



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 05:48 AM EDT

PDB ID : 7ML2 / pdb_00007ml2
EMDB ID : EMD-23906
Title : RNA polymerase II pre-initiation complex (PIC3)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 3.40 Å(reported)
Based on initial model : 5OQJ

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:

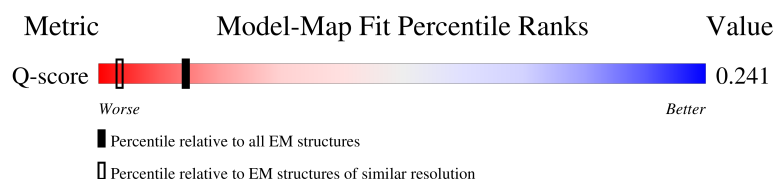
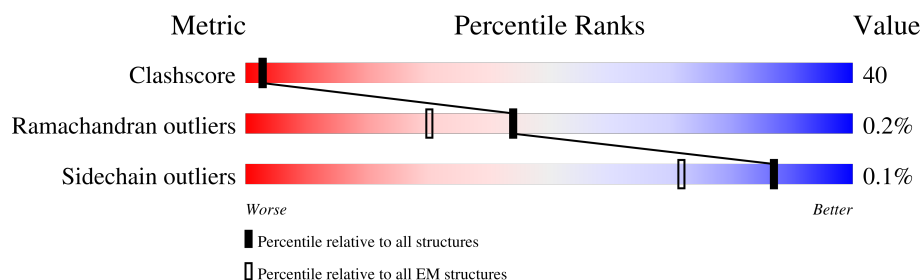
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

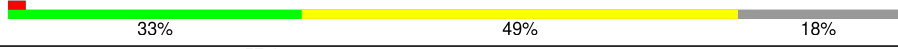
The reported resolution of this entry is 3.40 Å.

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



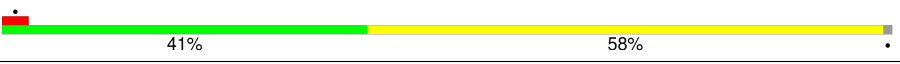
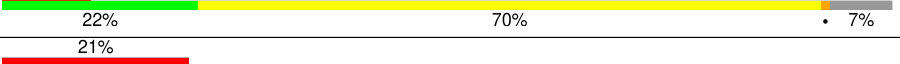
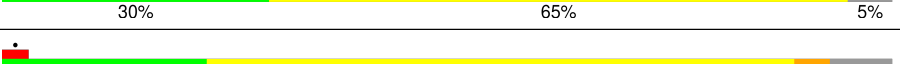
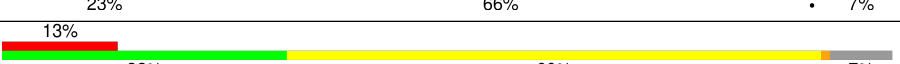
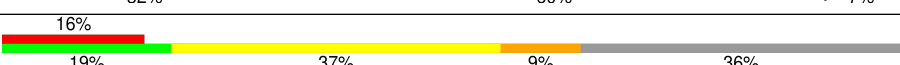
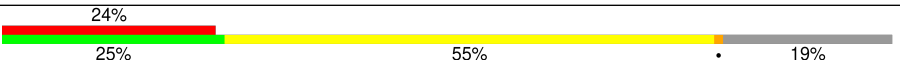
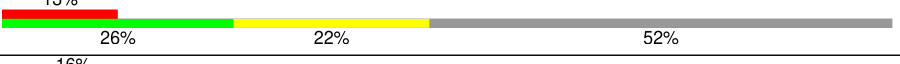
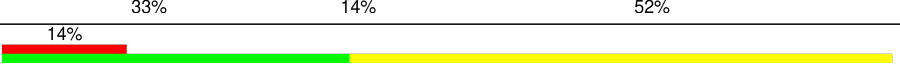
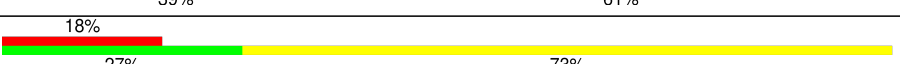
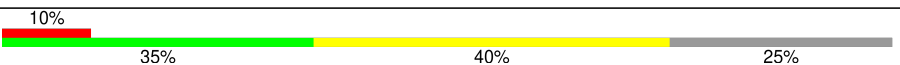
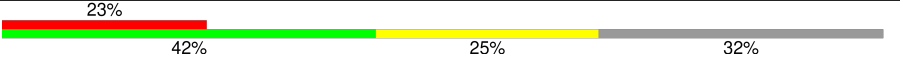
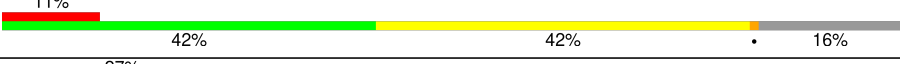
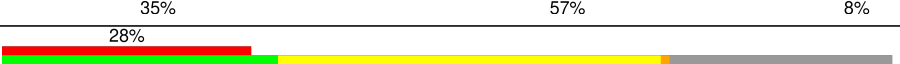
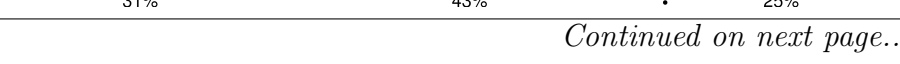
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	Q	735	
15	R	400	
16	U	286	
17	V	122	
18	W	482	
19	X	328	
20	T	56	
21	N	56	
22	O	240	
23	1	542	
24	4	338	
25	0	778	
26	6	461	
27	2	513	
28	5	72	
29	7	843	

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Mol	Chain	Length	Quality of chain
30	3	321	

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
33	SF4	0	801	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 64550 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	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	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 16 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	46	Total	C	N	O	S	0	0
			383	242	67	71	3		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	49	Total	C	N	O	S	0	0
			381	241	63	74	3		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 20 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	56	Total	C	N	O	P	0	0
			1140	550	188	346	56		

- Molecule 21 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	56	Total	C	N	O	P	0	0
			1156	552	222	326	56		

- Molecule 22 is a protein called BJ4_G0004860.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 23 is a protein called Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 24 is a protein called Tfb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 25 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 26 is a protein called General transcription and DNA repair factor IIH.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 30 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

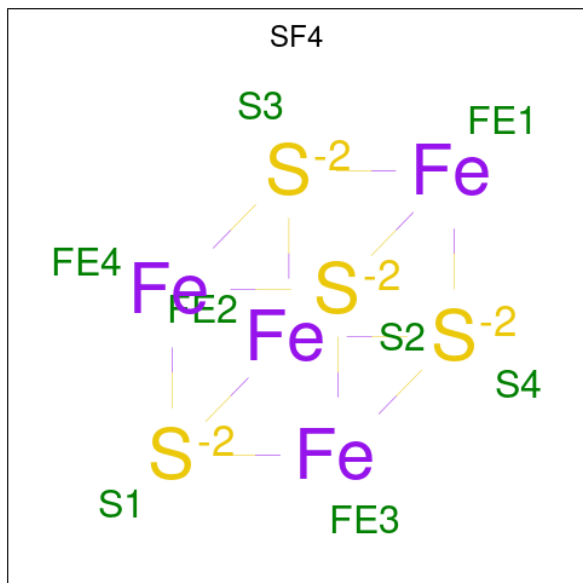
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	W	1	Total	Zn	0
			1	1	
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	
31	3	2	Total	Zn	0
			2	2	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Mg	0
			1	1	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

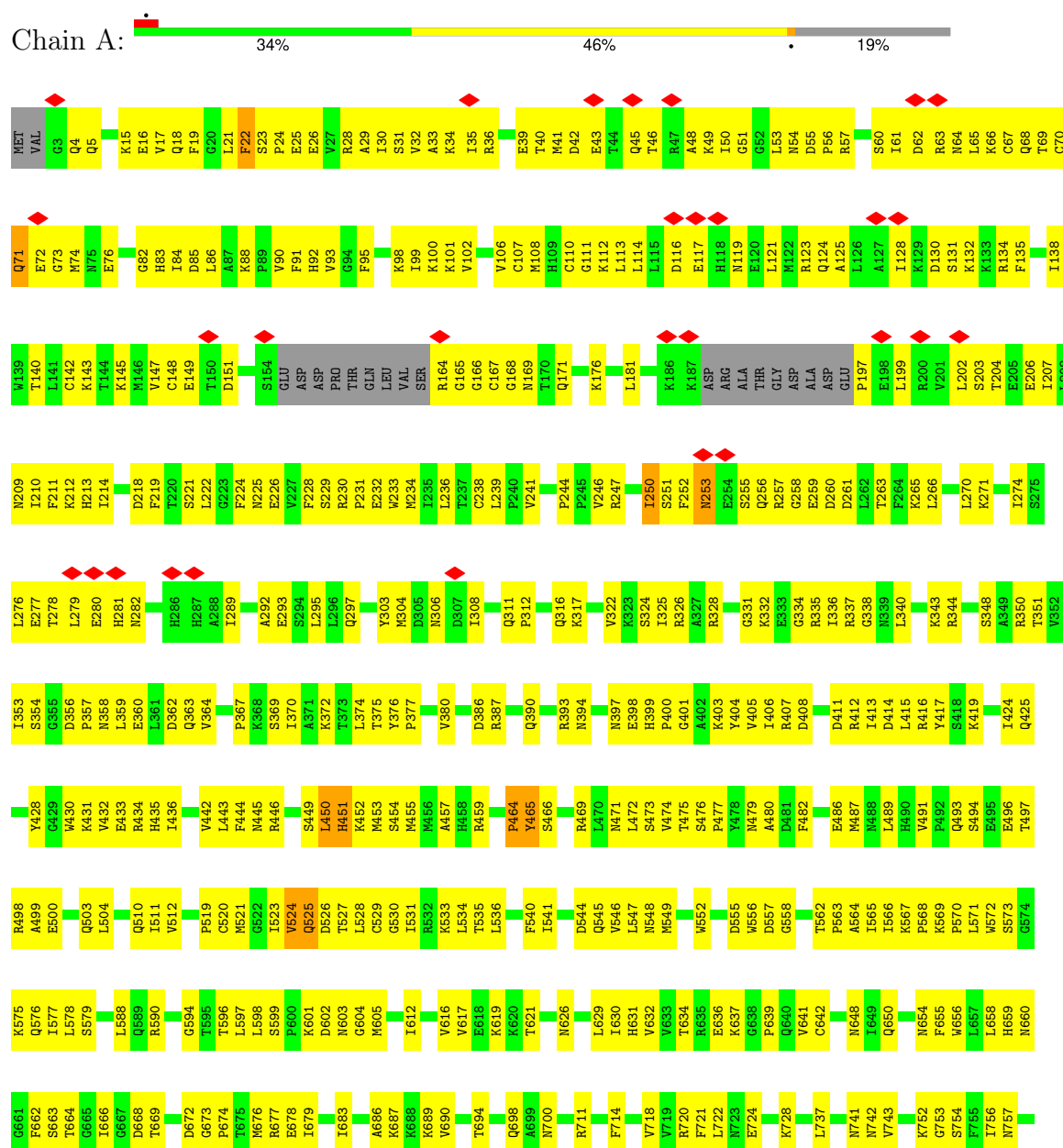


Mol	Chain	Residues	Atoms			AltConf
33	0	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

