wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 09:33 am BST

PDB ID	:	7O4L
EMDB ID	:	EMD-12722
Title	:	Yeast TFIIH in the expanded state within the pre-initiation complex
Authors	:	Schilbach, S.; Aibara, S.; Dienemann, C.; Grabbe, F.; Cramer, P.
Deposited on	:	2021-04-06
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:

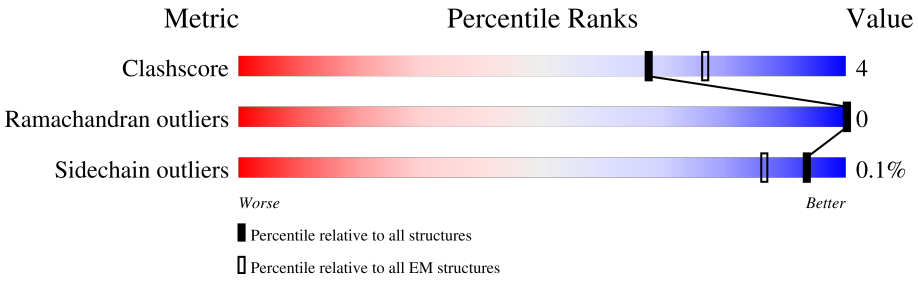
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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)
Clashscore	158937	4297
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 <=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	87% 10%
2	1	645	6% 76% 5% 19%
3	2	517	19% 76% 10% 14%
4	3	324	36% 60%
5	4	341	80% 6% 14%
6	5	76	32% 75% 11% 14%
7	6	464	9% 72% 9% 19%
8	7	843	62% 10% 28%

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Mol	Chain	Length	Quality of chain
9	A	1733	12% 87%
10	B	1224	6% 93%
11	D	221	66% 7% 27%
12	F	155	10% 33% 65%
13	G	177	85% 12%
14	N	106	9% 91%
15	T	106	8% 91%
16	W	492	9% 56% 7% 37%
17	X	328	38% 59%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 35159 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 IIH helicase subunit XPD.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	521	Total	C	N	O	S	0	0
			4206	2654	733	797	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-2	GLY	-	expression tag	UNP P32776
1	-1	GLY	-	expression tag	UNP P32776
1	0	SER	-	expression tag	UNP P32776

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	GLY	-	expression tag	UNP Q02939
2	-2	PRO	-	expression tag	UNP Q02939
2	-1	GLY	-	expression tag	UNP Q02939
2	0	SER	-	expression tag	UNP Q02939

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-2	GLY	-	expression tag	UNP Q03290
3	-1	PRO	-	expression tag	UNP Q03290
3	0	HIS	-	expression tag	UNP Q03290

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-2	SER	-	expression tag	UNP Q12004
4	-1	ASN	-	expression tag	UNP Q12004
4	0	ALA	-	expression tag	UNP Q12004

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	-3	GLY	-	expression tag	UNP Q3E7C1
5	-2	PRO	-	expression tag	UNP Q3E7C1
5	-1	GLY	-	expression tag	UNP Q3E7C1
5	0	SER	-	expression tag	UNP Q3E7C1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	-2	GLY	-	expression tag	UNP Q04673
6	-1	GLY	-	expression tag	UNP Q04673
6	0	SER	-	expression tag	UNP Q04673

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	227	Total	C	N	O	S	0	0
			1752	1102	301	330	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	81	Total	C	N	O	S	0	0
			644	409	114	113	8		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	162	Total	C	N	O	S	0	0
			1296	801	230	263	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	55	Total	C	N	O	S	0	0
			454	296	80	76	2		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

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 14 is a DNA chain called Nontemplate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	10	Total	C	N	O	P	0	0
			205	99	39	57	10		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	10	Total	C	N	O	P	0	0
			205	100	32	63	10		

- Molecule 16 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	311	Total	C	N	O	S	0	0
			2521	1589	438	487	7		

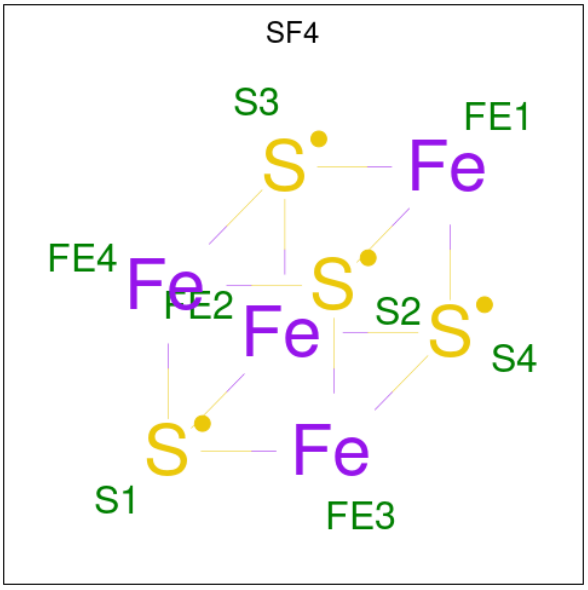
There are 10 discrepancies between the modelled and reference sequences:

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 17 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	135	Total	C	N	O	S	0	0
			1094	694	190	205	5		

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

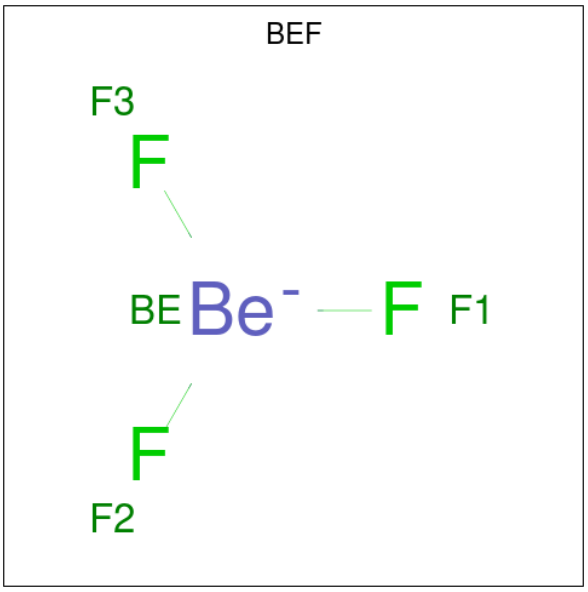


Mol	Chain	Residues	Atoms			AltConf
18	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	3	2	Total	Zn	0
			2	2	
19	4	1	Total	Zn	0
			1	1	
19	6	4	Total	Zn	0
			4	4	
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	W	1	Total	Zn	0
			1	1	

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

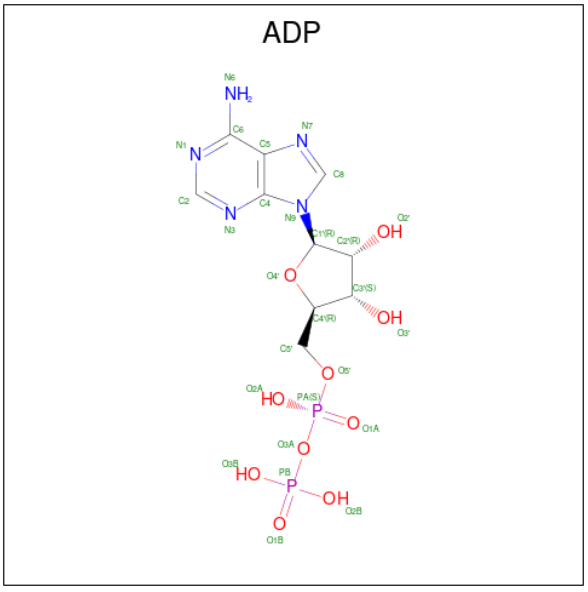


Mol	Chain	Residues	Atoms			AltConf
20	7	1	Total	Be	F	0
			4	1	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	7	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



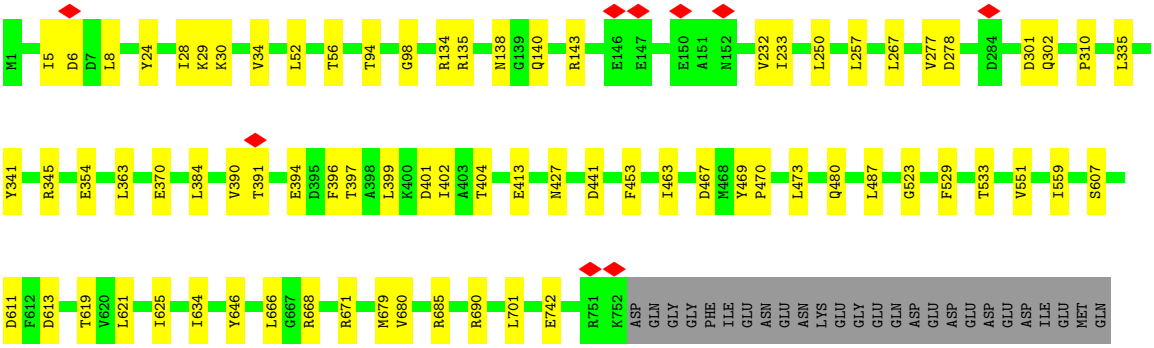
Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

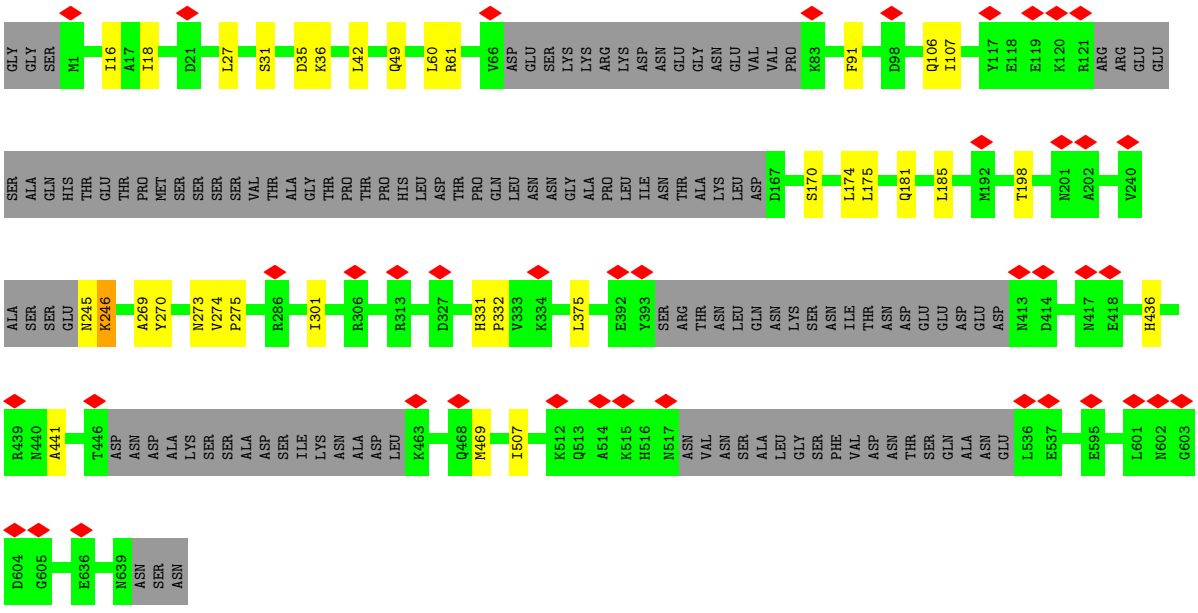
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 0:



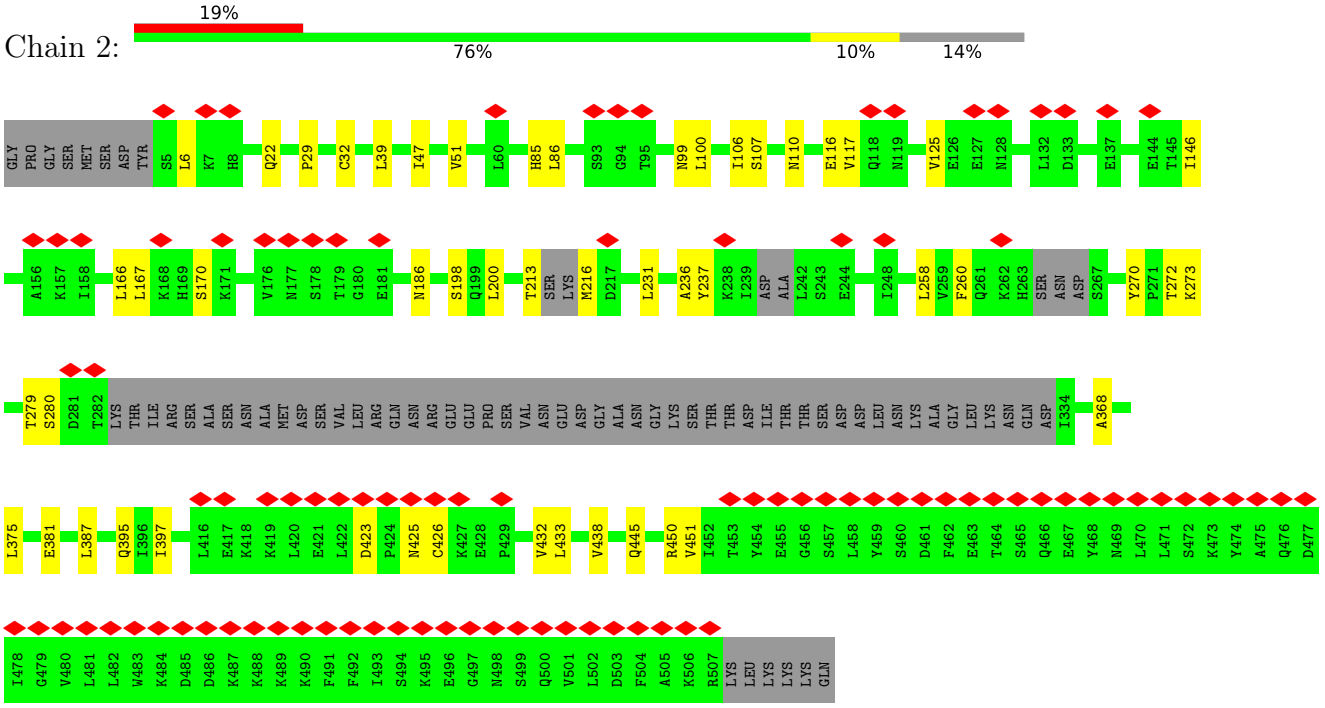
• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

Chain 1:



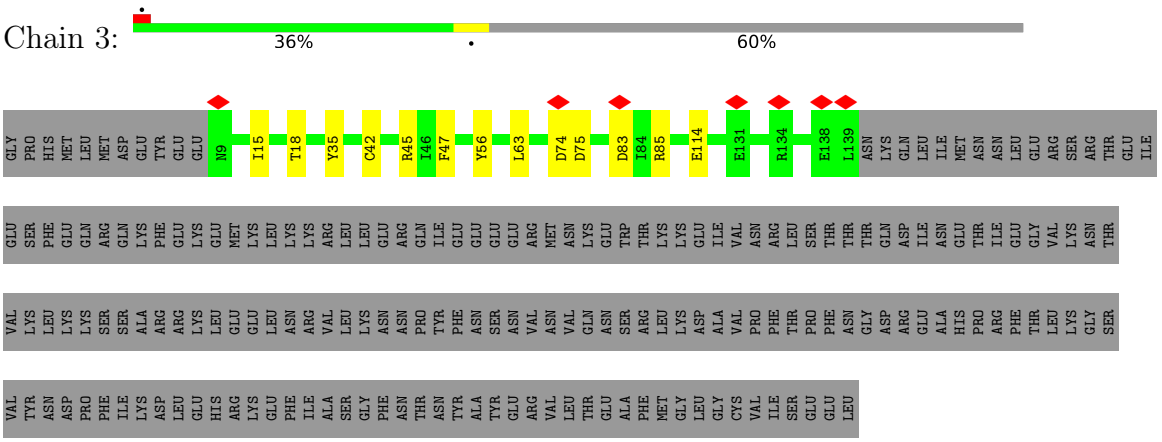
• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2

Chain 2:



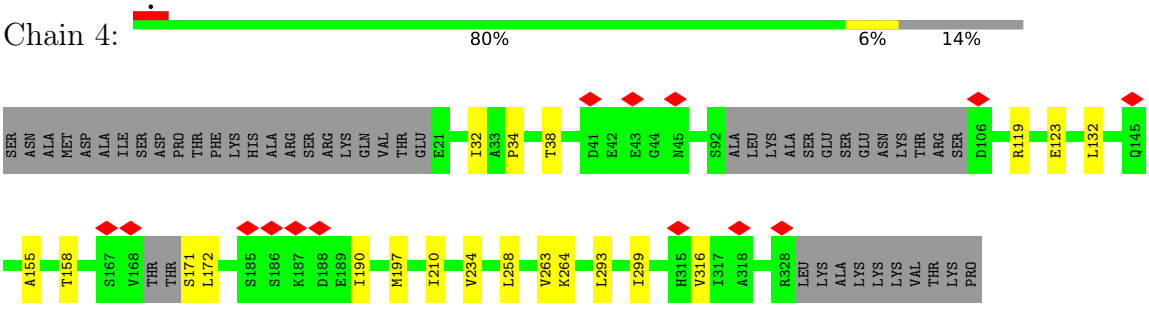
• Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain 3:



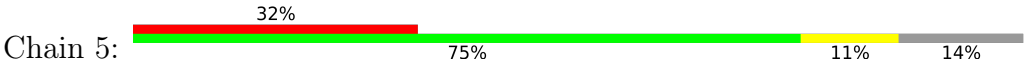
• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

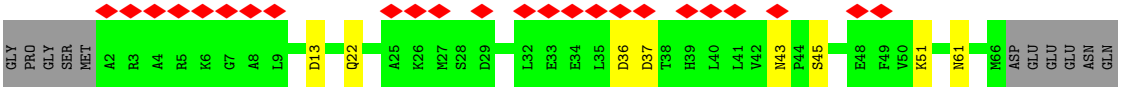
Chain 4:



• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

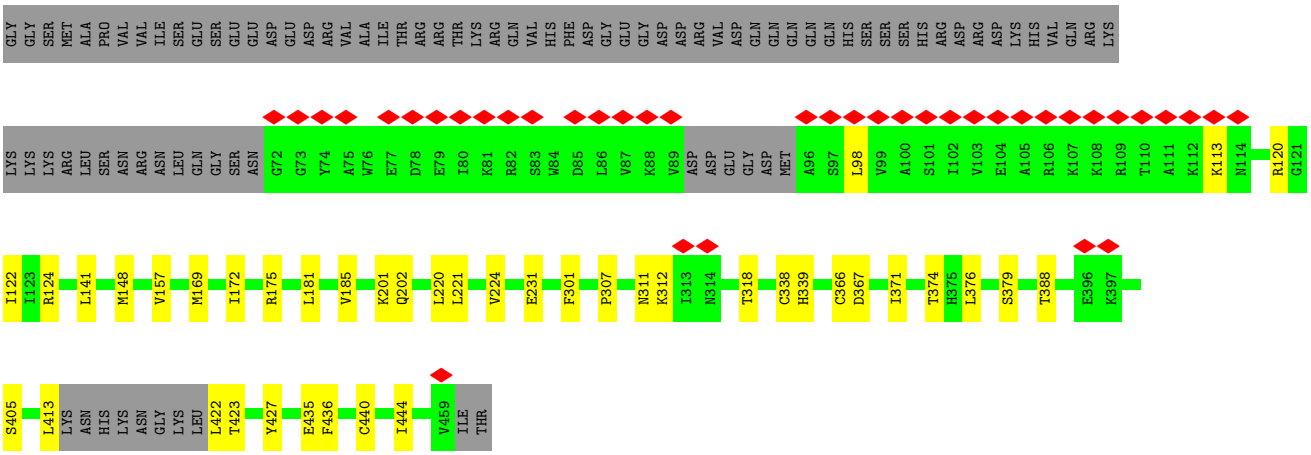
Chain 5:





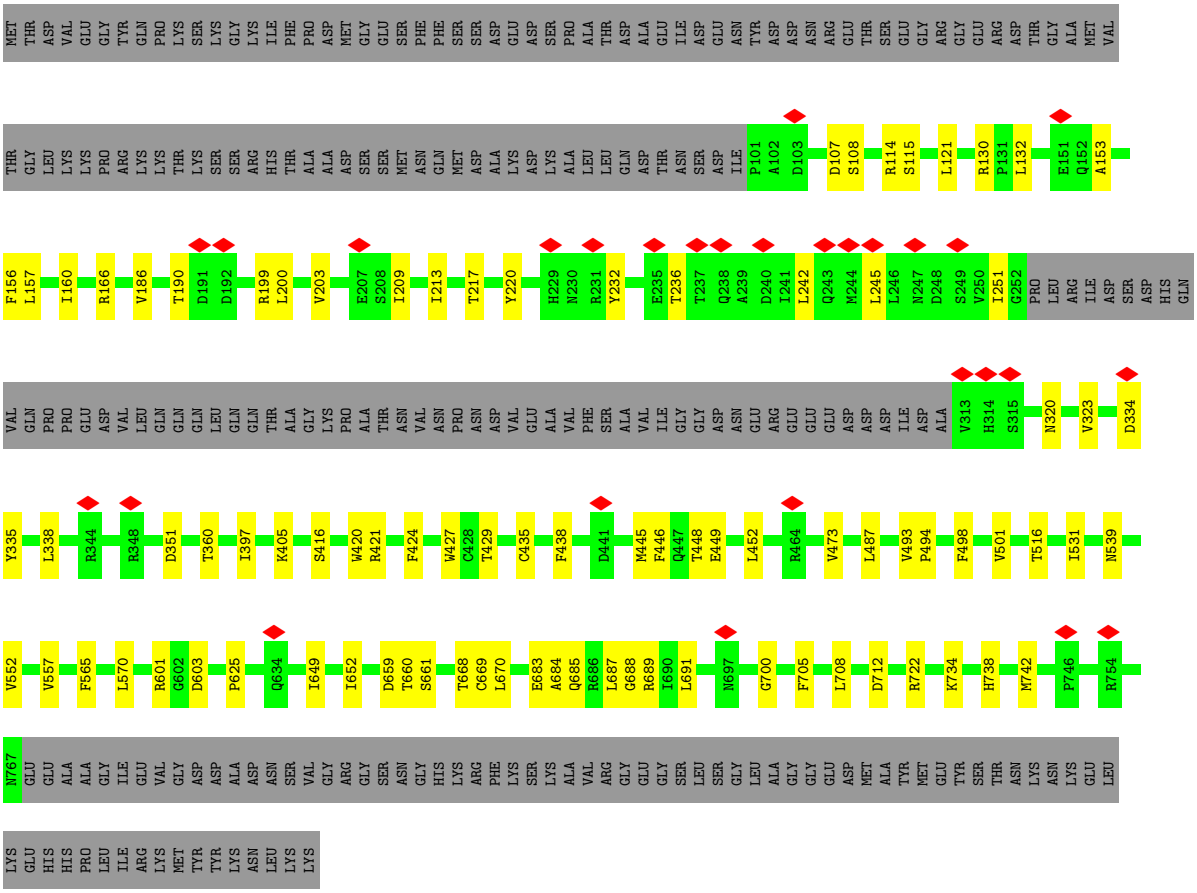
• Molecule 7: General transcription and DNA repair factor IIH subunit SSL1

Chain 6:



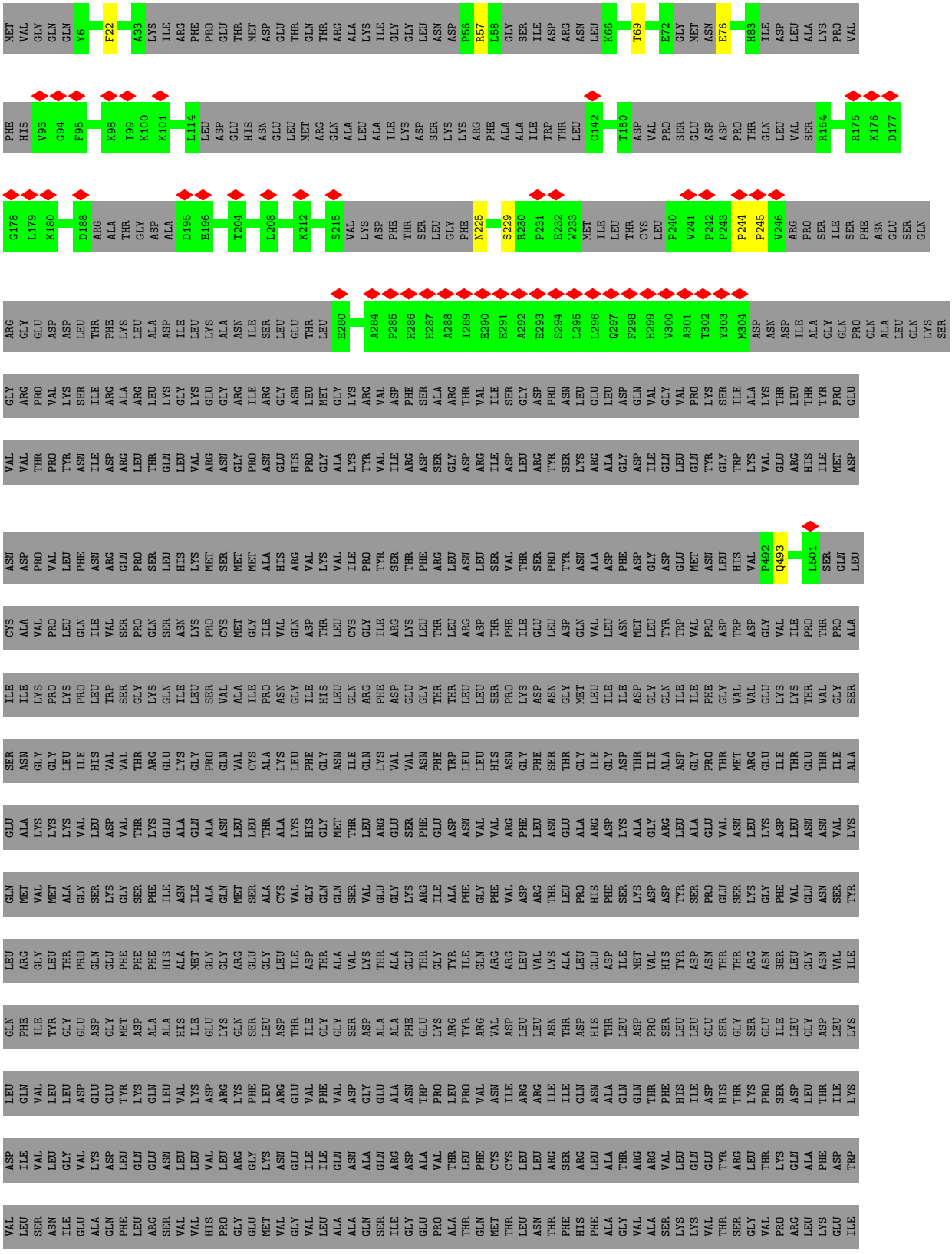
• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

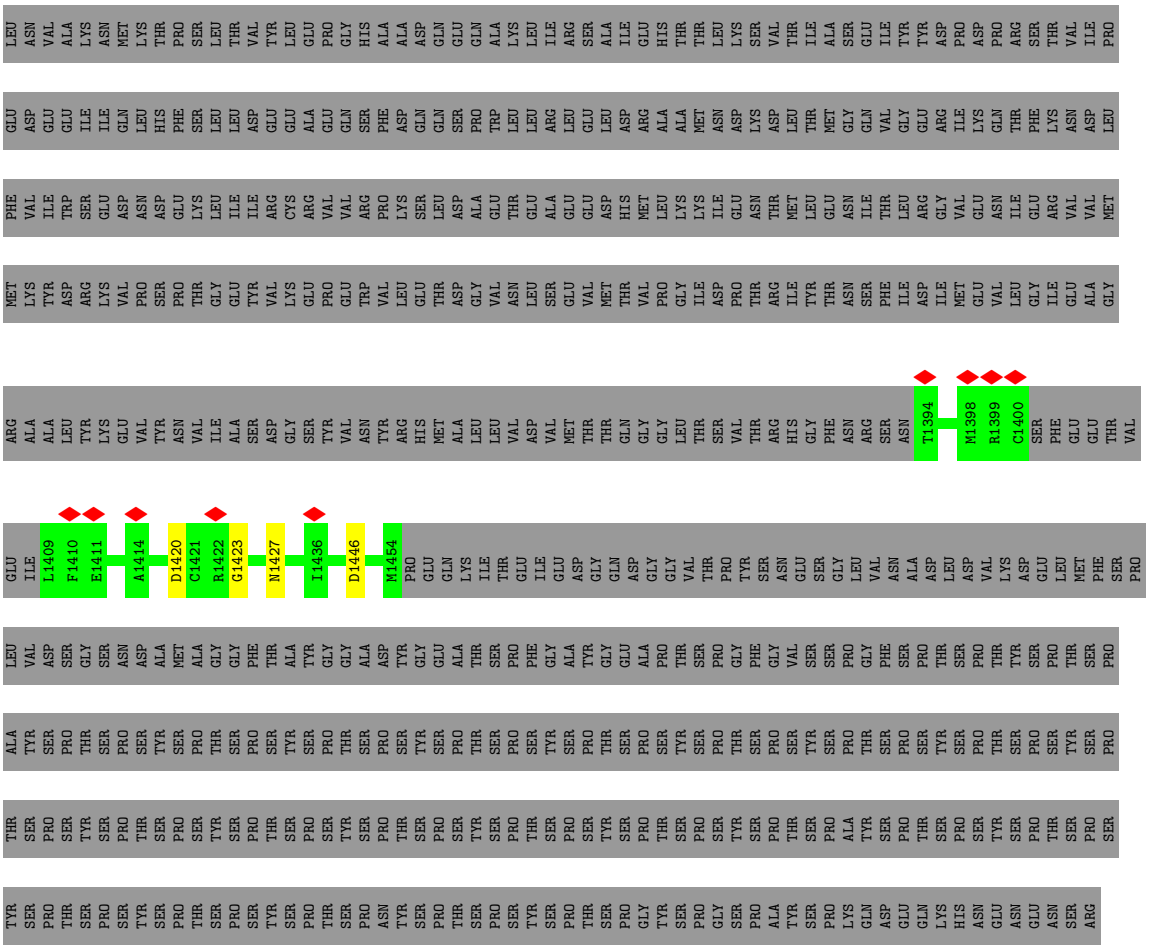
Chain 7:



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

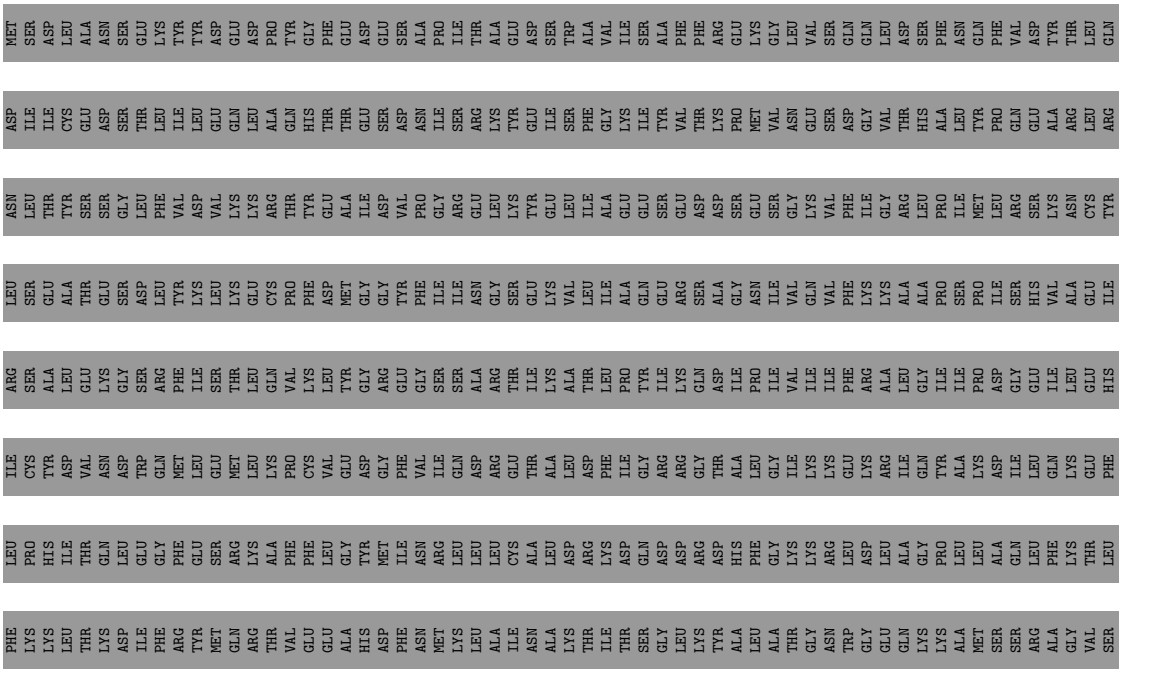
Chain A:

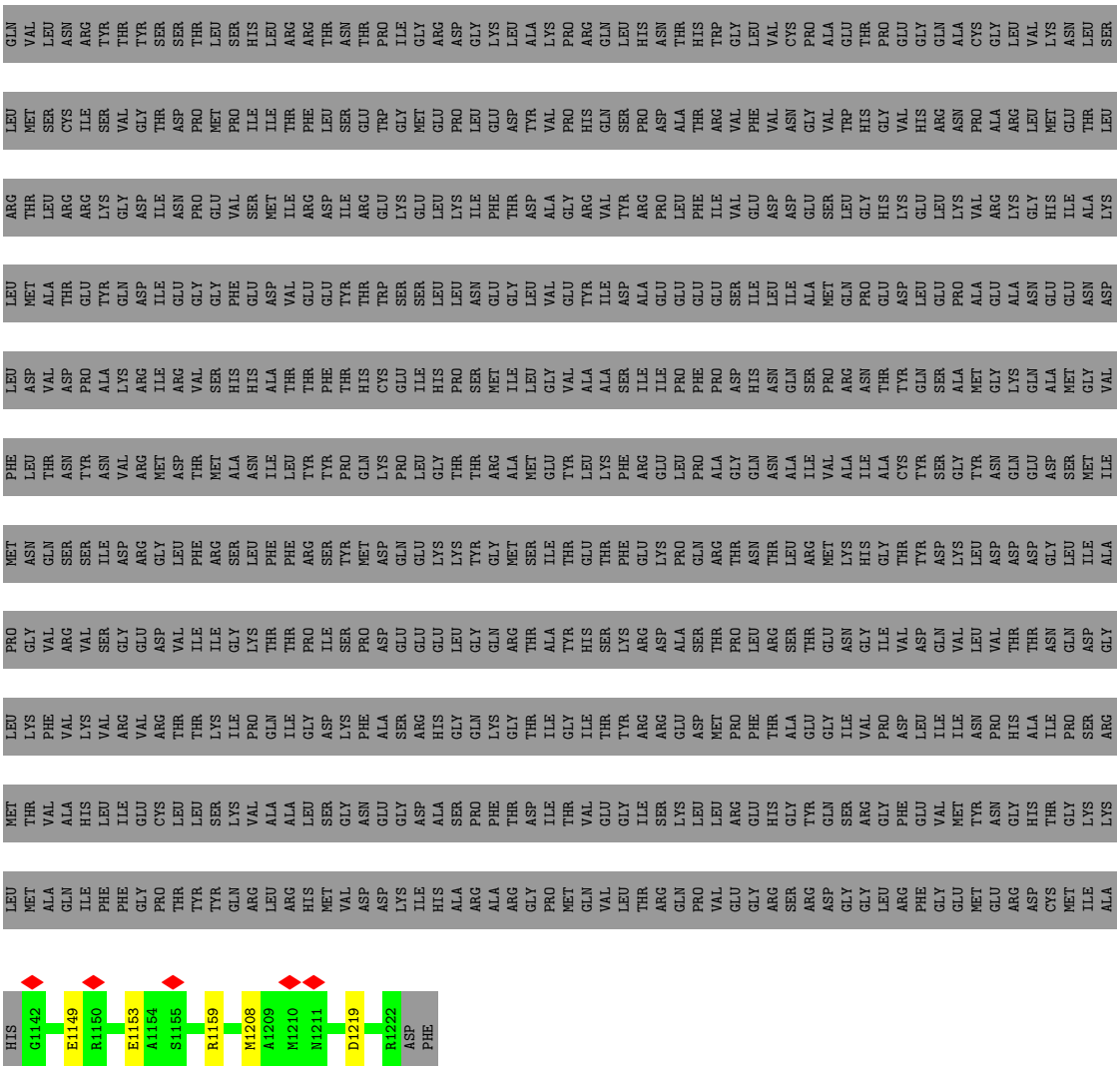




• Molecule 10: DNA-directed RNA polymerase II subunit RPB2

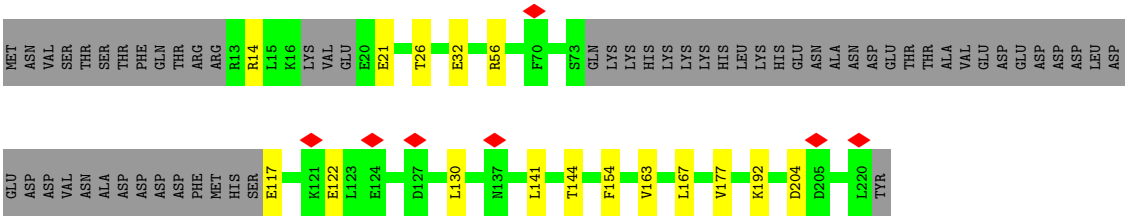
Chain B: 6% 93%





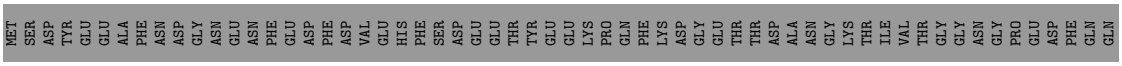
• Molecule 11: DNA-directed RNA polymerase II subunit RPB4

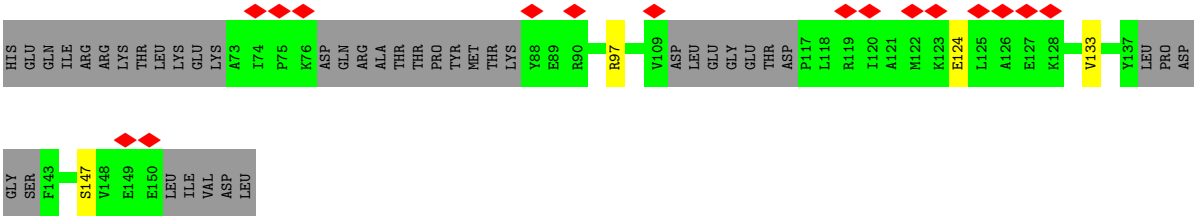
Chain D:



• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

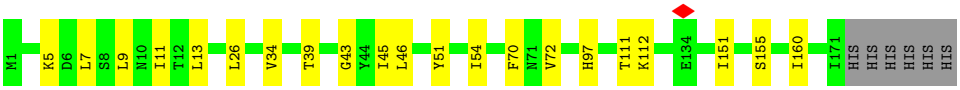
Chain F:





• Molecule 13: DNA-directed RNA polymerase II subunit RPB7

Chain G:

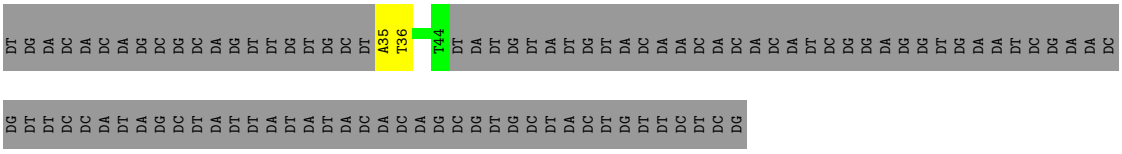


• Molecule 14: Nontemplate DNA

Chain N:

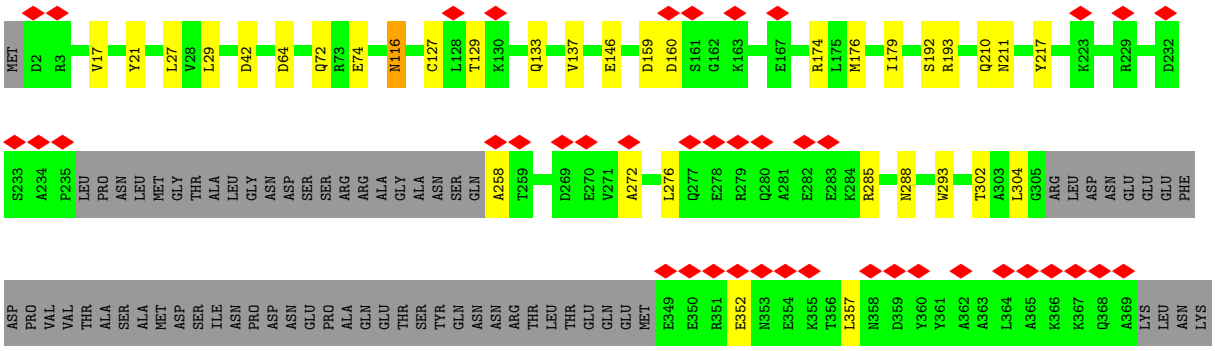
• Molecule 15: Template DNA

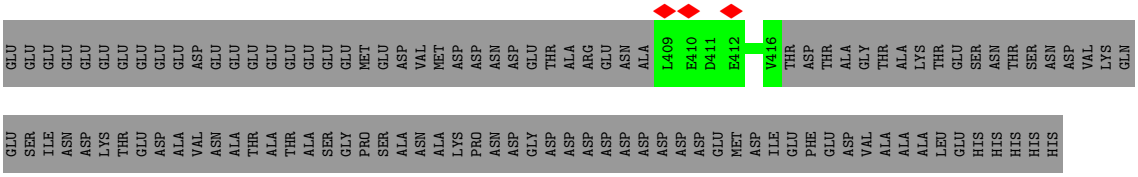
Chain T:



• Molecule 16: Transcription initiation factor IIE subunit alpha

Chain W:




GLU GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34198	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 ($e^-/Å^2$)	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	93.916	Depositor
Minimum map value	-66.865	Depositor
Average map value	0.052	Depositor
Map value standard deviation	1.010	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	398.99997, 398.99997, 398.99997	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SF4, MG, BEF, 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	0	0.24	0/6209	0.39	0/8384
2	1	0.23	0/4269	0.36	0/5744
3	2	0.24	0/3664	0.36	0/4952
4	3	0.24	0/1109	0.37	0/1492
5	4	0.24	0/2312	0.39	0/3127
6	5	0.22	0/520	0.38	0/701
7	6	0.25	0/3007	0.43	2/4066 (0.0%)
8	7	0.25	0/4984	0.42	2/6742 (0.0%)
9	A	0.23	0/1777	0.37	0/2378
10	B	0.25	0/655	0.41	0/879
11	D	0.23	0/1303	0.38	0/1747
12	F	0.23	0/460	0.35	0/614
13	G	0.25	0/1367	0.42	0/1844
14	N	0.49	0/230	0.91	0/352
15	T	0.57	0/228	1.09	0/350
16	W	0.23	0/2564	0.37	0/3459
17	X	0.24	0/1115	0.39	0/1502
All	All	0.25	0/35773	0.41	4/48333 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	6	301	PHE	CB-CG-CD1	-7.93	115.25	120.80
7	6	301	PHE	CB-CG-CD2	7.75	126.23	120.80
8	7	565	PHE	CB-CG-CD1	-7.43	115.60	120.80
8	7	565	PHE	CB-CG-CD2	7.04	125.72	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	6091	0	6155	46	0
2	1	4206	0	4277	27	0
3	2	3597	0	3687	35	0
4	3	1089	0	1069	8	0
5	4	2274	0	2332	16	0
6	5	514	0	541	7	0
7	6	2946	0	2958	26	0
8	7	4881	0	4867	62	0
9	A	1752	0	1719	9	0
10	B	644	0	649	5	0
11	D	1296	0	1311	10	0
12	F	454	0	480	3	0
13	G	1339	0	1357	17	0
14	N	205	0	114	0	0
15	T	205	0	117	1	0
16	W	2521	0	2516	26	0
17	X	1094	0	1114	9	0
18	0	8	0	0	0	0
19	3	2	0	0	0	0
19	4	1	0	0	0	0
19	6	4	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	W	1	0	0	0	0
20	7	4	0	0	0	0
21	7	1	0	0	0	0
22	7	27	0	12	0	0
All	All	35159	0	35275	275	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 4.

The worst 5 of 275 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)
8:7:424:PHE:CE2	8:7:452:LEU:HD22	1.93	1.04
8:7:397:ILE:HG12	8:7:424:PHE:CD1	2.01	0.96
1:0:52:LEU:HD21	1:0:233:ILE:HD13	1.50	0.94
8:7:424:PHE:CD2	8:7:452:LEU:HD22	2.04	0.92
5:4:293:LEU:HD11	7:6:376:LEU:HD22	1.52	0.89

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	0	750/778 (96%)	737 (98%)	13 (2%)	0	100	100
2	1	507/645 (79%)	494 (97%)	13 (3%)	0	100	100
3	2	435/517 (84%)	426 (98%)	9 (2%)	0	100	100
4	3	129/324 (40%)	125 (97%)	4 (3%)	0	100	100
5	4	287/341 (84%)	282 (98%)	5 (2%)	0	100	100
6	5	63/76 (83%)	62 (98%)	1 (2%)	0	100	100
7	6	368/464 (79%)	361 (98%)	7 (2%)	0	100	100
8	7	603/843 (72%)	581 (96%)	22 (4%)	0	100	100
9	A	199/1733 (12%)	196 (98%)	3 (2%)	0	100	100
10	B	79/1224 (6%)	77 (98%)	2 (2%)	0	100	100
11	D	156/221 (71%)	155 (99%)	1 (1%)	0	100	100
12	F	47/155 (30%)	46 (98%)	1 (2%)	0	100	100
13	G	169/177 (96%)	166 (98%)	3 (2%)	0	100	100
16	W	303/492 (62%)	297 (98%)	6 (2%)	0	100	100
17	X	131/328 (40%)	124 (95%)	7 (5%)	0	100	100
All	All	4226/8318 (51%)	4129 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	684/707 (97%)	684 (100%)	0	100 100
2	1	482/590 (82%)	481 (100%)	1 (0%)	93 98
3	2	408/470 (87%)	408 (100%)	0	100 100
4	3	125/305 (41%)	125 (100%)	0	100 100
5	4	260/302 (86%)	260 (100%)	0	100 100
6	5	59/68 (87%)	59 (100%)	0	100 100
7	6	338/419 (81%)	337 (100%)	1 (0%)	92 97
8	7	539/737 (73%)	539 (100%)	0	100 100
9	A	195/1520 (13%)	195 (100%)	0	100 100
10	B	69/1061 (6%)	69 (100%)	0	100 100
11	D	144/200 (72%)	143 (99%)	1 (1%)	84 92
12	F	48/137 (35%)	48 (100%)	0	100 100
13	G	152/158 (96%)	152 (100%)	0	100 100
16	W	280/436 (64%)	279 (100%)	1 (0%)	91 95
17	X	125/295 (42%)	124 (99%)	1 (1%)	81 91
All	All	3908/7405 (53%)	3903 (100%)	5 (0%)	93 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	246	LYS
7	6	201	LYS
11	D	14	ARG
16	W	116	ASN
17	X	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
7	6	192	HIS
7	6	445	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	BEF	7	901	22	0,3,3	-	-	-		
18	SF4	0	801	1	0,12,12	-	-	-		
22	ADP	7	903	20,21	24,29,29	0.68	0	29,45,45	0.68	0

