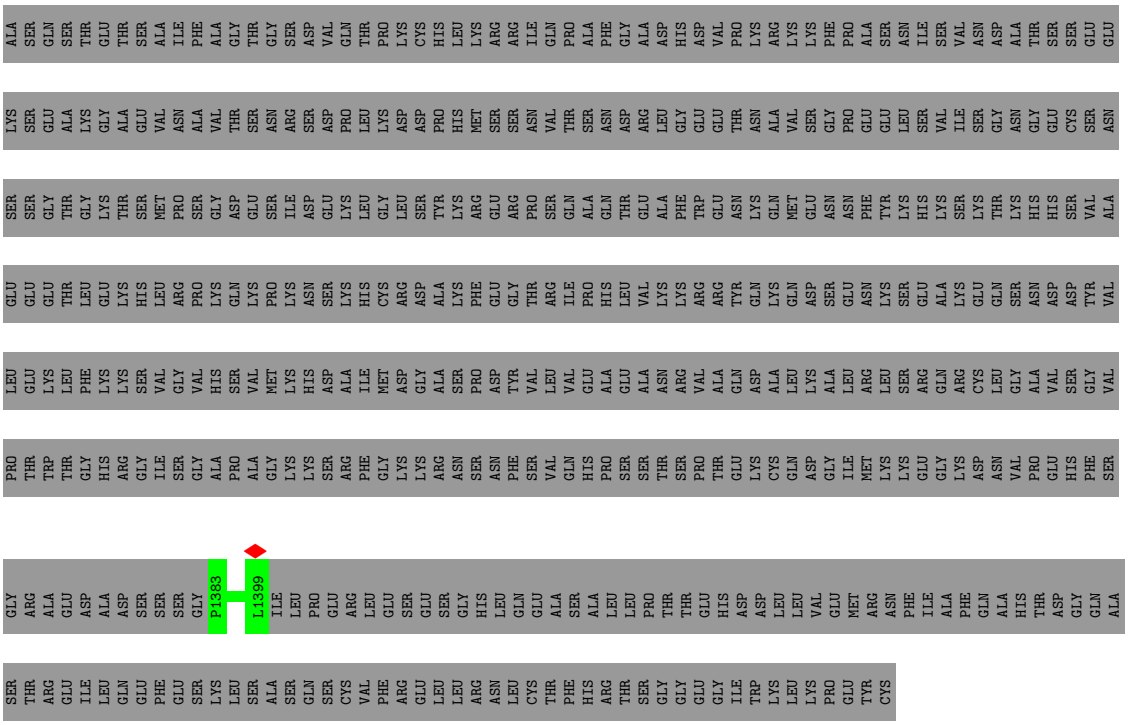
PRO VAL THR PRO PRO ALA PRO VAL GLN ASN LYS ASN LYS PRO ASN LYS LYS ALA ARG VAL LEU SER LYS LYS GLU GLU ARG LEU LYS LYS HIS ILE LYS LYS LEU GLN LYS ARG ALA LEU GLN PHE GLN GLY LYS VAL GLY LEU PRO LYS ALA ARG ARG PRO TRP GLU SER ASP MET ARG

PRO GLU ALA GLU GLY ASP SER GLU GLY GLU GLU SER GLU TYR PHE PRO THR GLU GLU GLU GLU GLU GLU GLU ASP ASP GLU VAL GLU GLY ALA GLU ALA ASP LEU SER GLY ASP GLY THR ASP TYR GLU LEU LYS PRO LEU PRO LYS GLY GLY LYS ARG GLN LYS LYS VAL PRO VAL GLN

GLU ILE ASP ASP PHE PHE PRO SER SER GLY GLU GLU ALA GLU ALA ALA SER VAL GLY GLU GLY GLY GLY GLY GLY ARG LYS VAL GLY ARG TYR ARG ASP ASP GLY ASP GLU ASP TYR TYR LYS GLN ARG LEU ARG ARG TRP ASN LYS LEU ARG LEU GLN ASP LYS GLU LYS ARG LEU

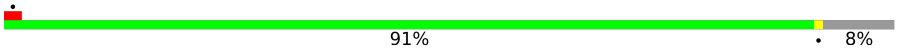
LYS LEU GLU ASP ASP SER GLU GLU SER D490 D494 E495 R555 THR ARG GLY SER ASN TYR R562 F563 E564 E608 R666 R670 M713 G714 G715 F779 E784 V785 I788 L789 N790 G791 E792 M793 L799 R803 F812 S813 G814 GLY PRO LYS ASN LEU LYS

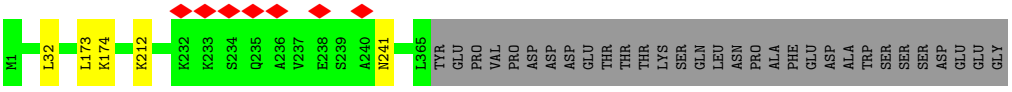
GLY LEU PRO ASP ASP GLU LEU E828 E829 D830 Q831 F832 G833 K840 G855 L868 K879 K884 I891 E903 D904 R915 V916 G917 G918 L919 G920 D935 G952 Q953 K954 R961 F996 K997 S998 N999 D1000 L1001 Y1002 E1003 L1004 F1005 T1006 L1007 T1008 S1009 P1010 D1011



• Molecule 20: DNA excision repair protein ERCC-8

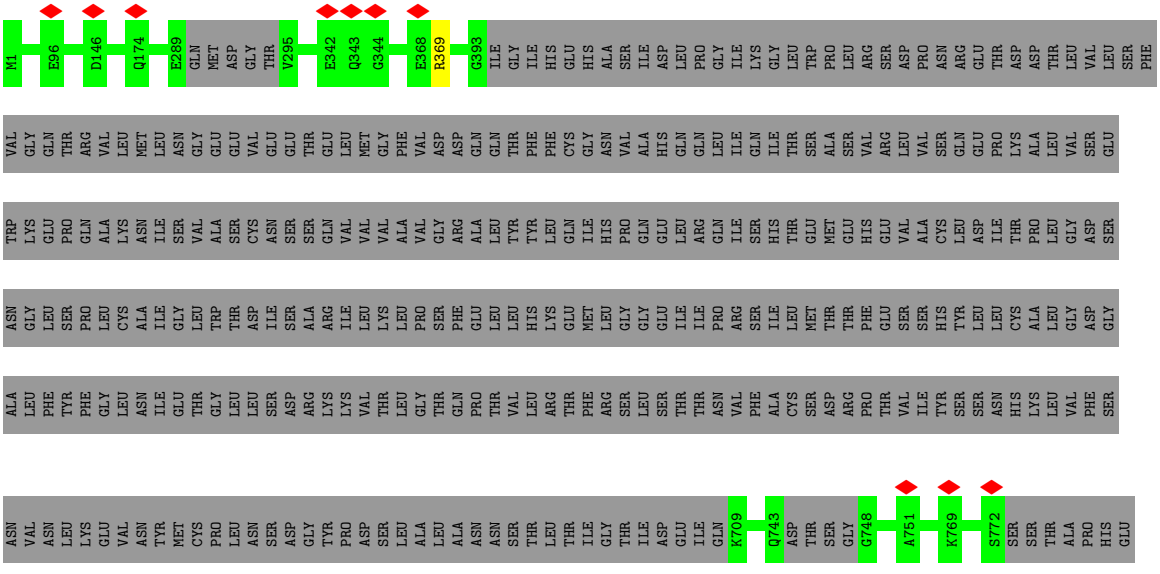
Chain a:

