



Full wwPDB EM Validation Report ⓘ

Apr 11, 2023 – 03:06 pm BST

PDB ID : 8CEN
EMDB ID : EMD-16610
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator
Authors : Wang, H.; Schilbach, S.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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.



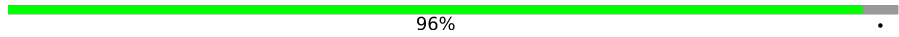


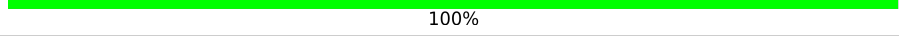

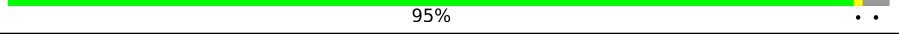
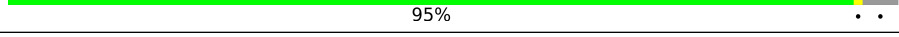
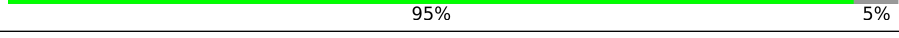
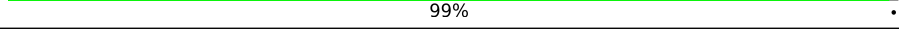
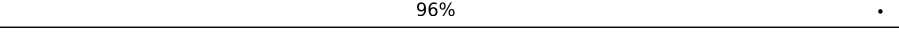
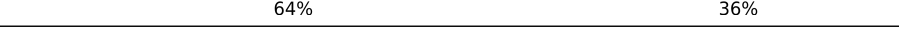
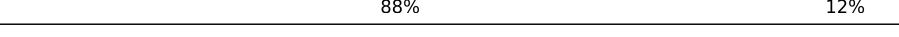

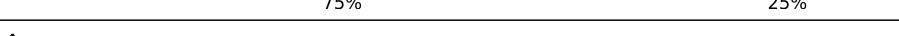


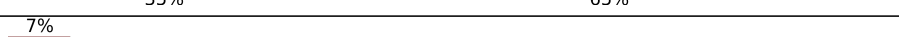

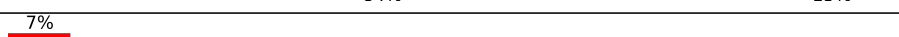






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	0	778	5% (red), 97% (green), . (grey)
2	1	642	18% (red), 81% (green), 19% (grey)
3	2	513	18% (red), 88% (green), 12% (grey)
4	3	321	41% (green), 59% (grey)
5	4	338	11% (red), 89% (green), . (grey), 11% (grey)
6	5	72	32% (red), 89% (green), . (grey), 10% (grey)
7	6	461	11% (red), 83% (green), 17% (grey)
8	7	843	7% (red), 73% (green), 27% (grey)
9	A	1733	. (red), 87% (green), 13% (grey)


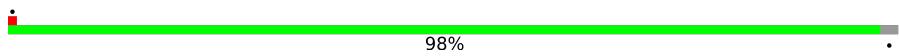




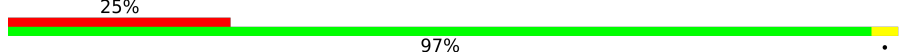


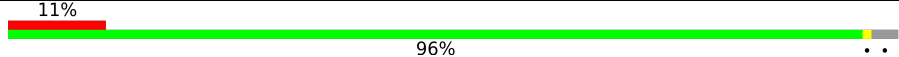


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Mol	Chain	Length	Quality of chain
10	B	1224	 96%
11	C	347	 77% 23%
12	D	221	 76% 24%
13	E	215	 100%
14	F	155	 76% 24%
15	G	177	 95%
16	H	146	 95%
17	I	122	 95% 5%
18	J	70	 99%
19	K	120	 96%
20	L	70	 64% 36%
21	M	352	 88% 12%
22	N	209	 35% 65%
23	O	240	 75% 25%
24	Q	735	 30% 70%
25	R	400	 67% 33%
26	T	209	 35% 65%
27	U	286	 7% 37% 63%
28	V	122	 8% 84% 15%
29	W	492	 7% 61% 38%
30	X	328	 7% 64% 36%
31	a	295	 7% 60% 40%
32	b	223	 7% 77% 22%
33	c	115	 7% 97%
34	d	687	 7% 73% 27%

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Mol	Chain	Length	Quality of chain
35	e	307	
36	f	210	
37	g	121	
38	h	284	
39	i	222	
40	j	149	
41	k	157	
42	l	745	
43	m	220	
44	n	140	
45	o	127	
46	p	566	

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 101943 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 General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	752	6091	3882	1029	1142	38	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	522	4214	2660	734	798	22	0	0

- Molecule 3 is a protein called General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	452	3647	2354	600	677	16	0	0

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	131	1089	692	180	209	8	0	0

- Molecule 5 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	302	2338	1492	390	442	14	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	65	514	326	90	95	3	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	383	3019	1915	523	552	29	0	0

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	615	4954	3153	860	914	27	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	1508	11815	7442	2042	2269	62	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	1180	9404	5946	1643	1760	55	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	266	2092	1315	348	416	13	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	initiating methionine	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370
C	-19	SER	-	expression tag	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370
C	2	SER	-	expression tag	UNP P16370
C	3	SER	-	expression tag	UNP P16370

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	167	1343	829	242	270	2	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	214	1752	1111	309	321	11	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	118	983	623	164	193	3	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	171	1339	861	222	248	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	140	1120	704	188	224	4	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	115	924	593	157	172	2	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	45	359	221	71	63	4	0	0

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	310	2379	1504	408	449	18	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	346	LYS	-	expression tag	UNP P29055
M	347	HIS	-	expression tag	UNP P29055
M	348	HIS	-	expression tag	UNP P29055
M	349	HIS	-	expression tag	UNP P29055
M	350	HIS	-	expression tag	UNP P29055
M	351	HIS	-	expression tag	UNP P29055
M	352	HIS	-	expression tag	UNP P29055

- Molecule 22 is a DNA chain called NONTEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	N	73	1495	717	270	436	72	0	0

- Molecule 23 is a protein called TATA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	181	1422	925	243	248	6	0	0

- Molecule 24 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	221	1871	1179	346	339	7	0	0

- Molecule 25 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	268	2230	1409	392	419	10	0	0

- Molecule 26 is a DNA chain called TEMPLATE DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	T	73	1495	716	268	438	73	0	0

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	107	885	559	147	176	3	0	0

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	104	815	511	136	164	4	0	0

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	304	2473	1558	431	477	7	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	211	1708	1089	293	320	6	0	0

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	a	178	1495	970	240	278	7	0	0

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	173	1414	900	241	270	3	0	0

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	111	902	566	154	178	4	0	0

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	501	4063	2613	684	752	14	0	0

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	256	2017	1280	336	390	11	0	0

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	206	1578	998	266	309	5	0	0

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	102	815	512	134	164	5	0	0

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	171	Total	C	N	O	S	0	0
			1394	884	234	271	5		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	181	Total	C	N	O	S	0	0
			1512	973	253	280	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	102	Total	C	N	O	S	0	0
			852	533	156	162	1		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	157	Total	C	N	O	S	0	0
			1259	777	222	257	3		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	535	Total	C	N	O	S	0	0
			4385	2846	759	763	17		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	130	Total	C	N	O	S	0	0
			1068	672	185	209	2		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	136	Total	C	N	O	S	0	0
			1095	685	185	220	5		

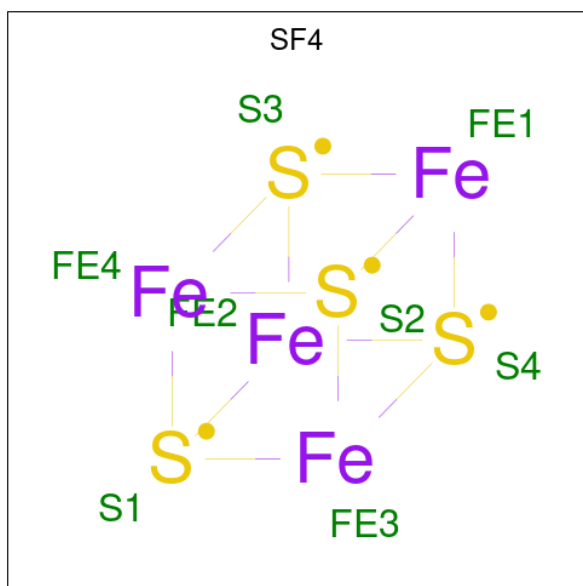
- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	110	922	607	143	166	6	0	0

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	225	1863	1193	298	366	6	0	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	0	1	8	4	4	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	3	2	2	2	0
48	4	1	1	1	0
48	6	4	4	4	0
48	A	2	2	2	0

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Mol	Chain	Residues	Atoms		AltConf
48	B	1	Total 1	Zn 1	0
48	C	1	Total 1	Zn 1	0
48	I	2	Total 2	Zn 2	0
48	J	1	Total 1	Zn 1	0
48	L	1	Total 1	Zn 1	0
48	M	1	Total 1	Zn 1	0
48	W	1	Total 1	Zn 1	0

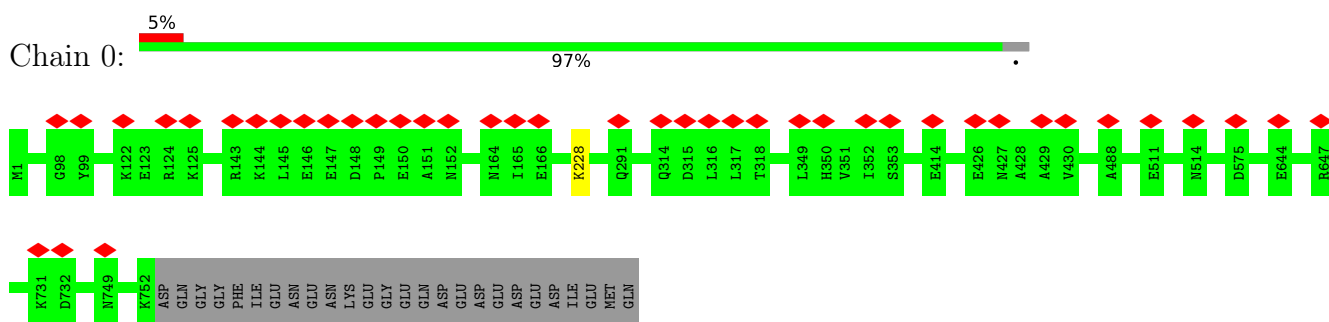
- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