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
18	SF4	0	801	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ADP	7	903	20,21	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

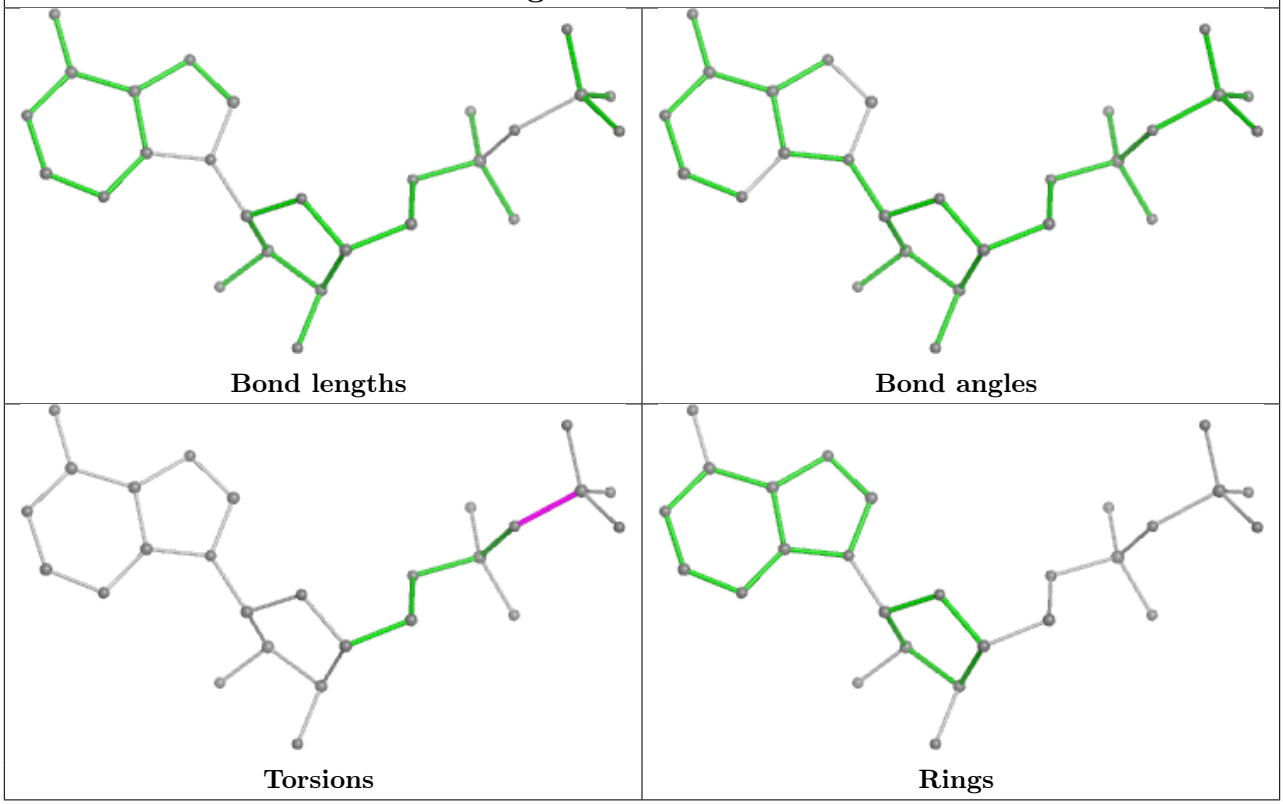
Mol	Chain	Res	Type	Atoms
22	7	903	ADP	PA-O3A-PB-O1B
22	7	903	ADP	PA-O3A-PB-O2B
22	7	903	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ADP 7 903



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

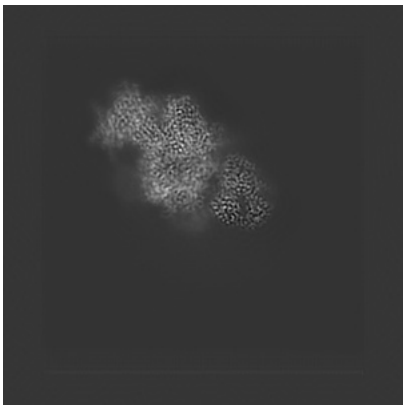
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12722. These allow visual inspection of the internal detail of the map and identification of artifacts.

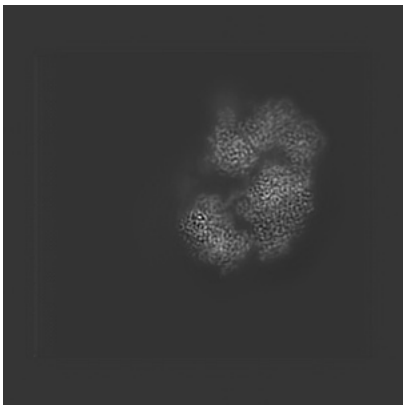
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

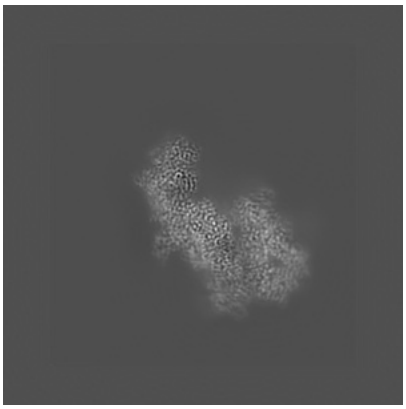
6.1.1 Primary map



X

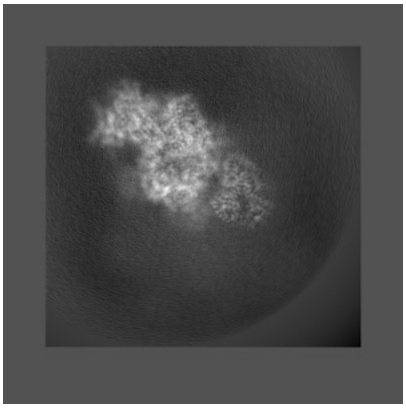


Y

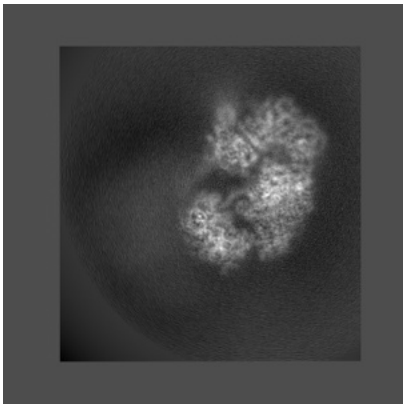


Z

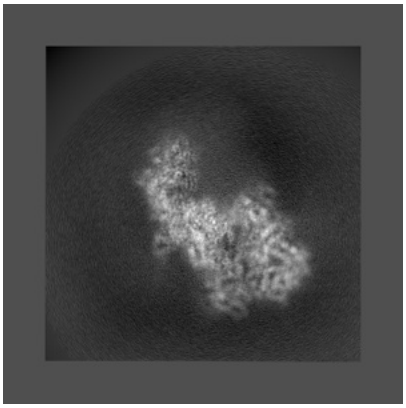
6.1.2 Raw map



X



Y

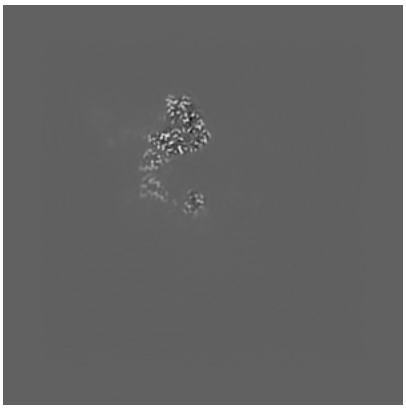


Z

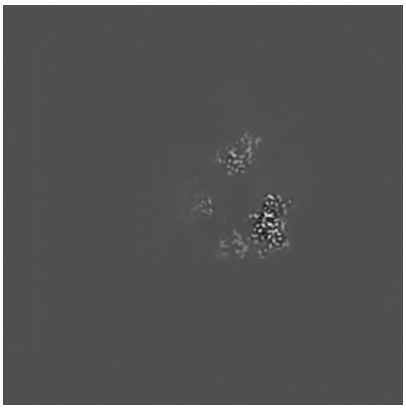
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

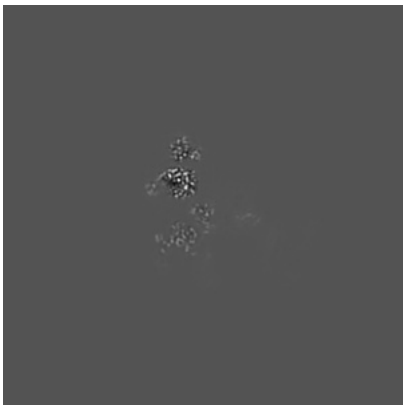
6.2.1 Primary map



X Index: 190

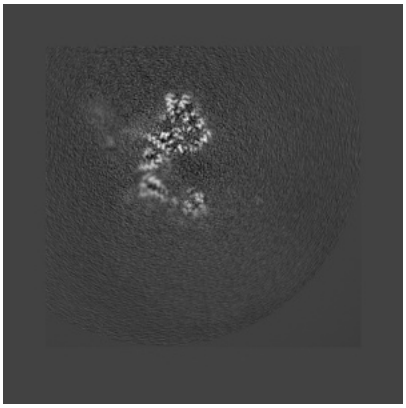


Y Index: 190

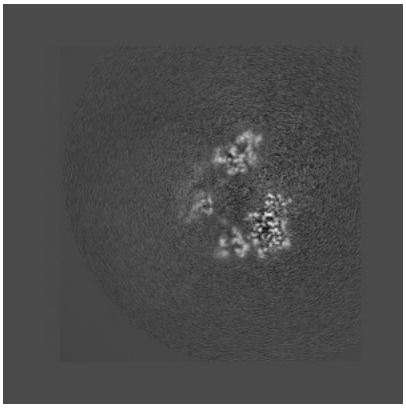


Z Index: 190

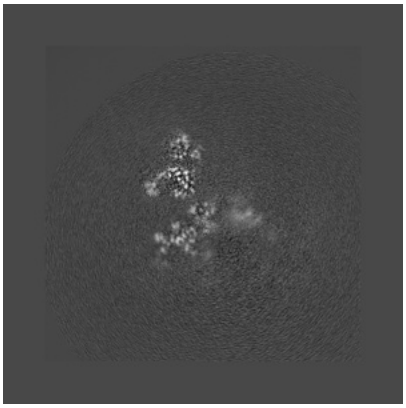
6.2.2 Raw map



X Index: 190



Y Index: 190



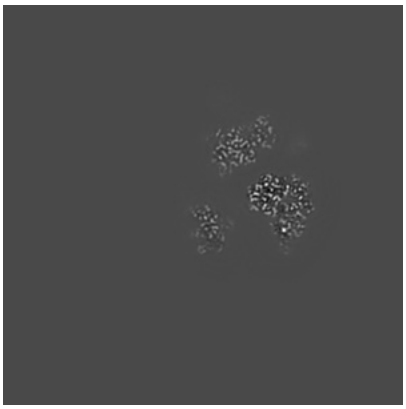
Z Index: 190

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

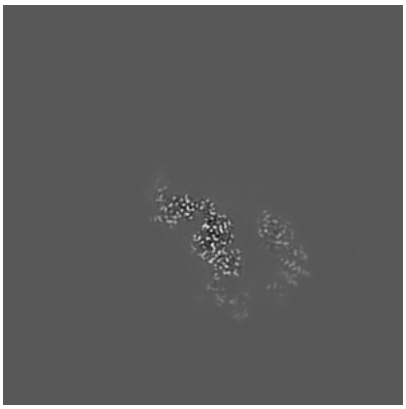
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 174