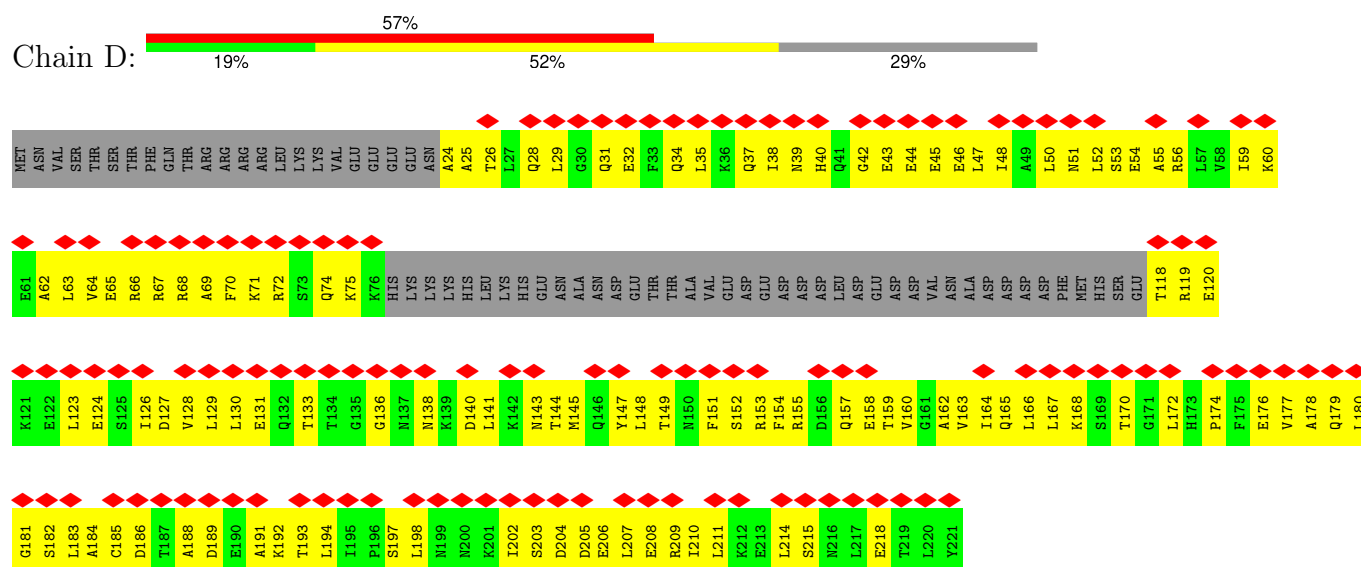
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



- Molecule 2: DNA-directed RNA polymerase subunit beta





Chain E:

41% 58%

Residues (from left to right):

- NET
- ASP
- Q3
- E6
- R7
- S10
- R11
- L12
- W13
- R14
- A15
- F16
- R17
- T18
- V19
- K20
- E21
- M22
- V23
- K24
- D25
- R26
- G27
- Y28
- F29
- I30
- T31
- Q32
- E33
- E34
- V35
- E36
- L39
- E40
- D41
- F42
- K43
- A44
- K45
- Y46
- C47
- D48
- S49
- M50
- G51
- R52
- P53
- Q54
- R55
- K56
- M57
- M58
- Q61
- A62
- M63
- P64

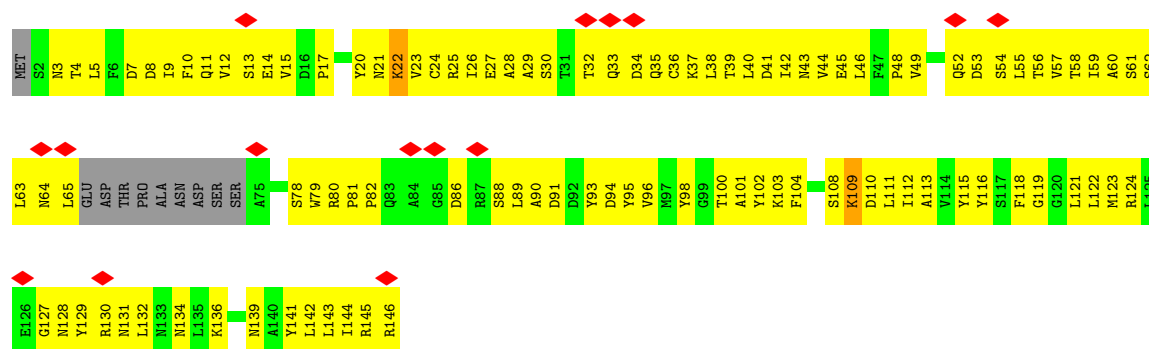
Chain F:

Amino Acid	Count
MET	1
SER	1
ASP	1
TYR	1
GLU	1
GLU	1
ALA	1
PHE	1
ASN	1
ASP	1
GLY	1
ASN	1
GLU	1
ASN	1
PHE	1
ASP	1
PHE	1
ASP	1
VAL	1
GLU	1
HIS	1
PHE	1
SER	1
ASP	1
GLU	1
THR	1
TYR	1
GLU	1
GLU	1
LYS	1
PRO	1
GLN	1
PHE	1
LYS	1
ASP	1
GLY	1
THR	1
THR	1
VAL	1
THR	1
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GLY	1
PRO	1
GLU	1
ASP	1
PHE	1
GLN	1
GLN	1

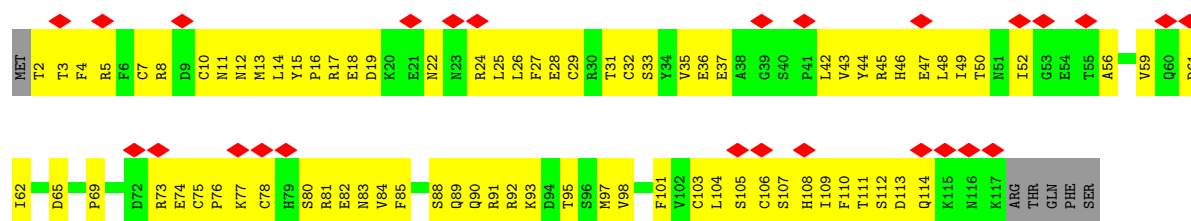
Chain G:

Element	Category
M1	Yellow
F2	Green
F3	Yellow
I4	Yellow
K5	Yellow
D6	Yellow
L9	Yellow
N10	Yellow
I11	Yellow
P15	Yellow
F18	Green
G19	Green
P20	Yellow
R21	Green
M22	Yellow
K23	Yellow
Q24	Yellow
Y25	Yellow
L26	Yellow
K27	Yellow
T28	Yellow
K29	Green
L30	Yellow
L31	Yellow
E32	Yellow
F33	Yellow
V34	Yellow
E35	Green
G36	Green
S37	Yellow
C38	Green
T39	Yellow
C40	Yellow
K41	Green
F42	Yellow
C43	Yellow
Y44	Yellow
I45	Yellow
L46	Yellow
C47	Yellow
V48	Yellow
L49	Yellow
D50	Green
Y51	Yellow
D52	Yellow
N53	Yellow
I54	Yellow
D55	Green
I56	Yellow
Q57	Yellow
R58	Yellow
G59	Yellow
R60	Yellow
I61	Yellow
L62	Yellow
P63	Green
T64	Yellow
D65	Yellow
G66	Yellow
S67	Yellow
A68	Green
E69	Yellow
F70	Yellow
M71	Yellow
V72	Yellow
K73	Yellow
Y74	Green
K75	Yellow
A76	Yellow
V77	Yellow
V78	Green
F79	Yellow
K80	Yellow
I81	Yellow
F82	Yellow
K83	Yellow
C84	Yellow
E85	Yellow
R86	Yellow
V87	Yellow
D88	Yellow
G89	Green
T90	Yellow
V91	Yellow
V92	Yellow
S93	Yellow
C94	Green
S95	Green
Q96	Yellow
H97	Yellow
G98	Yellow
F99	Yellow
I100	Yellow
V101	Yellow
Q102	Green
V103	Green
G104	Green
P105	Yellow
M106	Yellow
I107	Yellow
K108	Green
F109	Yellow
V110	Yellow
T111	Yellow
K112	Yellow
H113	Yellow
L114	Yellow
M115	Yellow
P116	Yellow
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T120	Yellow
F121	Yellow
M122	Yellow
A123	Yellow
C124	Green

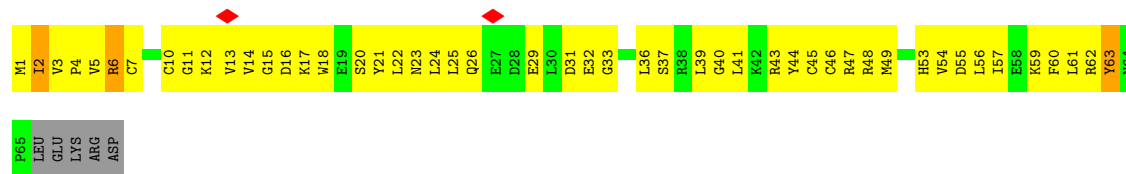
Chain H: 10% 22% 70% 7%



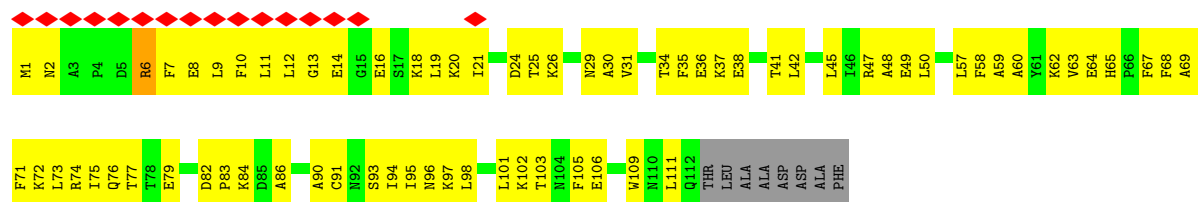
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



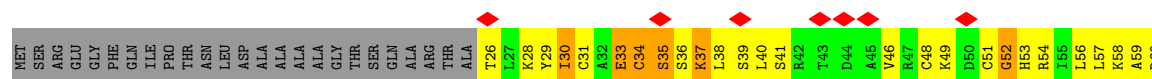
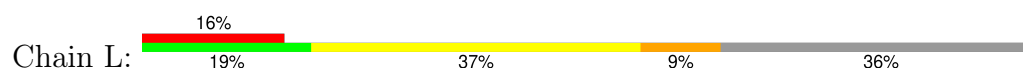
• Molecule 10: DNA-directed RNA polymerase II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