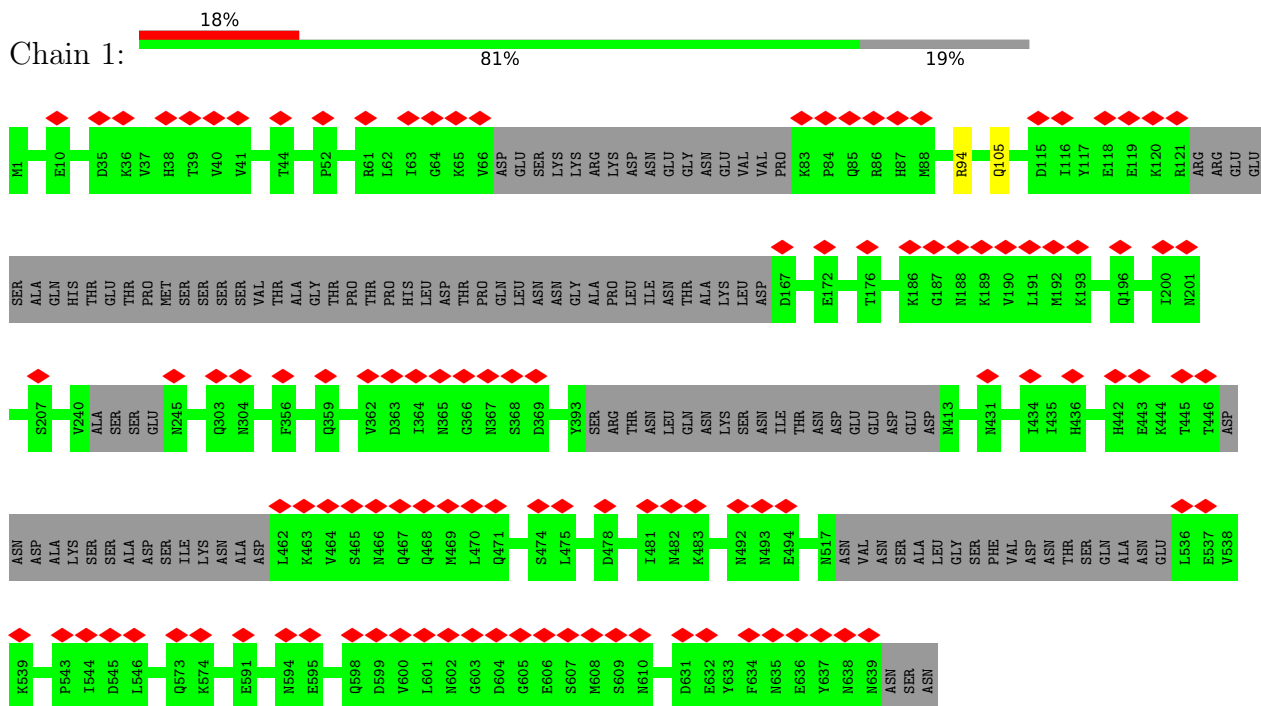
3 Residue-property plots [i](#)

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

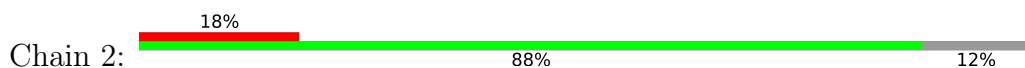
- Molecule 1: General transcription and DNA repair factor IIIH helicase subunit XPD

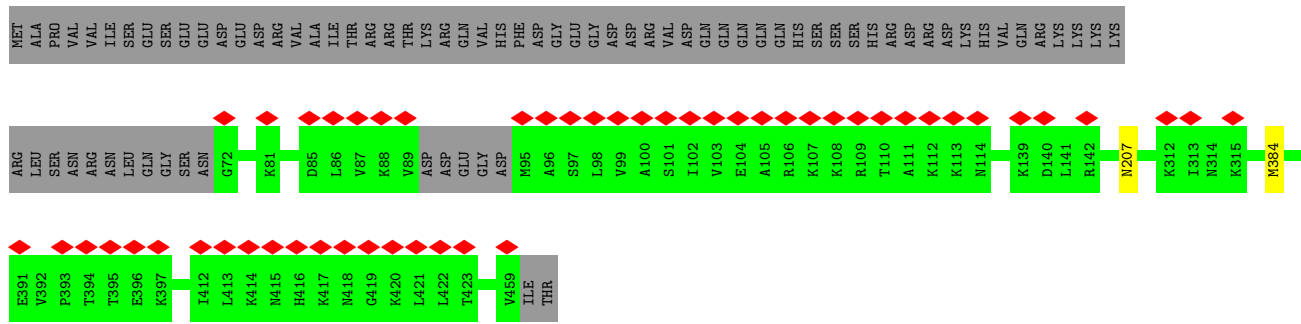


- Molecule 2: General transcription and DNA repair factor IIIH subunit TFB1



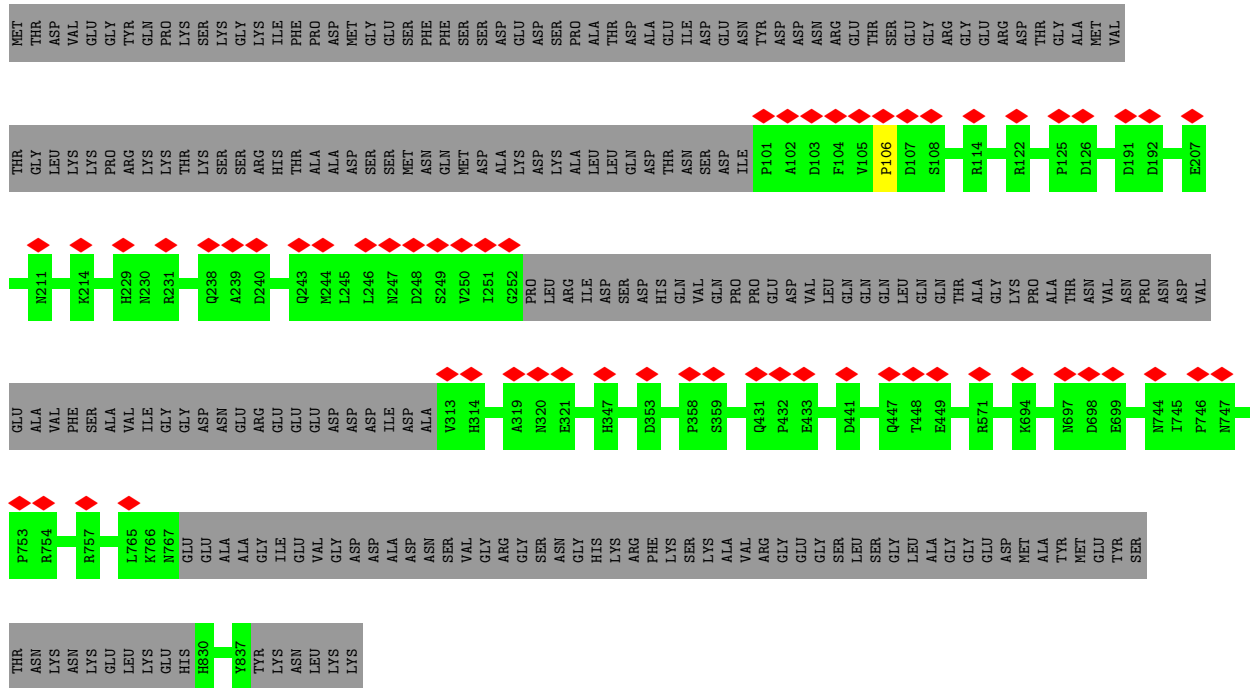
- Molecule 3: General transcription and DNA repair factor IIIH subunit TFB2





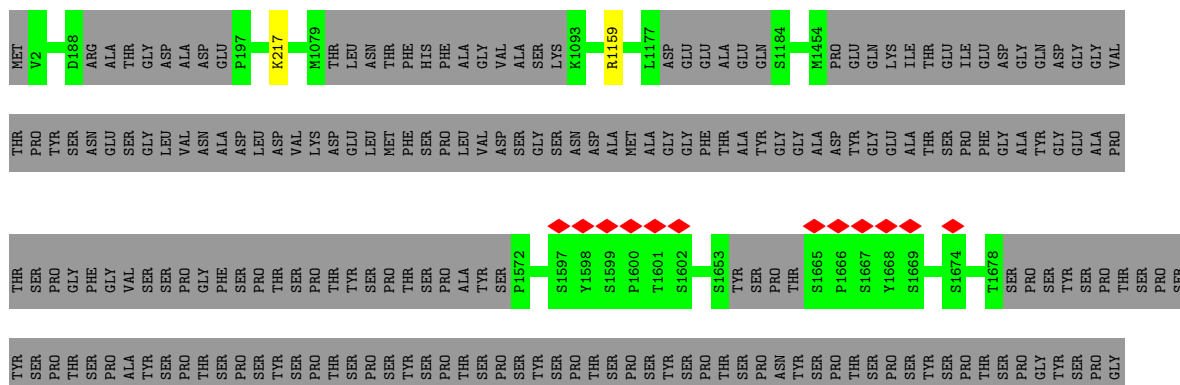
- Molecule 8: General transcription and DNA repair factor IIIH helicase subunit XPB

Chain 7: 7% 73% 27%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB1

Chain A: 87% 13%



SER
PRO
ALA
TYR
SER
PRO
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
GLU
ASN
SER
ARG


- Molecule 10: DNA-directed RNA polymerase II subunit RPB2

Chain B:  96%

MET
SER
SER
LEU
ASP
ALA
ASN
SER
GLU
LYS
TYR
TYR
ASP
GLU
ASP
PRO
TYR
GLY
F18
E157
ASP
SER
SER
GLU
SER
G163
E468
GLN
LYS
LYS
ALA
MET
SER
SER
R476
E502
GLY
ARG
ASP
G506
D568
I669
GLU
GLY
GLY
PHE
GLU
D675
E714
ALA
ASN
GLU
GLU
ASN
ASP

LEU
D722
M178
F1224


- Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C:  77%

MET
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
ASN
SER
GLY
LEU
ASN
ASP
ASP
ILE
PHE
GLY
ALA
GLN
LYS
LYS
ILE
GLU
TRP
HIS
GLU
ASP
THR
SER
S3
D268
LYS
VAL
ASN
PHE
ALA
SER
GLY
ASP
ASN
THR
ALA
SER
ASN
MET
LEU
GLY
SER
ASN
GLU
ASP
VAL
MET
MET
THR
GLY

ALA
GLU
GLN
ASP
PRO
TYR
SER
ASN
ALA
SER
GLN
MET
GLY
ASN
THR
GLY
SER
GLY
GLY
TYR
ASP
ASN
ALA
TRP

- Molecule 12: DNA-directed RNA polymerase II subunit RPB4

Chain D:  76%


MET
ASN
VAL
SER
THR
SER
THR
PHE
GLN
R11
S73
GLN
LYS
LYS
HIS
LYS
LYS
LYS
HIS
LYS
LYS
HIS
ASN
ALA
ASN
ASN
GLU
GLY
THR
THR
ALA
VAL
ASP
GLU
GLY
GLY
ASP
ASP
LEU
ASP
GLY
ASN
ASP
VAL
ASN
ALA
ASP
ASP
ASP
ASP
PHE
MET
HIS
SER
E117
L220
TYR

- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  100%

MET
D2
M215

- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

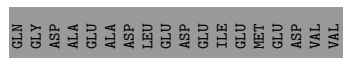
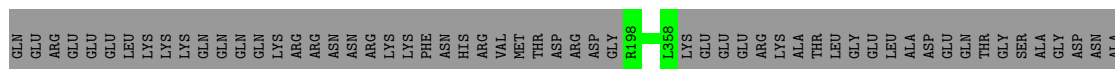
Chain F:  76%

MET
SER
TYR
GLU
ALA
PHE
ASN
ASP
GLY
H12
F18
D19
V20
E21
E35
LYS
ASP
GLY
GLU
THR
THR
ASP
ALA
ASN
ASN
GLY
LYS
THR
THR
ILE
VAL
THR
THR
GLY
GLY
ASN
GLY
PRO
GLU
ASP
PHE
GLN
GLN
HIS
E62
L155

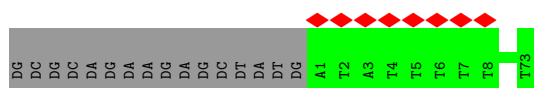
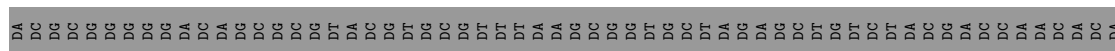
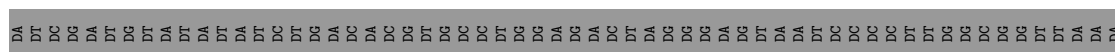
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:  95%