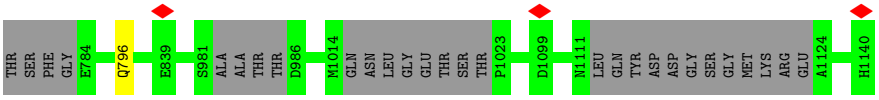




• Molecule 21: DNA damage-binding protein 1

Chain d:




THR
SER
PHE
GLY
E784
Q796
E839
S981
ALA
ALA
THR
THR
D936
M1014
GLN
ASN
LEU
GLY
GLU
THR
SER
THR
P1023
D1099
N1111
LEU
GLN
TYR
ASP
ASP
GLY
SER
GLY
MET
LYS
ARG
GLU
A1124
H1140

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	39.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.590	Depositor
Minimum map value	-3.746	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.873	Depositor
Map size (Å)	442.80002, 442.80002, 442.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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, MG, BEF, ADP

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	P	1.44	0/344	2.42	5/535 (0.9%)
2	Q	0.39	0/1784	0.54	0/2416
3	A	0.61	0/11373	0.62	0/15353
4	B	0.73	1/9229 (0.0%)	0.64	4/12458 (0.0%)
5	C	0.74	0/2132	0.61	0/2896
6	D	0.28	0/1027	0.47	0/1384
7	E	0.56	0/1751	0.60	0/2366
8	F	0.67	0/667	0.54	0/901
9	G	0.37	0/1365	0.61	1/1853 (0.1%)
10	H	0.69	0/1207	0.55	0/1628
11	I	0.51	1/972 (0.1%)	0.60	0/1316
12	J	0.75	0/542	0.66	0/730
13	K	0.62	0/939	0.55	0/1271
14	L	0.62	0/394	0.63	0/524
15	N	0.70	0/932	0.92	0/1435
16	T	1.13	1/1102 (0.1%)	1.06	1/1682 (0.1%)
17	M	0.33	0/1238	0.49	0/1664
17	c	0.28	0/741	0.57	0/976
18	O	0.50	0/515	0.51	0/700
19	b	0.32	0/4362	0.51	0/5890
20	a	0.60	0/2908	0.60	1/3939 (0.0%)
21	d	0.36	0/6268	0.52	0/8466
All	All	0.60	3/51792 (0.0%)	0.64	12/70383 (0.0%)

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
2	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	2
20	a	0	3
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	24	LEU	C-N	-7.90	1.15	1.34
16	T	28	DT	C4-C5	-5.71	1.39	1.45
4	B	1047	TYR	CD1-CE1	-5.05	1.31	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	36	A	O5'-P-OP2	-36.55	66.83	110.70
1	P	36	A	OP1-P-OP2	-28.46	76.90	119.60
1	P	36	A	O5'-P-OP1	15.48	129.28	110.70
1	P	35	A	OP2-P-O3'	14.86	137.90	105.20
1	P	35	A	OP1-P-O3'	-7.84	87.95	105.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	538	VAL	Peptide
4	B	1048	TYR	Sidechain
4	B	959	GLU	Peptide
2	Q	233	ARG	Peptide
20	a	173	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	306	152	153	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1752	1782	1787	16	0
3	A	11170	11308	11311	146	0
4	B	9048	9084	9084	115	0
5	C	2089	2031	2031	20	0
6	D	1013	972	972	17	0
7	E	1720	1737	1737	22	0
8	F	657	684	684	14	0
9	G	1334	1333	1333	25	0
10	H	1186	1147	1147	14	0
11	I	949	879	878	21	0
12	J	533	553	553	8	0
13	K	920	942	942	9	0
14	L	388	393	393	3	0
15	N	829	449	450	2	0
16	T	991	553	553	1	0
17	M	1215	1234	1235	27	0
17	c	731	634	633	0	0
18	O	505	463	463	2	0
19	b	4259	4299	4302	0	0
20	a	2849	2769	2778	0	0
21	d	6161	6159	6159	0	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	O	1	0	0	0	0
22	c	2	0	0	0	0
23	A	1	0	0	0	0
23	b	1	0	0	0	0
24	b	27	12	11	0	0
25	b	4	0	0	0	0
All	All	50649	49569	49589	418	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.

The worst 5 of 418 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)
2:Q:318:TYR:OH	17:M:41:ARG:NH1	2.06	0.89
5:C:190:ASN:O	5:C:193:ARG:NH1	2.13	0.81
5:C:152:LYS:NZ	12:J:57:GLU:OE2	2.13	0.81
3:A:927:GLU:OE2	3:A:931:ARG:NH2	2.13	0.81
8:F:53:THR:OG1	8:F:116:GLU:OE2	1.98	0.81

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	
2	Q	222/258 (86%)	212 (96%)	10 (4%)	0	100	100
3	A	1400/1984 (71%)	1294 (92%)	106 (8%)	0	100	100
4	B	1122/1167 (96%)	1031 (92%)	91 (8%)	0	100	100
5	C	256/275 (93%)	238 (93%)	18 (7%)	0	100	100
6	D	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
7	E	207/210 (99%)	193 (93%)	14 (7%)	0	100	100
8	F	80/127 (63%)	74 (92%)	6 (8%)	0	100	100
9	G	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
10	H	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
11	I	115/125 (92%)	105 (91%)	10 (9%)	0	100	100
12	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
13	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
14	L	44/58 (76%)	35 (80%)	9 (20%)	0	100	100
17	M	146/709 (21%)	142 (97%)	4 (3%)	0	100	100
17	c	104/709 (15%)	101 (97%)	3 (3%)	0	100	100
18	O	62/64 (97%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	b	512/1493 (34%)	484 (94%)	28 (6%)	0	100	100
20	a	363/396 (92%)	316 (87%)	47 (13%)	0	100	100
21	d	765/1140 (67%)	722 (94%)	43 (6%)	0	100	100
All	All	6017/9363 (64%)	5593 (93%)	424 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	Q	188/218 (86%)	188 (100%)	0	100	100
3	A	1242/1763 (70%)	1241 (100%)	1 (0%)	92	96
4	B	992/1021 (97%)	991 (100%)	1 (0%)	92	96
5	C	237/252 (94%)	237 (100%)	0	100	100
6	D	108/126 (86%)	108 (100%)	0	100	100
7	E	191/192 (100%)	191 (100%)	0	100	100
8	F	71/111 (64%)	71 (100%)	0	100	100
9	G	147/153 (96%)	147 (100%)	0	100	100
10	H	129/131 (98%)	129 (100%)	0	100	100
11	I	105/112 (94%)	104 (99%)	1 (1%)	73	84
12	J	56/56 (100%)	56 (100%)	0	100	100
13	K	104/106 (98%)	104 (100%)	0	100	100
14	L	43/55 (78%)	43 (100%)	0	100	100
17	M	132/608 (22%)	130 (98%)	2 (2%)	60	77
17	c	60/608 (10%)	60 (100%)	0	100	100
18	O	59/59 (100%)	59 (100%)	0	100	100
19	b	466/1297 (36%)	464 (100%)	2 (0%)	89	93
20	a	320/348 (92%)	319 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	d	685/999 (69%)	683 (100%)	2 (0%)	91 94
All	All	5335/8215 (65%)	5325 (100%)	10 (0%)	91 95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	a	212	LYS
21	d	369	ARG
21	d	796	GLN
17	M	41	ARG
17	M	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
19	b	956	GLN
21	d	241	ASN
21	d	796	GLN
7	E	148	HIS
14	L	23	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	13/14 (92%)	6 (46%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	33	A
1	P	34	A
1	P	35	A
1	P	36	A
1	P	39	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 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	BEF	b	1502	-	0,3,3	-	-	-		
24	ADP	b	1501	23	24,29,29	5.13	10 (41%)	29,45,45	1.99	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	ADP	b	1501	23	-	1/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	1501	ADP	C2'-C1'	-17.16	1.27	1.53
24	b	1501	ADP	O4'-C1'	15.21	1.62	1.41
24	b	1501	ADP	O4'-C4'	-5.79	1.32	1.45
24	b	1501	ADP	C6-N6	3.44	1.46	1.34
24	b	1501	ADP	O3'-C3'	-3.26	1.35	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	1501	ADP	C5-C6-N6	6.28	129.90	120.35
24	b	1501	ADP	N3-C2-N1	-5.49	120.10	128.68
24	b	1501	ADP	N6-C6-N1	-4.02	110.24	118.57
24	b	1501	ADP	PA-O3A-PB	-3.61	120.44	132.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

