Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 05:51 am BST

PDB ID	:	7O73
EMDB ID	:	EMD-12744
Title	:	Yeast RNA polymerase II transcription pre-initiation complex with closed distorted promoter DNA
Authors	:	Schilbach, S.; Aibara, S.; Dienemann, C.; Grabbe, F.; Cramer, P.
Deposited on	:	2021-04-12
Resolution	:	3.40 Å(reported)
Based on initial model	:	5OQJ

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:

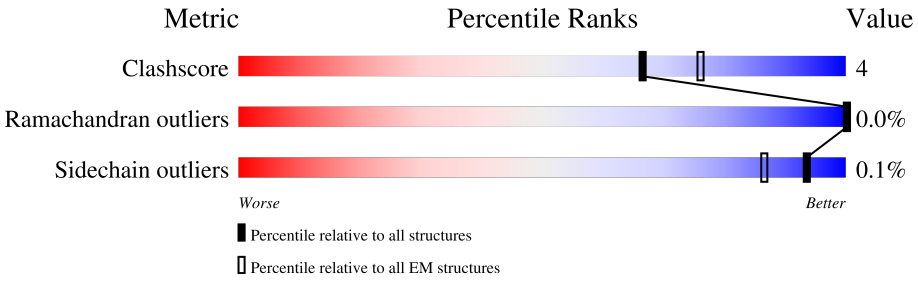
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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	85% 12% ·
2	1	645	· 75% 6% 19%
3	2	517	13% 77% 9% 14%
4	3	324	36% · 60%
5	4	341	· 75% 11% 14%
6	5	76	14% 83% · 14%
7	6	464	· 70% 7% 23%
8	7	843	12% 65% 8% 27%

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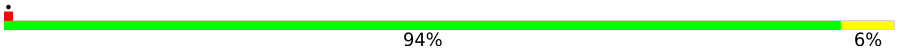
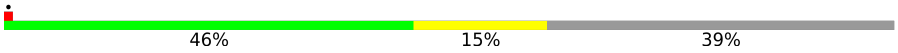
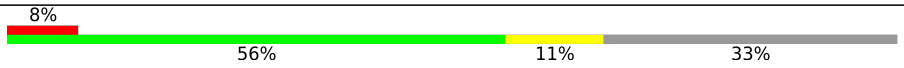
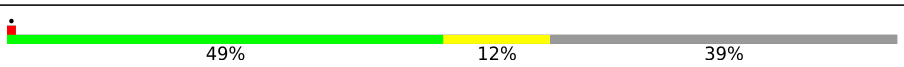
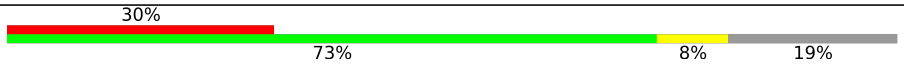
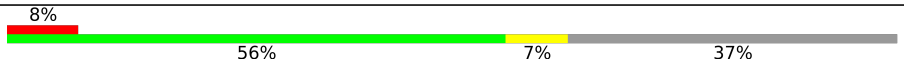
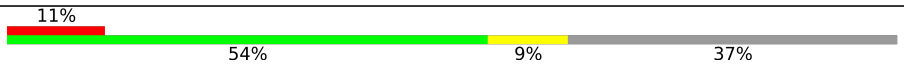
Mol	Chain	Length	Quality of chain
9	A	1733	
10	B	1224	
11	C	347	
12	D	221	
13	E	215	
14	F	155	
15	G	177	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	352	
22	N	106	
23	O	247	
24	Q	738	
25	R	400	
26	T	106	
27	U	286	
28	V	129	
29	W	492	
30	X	328	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 73768 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	522	Total	C	N	O	S	0	0
			4214	2660	734	798	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	356	Total	C	N	O	S	0	0
			2794	1771	482	513	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	615	Total	C	N	O	S	0	0
			4954	3153	860	914	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1428	Total	C	N	O	S	0	0
			11238	7079	1962	2135	62		