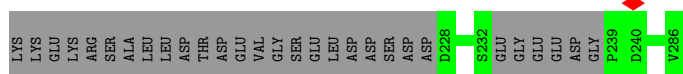
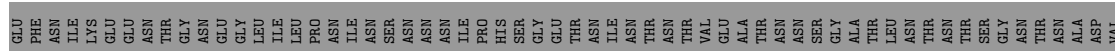
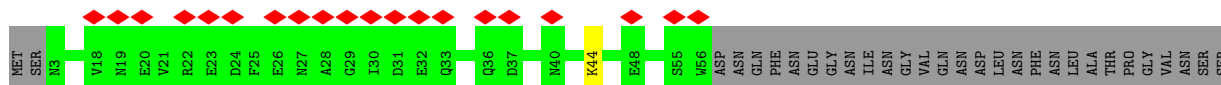
H1
Q96
K112
K114
HIS
HIS
HIS
HIS
HIS



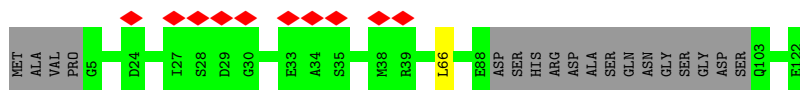
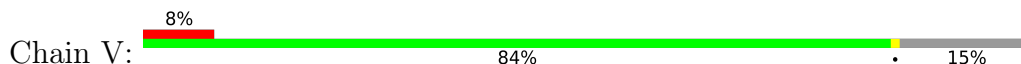
• Molecule 26: TEMPLATE DNA (209-MER)



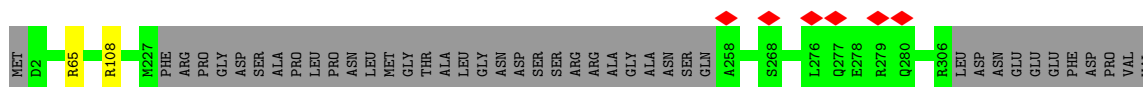
• Molecule 27: Transcription initiation factor IIA large subunit

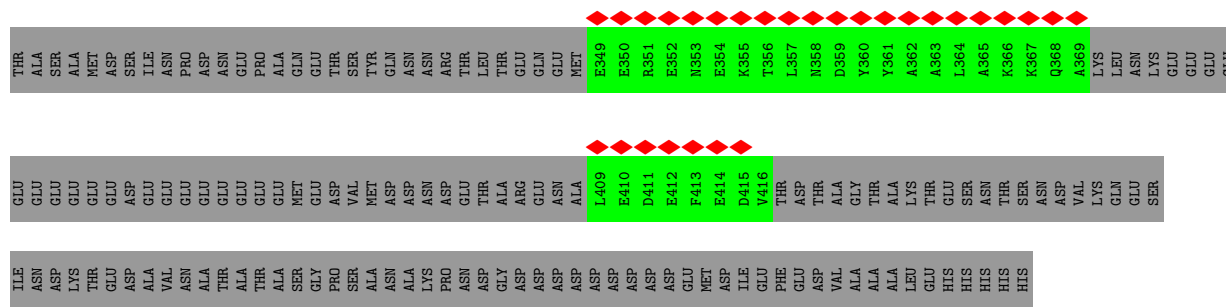


• Molecule 28: Transcription initiation factor IIA subunit 2

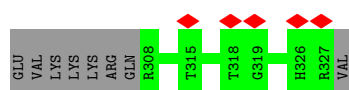
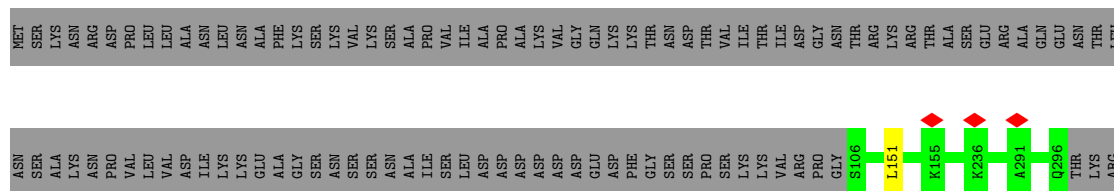


• Molecule 29: Transcription initiation factor IIE subunit alpha

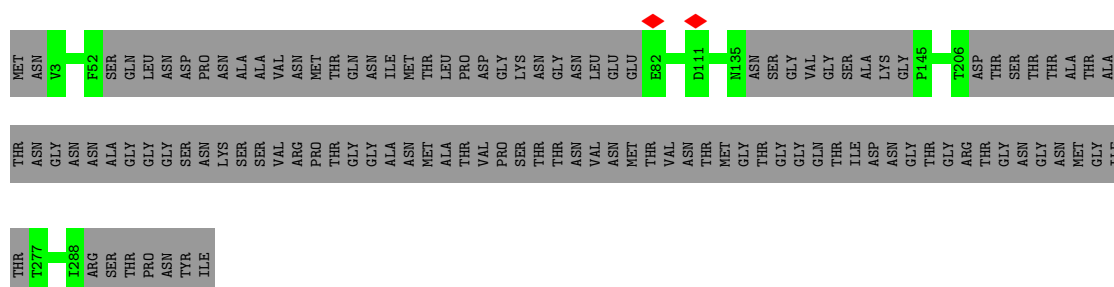




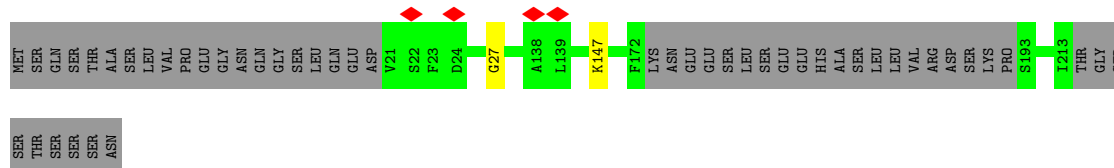
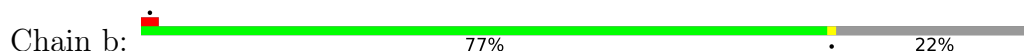
- Molecule 30: Transcription initiation factor IIE subunit beta



- Molecule 31: Mediator of RNA polymerase II transcription subunit 6

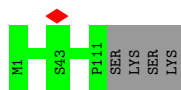


- Molecule 32: Mediator of RNA polymerase II transcription subunit 8

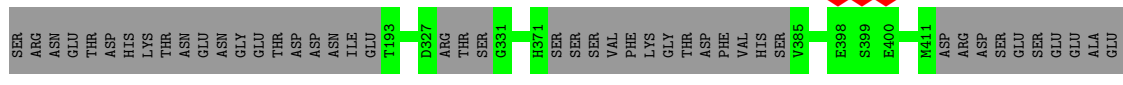
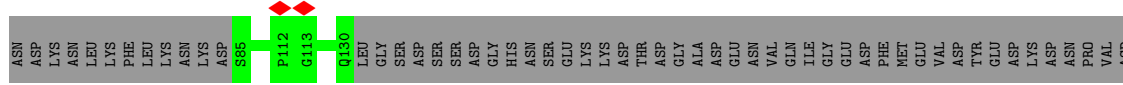
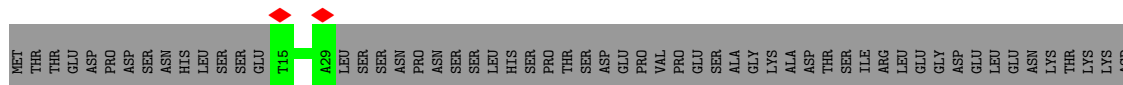


- Molecule 33: Mediator of RNA polymerase II transcription subunit 11

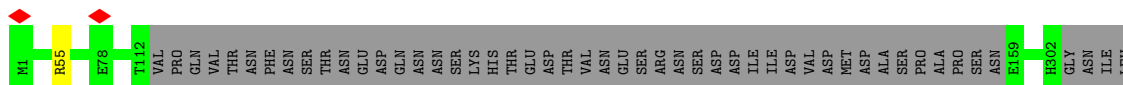
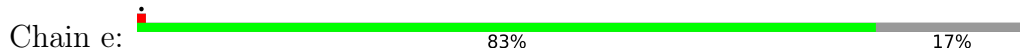




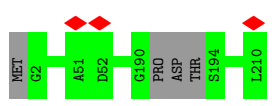
• Molecule 34: Mediator of RNA polymerase II transcription subunit 17



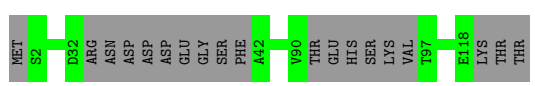
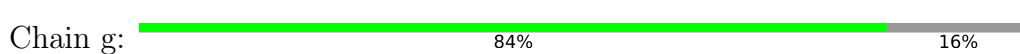
• Molecule 35: Mediator of RNA polymerase II transcription subunit 18



• Molecule 36: Mediator of RNA polymerase II transcription subunit 20

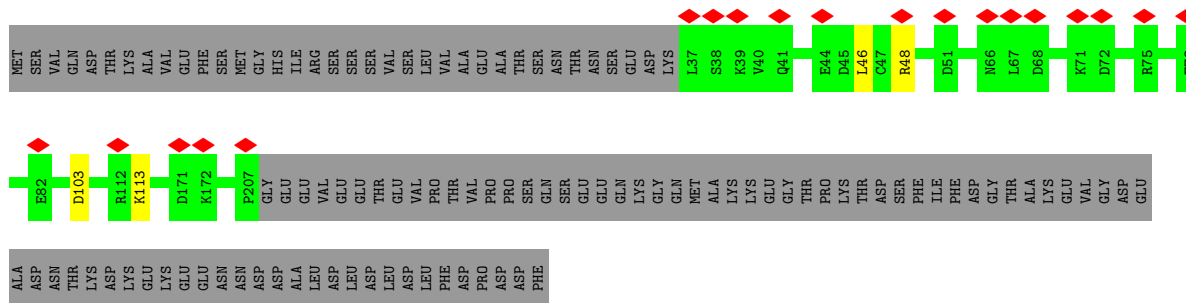


• Molecule 37: Mediator of RNA polymerase II transcription subunit 22

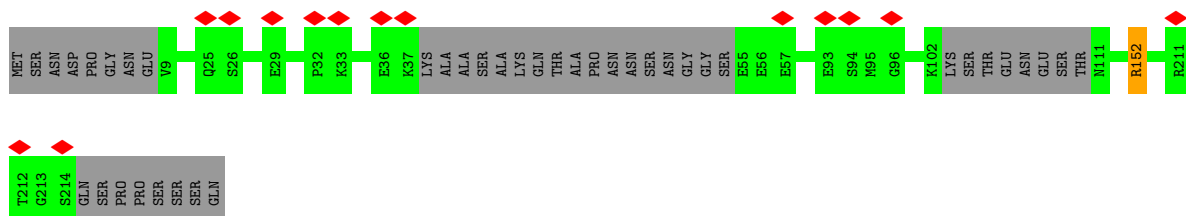
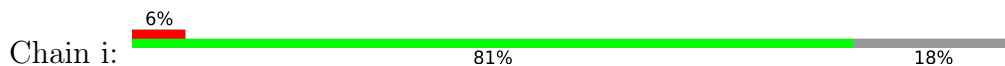


• Molecule 38: Mediator of RNA polymerase II transcription subunit 4

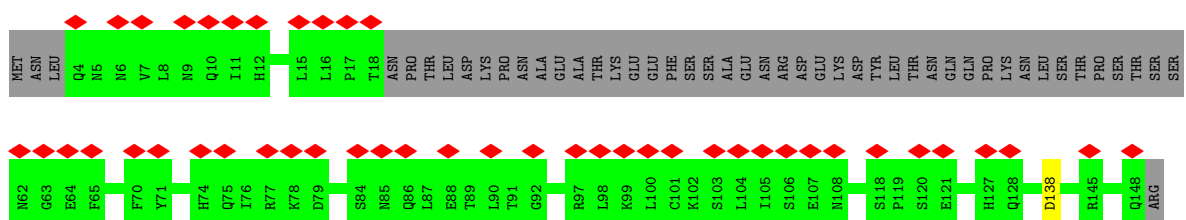




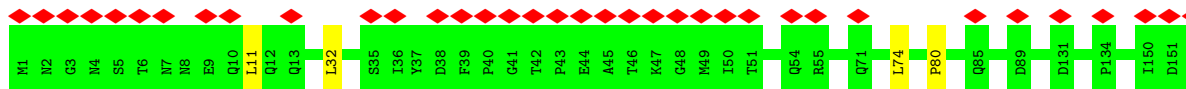
• Molecule 39: Mediator of RNA polymerase II transcription subunit 7