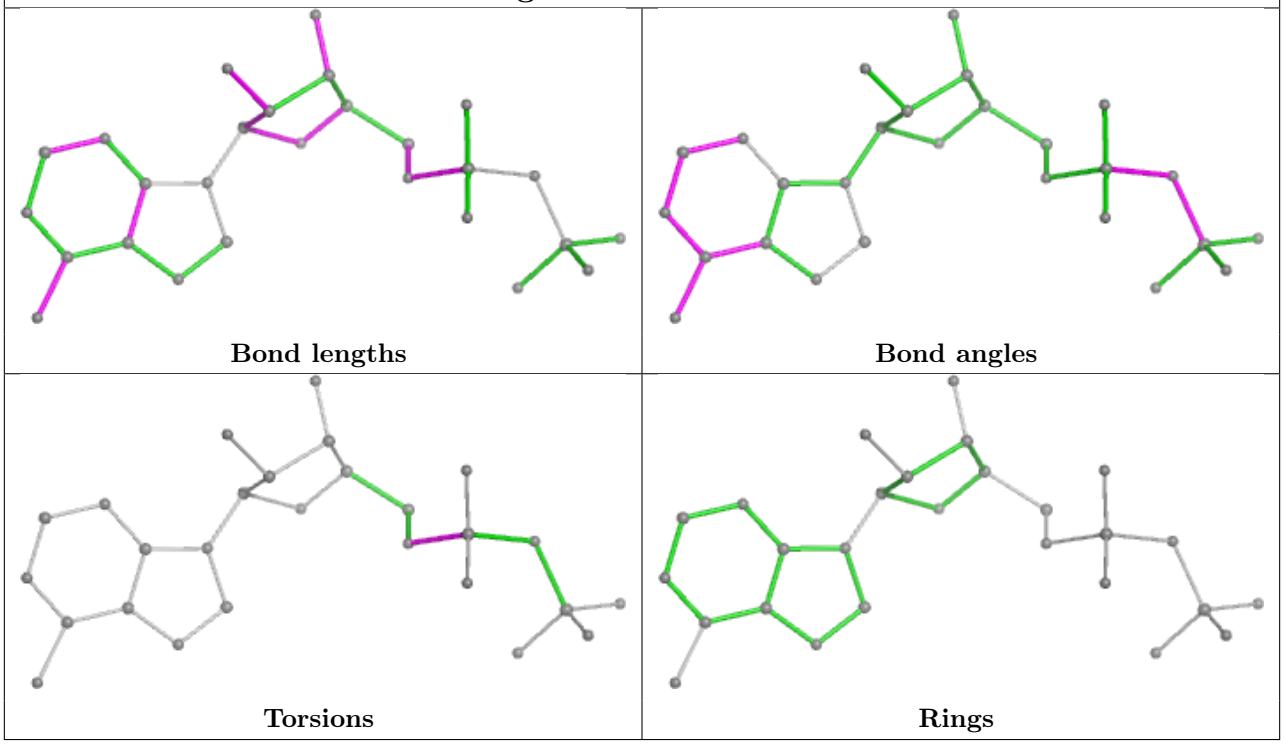
Mol	Chain	Res	Type	Atoms
24	b	1501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ADP b 1501



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
11	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	24:LEU	C	25:TYR	N	1.15

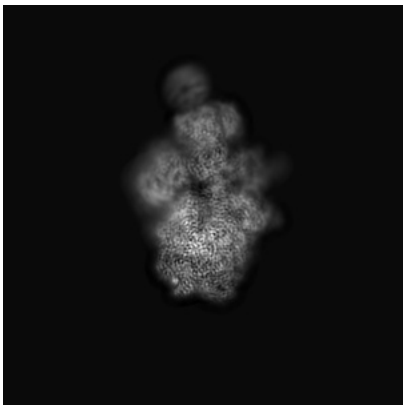
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19909. These allow visual inspection of the internal detail of the map and identification of artifacts.

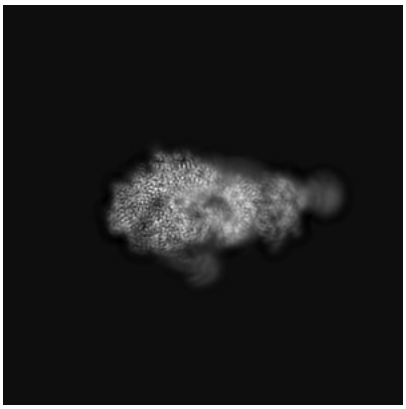
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

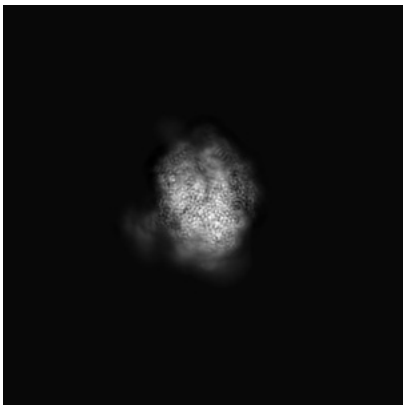
6.1.1 Primary map



X

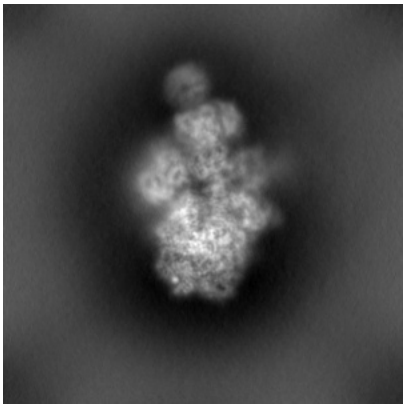


Y

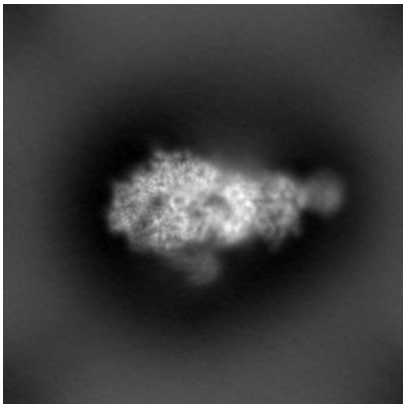


Z

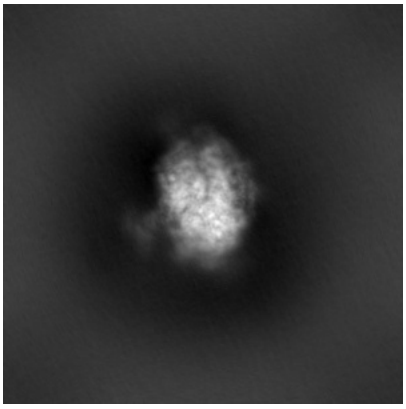
6.1.2 Raw map



X



Y

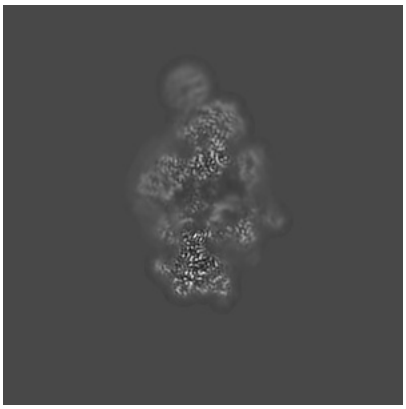


Z

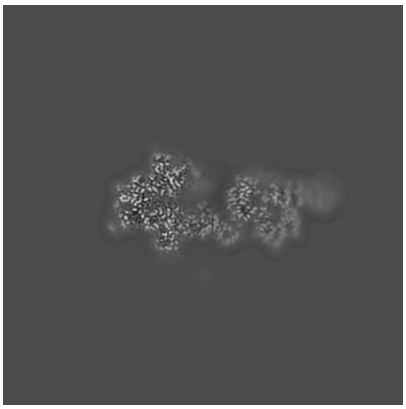
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