• Molecule 12: DNA-directed RNA polymerase II subunit RPABC4



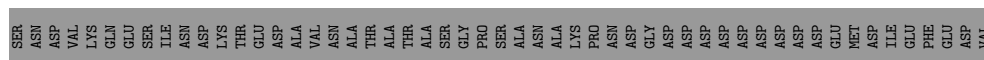
E241	N242	L243	M244	L245	C246	L247	Y248	D249	K250	V251	T252	R253	T254	K255	A256	R257	W258	K259	C260	S261	L262	K263	D264	G265	V266	V267	T268	L269	N270	N271	N272	D273	Y274	T275	F276	Q277	K278	A279	Q280	V281	E282	A283	E284	W285	V286
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain V: 14% 36% 26% 60%

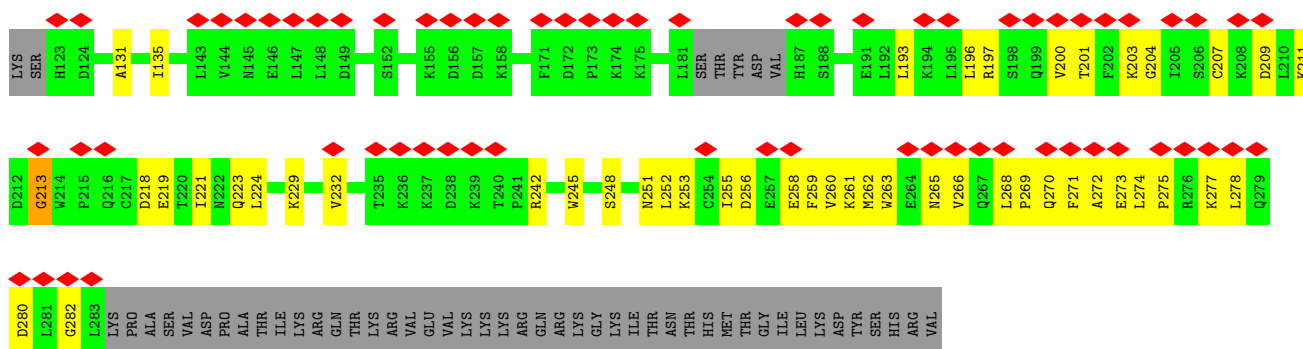
SER GLU																													MET																																																					
	T61	V62	K63	G64	N65	L66	D67	T68	V69	G70	F71	C72	D73	V74	V75	W76	T77	F78	I79	V80	K81	N82	C83	Q84	V85	T86	V87	E88		ASP	SER	HIS	ASP	ASP	ALA	SER	GLN	ASN	GLY	ASP	SER	GLY	ASP	SER	GLN	S104	V105	I106	S107	V108	D109	K110	L111	R112	T113	V114	A115	C116	N117	S118	K119	LVS																				
																												ALA	VAL	PRO	GLY	TYR	GLU	TYR	ARG	ARG	SER	THR	ILE	GLY	ASN	SER	LEU	VAL	ASP	ALA	LEU	THR	ASP	LEU	ALA	SER	LEU	ALA	MET	MET	ARG	VAL	LEU	GLU	THR	PHE	ASP	LYS	VAL	VAL	ALA	GLU	THR	LEU	LYS	ASP	ASN	T56	Q57	S58	K59	L60				

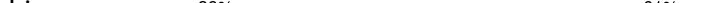
Chain W: 23% 19% 21% 60%

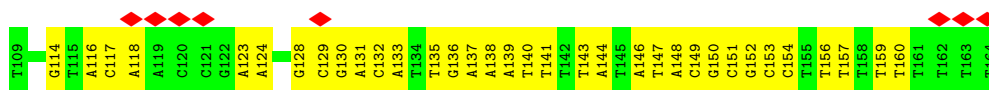
[illegible]

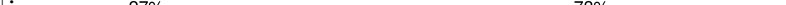


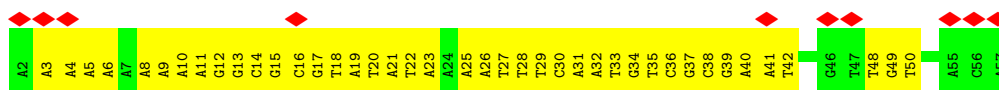
Chain X: 

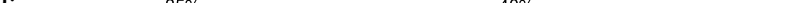


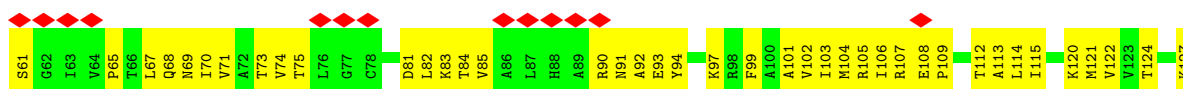
Chain T: 

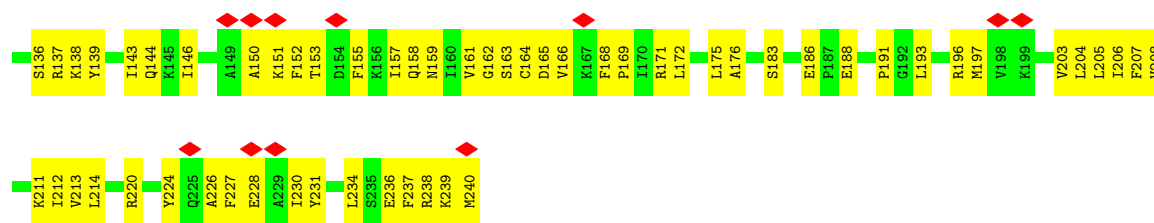


Chain N:  18% 27% 73%

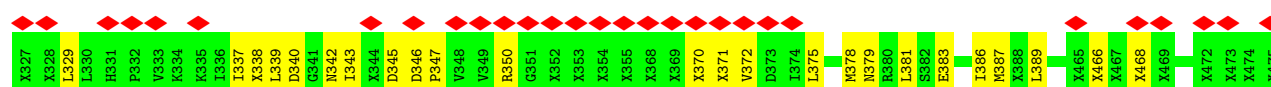
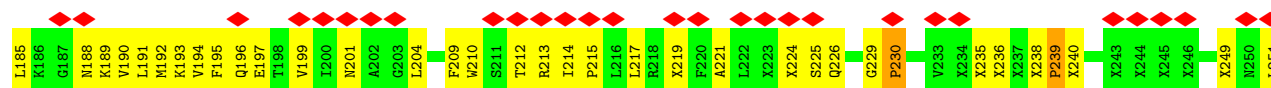
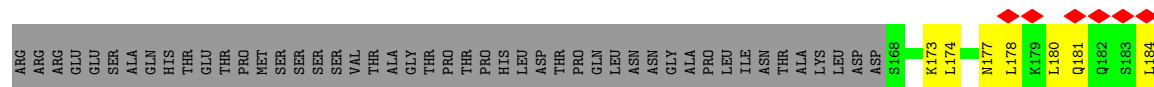
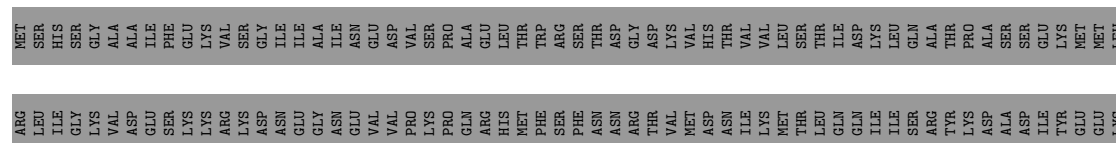
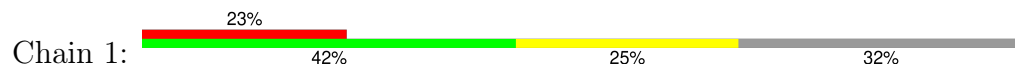


Chain O: 

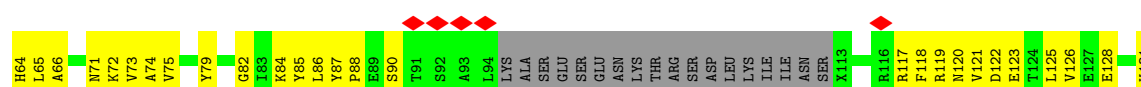
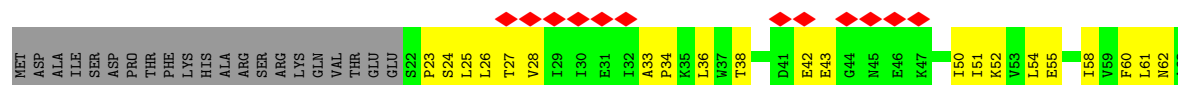