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP P16370
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
12	D	163	Total	C	N	O	S	0	0
			1307	807	234	264	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	308	Total	C	N	O	S	0	0
			2360	1489	406	447	18		

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 Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	65	Total	C	N	O	P	0	0
			1332	637	236	394	65		

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

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	241	LYS	-	expression tag	UNP P13393
O	242	HIS	-	expression tag	UNP P13393
O	243	HIS	-	expression tag	UNP P13393
O	244	HIS	-	expression tag	UNP P13393
O	245	HIS	-	expression tag	UNP P13393
O	246	HIS	-	expression tag	UNP P13393
O	247	HIS	-	expression tag	UNP P13393

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-2	GLY	-	expression tag	UNP P41895
Q	-1	PRO	-	expression tag	UNP P41895
Q	0	GLY	-	expression tag	UNP P41895

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

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

- Molecule 26 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	65	Total	C	N	O	P	0	0
			1330	636	246	384	64		

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

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

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

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	123	LYS	-	expression tag	UNP P32774
V	124	HIS	-	expression tag	UNP P32774
V	125	HIS	-	expression tag	UNP P32774

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Chain	Residue	Modelled	Actual	Comment	Reference
V	126	HIS	-	expression tag	UNP P32774
V	127	HIS	-	expression tag	UNP P32774
V	128	HIS	-	expression tag	UNP P32774
V	129	HIS	-	expression tag	UNP P32774

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	312	Total	C	N	O	S	0	0
			2532	1595	442	488	7		

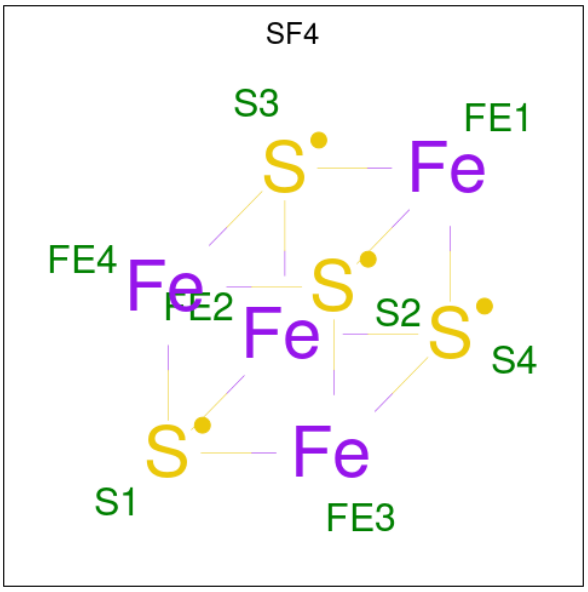
There are 10 discrepancies between the modelled and reference sequences:

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	207	Total	C	N	O	S	0	0
			1661	1061	281	313	6		

- Molecule 31 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

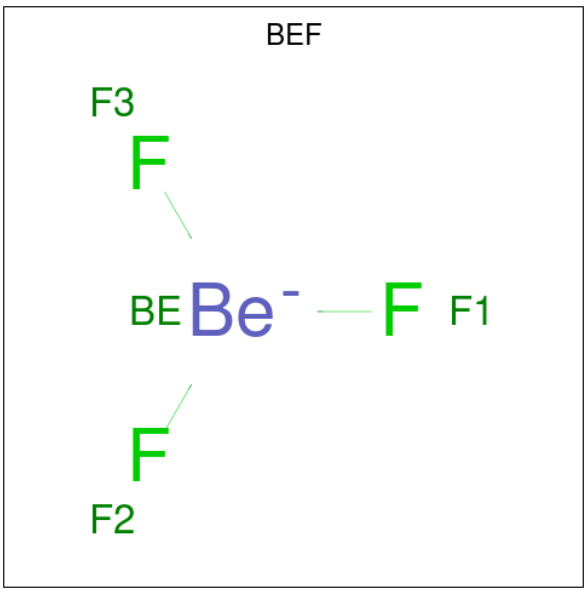


Mol	Chain	Residues	Atoms	AltConf
31	0	1	Total Fe S 8 4 4	0

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
32	3	2	Total Zn 2 2	0
32	4	1	Total Zn 1 1	0
32	6	4	Total Zn 4 4	0
32	A	2	Total Zn 2 2	0
32	B	1	Total Zn 1 1	0
32	C	1	Total Zn 1 1	0
32	I	2	Total Zn 2 2	0
32	J	1	Total Zn 1 1	0
32	L	1	Total Zn 1 1	0
32	M	1	Total Zn 1 1	0
32	W	1	Total Zn 1 1	0