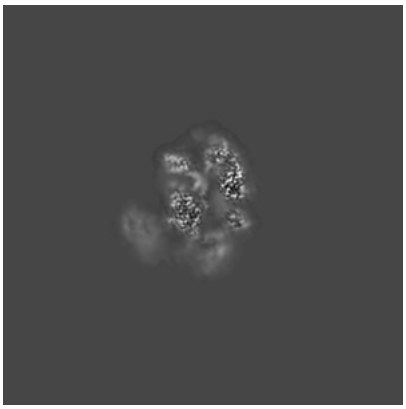
6.2.1 Primary map



X Index: 180

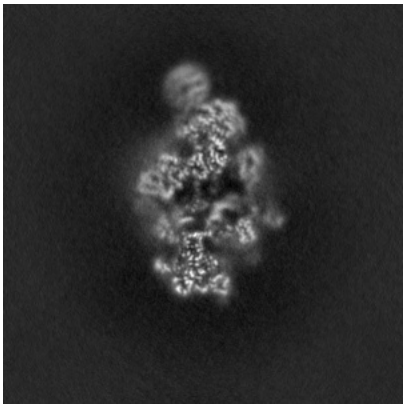


Y Index: 180

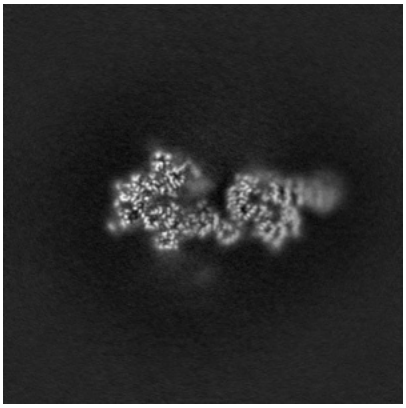


Z Index: 180

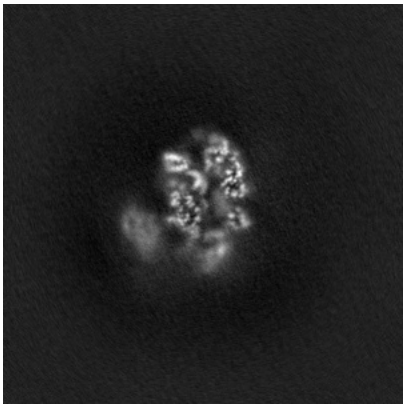
6.2.2 Raw map



X Index: 180



Y Index: 180

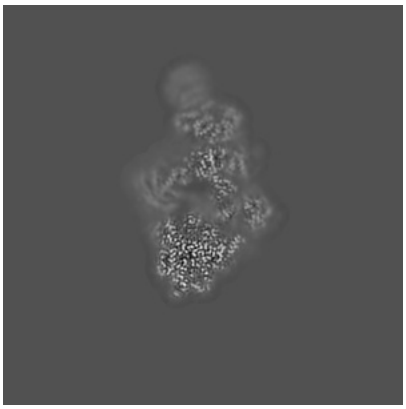


Z Index: 180

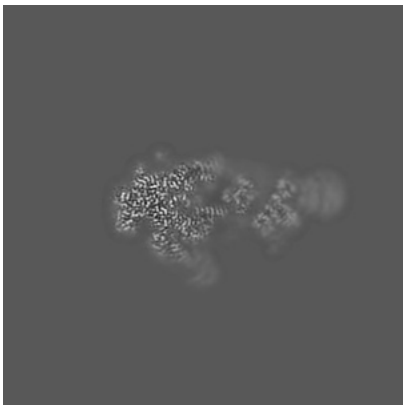
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

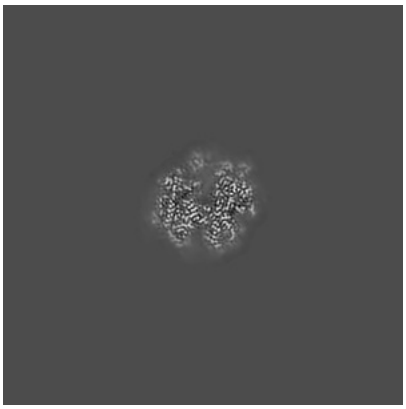
6.3.1 Primary map



X Index: 194

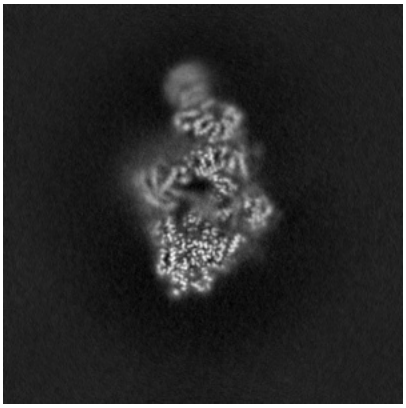


Y Index: 168

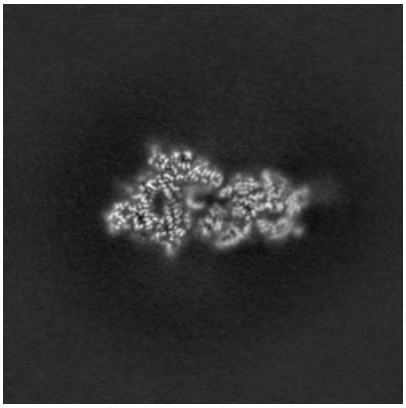


Z Index: 145

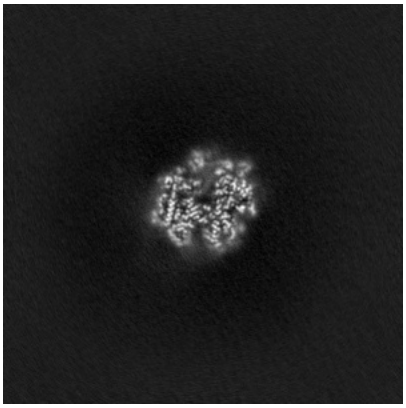
6.3.2 Raw map



X Index: 194



Y Index: 189

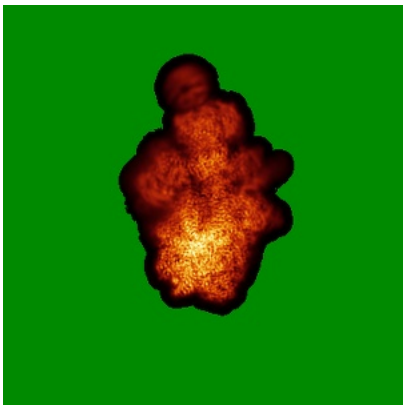


Z Index: 145

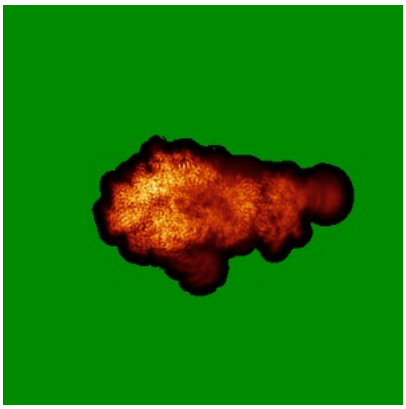
The images above show the largest variance slices of the map in three orthogonal directions.