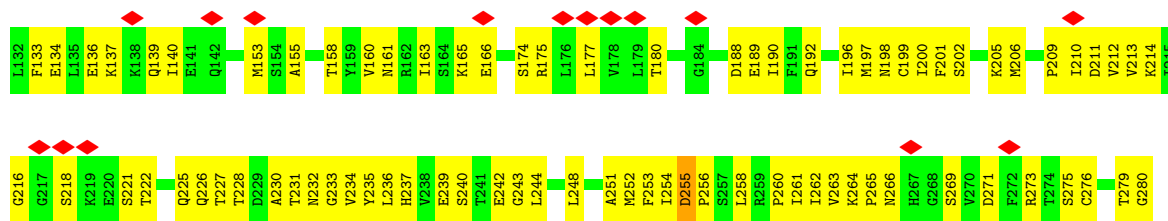


• Molecule 23: Tfb1

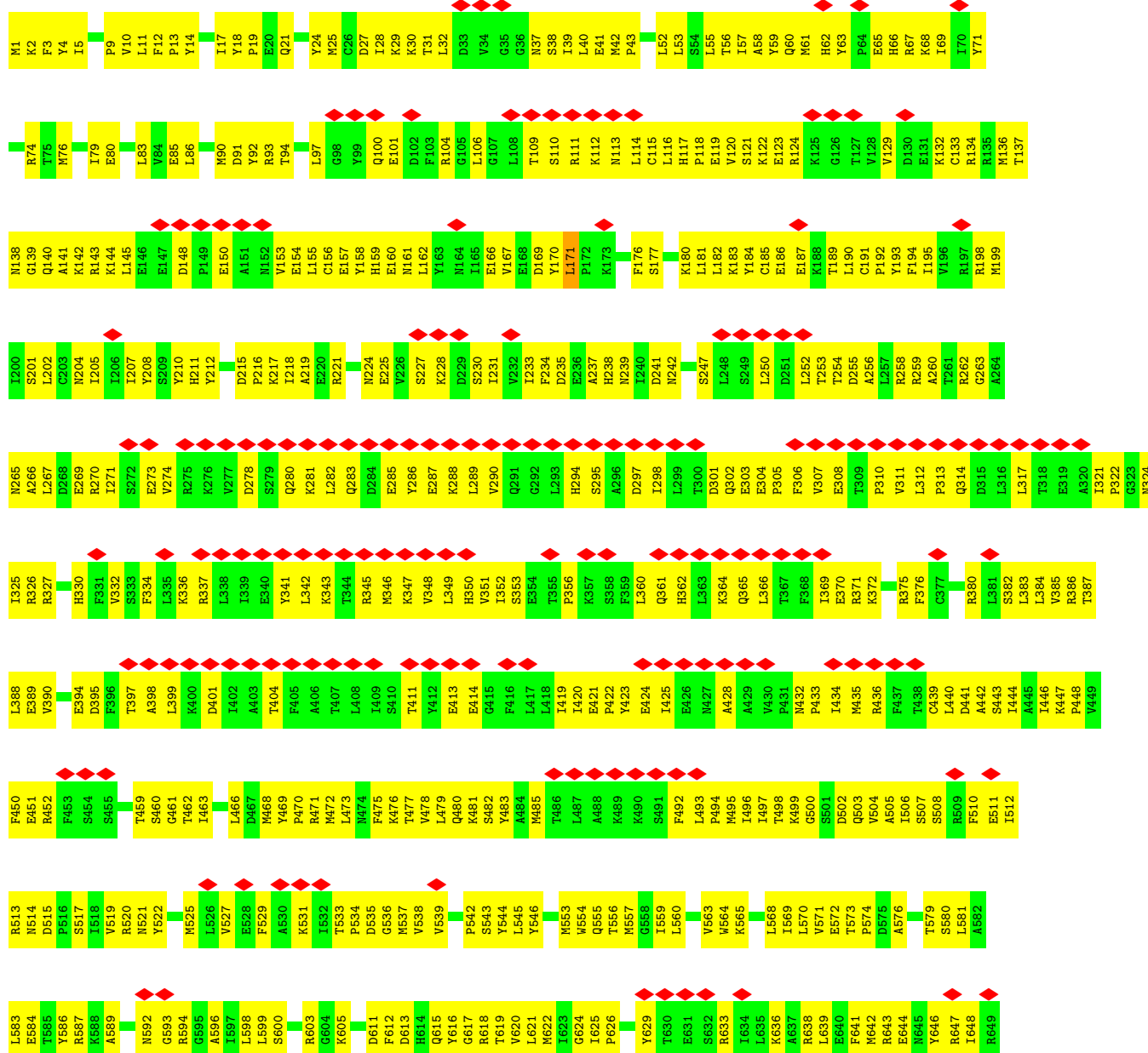


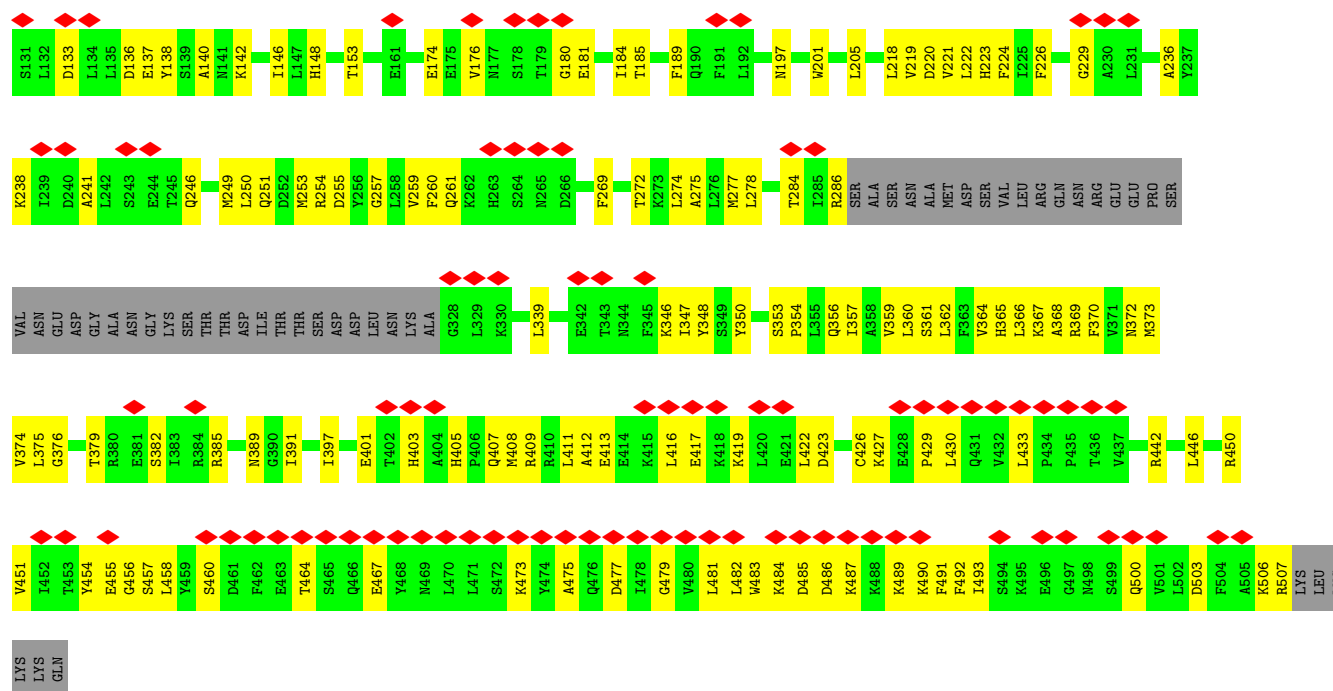
• Molecule 24: Tfb4



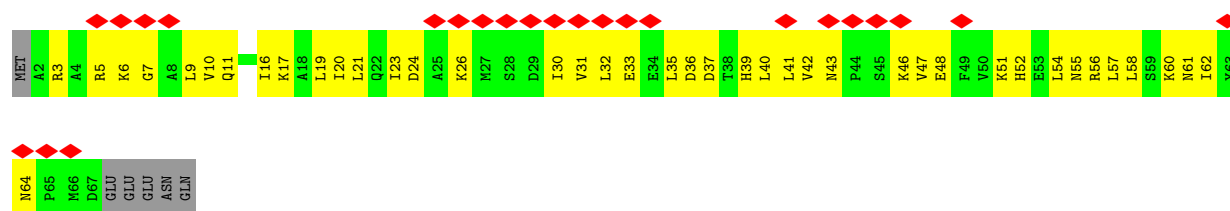


• Molecule 25: General transcription and DNA repair factor IIH helicase subunit XPD