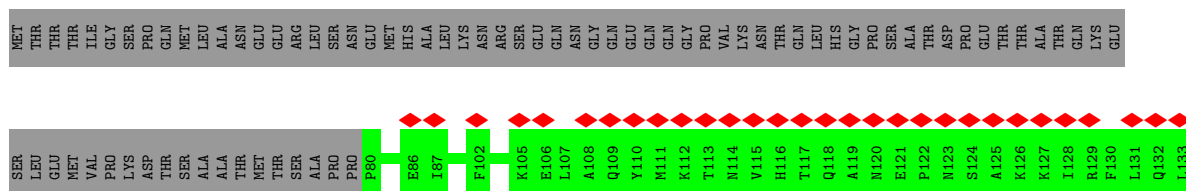
• Molecule 40: Mediator of RNA polymerase II transcription subunit 9



• Molecule 41: Mediator of RNA polymerase II transcription subunit 10



• Molecule 42: Mediator of RNA polymerase II transcription subunit 14



Y125	L126	L127	D128	A129	Y130	S131	HIS	ILE	GLU	SER	ASP	SER	THR	HIS	HIS	ASN	ASN	GLY	SER	SER	SER	ASP	LYS	SER	LEU	SER	SER	ALA	ASN	GLN	GLY	K161	L162	D163	L164	F165	K166	Y167	F168	T169	E170	L171	S172	H173	Y174	I175	R176	Q177	C178	F179	Q180	D181	N182	C183	C184				
D185	F186	K187	V188	R189	T190	N191	L192	N193	D194	K195	F196	G197	I198	Y199	I200	L201	T202	Q203	G204	I205	N206	G207	K208	E209	V210	P211	L212	A213	K214	I215	Y216	L217	E218	E219	N220	K221	S222	D223	S224	Q225	Y226	R227	F228	Y229	E230	Y231	I232	Y233	S234	Q235	E236	T237	K238	S239	W240	I241	N242	E243	S244
A245	E246	N247	F248	S249	N250	G251	I252	S253	L254	V255	M256	E257	I258	V259	ALA	ASN	ALA	LYS	GLU	SER	ASN	TYR	THR	ASP	LEU	ILE	TRP	PHE	PRO	GLU	ASP	ILE	E219	N220	K221	S222	D223	S224	Q225	Y226	R227	F228	Y229	E230	Y231	I232	Y233	S234	Q235	E236	T237	K238	S239	W240	I241	N242	E243	S244	
ASN	ASN	ASN	TYR	ASN	SER	ARG	ILE	GLN	MET	ASN	ASP	THR	LYS	LEU	ILE	ASN	ALA	LYS	LYS	PHE	GLU	ASN	TYR	ASP	LEU	ASP	TRP	PRO	GLU	VAL	TRP	SER	ARG	LYS	VAL	THR	CYS	SER	VAL	ASN	ASN	SER	SER	SER	PRO	PRO	ILE	ASP	LEU	PHE	SER								
ASN	SER	ASN	SER	GLU	LEU	GLU	PRO	TYR	GLN	ALA	PRO	PHE	THR	THR	LYS	THR	ILE	LYS	ASP	ASN	LYS	GLU	THR	THR	ILE	PRO	ARG	ILE	GLU	VAL	TRP	SER	ARG	VAL	ARG	THR	ARG	ASN	VAL	THR	ASN	LYS	LEU	VAL	LYS	THR	ARG	PRO	SER	ILE									
THR	GLU	ALA	MET	ASP	HIS	GLY	GLN	GLN	THR	PHE	ASN	LEU	HIS	GLY	THR	ILE	LEU	SER	ALA	GLU	PRO	ASP	ALA	THR	ILE	GLU	GLU	ASN	GLY	ASP	ILE	THR	GLY	HIS	ASN	ARG	THR	THR	THR	GLY	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR							
ASP	ILE	VAL	MET	GLU	ASP	HIS	GLY	VAL	LEU	THR	GLN	ASN	TYR	GLY	THR	ALA	ALA	THR	ASP	ILE	GLU	GLU	MET	LYS	ASP	VAL	SER	ILE	SER	PRO	LYS	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR						
CYS	ASN	LEU	TYR	ASP	ASP	VAL	LYS	CYS	TRP	SER	THR	PHE	ILE	GLU	LYS	PHE	GLN	GLY	THR	ASP	ILE	VAL	SER																																				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186599	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0	0.27	0/6209	0.57	0/8384
2	1	0.26	0/4277	0.53	0/5755
3	2	0.28	0/3717	0.56	0/5028
4	3	0.27	0/1109	0.53	0/1492
5	4	0.28	0/2377	0.54	0/3216
6	5	0.27	0/520	0.60	0/701
7	6	0.27	0/3082	0.55	1/4165 (0.0%)
8	7	0.27	0/5059	0.55	1/6841 (0.0%)
9	A	0.28	0/12048	0.54	0/16321
10	B	0.28	0/9589	0.55	1/12934 (0.0%)
11	C	0.28	0/2130	0.51	0/2887
12	D	0.28	0/1351	0.60	0/1811
13	E	0.27	0/1788	0.55	0/2406
14	F	0.28	0/1001	0.55	0/1347
15	G	0.28	0/1367	0.53	0/1844
16	H	0.26	0/1139	0.55	0/1544
17	I	0.28	0/962	0.61	0/1295
18	J	0.30	0/578	0.61	0/775
19	K	0.27	0/942	0.54	0/1272
20	L	0.25	0/361	0.63	0/478
21	M	0.27	0/2408	0.54	0/3241
22	N	0.55	0/1677	0.95	0/2587
23	O	0.27	0/1449	0.57	0/1952
24	Q	0.27	0/1907	0.60	1/2556 (0.0%)
25	R	0.25	0/2270	0.56	0/3052
26	T	0.53	0/1676	0.95	0/2584
27	U	0.28	0/898	0.63	0/1212
28	V	0.28	0/822	0.61	1/1109 (0.1%)
29	W	0.28	0/2513	0.57	0/3388
30	X	0.26	0/1739	0.59	1/2339 (0.0%)
31	a	0.29	0/1531	0.56	0/2072
32	b	0.27	0/1443	0.58	0/1957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.27	0/913	0.59	0/1228
34	d	0.27	0/4118	0.55	0/5532
35	e	0.26	0/2054	0.54	0/2782
36	f	0.28	0/1602	0.57	0/2169
37	g	0.25	0/818	0.54	0/1104
38	h	0.29	0/1415	0.66	2/1907 (0.1%)
39	i	0.27	0/1543	0.54	1/2084 (0.0%)
40	j	0.26	0/865	0.67	1/1166 (0.1%)
41	k	0.31	0/1277	0.75	5/1727 (0.3%)
42	l	0.27	0/4468	0.58	0/6048
43	m	0.32	0/1093	0.70	1/1481 (0.1%)
44	n	0.30	0/1106	0.61	2/1488 (0.1%)
45	o	0.28	0/949	0.48	0/1294
46	p	0.37	1/1898 (0.1%)	0.74	3/2559 (0.1%)
All	All	0.29	1/104058 (0.0%)	0.59	21/141114 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	p	211	PRO	CG-CD	-10.57	1.15	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	p	211	PRO	N-CD-CG	-16.42	78.57	103.20
46	p	211	PRO	CA-CB-CG	-14.02	77.37	104.00
8	7	106	PRO	CA-N-CD	-8.05	100.23	111.50
41	k	11	LEU	CA-CB-CG	7.94	133.55	115.30
41	k	32	LEU	CA-CB-CG	7.92	133.52	115.30
41	k	80	PRO	CA-N-CD	-7.43	101.10	111.50
10	B	568	ASP	CB-CG-OD1	7.34	124.91	118.30
30	X	151	LEU	CA-CB-CG	7.08	131.59	115.30
43	m	93	LEU	CA-CB-CG	6.33	129.85	115.30
38	h	46	LEU	CA-CB-CG	6.32	129.83	115.30
41	k	74	LEU	CA-CB-CG	5.80	128.65	115.30
40	j	138	ASP	CB-CG-OD1	5.79	123.51	118.30
28	V	66	LEU	CA-CB-CG	5.73	128.47	115.30
38	h	103	ASP	CB-CG-OD1	5.68	123.41	118.30
44	n	13	ASP	CB-CG-OD1	5.52	123.27	118.30
44	n	44	ASP	CB-CG-OD1	5.52	123.27	118.30
46	p	211	PRO	CA-N-CD	-5.26	104.14	111.50
39	i	152	ARG	CA-CB-CG	5.17	124.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	143	ASP	CB-CG-OD1	5.16	122.94	118.30
7	6	384	MET	CA-CB-CG	5.08	121.93	113.30
41	k	11	LEU	CB-CG-CD2	5.02	119.54	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100
2	1	508/642 (79%)	502 (99%)	6 (1%)	0	100	100
3	2	448/513 (87%)	441 (98%)	7 (2%)	0	100	100
4	3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
5	4	298/338 (88%)	289 (97%)	9 (3%)	0	100	100
6	5	63/72 (88%)	60 (95%)	3 (5%)	0	100	100
7	6	379/461 (82%)	366 (97%)	13 (3%)	0	100	100
8	7	609/843 (72%)	585 (96%)	24 (4%)	0	100	100
9	A	1494/1733 (86%)	1443 (97%)	51 (3%)	0	100	100
10	B	1168/1224 (95%)	1130 (97%)	38 (3%)	0	100	100
11	C	264/347 (76%)	257 (97%)	7 (3%)	0	100	100
12	D	163/221 (74%)	159 (98%)	4 (2%)	0	100	100
13	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	F	114/155 (74%)	108 (95%)	6 (5%)	0	100	100
15	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
20	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	168 (94%)	11 (6%)	0	100	100
24	Q	215/735 (29%)	208 (97%)	7 (3%)	0	100	100
25	R	264/400 (66%)	259 (98%)	5 (2%)	0	100	100
27	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100
28	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
29	W	296/492 (60%)	290 (98%)	6 (2%)	0	100	100
30	X	207/328 (63%)	197 (95%)	10 (5%)	0	100	100
31	a	170/295 (58%)	163 (96%)	7 (4%)	0	100	100
32	b	169/223 (76%)	163 (96%)	5 (3%)	1 (1%)	25	64
33	c	109/115 (95%)	107 (98%)	2 (2%)	0	100	100
34	d	481/687 (70%)	470 (98%)	11 (2%)	0	100	100
35	e	252/307 (82%)	246 (98%)	6 (2%)	0	100	100
36	f	202/210 (96%)	196 (97%)	6 (3%)	0	100	100
37	g	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
38	h	169/284 (60%)	166 (98%)	3 (2%)	0	100	100
39	i	175/222 (79%)	173 (99%)	2 (1%)	0	100	100
40	j	98/149 (66%)	94 (96%)	4 (4%)	0	100	100
41	k	155/157 (99%)	152 (98%)	3 (2%)	0	100	100
42	l	521/745 (70%)	506 (97%)	14 (3%)	1 (0%)	47	82
43	m	126/220 (57%)	122 (97%)	4 (3%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	107 (99%)	1 (1%)	0	100	100
46	p	221/566 (39%)	210 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12095/16091 (75%)	11739 (97%)	354 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	b	27	GLY
42	l	648	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	684/707 (97%)	683 (100%)	1 (0%)	93	98
2	1	483/589 (82%)	481 (100%)	2 (0%)	91	97
3	2	414/468 (88%)	414 (100%)	0	100	100
4	3	125/303 (41%)	125 (100%)	0	100	100
5	4	267/300 (89%)	265 (99%)	2 (1%)	84	94
6	5	59/66 (89%)	58 (98%)	1 (2%)	60	85
7	6	346/418 (83%)	345 (100%)	1 (0%)	92	97
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1330/1520 (88%)	1328 (100%)	2 (0%)	93	98
10	B	1024/1061 (96%)	1023 (100%)	1 (0%)	93	98
11	C	234/299 (78%)	234 (100%)	0	100	100
12	D	149/200 (74%)	149 (100%)	0	100	100
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	108/137 (79%)	108 (100%)	0	100	100
15	G	152/158 (96%)	150 (99%)	2 (1%)	69	89
16	H	123/128 (96%)	122 (99%)	1 (1%)	81	93
17	I	110/116 (95%)	110 (100%)	0	100	100
18	J	64/65 (98%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	K	99/102 (97%)	99 (100%)	0	100	100
20	L	40/57 (70%)	40 (100%)	0	100	100
21	M	267/306 (87%)	267 (100%)	0	100	100
23	O	153/205 (75%)	153 (100%)	0	100	100
24	Q	204/641 (32%)	202 (99%)	2 (1%)	76	91
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	98 (99%)	1 (1%)	76	91
28	V	94/108 (87%)	94 (100%)	0	100	100
29	W	275/436 (63%)	273 (99%)	2 (1%)	84	94
30	X	193/295 (65%)	193 (100%)	0	100	100
31	a	170/259 (66%)	170 (100%)	0	100	100
32	b	162/207 (78%)	161 (99%)	1 (1%)	86	95
33	c	104/108 (96%)	104 (100%)	0	100	100
34	d	469/642 (73%)	469 (100%)	0	100	100
35	e	232/280 (83%)	231 (100%)	1 (0%)	91	97
36	f	174/178 (98%)	174 (100%)	0	100	100
37	g	95/113 (84%)	95 (100%)	0	100	100
38	h	158/258 (61%)	156 (99%)	2 (1%)	69	89
39	i	174/208 (84%)	173 (99%)	1 (1%)	86	95
40	j	100/144 (69%)	100 (100%)	0	100	100
41	k	145/145 (100%)	145 (100%)	0	100	100
42	l	505/688 (73%)	504 (100%)	1 (0%)	93	98
43	m	119/195 (61%)	117 (98%)	2 (2%)	60	85
44	n	128/132 (97%)	128 (100%)	0	100	100
45	o	103/117 (88%)	103 (100%)	0	100	100
46	p	212/528 (40%)	211 (100%)	1 (0%)	88	96
All	All	11141/14444 (77%)	11114 (100%)	27 (0%)	93	98