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

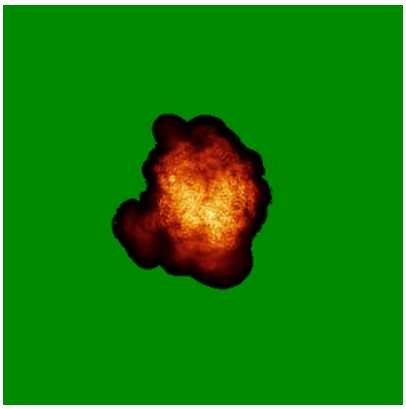
6.4.1 Primary map



X

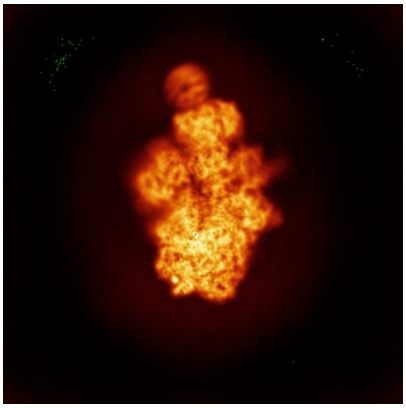


Y

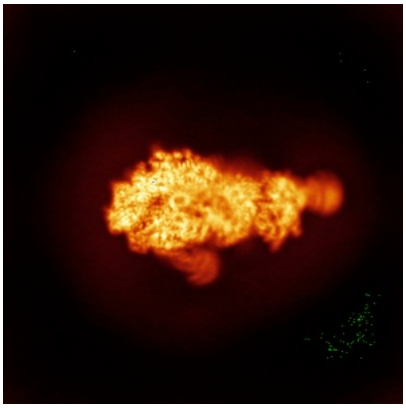


Z

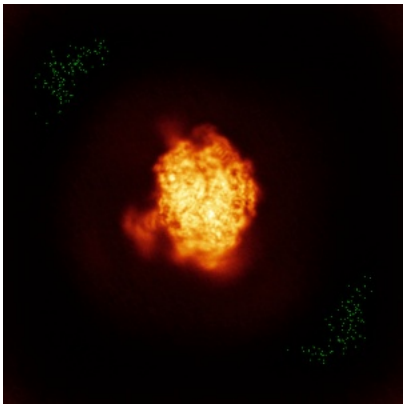
6.4.2 Raw map



X



Y

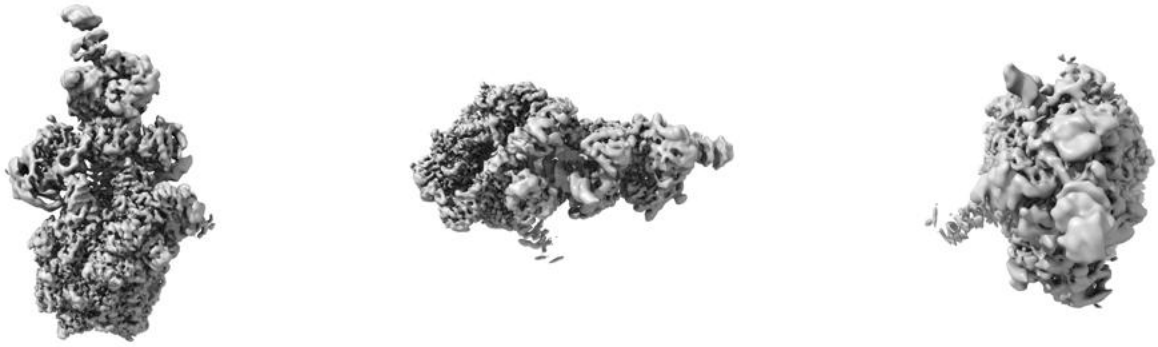


Z

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)

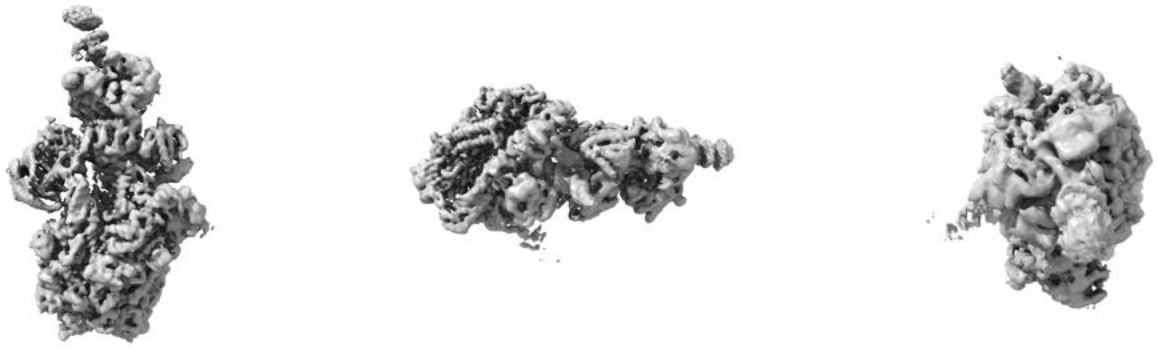
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.873. 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.

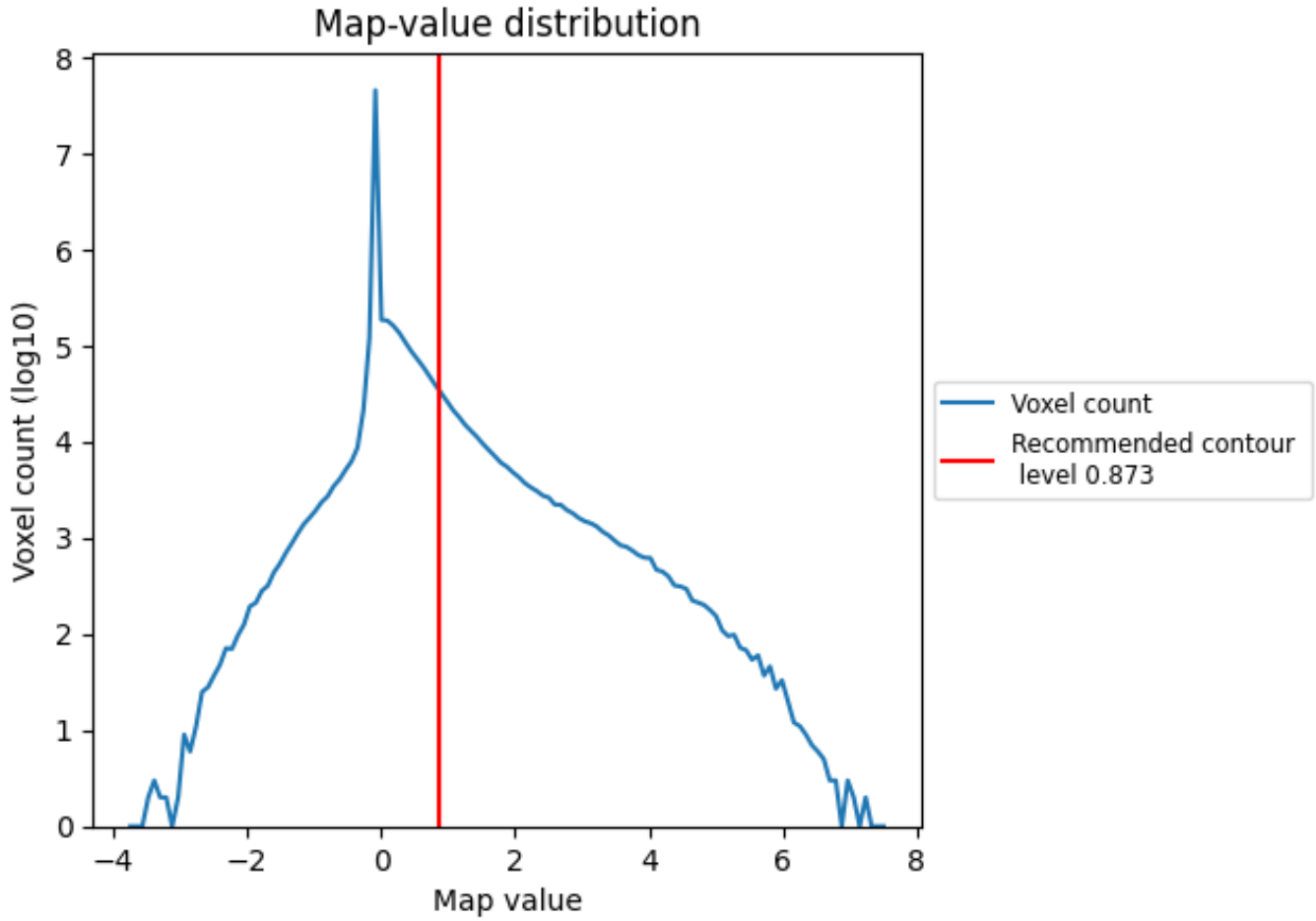
6.6 Mask visualisation (i)