- Molecule 33 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

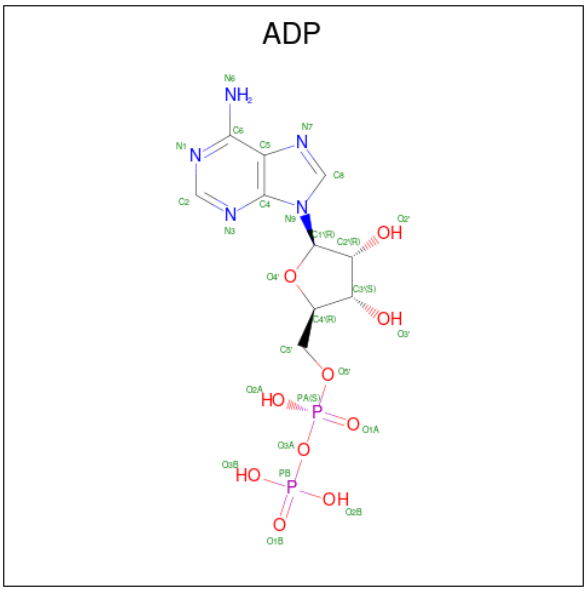


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
33	7	1	4	1	3	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	7	1	1	1	0
			Total	Mg	
34	A	1	1	1	0

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



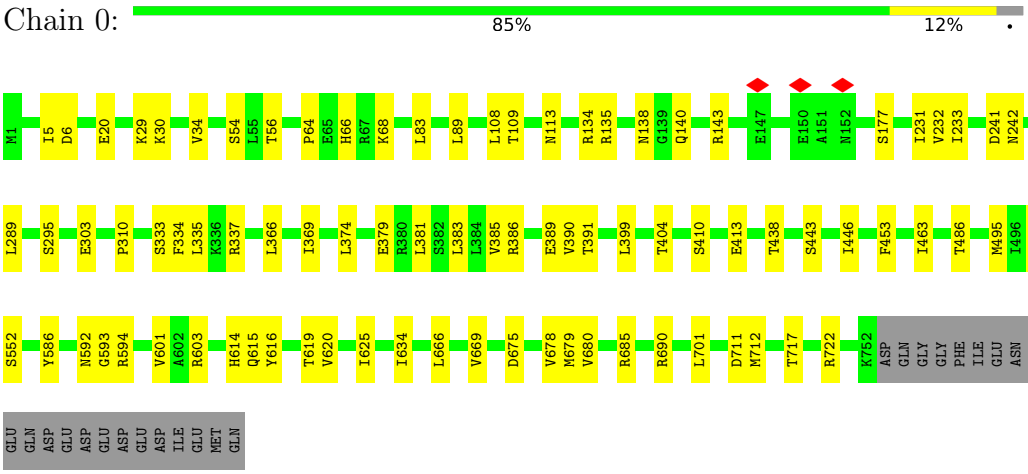
Mol	Chain	Residues	Atoms					AltConf
35	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