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	228	LYS
2	1	94	ARG

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Mol	Chain	Res	Type
2	1	105	GLN
5	4	117	ARG
5	4	119	ARG
6	5	5	ARG
7	6	207	ASN
9	A	217	LYS
9	A	1159	ARG
10	B	1178	ASN
15	G	96	GLN
15	G	112	LYS
16	H	130	ARG
24	Q	145	ARG
24	Q	369	ASN
27	U	44	LYS
29	W	65	ARG
29	W	108	ARG
32	b	147	LYS
35	e	55	ARG
38	h	48	ARG
38	h	113	LYS
39	i	152	ARG
42	l	581	LYS
43	m	67	GLN
43	m	95	GLN
46	p	211	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	468	GLN
3	2	395	GLN
8	7	584	ASN
9	A	171	GLN
9	A	316	GLN
10	B	1013	ASN
10	B	1093	GLN
24	Q	140	HIS
25	R	43	ASN
34	d	255	ASN
40	j	148	GLN
43	m	67	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
47	SF4	0	801	1	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
47	SF4	0	801	1	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1614:PRO	C	1629:THR	N	23.05

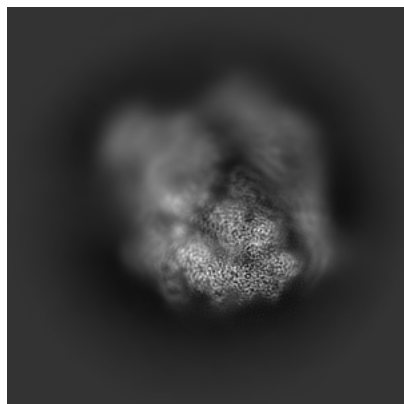
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16610. These allow visual inspection of the internal detail of the map and identification of artifacts.

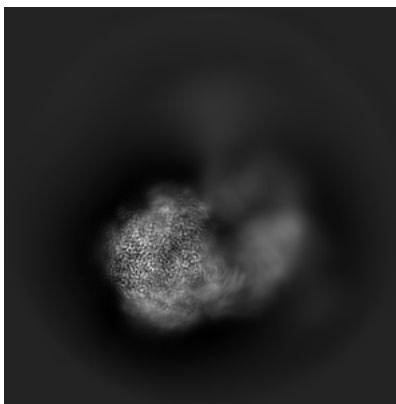
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

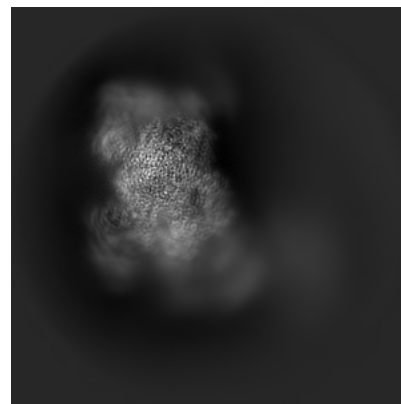
6.1.1 Primary map



X

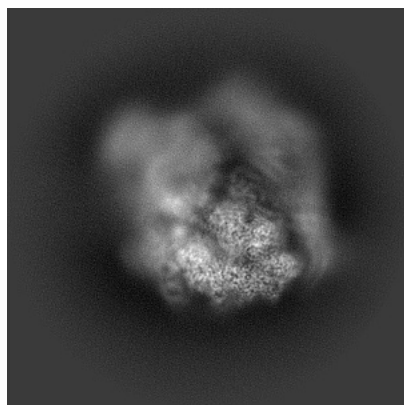


Y

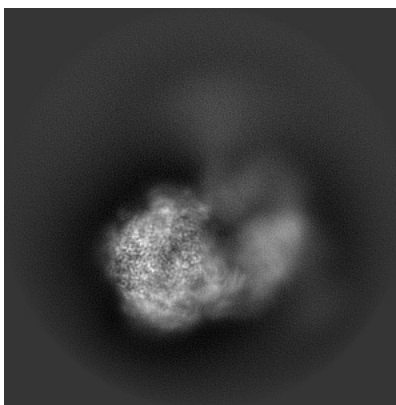


Z

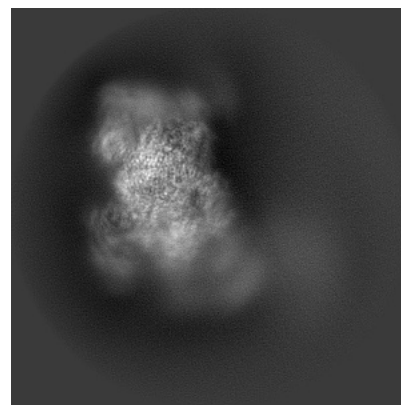
6.1.2 Raw map



X



Y



Z

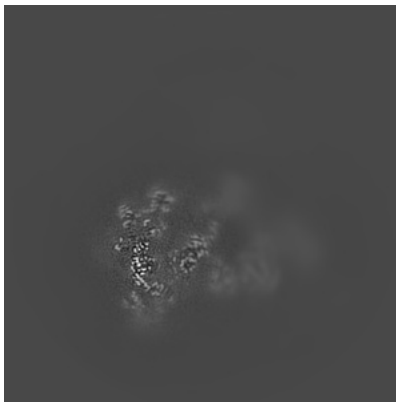
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

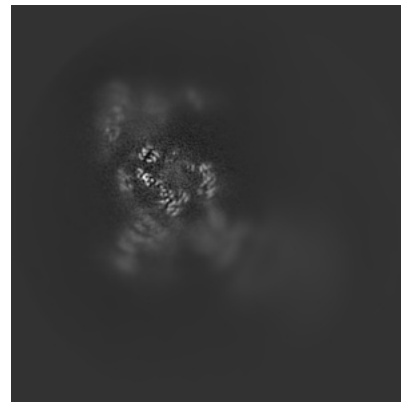
6.2.1 Primary map



X Index: 200

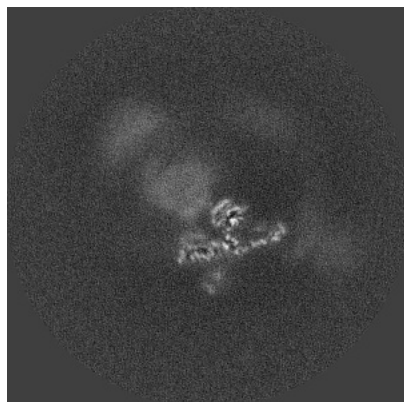


Y Index: 200

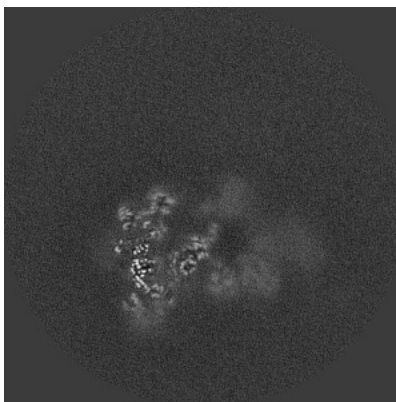


Z Index: 200

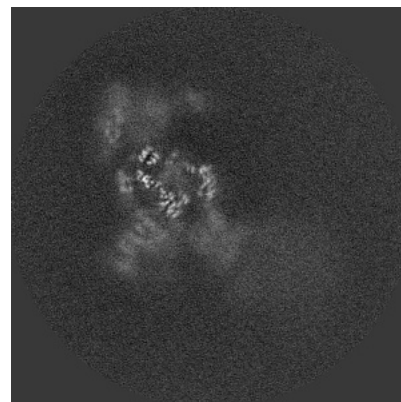
6.2.2 Raw map



X Index: 200



Y Index: 200

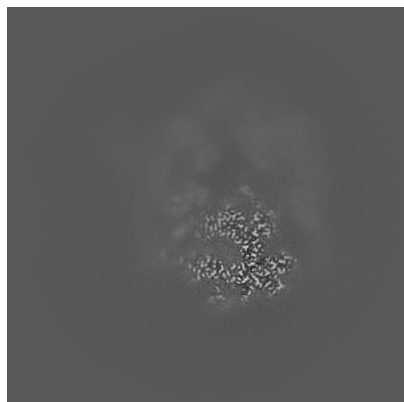


Z Index: 200

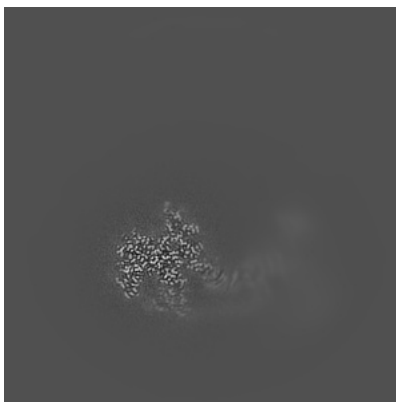
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