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

7 Map analysis

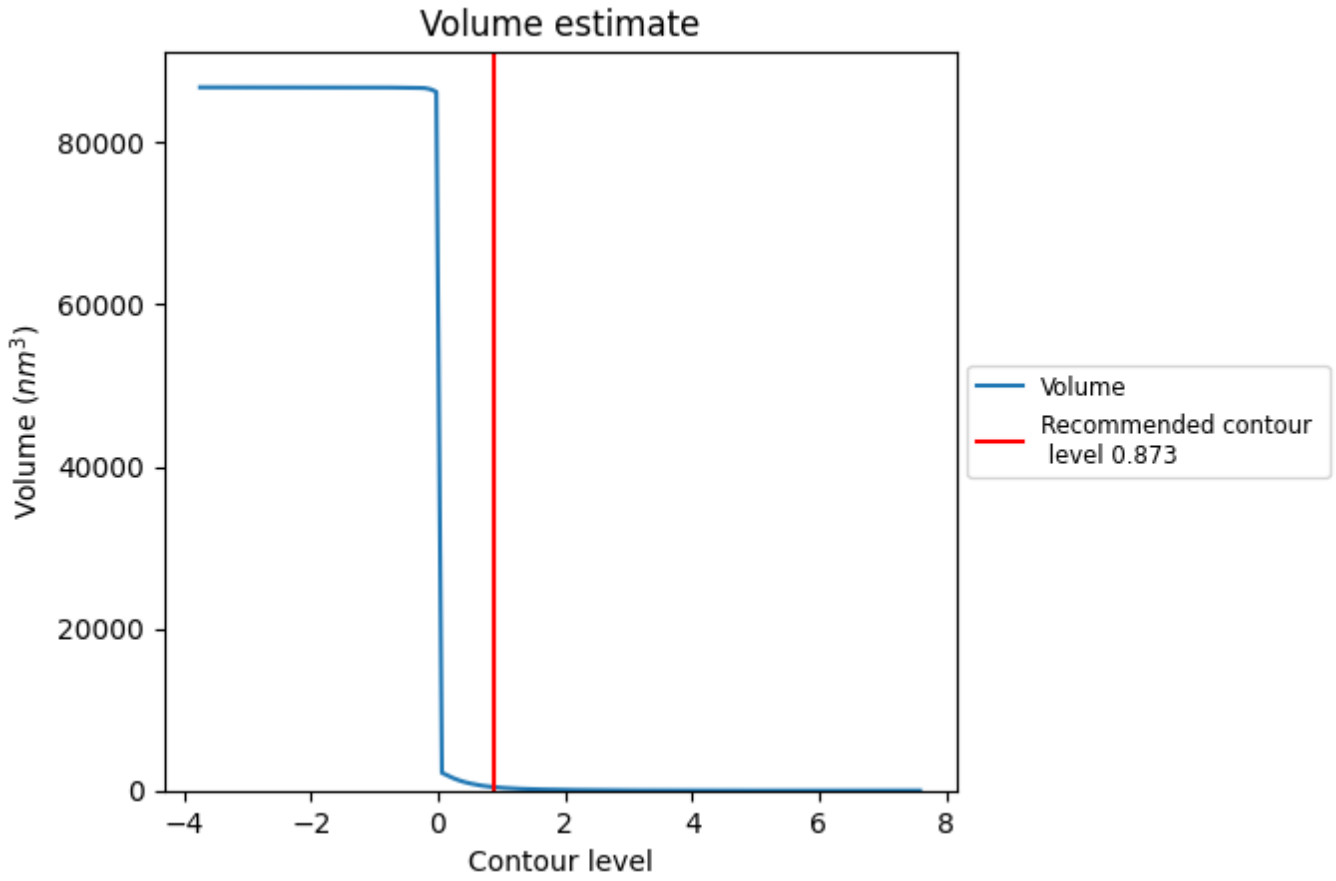
This section contains the results of statistical analysis of the map.

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.

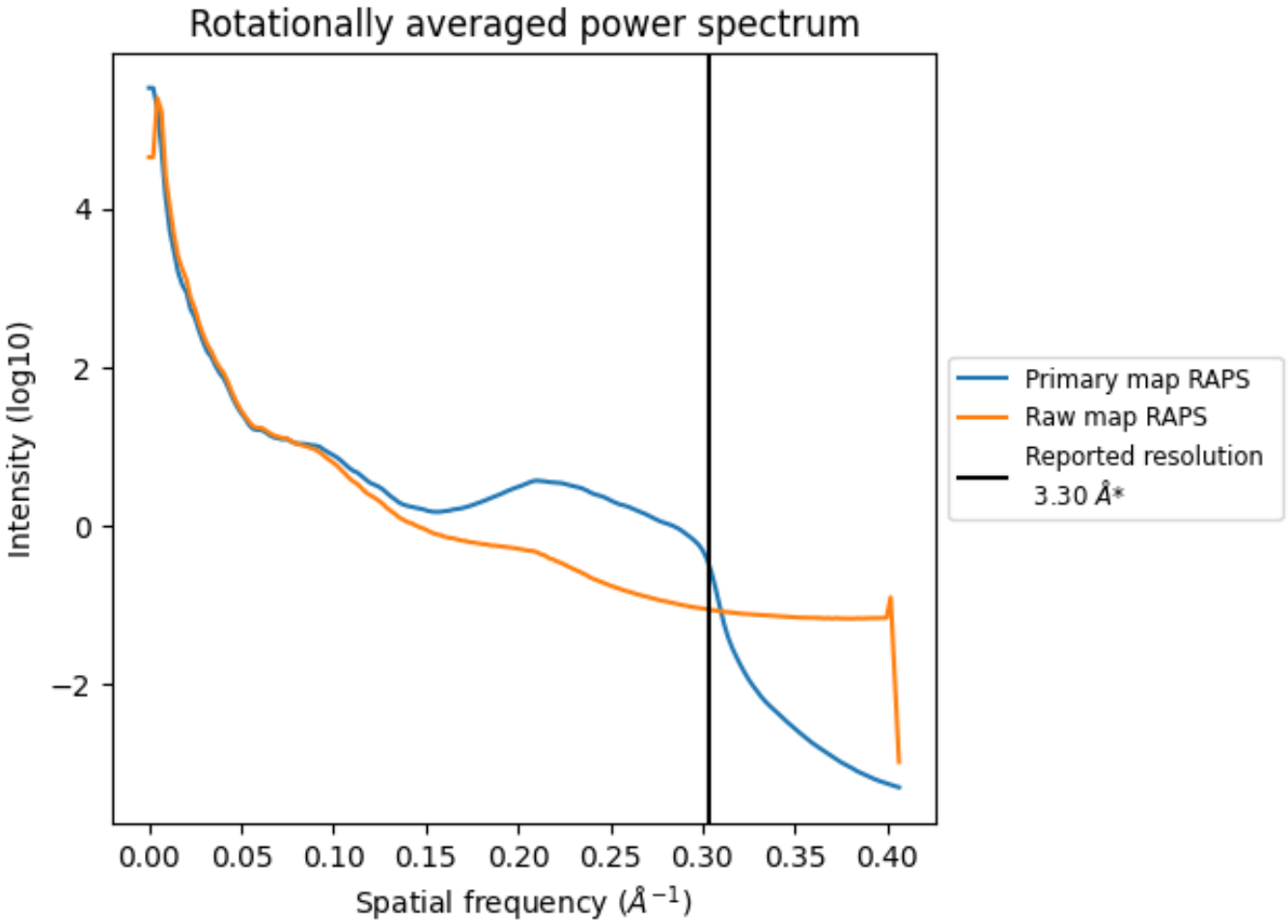
7.2 Volume estimate (i)