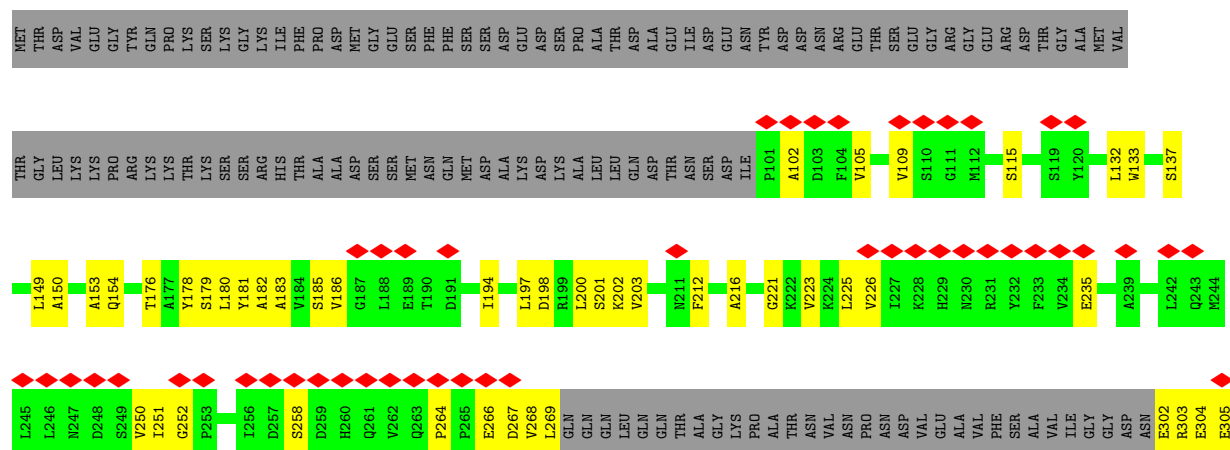


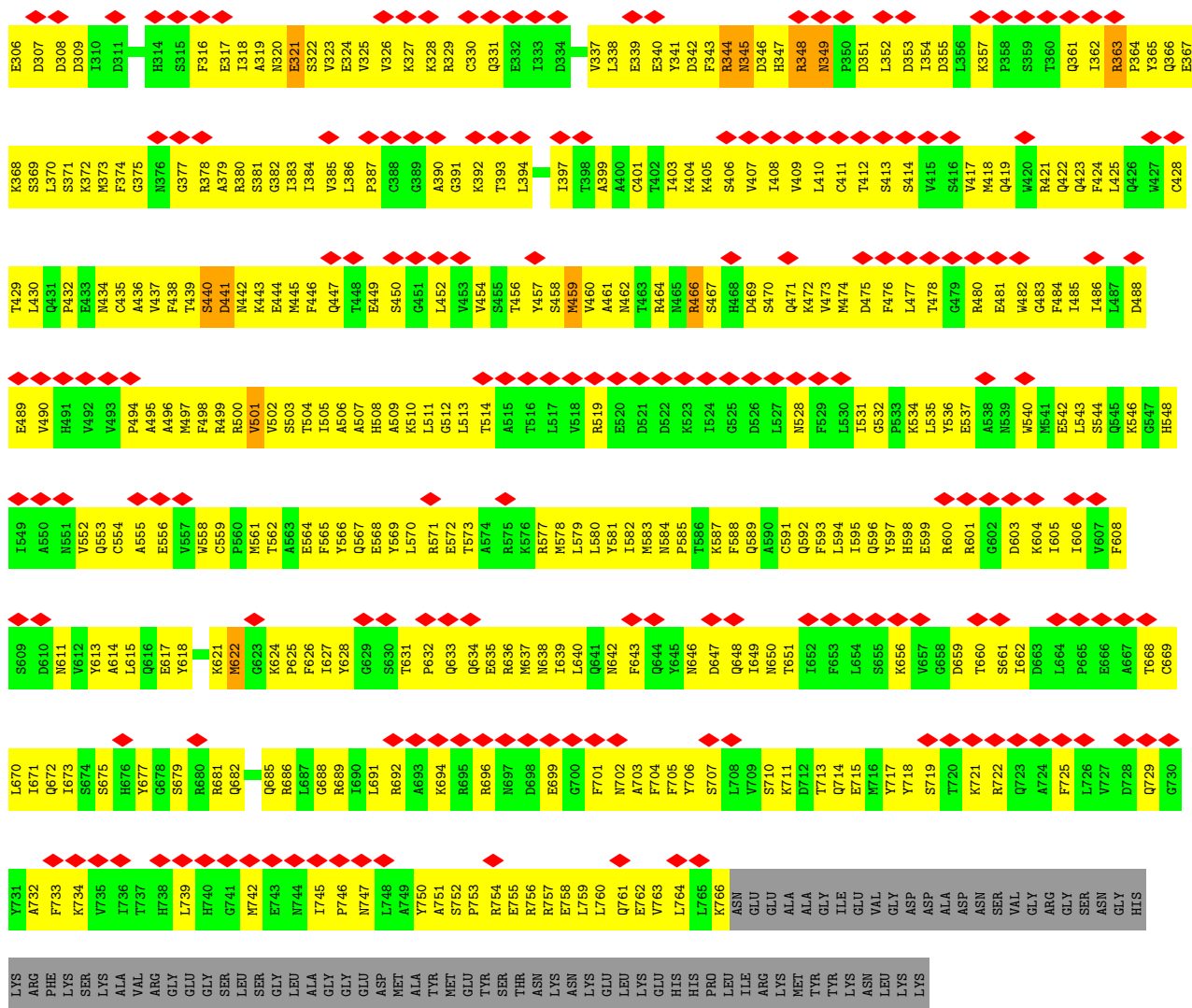


- Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

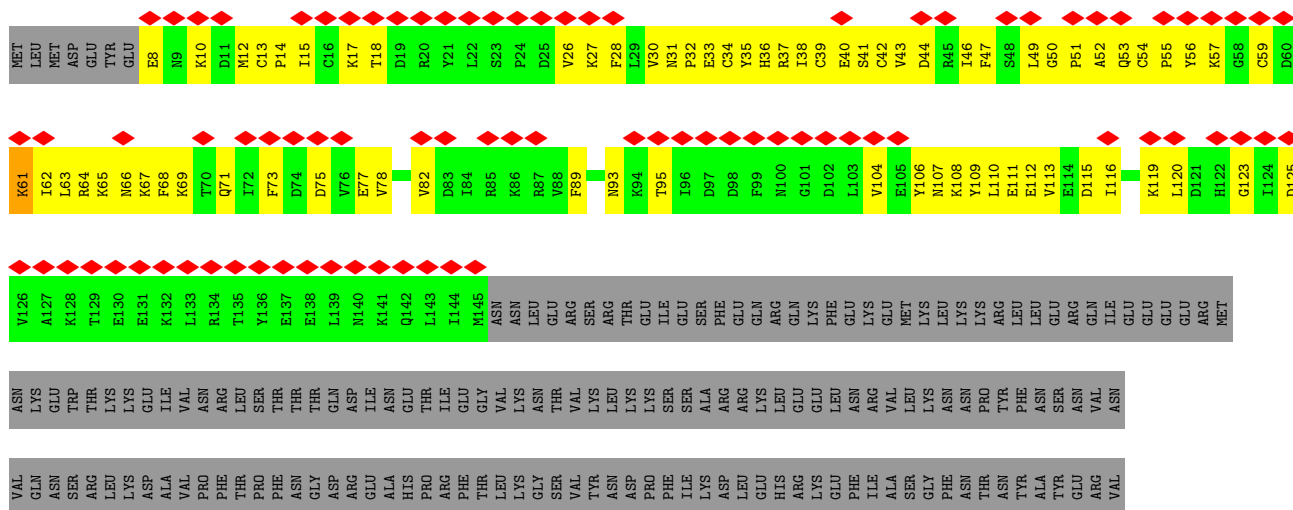


- Molecule 29: General transcription and DNA repair factor IIH helicase subunit XPB





• Molecule 30: BJ4_G0050160.mRNA.1.CDS.1



LEU
THR
GLU
ALA
PHE
MET
GLY
LEU
GLY
CYS
VAL
ILE
SER
GLU
GLU
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	474.87997, 501.37997, 473.81998	wwPDB
Map dimensions	448, 473, 447	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	1/11192 (0.0%)	0.71	8/15128 (0.1%)
2	B	0.48	1/9357 (0.0%)	0.70	1/12618 (0.0%)
3	C	0.53	1/2099 (0.0%)	0.76	0/2845
4	D	0.31	0/1262	0.65	0/1693
5	E	0.41	0/1780	0.69	0/2395
6	F	0.59	1/682 (0.1%)	0.89	0/922
7	G	0.32	0/1368	0.62	0/1844
8	H	0.47	0/1107	0.79	0/1499
9	I	0.40	0/962	0.83	0/1295
10	J	0.55	0/541	1.03	3/727 (0.4%)
11	K	0.53	0/922	0.88	2/1244 (0.2%)
12	L	0.39	0/360	0.94	0/478
13	M	0.32	0/2204	0.69	0/2963
14	Q	0.26	0/1168	0.52	0/1579
15	R	0.24	0/1312	0.51	0/1777
16	U	0.16	0/389	0.47	0/523
17	V	0.18	0/384	0.39	0/518
18	W	0.21	0/1490	0.47	0/2014
19	X	0.17	0/993	0.47	0/1357
20	T	0.41	0/1273	0.55	0/1962
21	N	0.42	0/1301	0.60	0/2006
22	O	0.24	0/1443	0.49	0/1942
23	1	0.20	0/1896	0.48	0/2543
24	4	0.26	0/2062	0.58	0/2805
25	0	0.26	0/6226	0.57	1/8407 (0.0%)
26	6	0.25	0/2506	0.56	0/3402
27	2	0.23	0/3057	0.53	1/4071 (0.0%)
28	5	0.23	0/502	0.53	0/677
29	7	0.32	0/4521	0.67	4/6036 (0.1%)
30	3	0.49	1/870 (0.1%)	0.71	2/1190 (0.2%)
All	All	0.38	5/65229 (0.0%)	0.65	22/88460 (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
1	A	0	7
2	B	0	4
8	H	0	3
9	I	0	1
10	J	0	1
13	M	0	3
18	W	0	1
19	X	0	1
24	4	0	2
25	0	0	2
26	6	0	1
29	7	0	8
30	3	0	2
All	All	0	36

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	61	LYS	CE-NZ	-6.75	1.29	1.49
1	A	1074	GLU	CD-OE2	-5.86	1.14	1.25
6	F	135	ARG	CA-CB	-5.54	1.39	1.53
3	C	166	GLU	CA-CB	-5.31	1.44	1.53
2	B	112	LEU	C-N	-5.14	1.23	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	501	VAL	N-CA-C	-11.57	101.38	112.83
27	2	70	GLY	N-CA-C	-8.83	103.97	114.48
10	J	63	TYR	CA-C-N	-8.14	108.93	120.49
10	J	63	TYR	C-N-CA	-8.14	108.93	120.49
10	J	6	ARG	N-CA-C	7.68	121.11	110.35

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	250	ILE	Peptide
1	A	450	LEU	Peptide
1	A	465	TYR	Peptide
1	A	71	GLN	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	10997	0	11081	837	0
2	B	9178	0	9195	650	0
3	C	2061	0	2029	162	0
4	D	1253	0	1275	133	0
5	E	1744	0	1772	126	0
6	F	670	0	690	66	0
7	G	1340	0	1357	138	0
8	H	1089	0	1062	129	0
9	I	944	0	899	106	0
10	J	532	0	542	65	0
11	K	904	0	911	93	0
12	L	358	0	383	39	0
13	M	2175	0	2283	231	0
14	Q	1144	0	1034	115	0
15	R	1303	0	1110	125	0
16	U	383	0	384	25	0
17	V	381	0	388	35	0
18	W	1469	0	1432	112	0
19	X	984	0	722	60	0
20	T	1140	0	641	73	0
21	N	1156	0	631	87	0
22	O	1416	0	1493	105	0
23	1	2411	0	1881	126	0
24	4	2041	0	1954	147	0
25	0	6108	0	6168	577	0
26	6	2527	0	2321	226	0
27	2	3011	0	2600	229	0
28	5	498	0	506	59	0
29	7	4447	0	3905	498	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	860	0	623	103	0
31	3	2	0	0	0	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	W	1	0	0	0	0
32	A	1	0	0	0	0
33	0	8	0	0	3	0
All	All	64550	0	61272	5031	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 40.

The worst 5 of 5031 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)
12:L:48:CYS:SG	12:L:53:HIS:HB3	1.70	1.32
12:L:34:CYS:SG	12:L:36:SER:OG	1.98	1.18
2:B:649:LYS:NZ	2:B:736:THR:O	1.83	1.11
25:0:162:LEU:HD22	25:0:194:PHE:HB3	1.27	1.09
1:A:253:ASN:HA	2:B:935:ARG:HH12	1.17	1.07

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	1386/1733 (80%)	1192 (86%)	189 (14%)	5 (0%)	30	59
2	B	1136/1224 (93%)	987 (87%)	146 (13%)	3 (0%)	36	65
3	C	260/318 (82%)	214 (82%)	46 (18%)	0	100	100
4	D	153/221 (69%)	135 (88%)	18 (12%)	0	100	100
5	E	211/215 (98%)	193 (92%)	18 (8%)	0	100	100
6	F	81/155 (52%)	69 (85%)	12 (15%)	0	100	100
7	G	169/171 (99%)	152 (90%)	17 (10%)	0	100	100
8	H	132/146 (90%)	106 (80%)	24 (18%)	2 (2%)	8	30
9	I	114/122 (93%)	94 (82%)	20 (18%)	0	100	100
10	J	63/70 (90%)	44 (70%)	19 (30%)	0	100	100
11	K	110/120 (92%)	95 (86%)	15 (14%)	0	100	100
12	L	43/70 (61%)	33 (77%)	7 (16%)	3 (7%)	1	6
13	M	273/345 (79%)	221 (81%)	52 (19%)	0	100	100
14	Q	140/735 (19%)	120 (86%)	20 (14%)	0	100	100
15	R	176/400 (44%)	163 (93%)	13 (7%)	0	100	100
16	U	44/286 (15%)	38 (86%)	6 (14%)	0	100	100
17	V	45/122 (37%)	44 (98%)	1 (2%)	0	100	100
18	W	189/482 (39%)	182 (96%)	7 (4%)	0	100	100
19	X	152/328 (46%)	136 (90%)	16 (10%)	0	100	100
22	O	178/240 (74%)	167 (94%)	11 (6%)	0	100	100
23	1	256/542 (47%)	234 (91%)	19 (7%)	3 (1%)	10	35
24	4	279/338 (82%)	222 (80%)	57 (20%)	0	100	100
25	0	752/778 (97%)	670 (89%)	82 (11%)	0	100	100
26	6	336/461 (73%)	298 (89%)	36 (11%)	2 (1%)	21	50
27	2	456/513 (89%)	390 (86%)	66 (14%)	0	100	100
28	5	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
29	7	630/843 (75%)	539 (86%)	90 (14%)	1 (0%)	43	71
30	3	136/321 (42%)	105 (77%)	31 (23%)	0	100	100
All	All	7964/11371 (70%)	6901 (87%)	1044 (13%)	19 (0%)	44	71