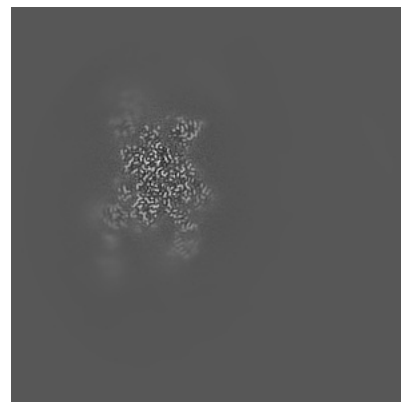
6.3.1 Primary map



X Index: 145

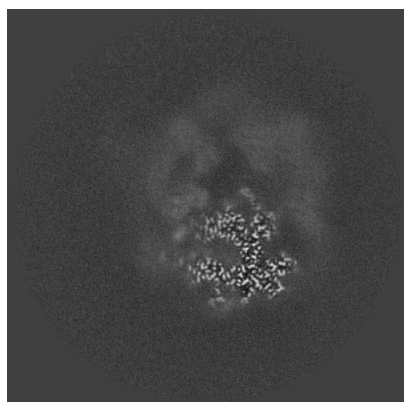


Y Index: 248

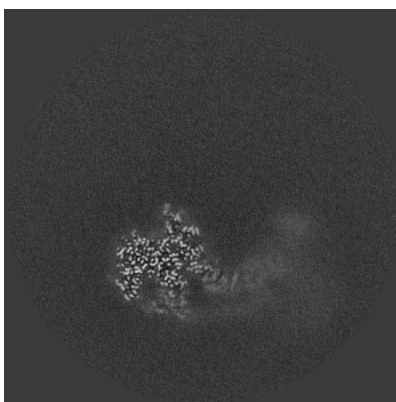


Z Index: 133

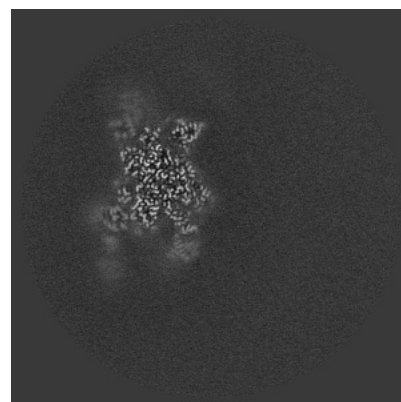
6.3.2 Raw map



X Index: 145



Y Index: 248

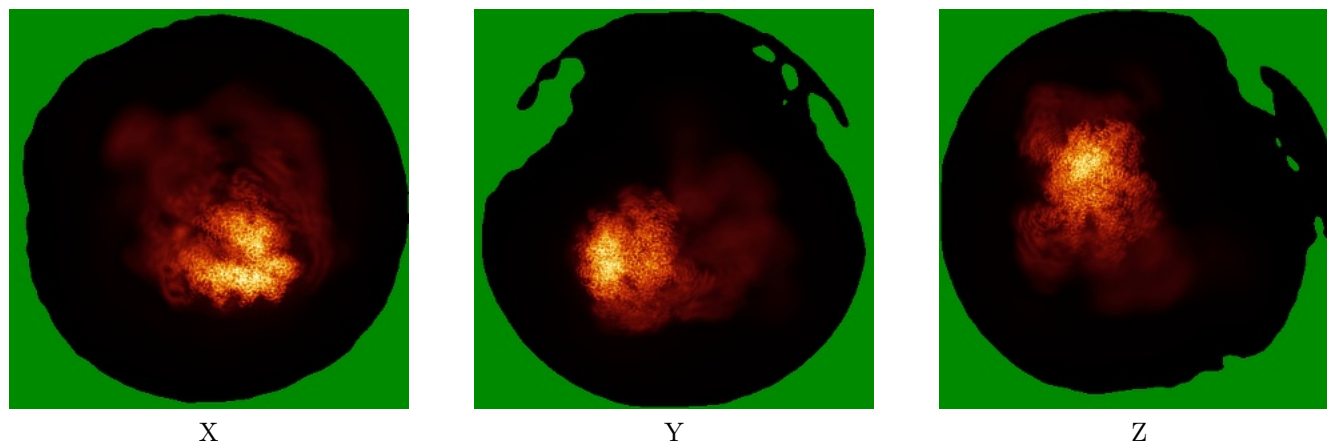


Z Index: 133

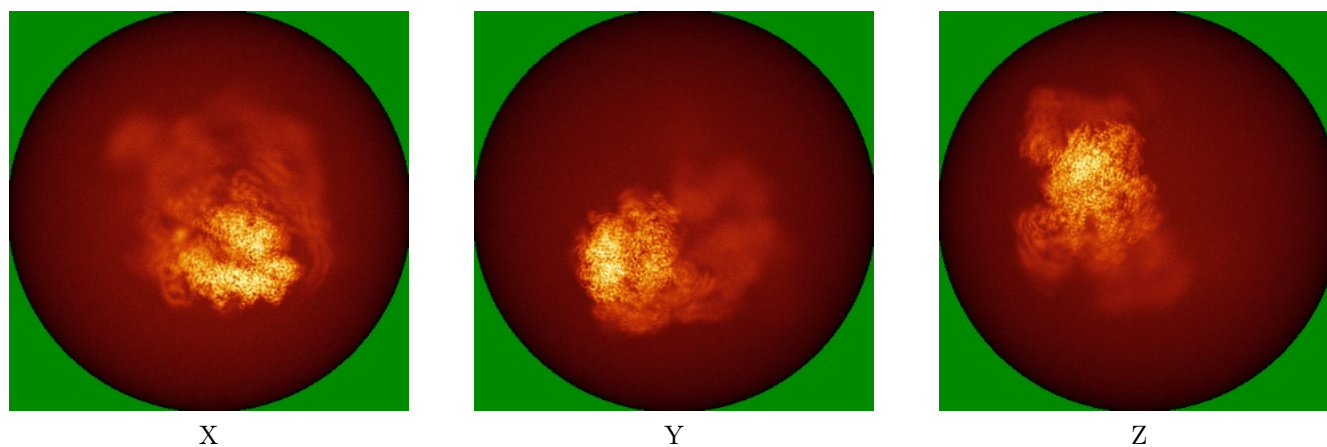
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



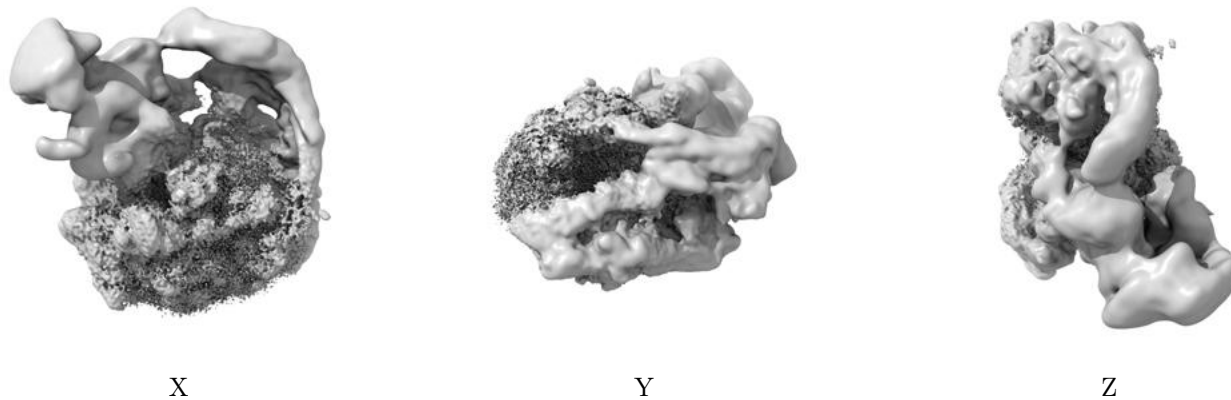
6.4.2 Raw map



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.

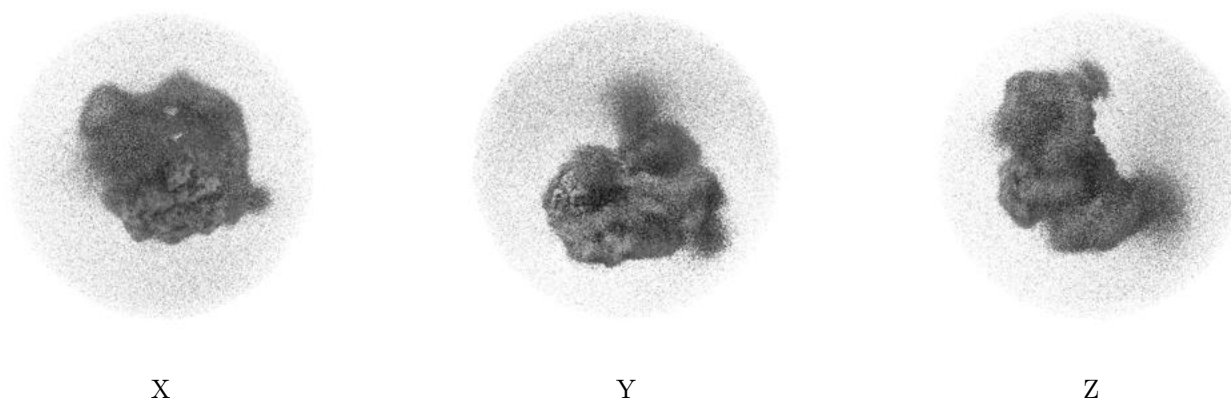
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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



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.

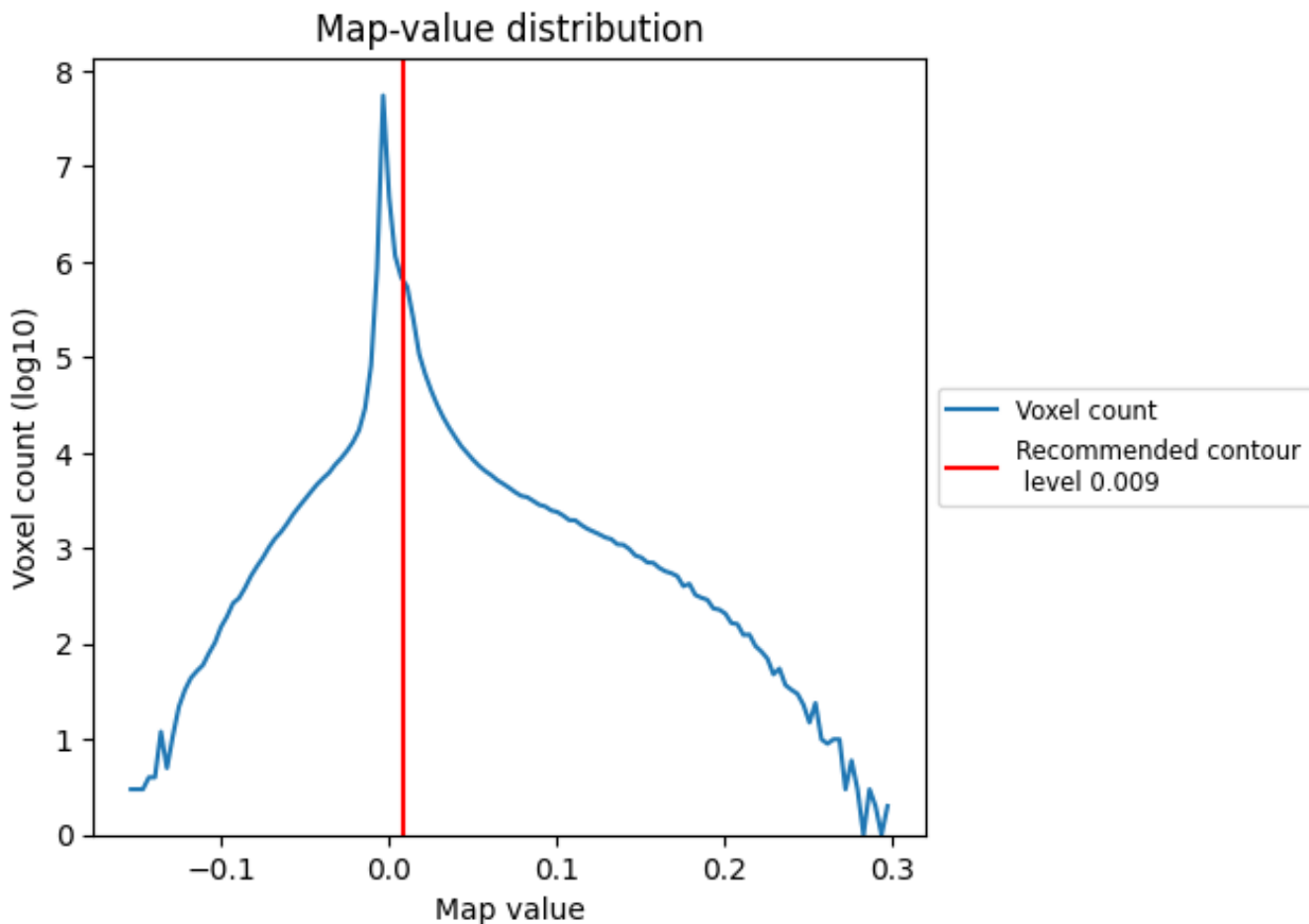
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