The volume at the recommended contour level is 432 nm^3; this corresponds to an approximate mass of 390 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)

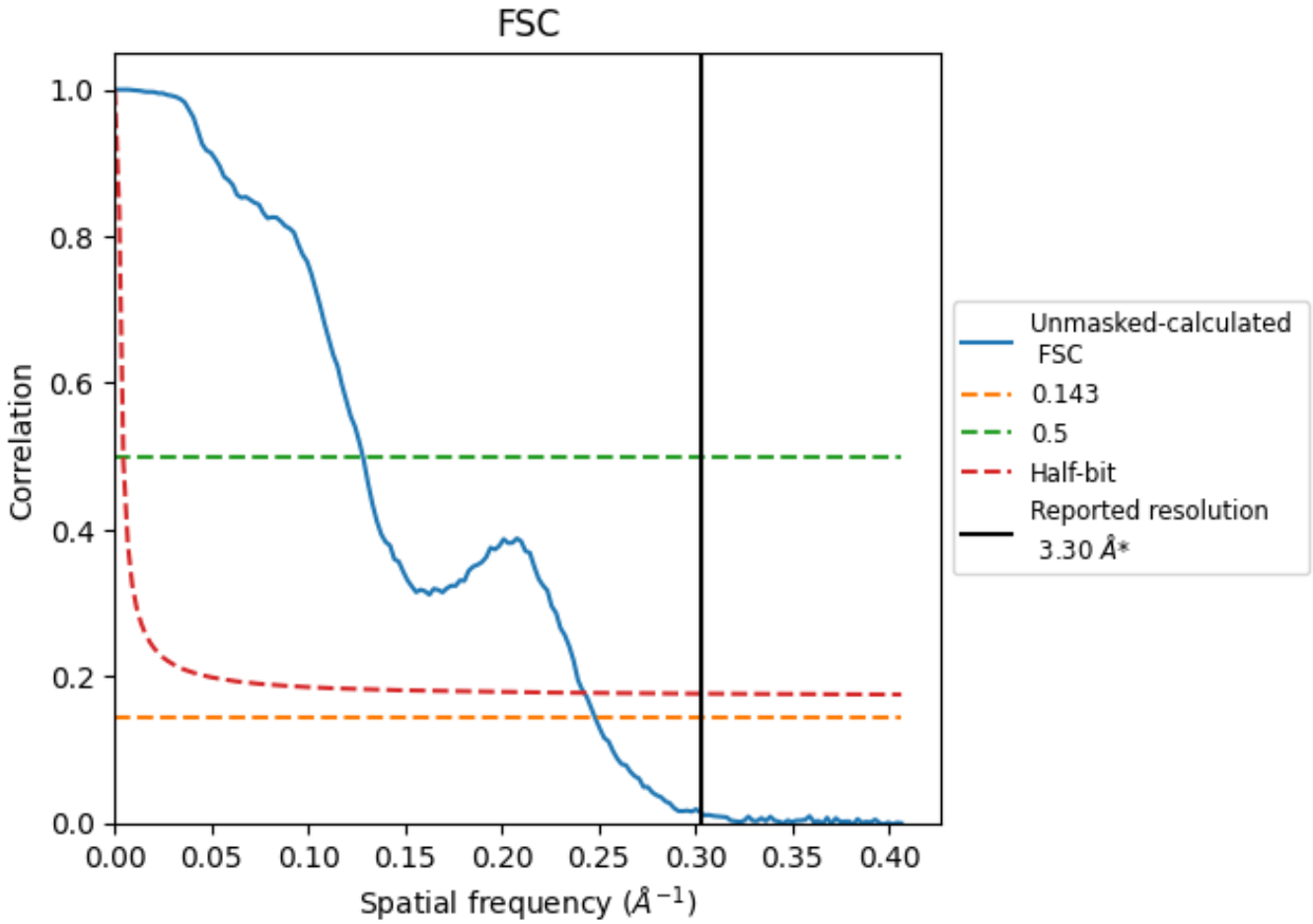


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

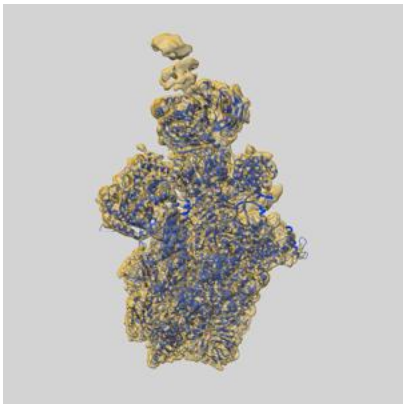
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.80	4.12

*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 4.03 differs from the reported value 3.3 by more than 10 %

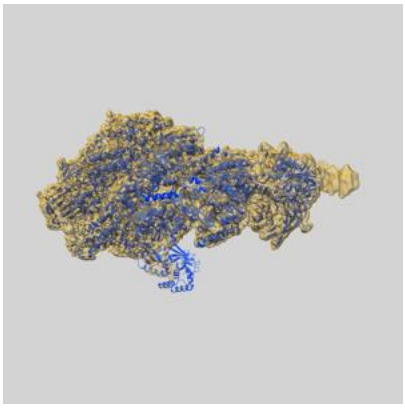
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19909 and PDB model 9ER2. Per-residue inclusion information can be found in section 3 on page 9.