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
2	B	364	ILE
8	H	110	ASP
26	6	411	PRO
29	7	349	ASN

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	1221/1520 (80%)	1221 (100%)	0	100	100
2	B	1000/1061 (94%)	1000 (100%)	0	100	100
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	11
13	M	245/299 (82%)	245 (100%)	0	100	100
14	Q	109/641 (17%)	109 (100%)	0	100	100
15	R	107/363 (30%)	107 (100%)	0	100	100
16	U	42/260 (16%)	42 (100%)	0	100	100
17	V	46/108 (43%)	46 (100%)	0	100	100
18	W	155/429 (36%)	155 (100%)	0	100	100
19	X	62/295 (21%)	62 (100%)	0	100	100
22	O	152/205 (74%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1	169/395 (43%)	169 (100%)	0	100	100
24	4	198/298 (66%)	198 (100%)	0	100	100
25	0	686/707 (97%)	686 (100%)	0	100	100
26	6	247/406 (61%)	247 (100%)	0	100	100
27	2	258/468 (55%)	258 (100%)	0	100	100
28	5	53/66 (80%)	53 (100%)	0	100	100
29	7	414/737 (56%)	414 (100%)	0	100	100
30	3	53/303 (18%)	53 (100%)	0	100	100
All	All	6432/9989 (64%)	6426 (100%)	6 (0%)	87	89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	35	SER
12	L	38	LEU
12	L	40	LEU
12	L	33	GLU
12	L	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
25	0	224	ASN
27	2	500	GLN
25	0	699	GLN
26	6	249	GLN
29	7	589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 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	$\# Z > 2$
33	SF4	0	801	25	0,12,12	-	-	-		

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
33	SF4	0	801	25	-	-	0/6/5/5

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	801	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.96
1	1	519:UNK	C	537:GLU	N	11.53
1	1	355:UNK	C	368:UNK	N	10.44

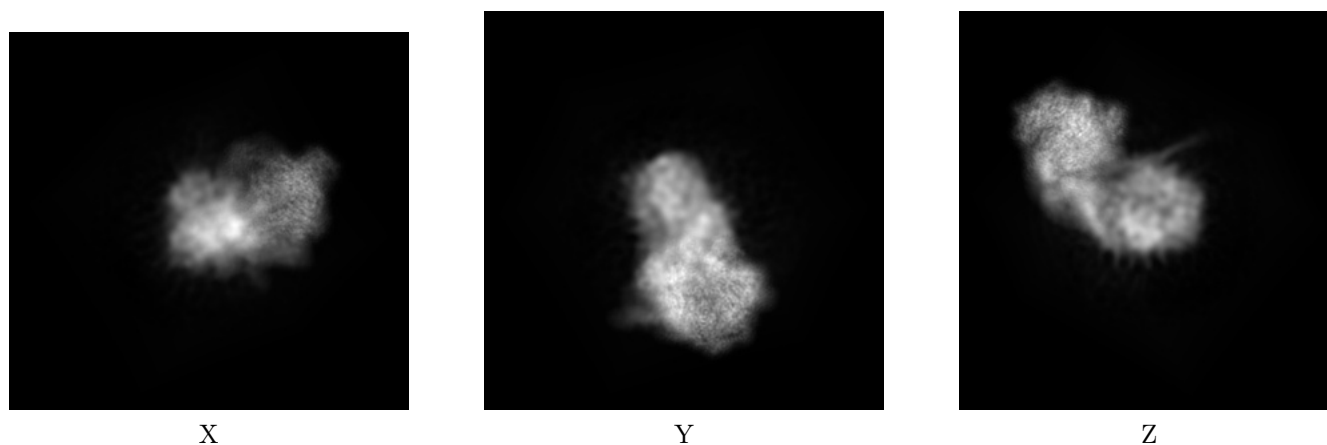
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23906. 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](#)

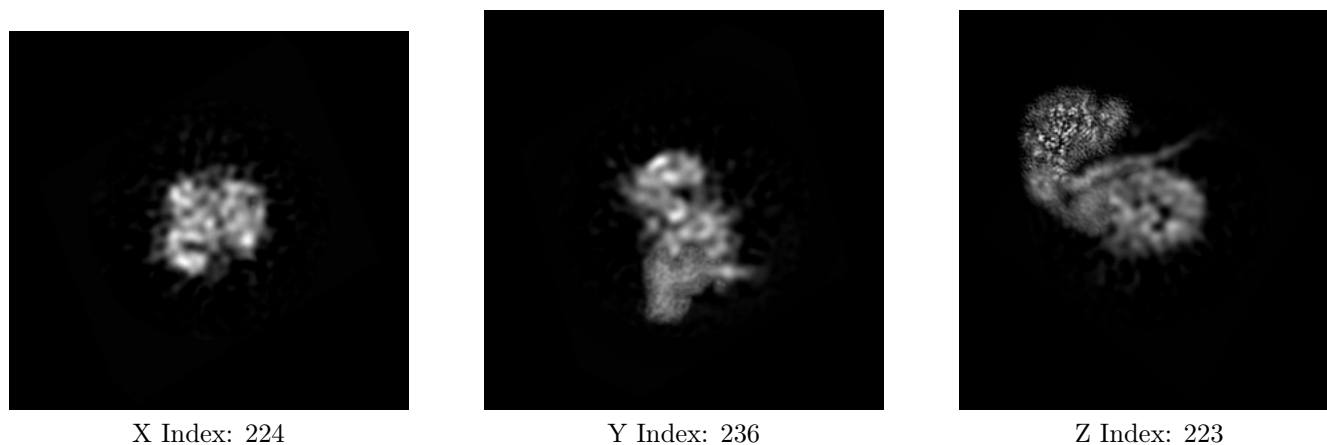
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



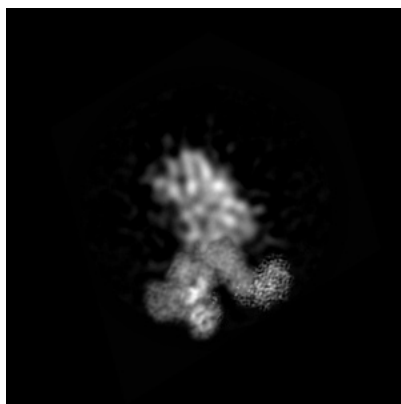
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

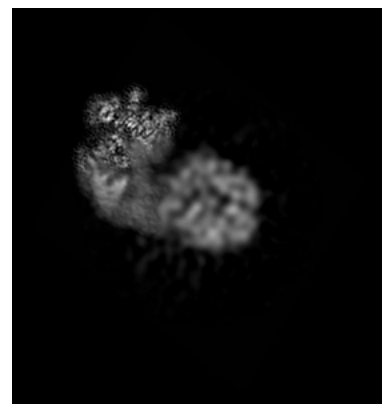
6.3.1 Primary map



X Index: 152



Y Index: 263

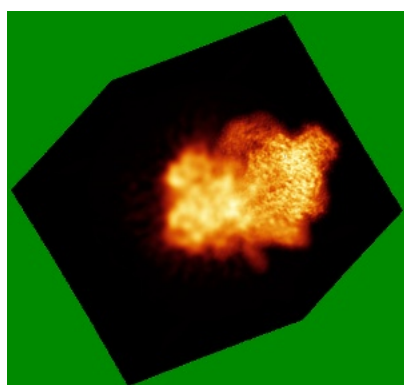


Z Index: 210

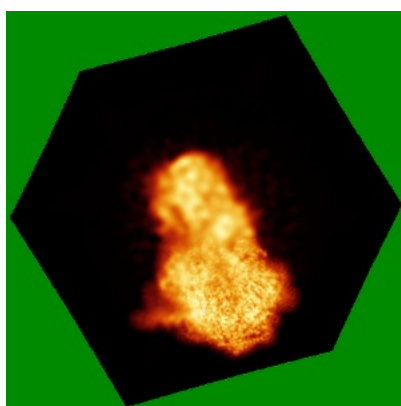
The images above show the largest variance slices of the map in three orthogonal directions.

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

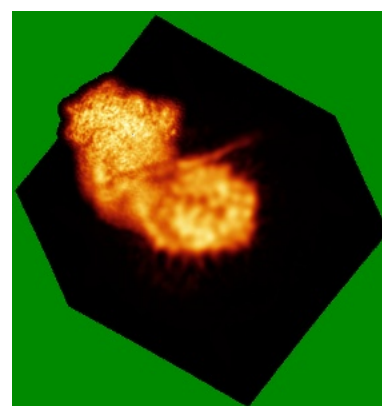
6.4.1 Primary map



X



Y

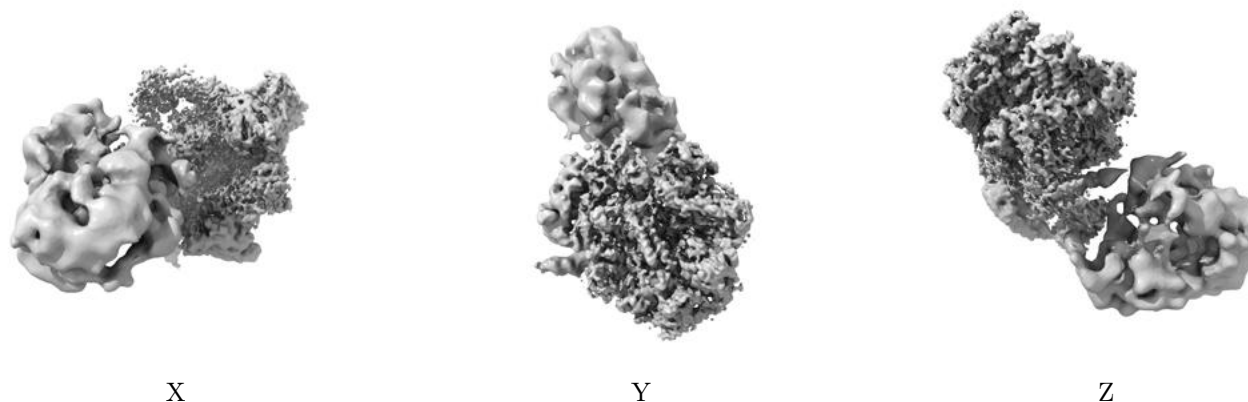


Z

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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