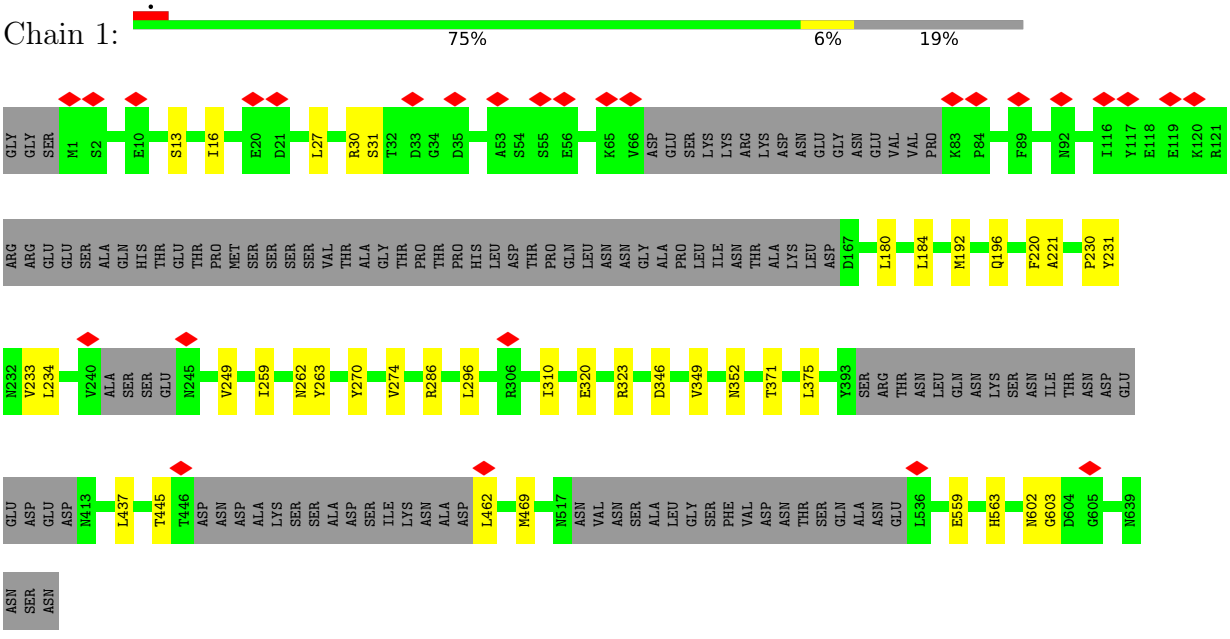
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 0:

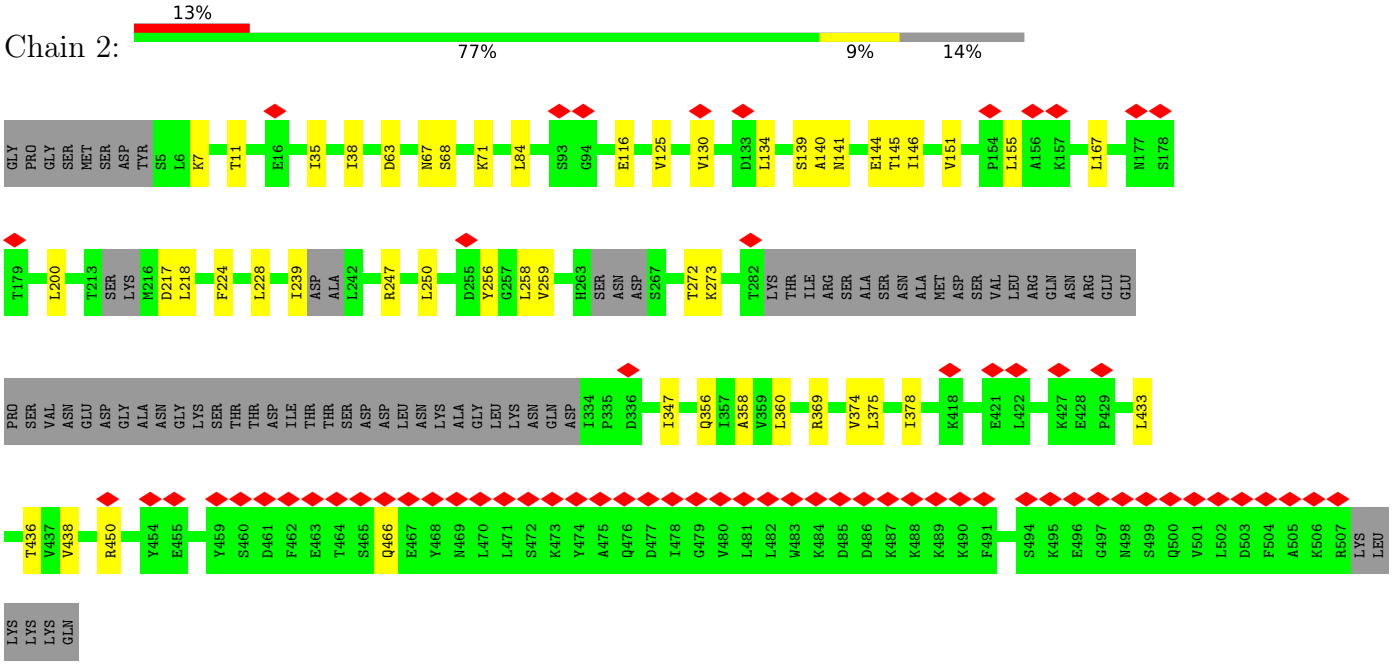


• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

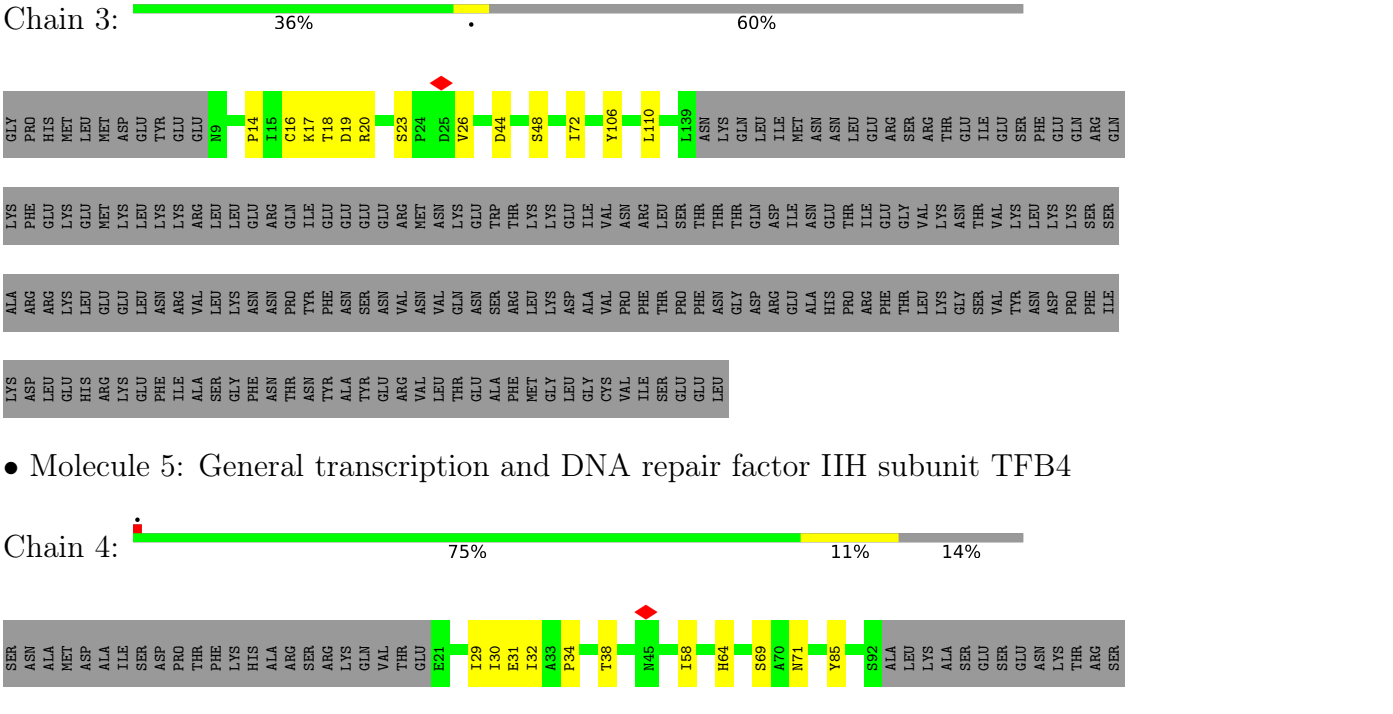
Chain 1:



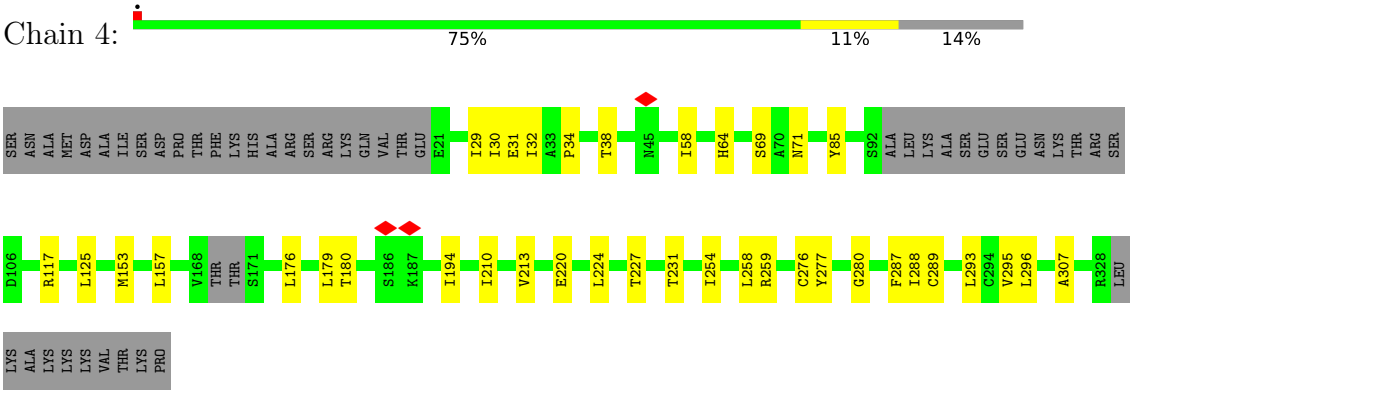
• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2



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

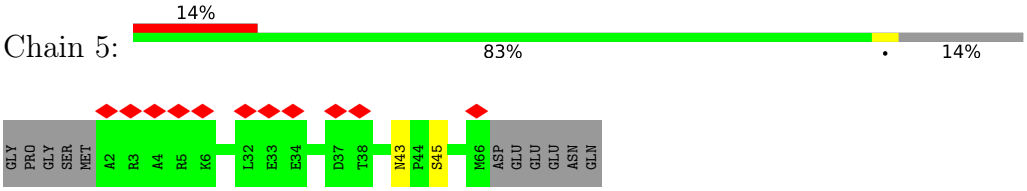


• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4



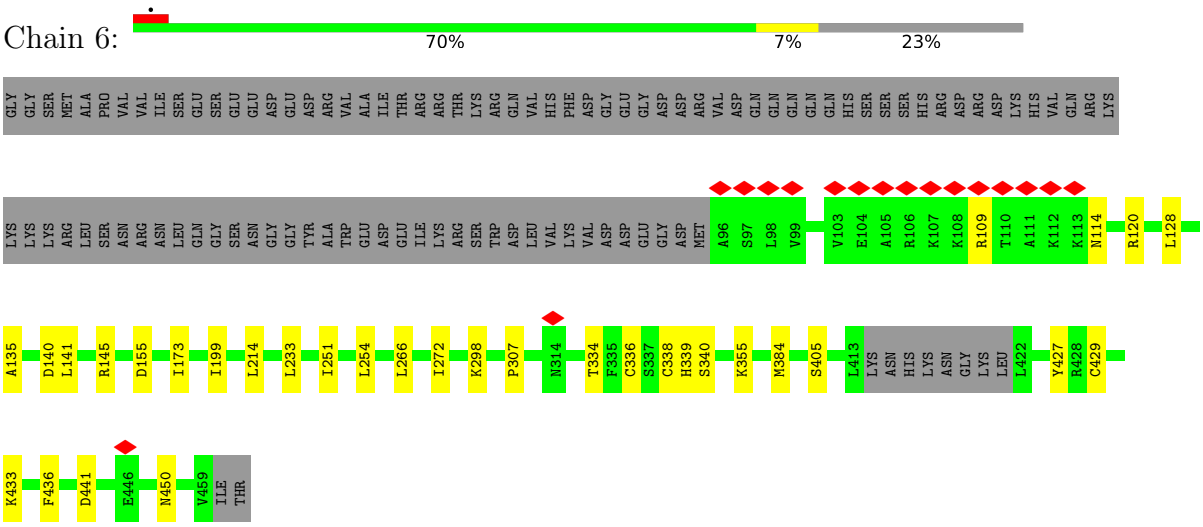
• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