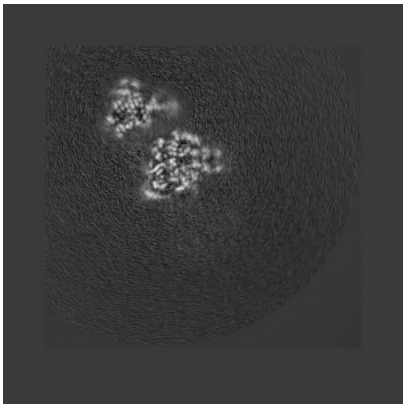


Y Index: 160

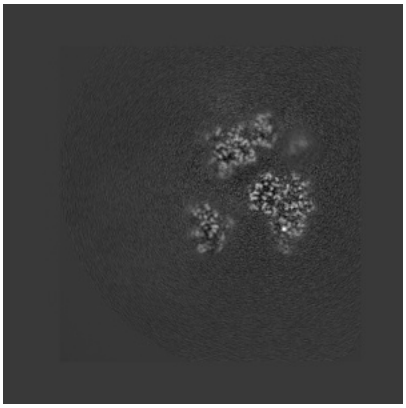


Z Index: 252

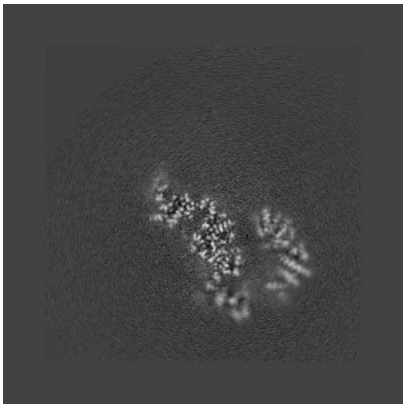
6.3.2 Raw map



X Index: 249



Y Index: 160

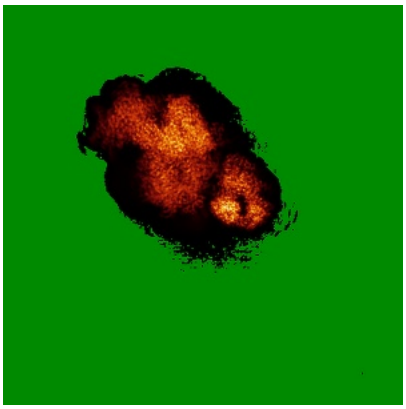


Z Index: 252

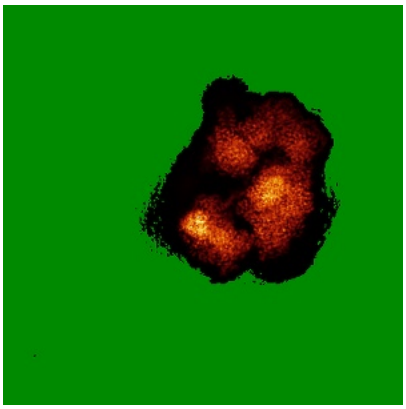
The images above show the largest variance slices of the map in three orthogonal directions.

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

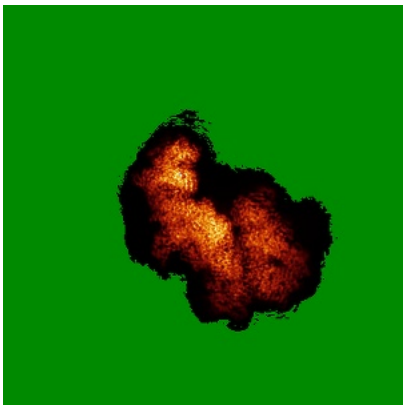
6.4.1 Primary map



X

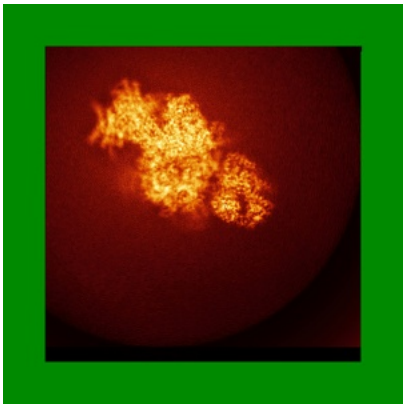


Y

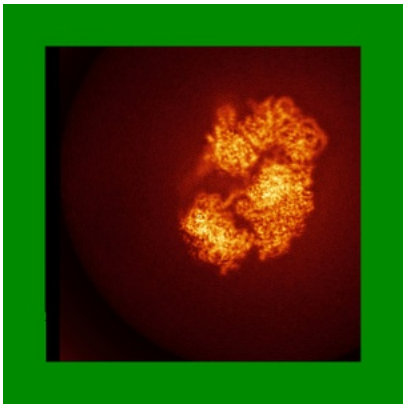


Z

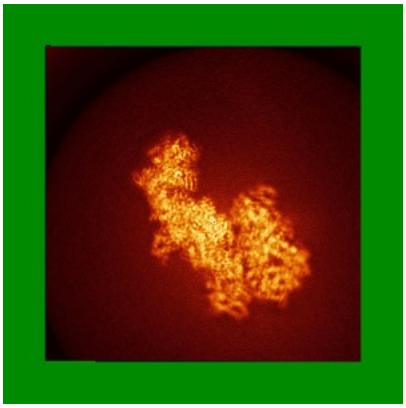
6.4.2 Raw map



X



Y

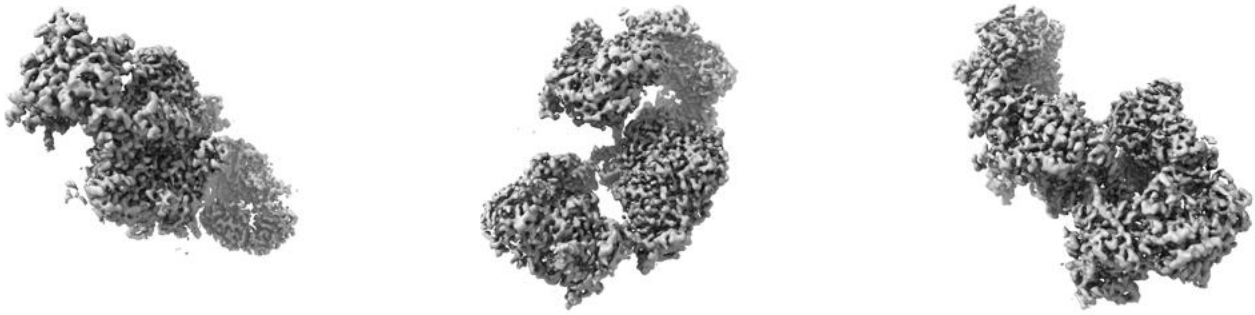


Z

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

6.5 Orthogonal surface views (i)

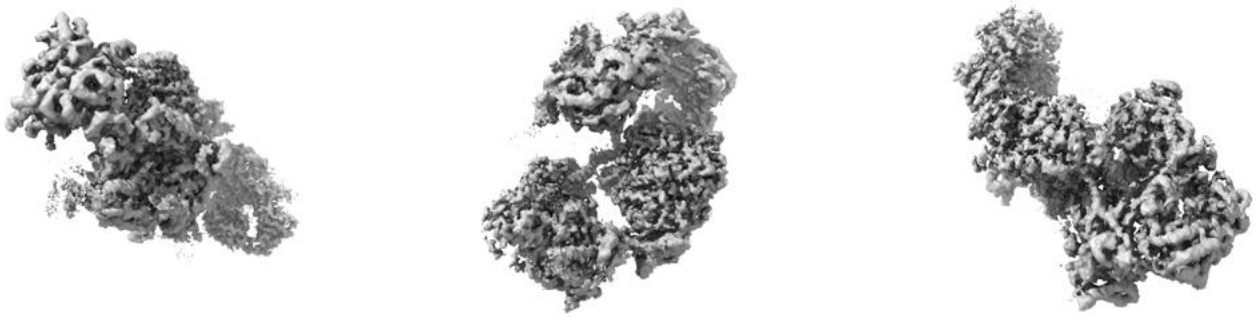
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

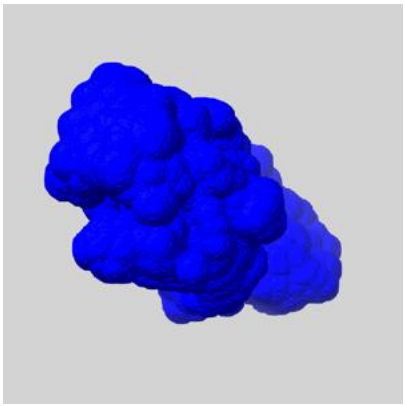
6.6 Mask visualisation (i)

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

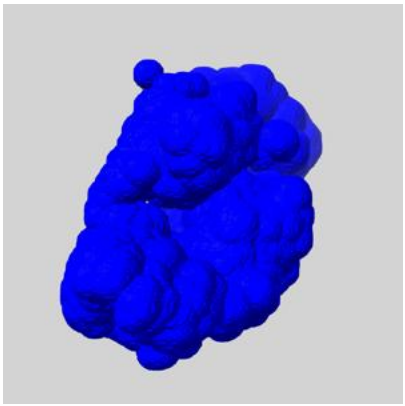
A mask typically either:

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

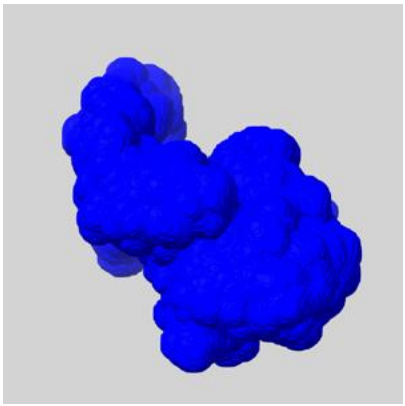
6.6.1 emd_12722_msk_1.map (i)