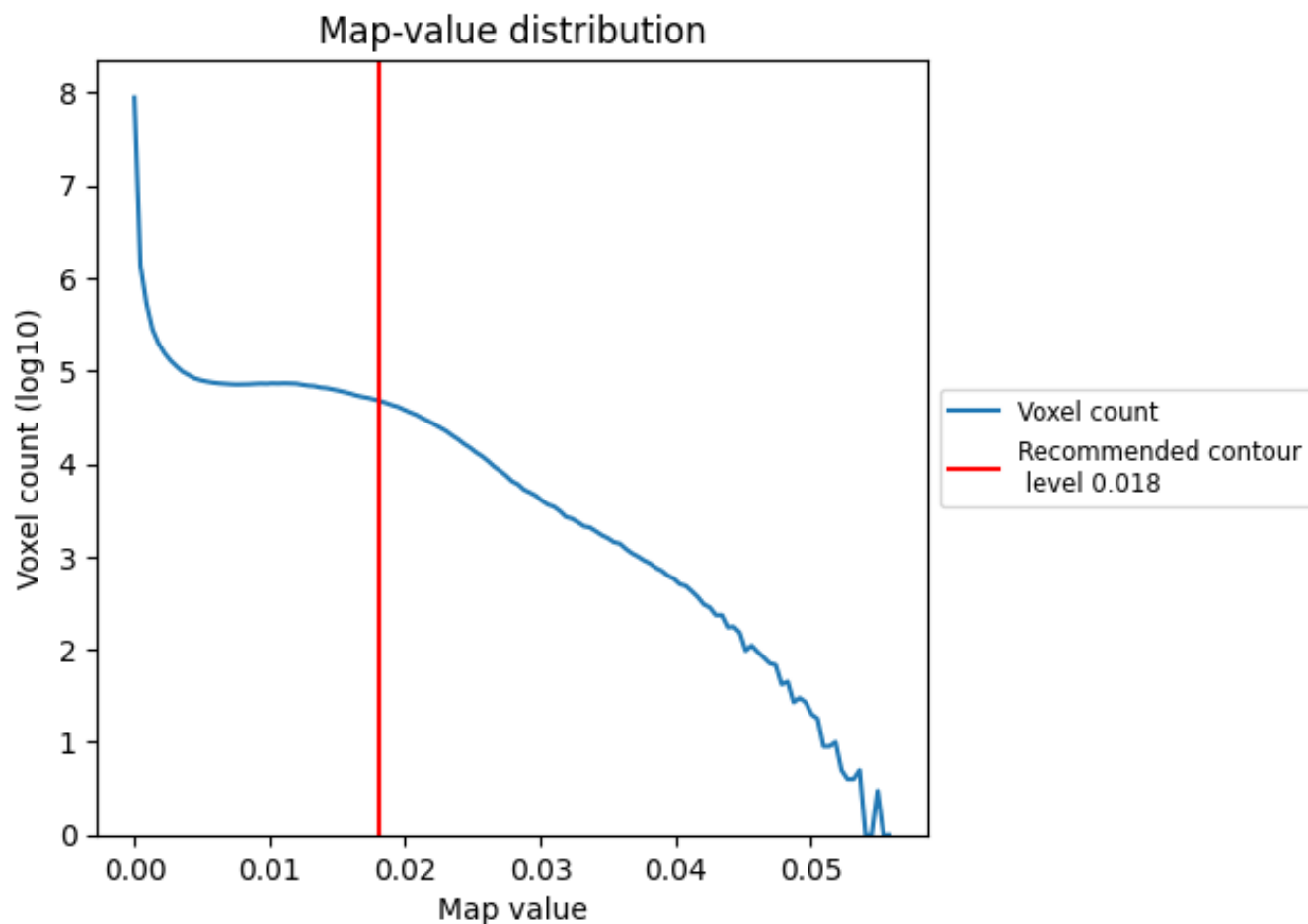
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

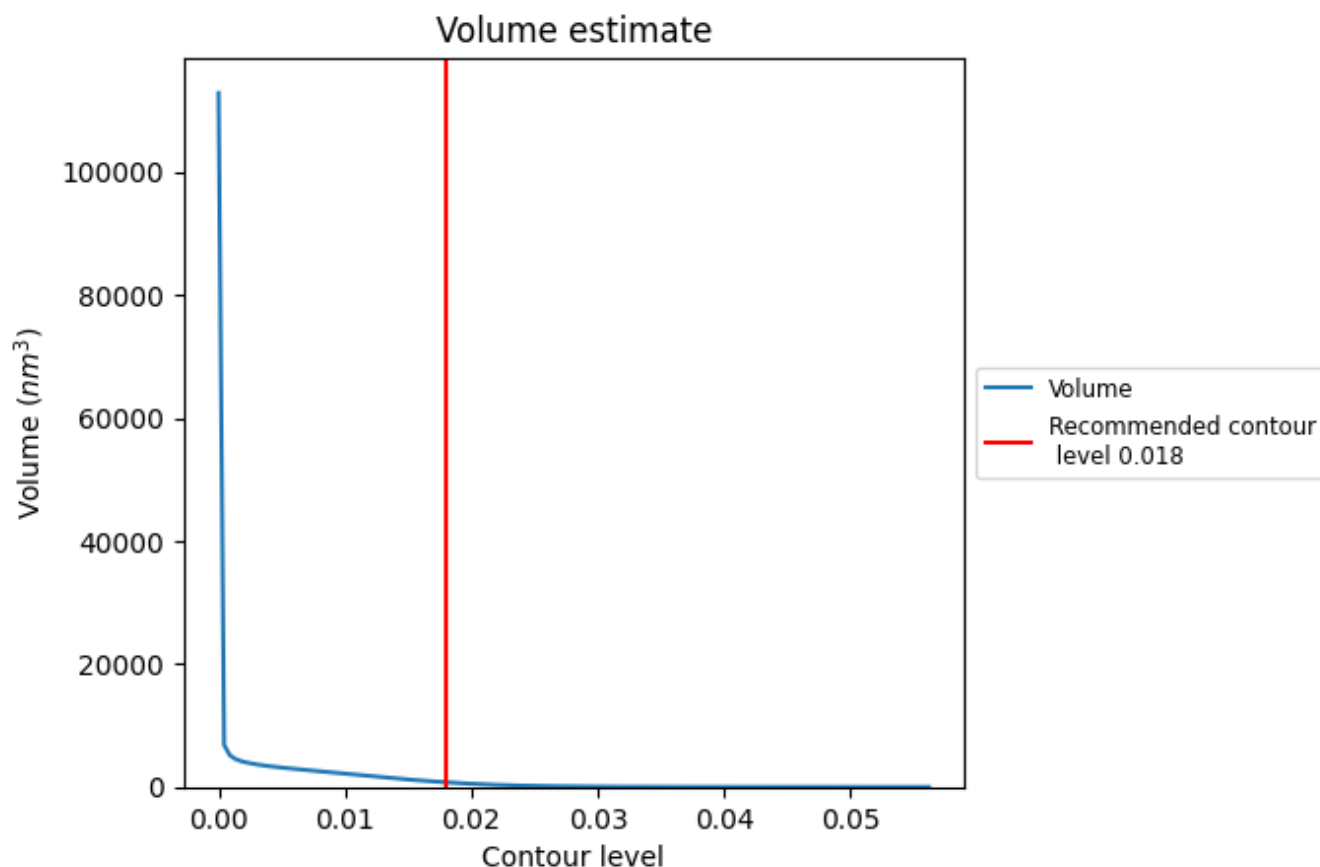
This section contains the results of statistical analysis of the map.

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 762 nm^3 ; this corresponds to an approximate mass of 688 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.

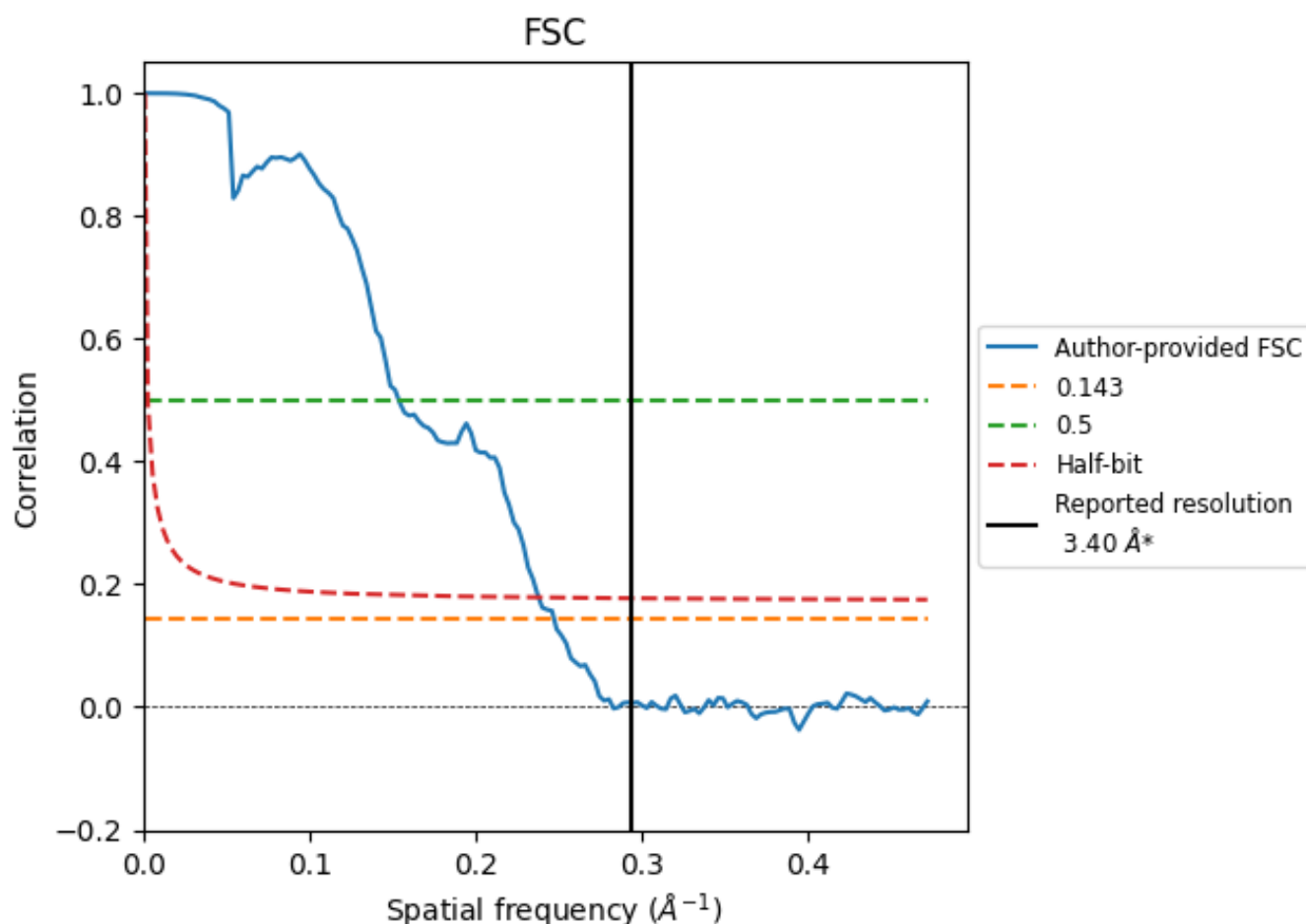
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