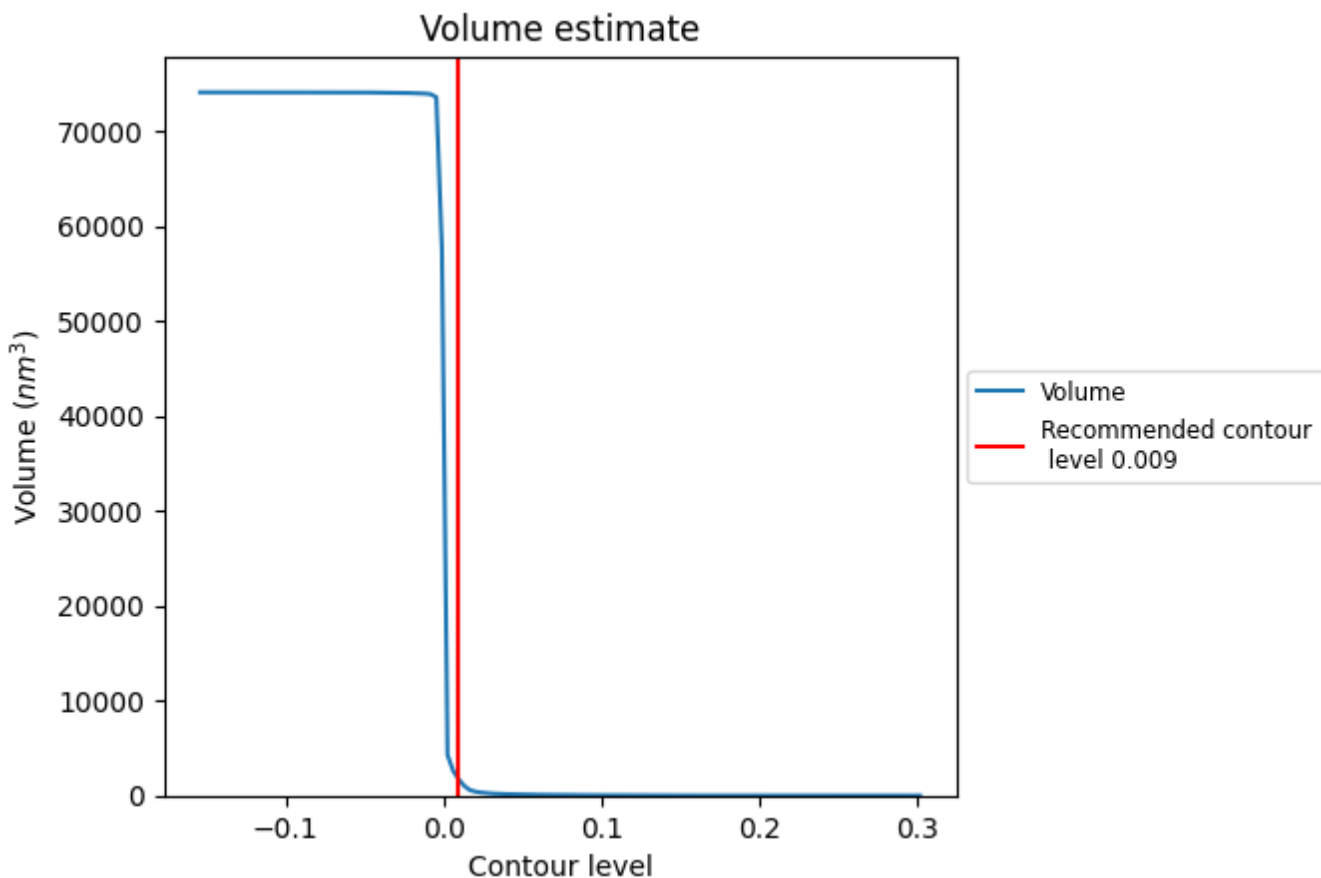
This section contains the results of statistical analysis of the map.

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.

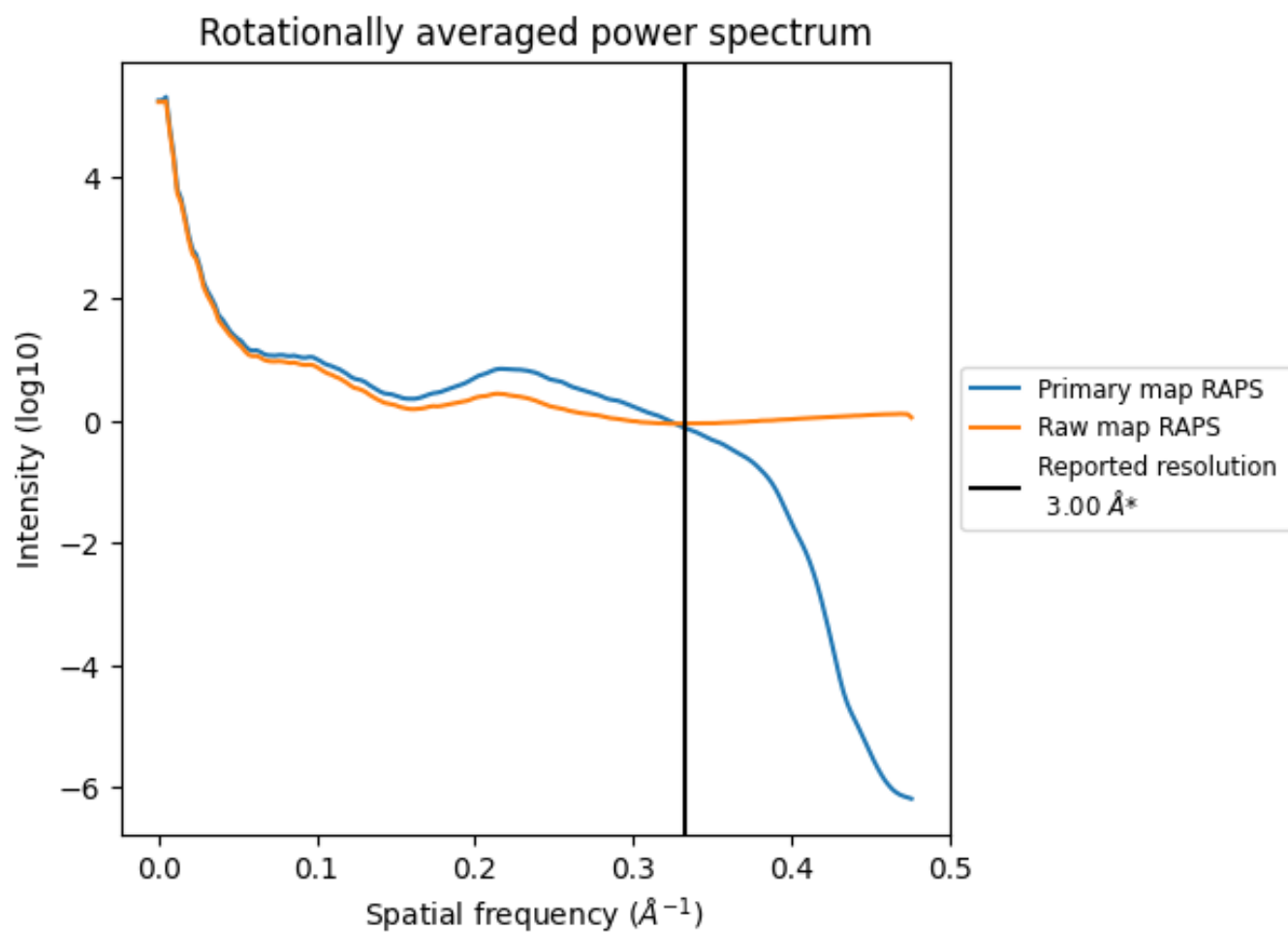
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1864 nm³; this corresponds to an approximate mass of 1684 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