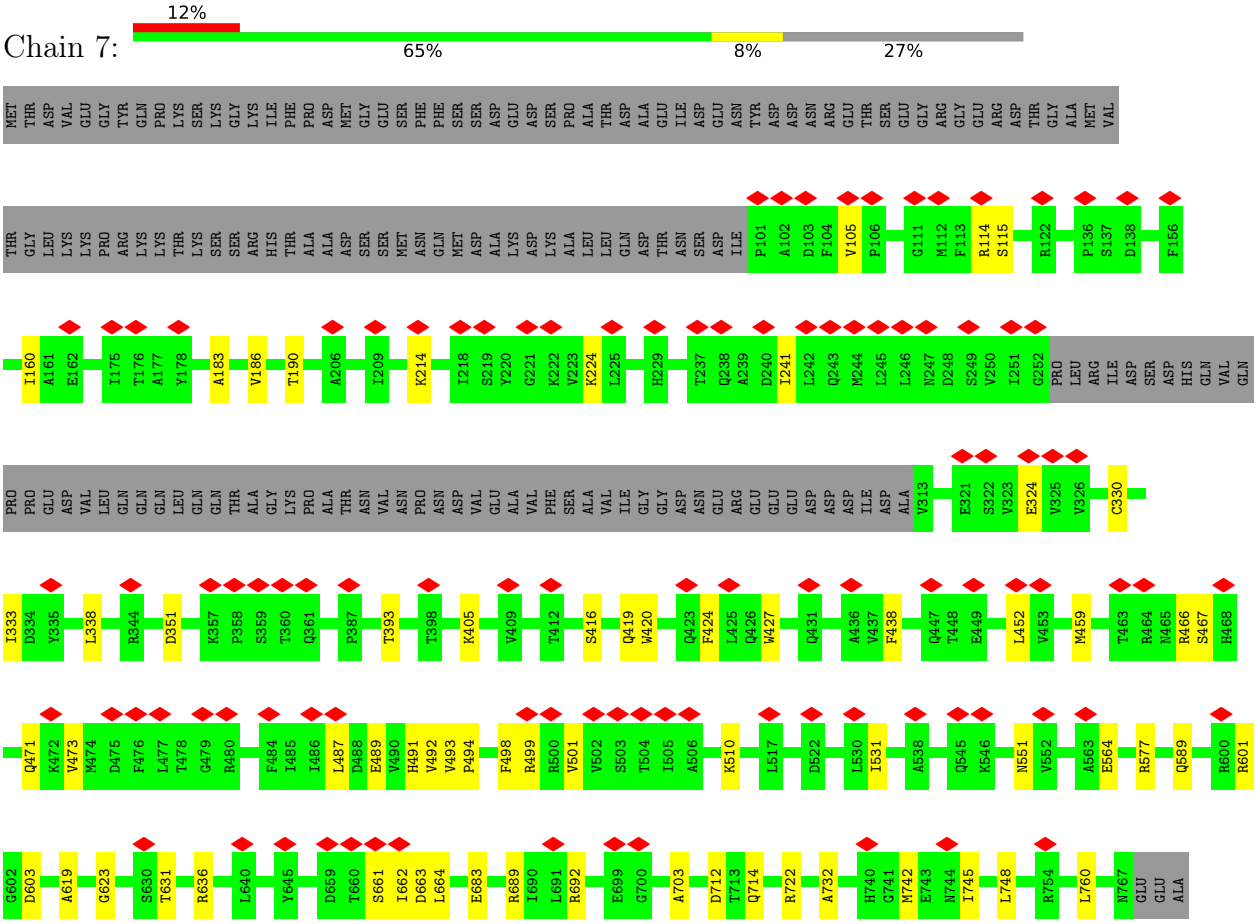
• Molecule 7: General transcription and DNA repair factor IIH subunit SSL1