X



Y

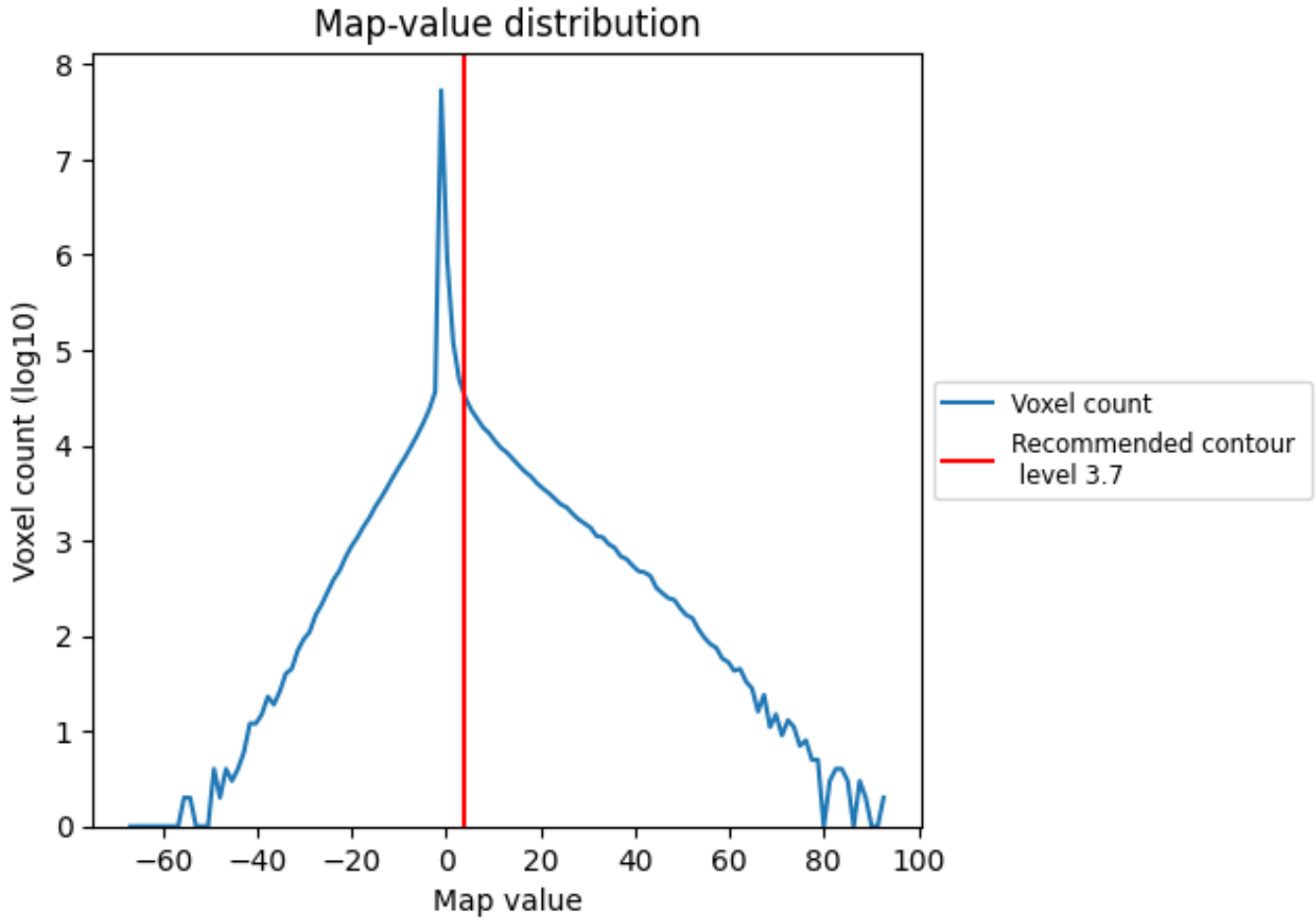


Z

7 Map analysis

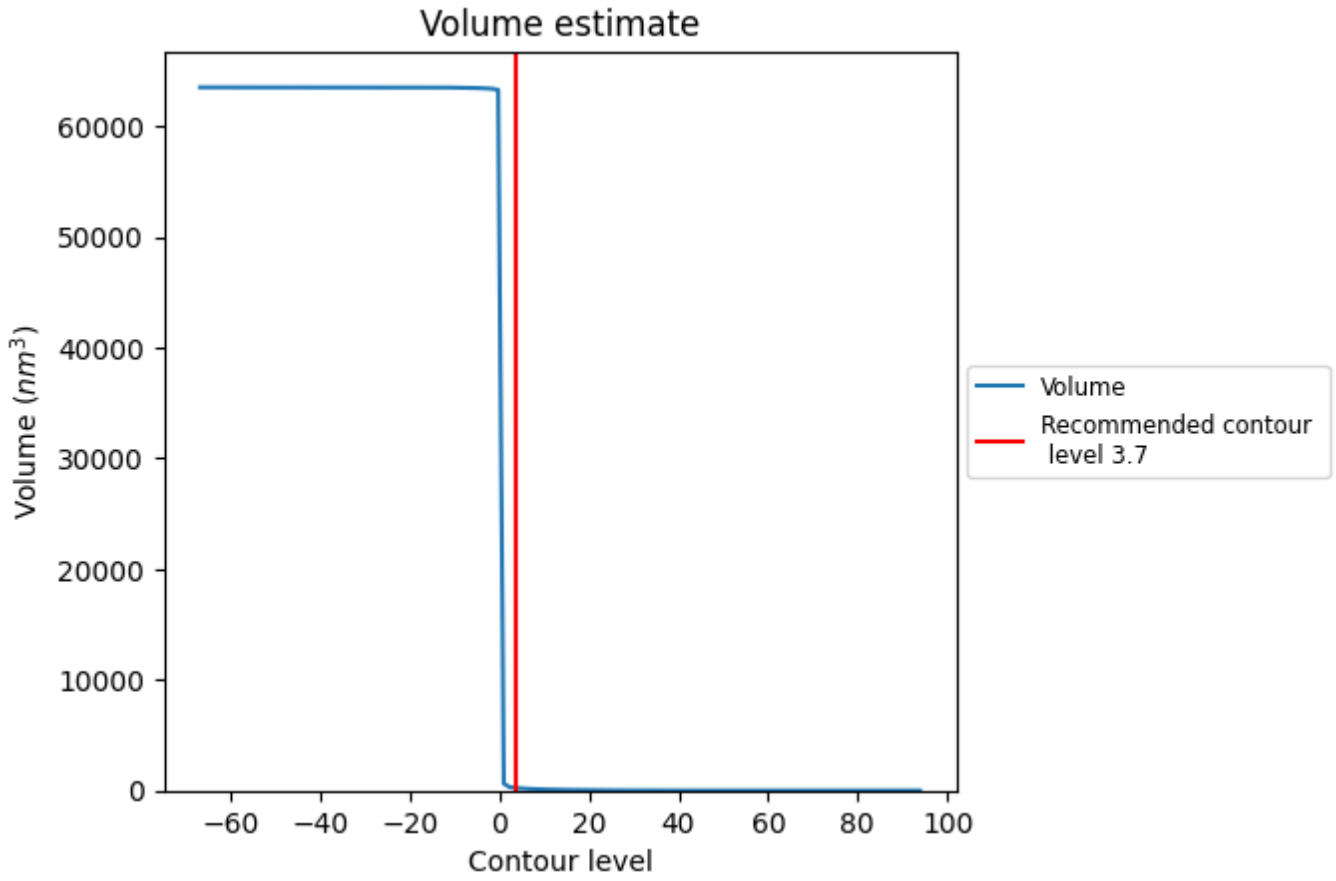
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

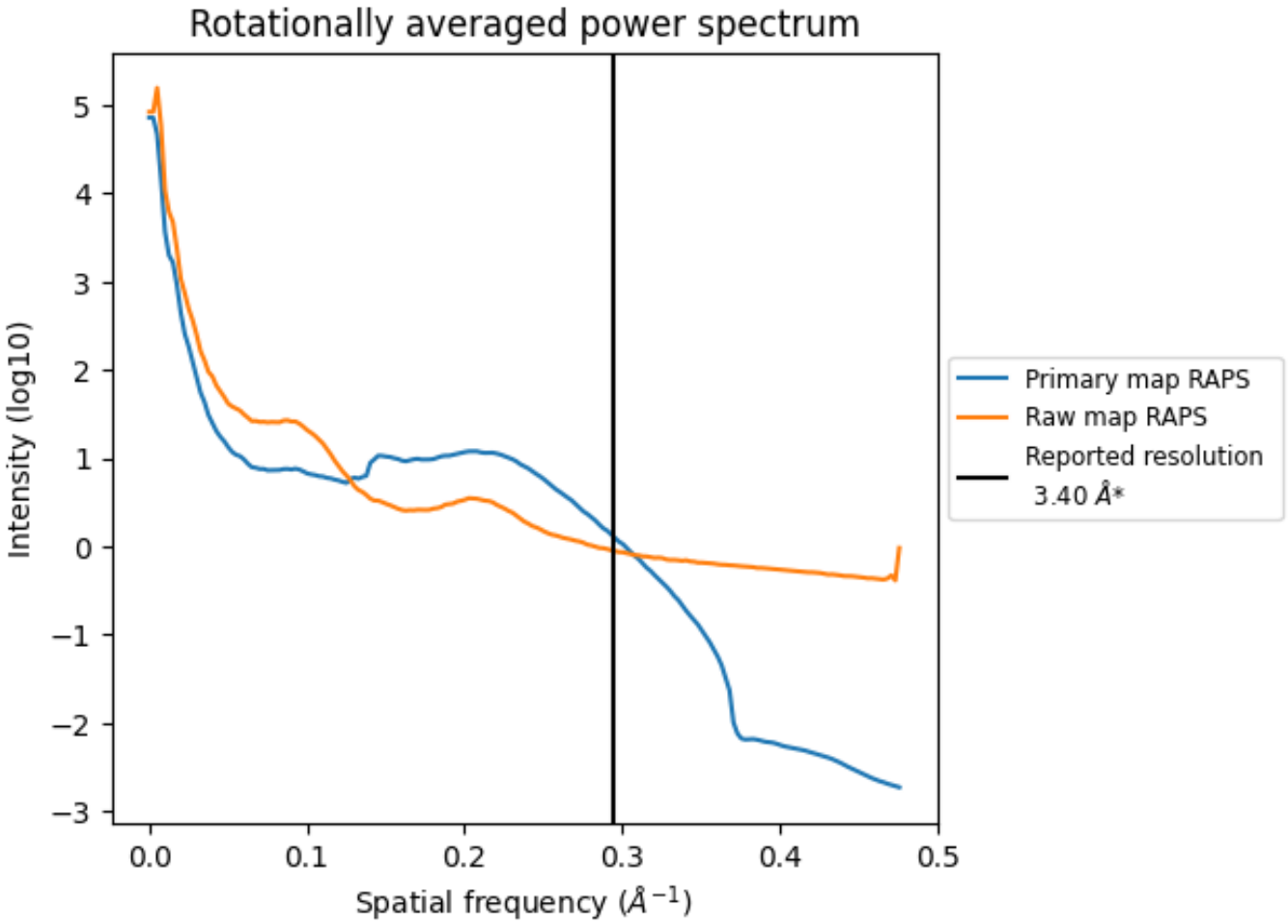
7.2 Volume estimate (i)



The volume at the recommended contour level is 233 nm^3; this corresponds to an approximate mass of 211 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)