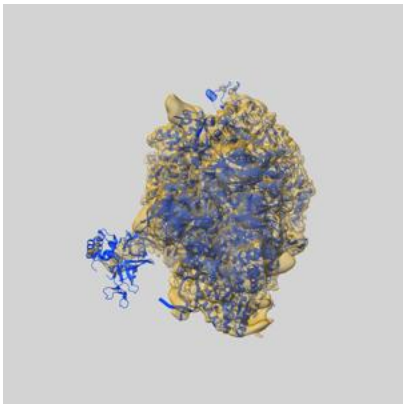
9.1 Map-model overlay



X



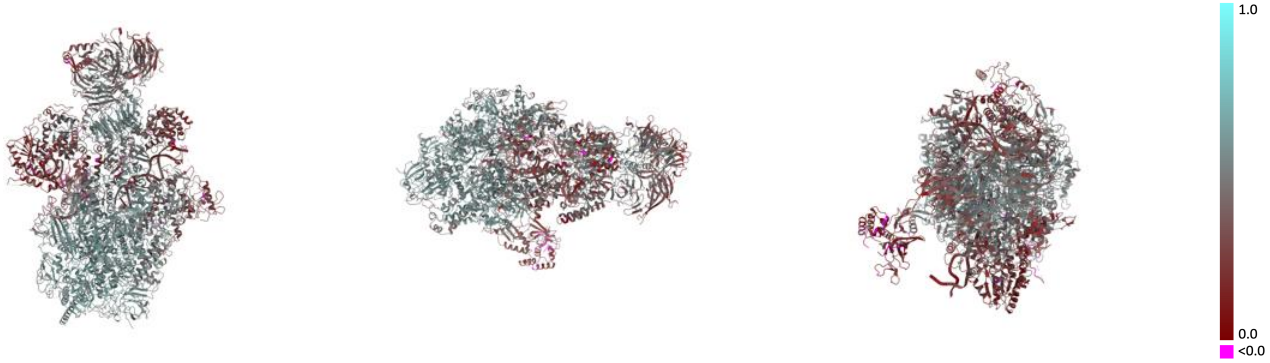
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.873 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.

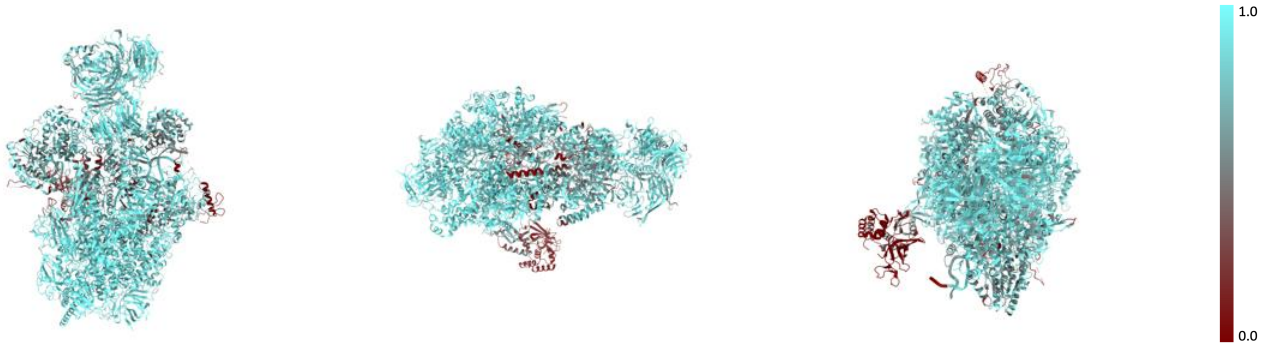
9.2 Q-score mapped to coordinate model



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.

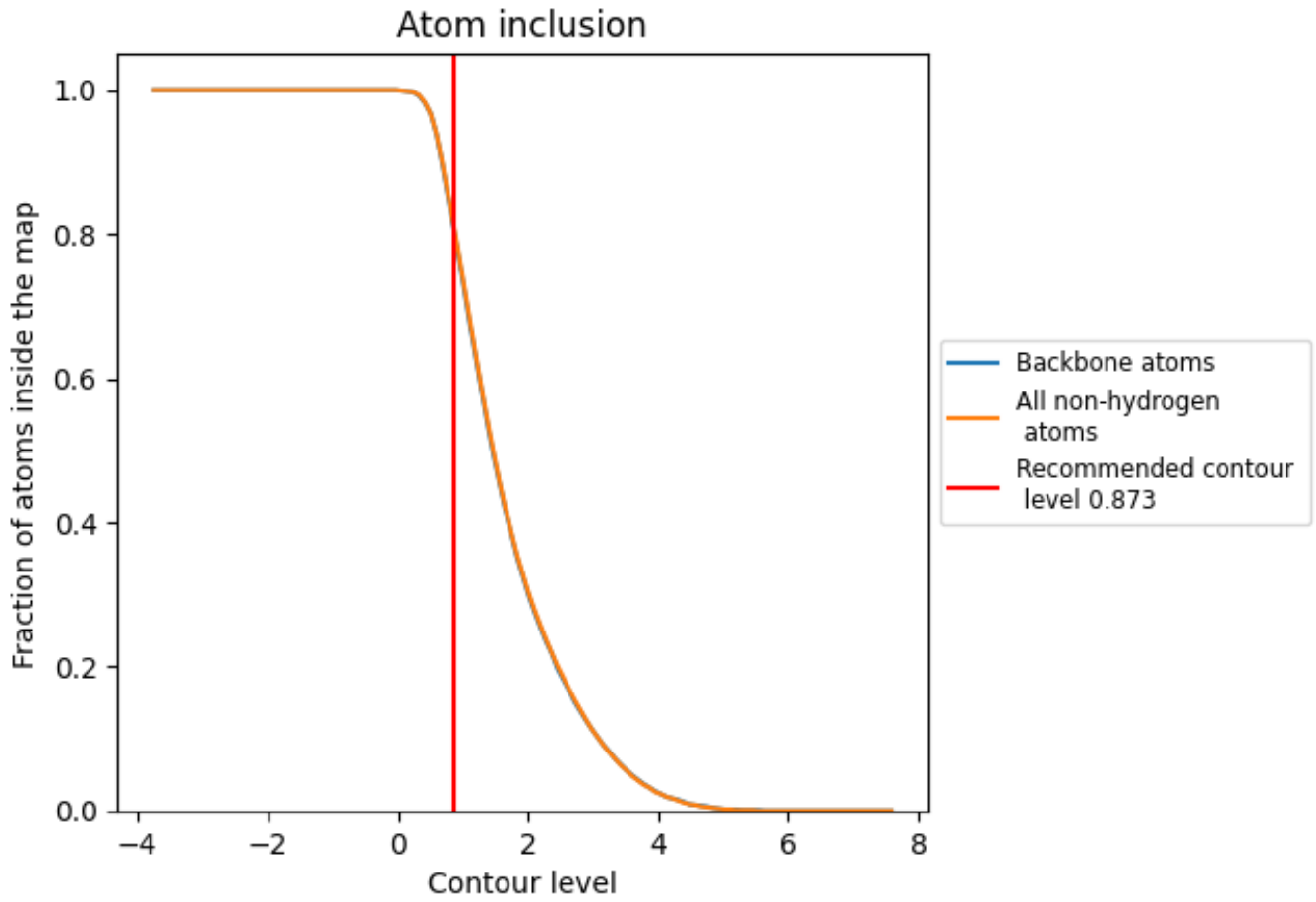
9.3 Atom inclusion mapped to coordinate model



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 (0.873).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.873) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.4480
A	0.8620	0.5050
B	0.8960	0.5290
C	0.9420	0.5440
D	0.0910	0.1640
E	0.8930	0.4760
F	0.8970	0.5420
G	0.2930	0.2570
H	0.9350	0.5320
I	0.7570	0.4490
J	0.9560	0.5740
K	0.9450	0.5510
L	0.8980	0.4830
M	0.6460	0.2760
N	0.7470	0.2810
O	0.8400	0.4930
P	0.7650	0.4700
Q	0.7610	0.3910
T	0.8530	0.3680
a	0.9020	0.5180
b	0.7170	0.3140
c	0.3100	0.2670
d	0.8320	0.3790