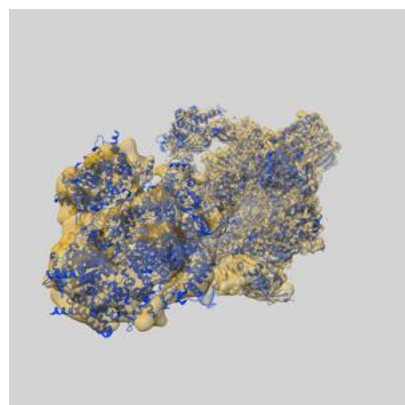
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	4.05	6.50	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.4 by more than 10 %

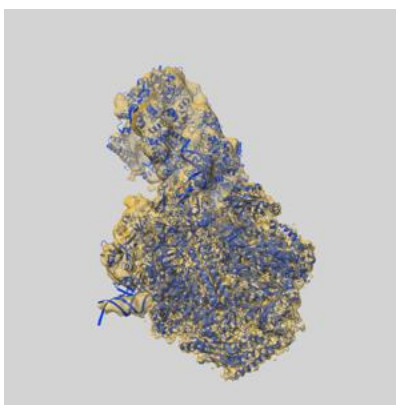
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23906 and PDB model 7ML2. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

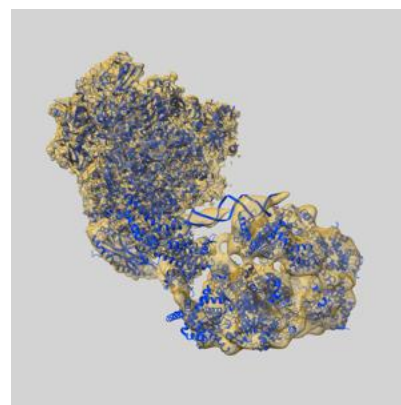
9.1 Map-model overlay [i](#)



X



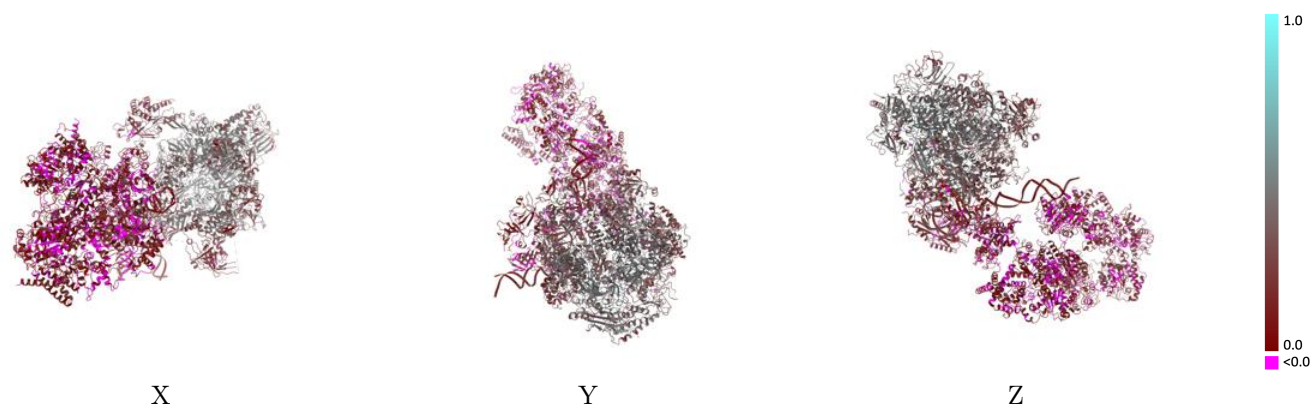
Y



Z

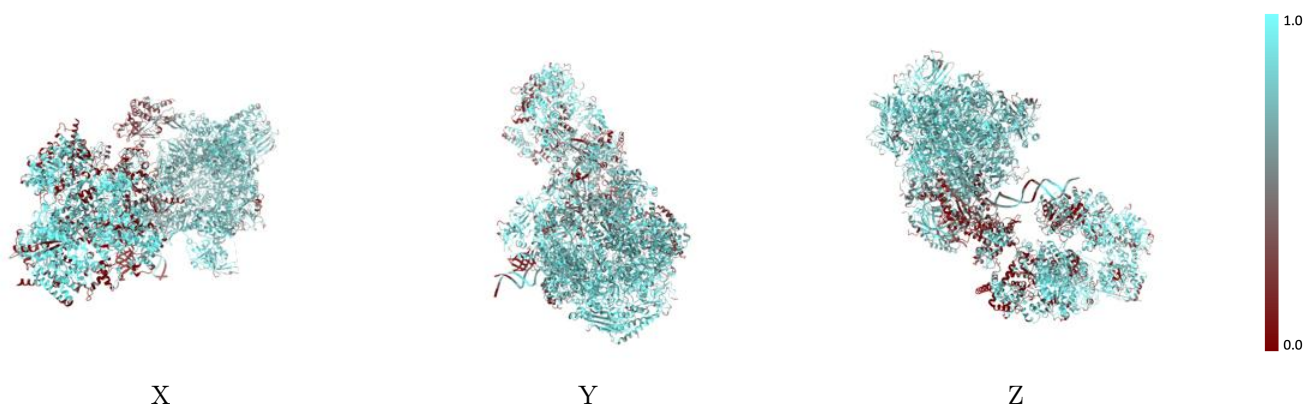
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



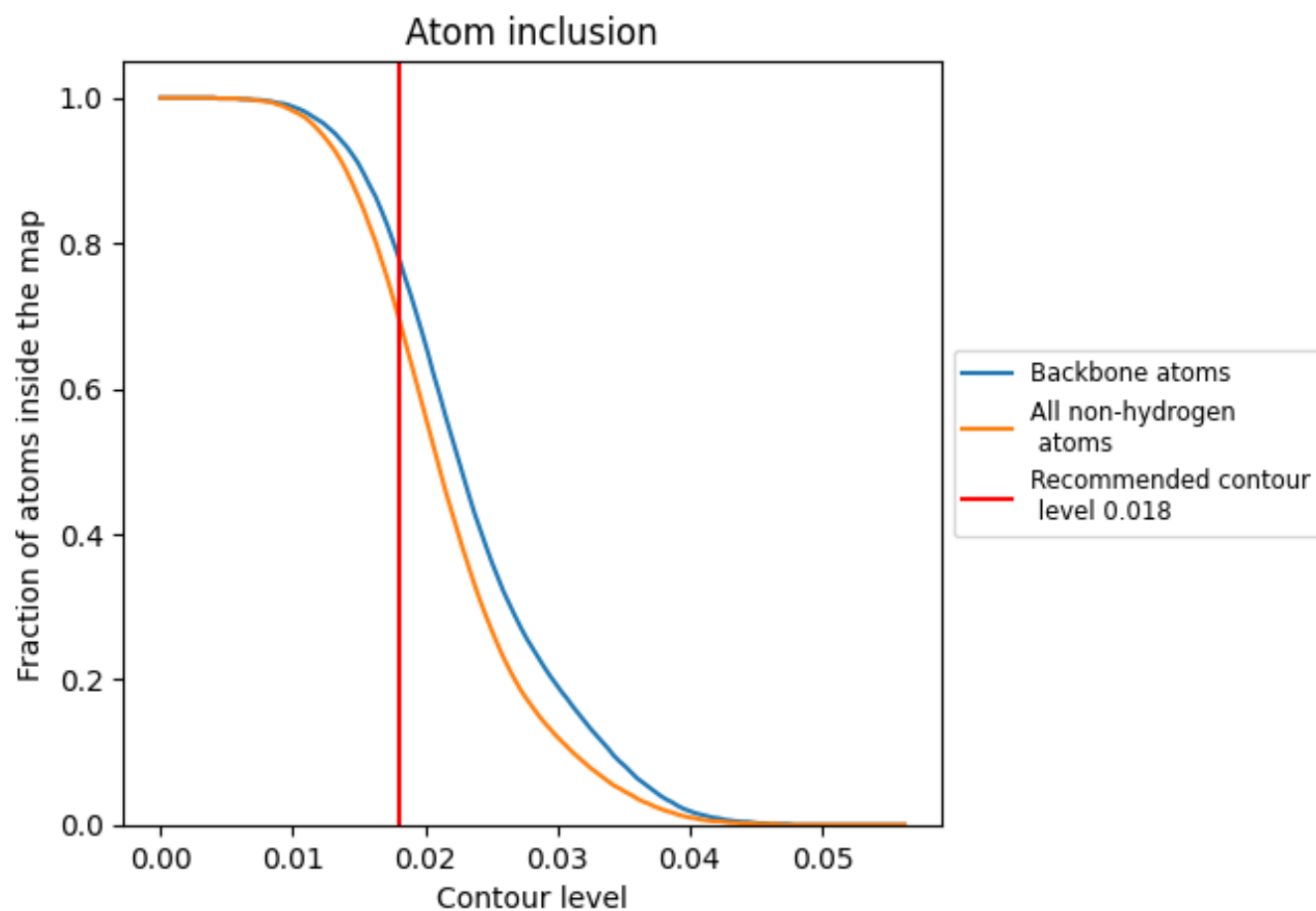
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.2410
0	 0.6760	 0.0760
1	 0.6300	 0.0700
2	 0.6610	 0.0730
3	 0.3780	 0.0870
4	 0.8350	 0.0840
5	 0.6360	 0.0880
6	 0.8020	 0.0860
7	 0.5850	 0.0670
A	 0.7980	 0.4070
B	 0.8270	 0.4220
C	 0.8410	 0.4250
D	 0.2470	 0.2040
E	 0.7770	 0.3820
F	 0.7930	 0.3810
G	 0.4360	 0.2550
H	 0.7370	 0.3440
I	 0.6100	 0.2690
J	 0.8380	 0.4100
K	 0.7150	 0.3710
L	 0.6970	 0.2880
M	 0.5480	 0.2340
N	 0.6980	 0.1450
O	 0.7610	 0.1580
Q	 0.8080	 0.2110
R	 0.6770	 0.1820
T	 0.7070	 0.1650
U	 0.0290	 0.0510
V	 0.1140	 0.0470
W	 0.4040	 0.0900
X	 0.5360	 0.0920