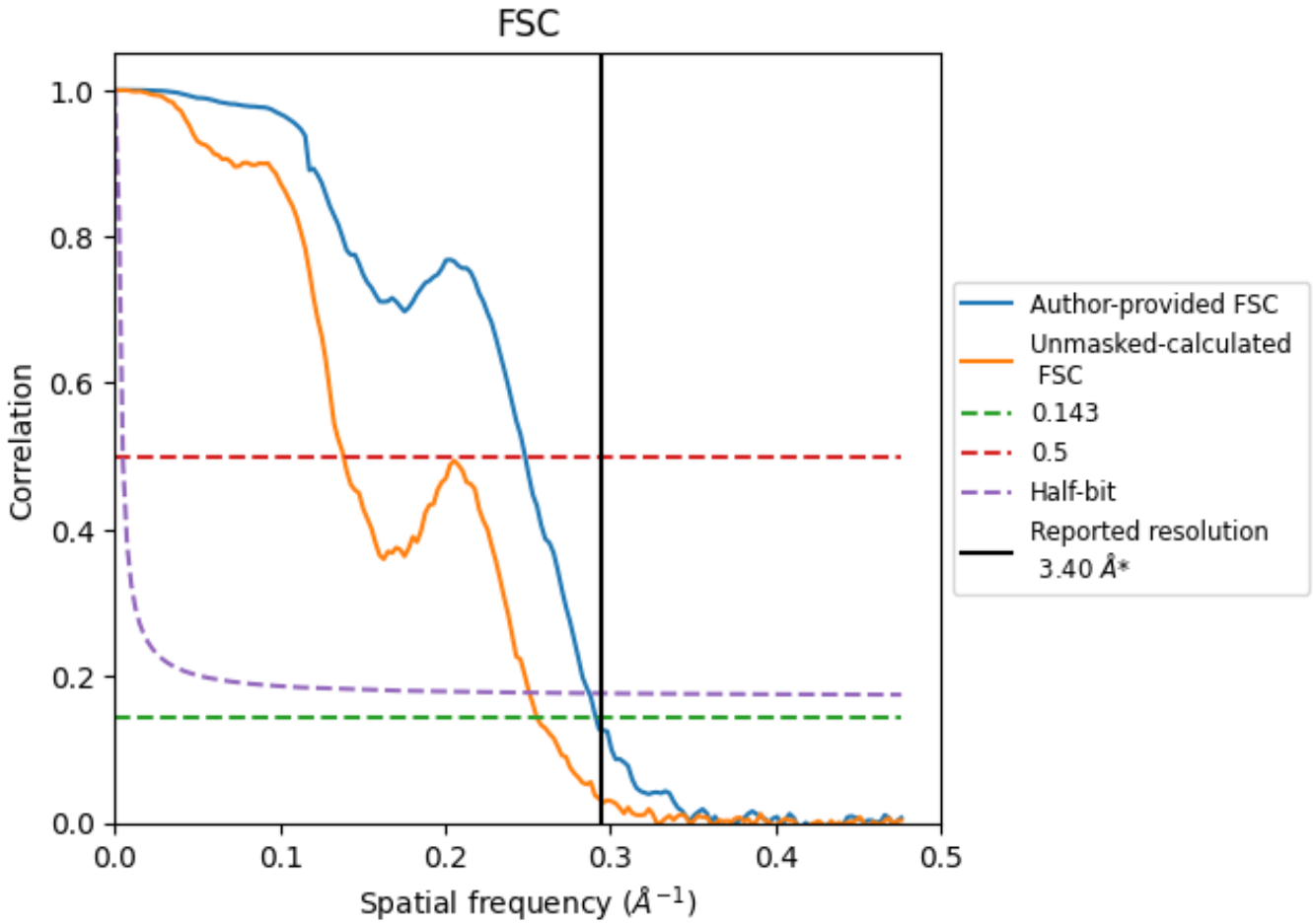


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8.2 Resolution estimates (i)

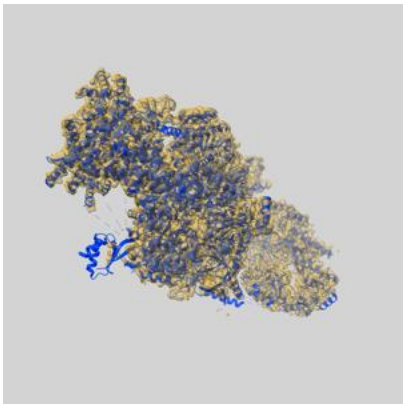
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.03	3.48
Unmasked-calculated*	3.91	7.22	3.98

*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 3.91 differs from the reported value 3.4 by more than 10 %

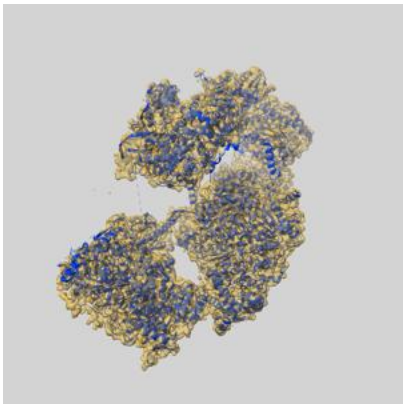
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12722 and PDB model 7O4L. Per-residue inclusion information can be found in section 3 on page 11.

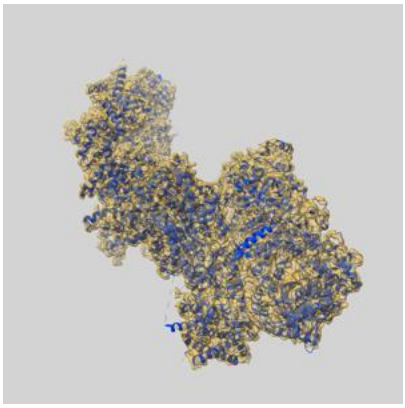
9.1 Map-model overlay



X



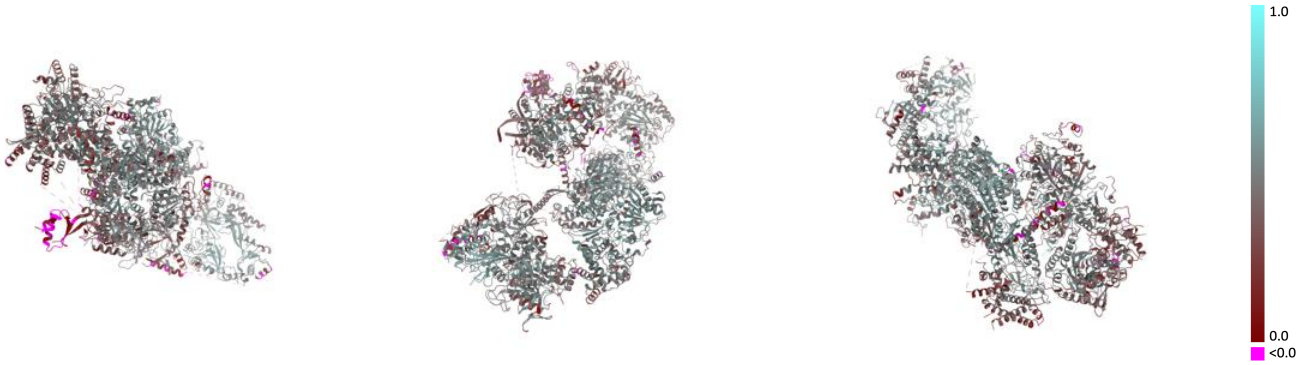
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

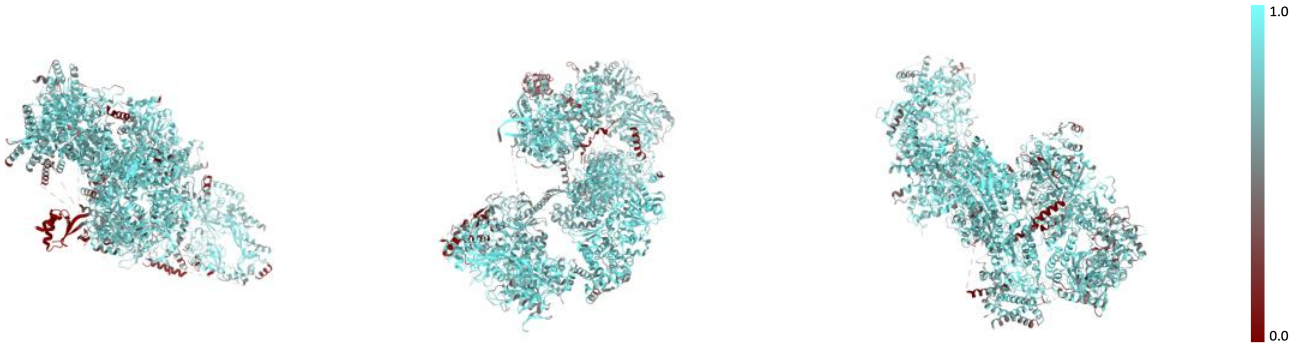
9.2 Q-score mapped to coordinate model



X Y Z

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

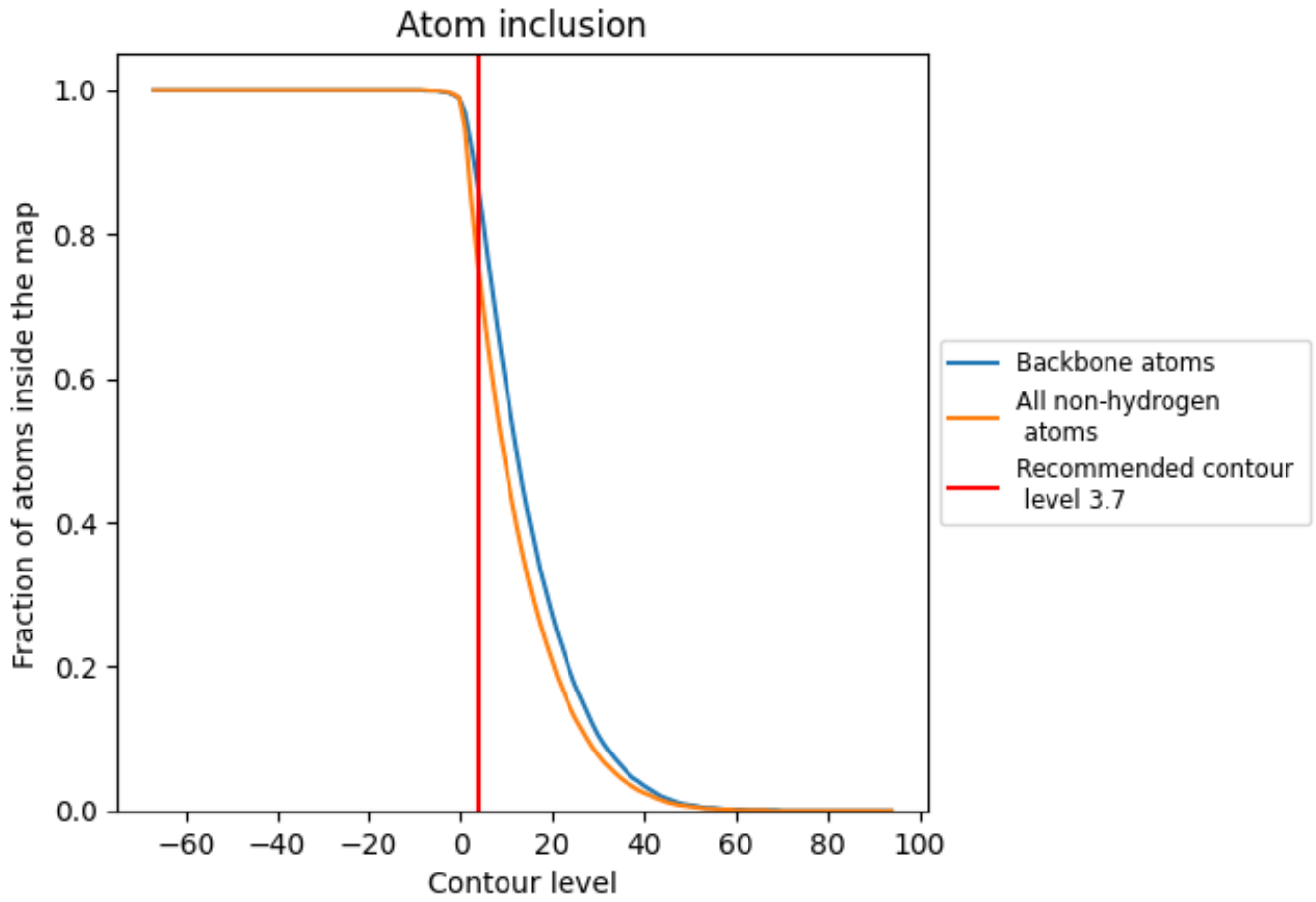
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.4400
0	0.8690	0.5220
1	0.7100	0.3970
2	0.6330	0.3530
3	0.7590	0.4240
4	0.7970	0.4570
5	0.5340	0.3030
6	0.7760	0.4640
7	0.8110	0.4340
A	0.6080	0.4190
B	0.8500	0.5480
D	0.7570	0.4470
F	0.6350	0.4430
G	0.8890	0.5230
N	0.8540	0.3640
T	0.8540	0.3770
W	0.7100	0.4080
X	0.7270	0.4130