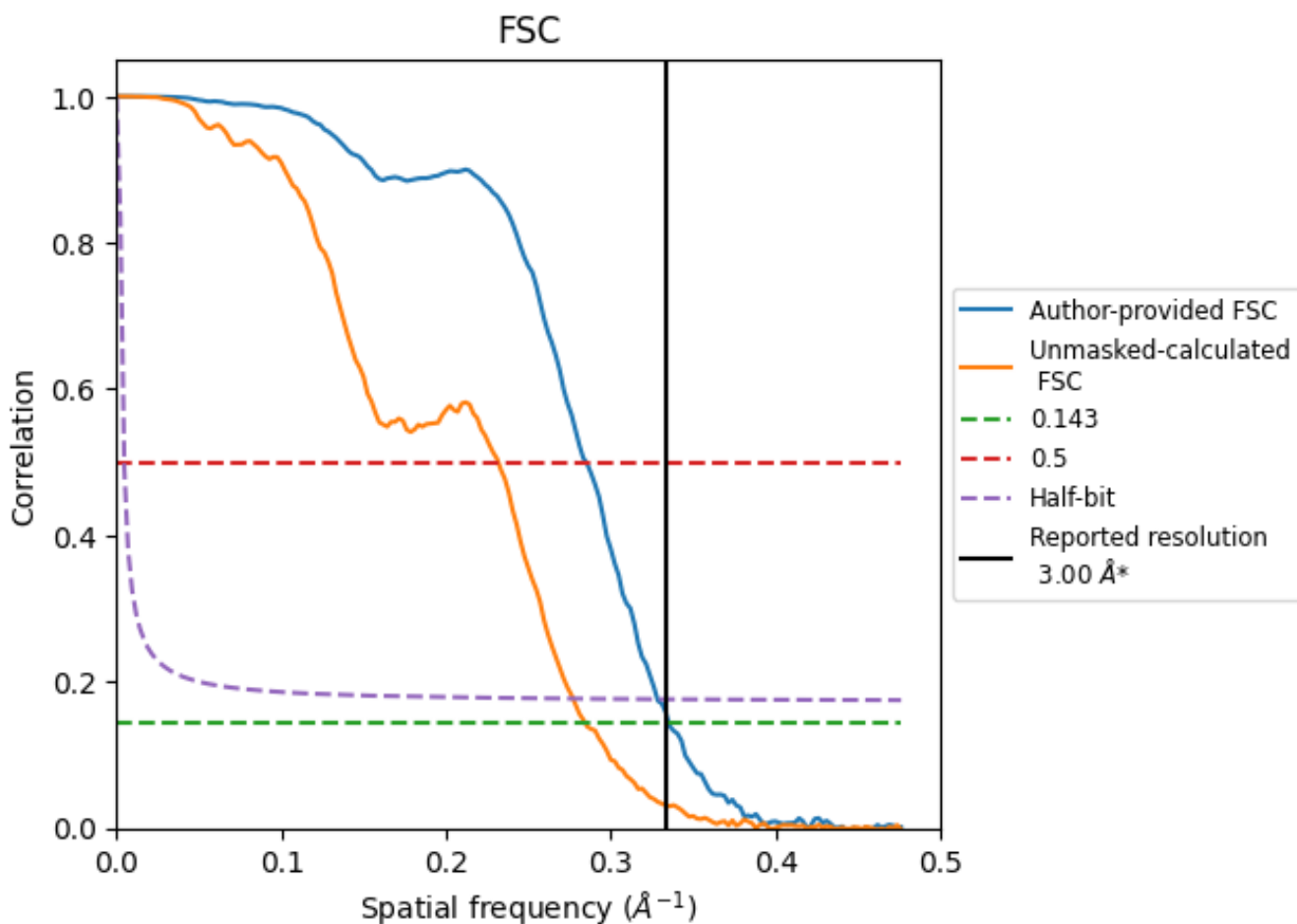


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333\AA^{-1}

8.2 Resolution estimates [i](#)

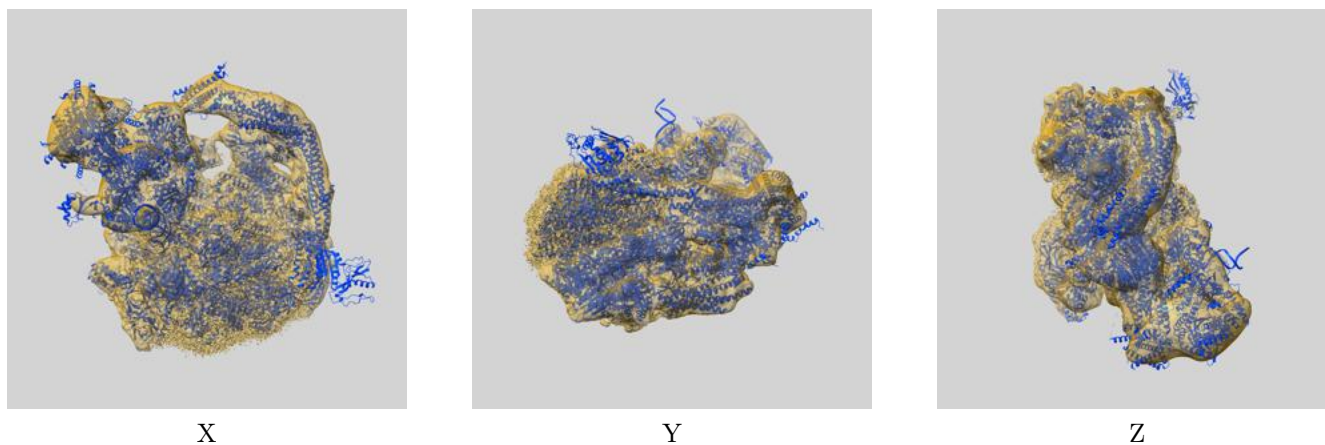
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.51	3.05
Unmasked-calculated*	3.51	4.32	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

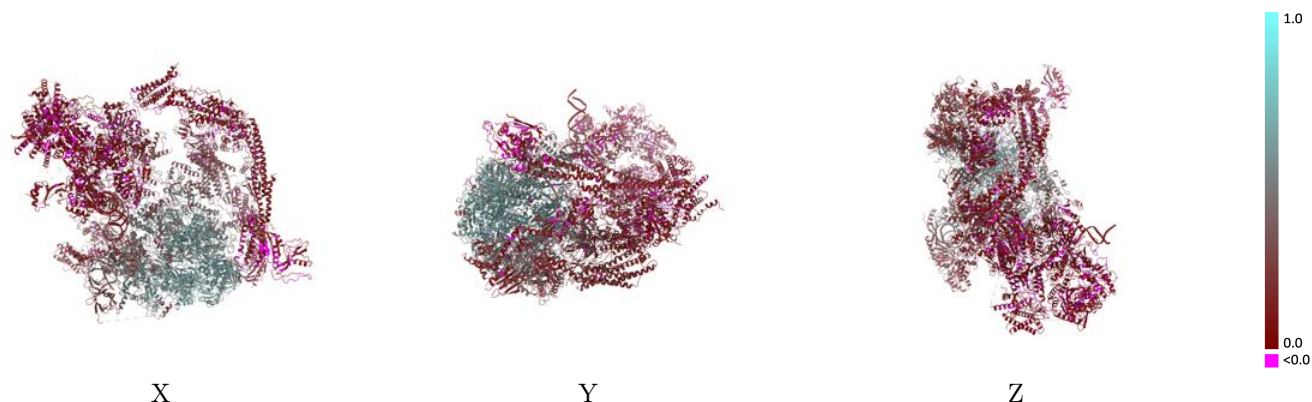
This section contains information regarding the fit between EMDB map EMD-16610 and PDB model 8CEN. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



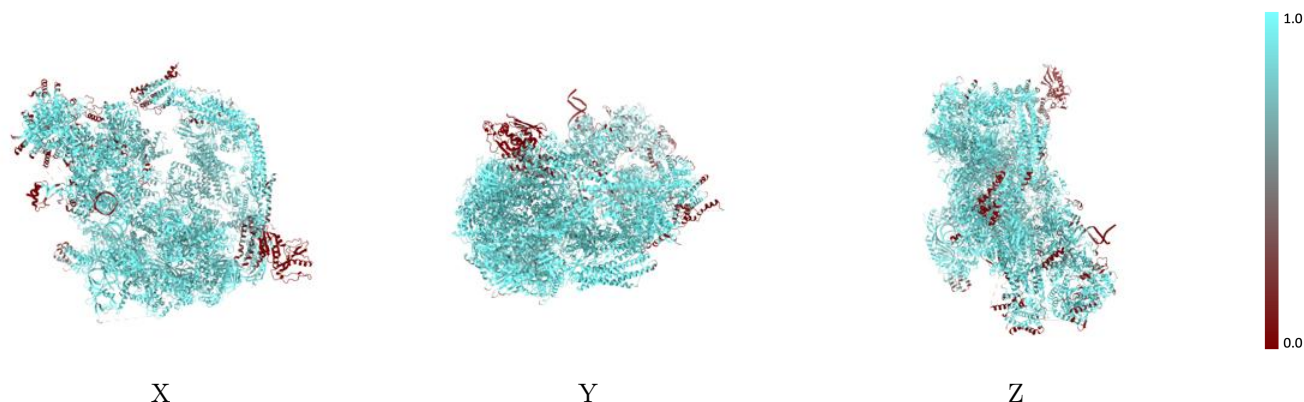
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



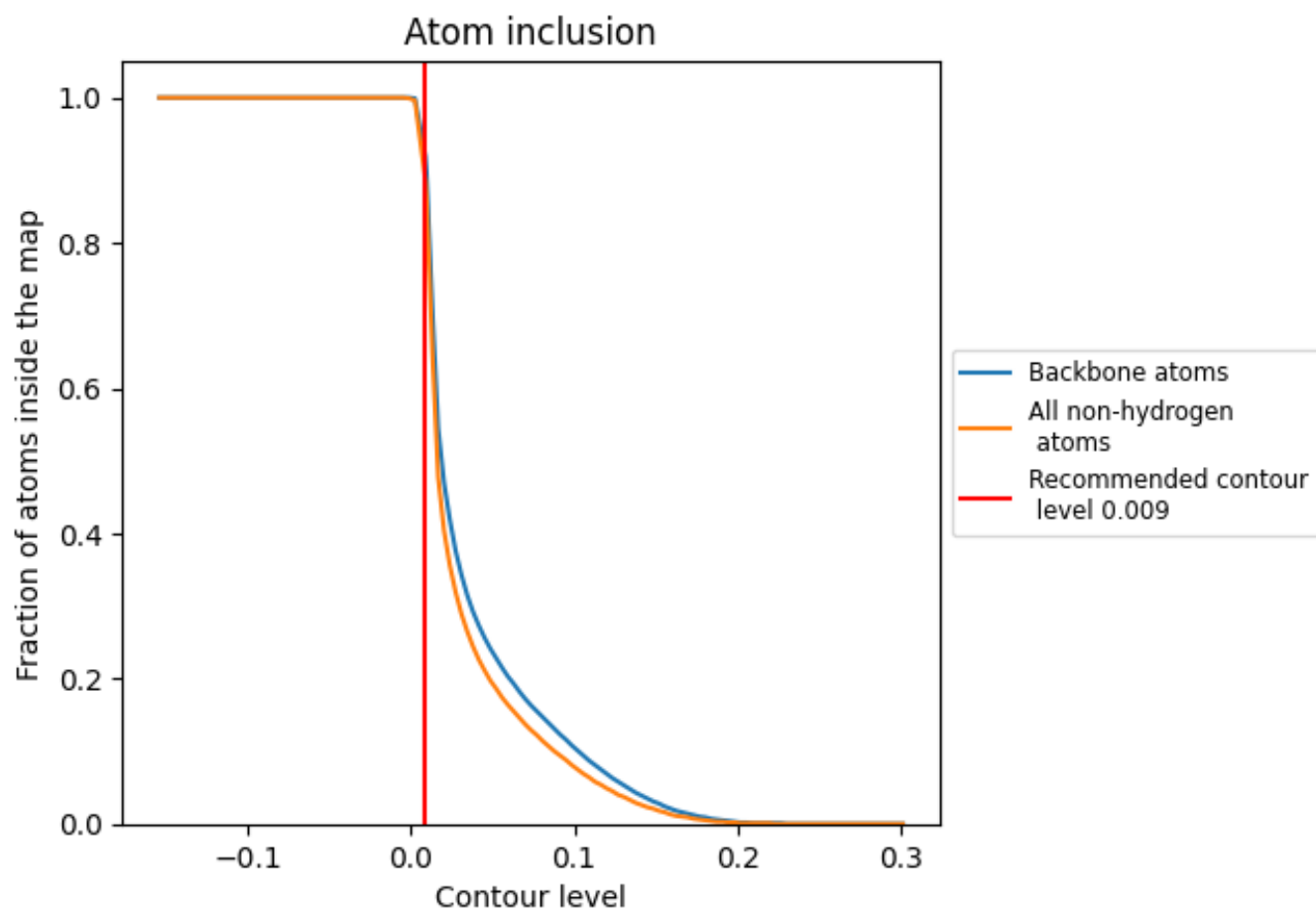
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.2690
0	 0.9110	 0.1000
1	 0.7380	 0.0770
2	 0.7750	 0.0740
3	 0.9280	 0.1710
4	 0.8560	 0.0600
5	 0.6250	 0.0530
6	 0.8420	 0.0690
7	 0.8850	 0.0880
A	 0.9700	 0.5110
B	 0.9810	 0.5560
C	 0.9810	 0.5870
D	 0.9060	 0.2590
E	 0.9770	 0.4580
F	 0.8920	 0.4250
G	 0.9560	 0.3940
H	 0.9770	 0.5400
I	 0.9700	 0.4300
J	 0.9840	 0.5910
K	 0.9860	 0.6000
L	 0.9860	 0.5190
M	 0.9510	 0.4190
N	 0.8850	 0.2060
O	 0.9740	 0.2610
Q	 0.9500	 0.3050
R	 0.9700	 0.2540
T	 0.8720	 0.2020
U	 0.7770	 0.1330
V	 0.8540	 0.1470
W	 0.8560	 0.1750
X	 0.9280	 0.1670
a	 0.9370	 0.1280
b	 0.9230	 0.1850
c	 0.9600	 0.2130
d	 0.9460	 0.1830



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Chain	Atom inclusion	Q-score
e	 0.9380	 0.4110
f	 0.9320	 0.4000
g	 0.9650	 0.1930
h	 0.8090	 0.1300
i	 0.9070	 0.1280
j	 0.4600	 0.0860
k	 0.7230	 0.0910
l	 0.8690	 0.1220
m	 0.4290	 0.0590
n	 0.8320	 0.1050
o	 0.9170	 0.1230
p	 0.0380	 0.0530