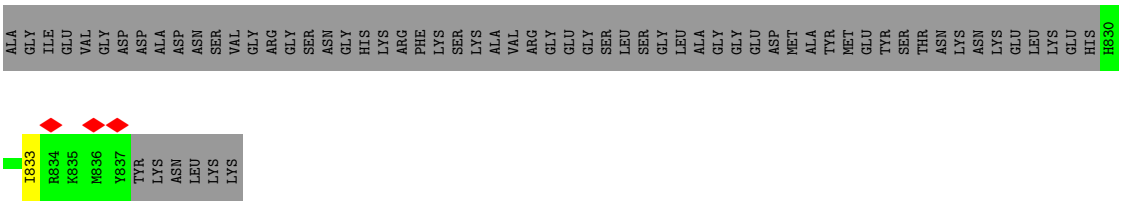
Chain 6:



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

Chain 7:



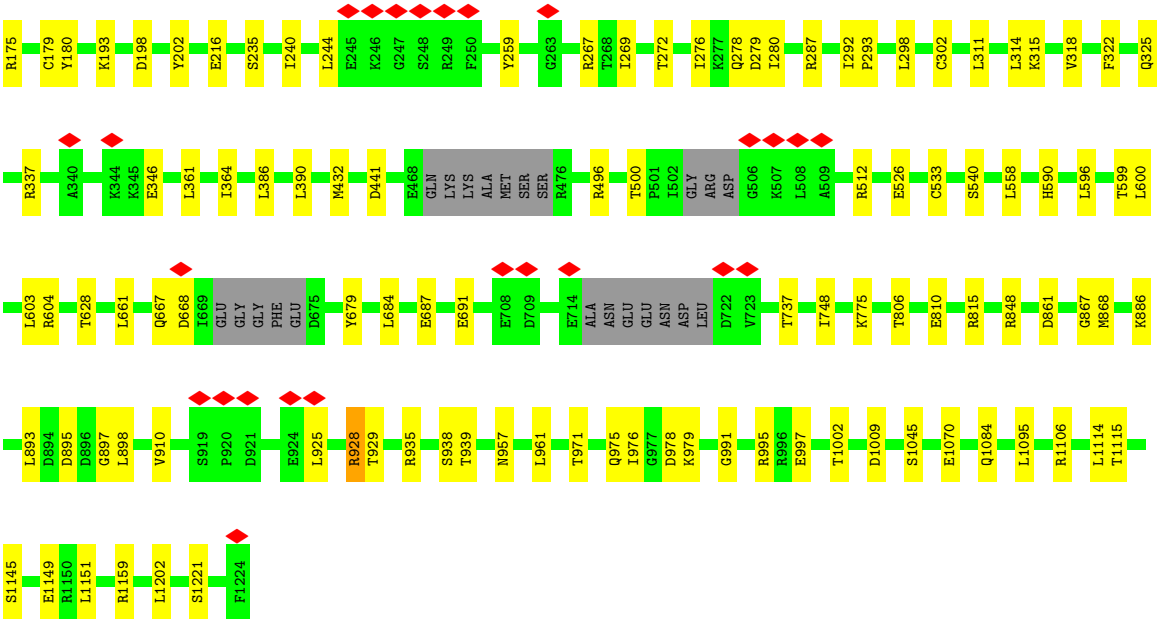


• Molecule 9: DNA-directed RNA polymerase II subunit RPB1

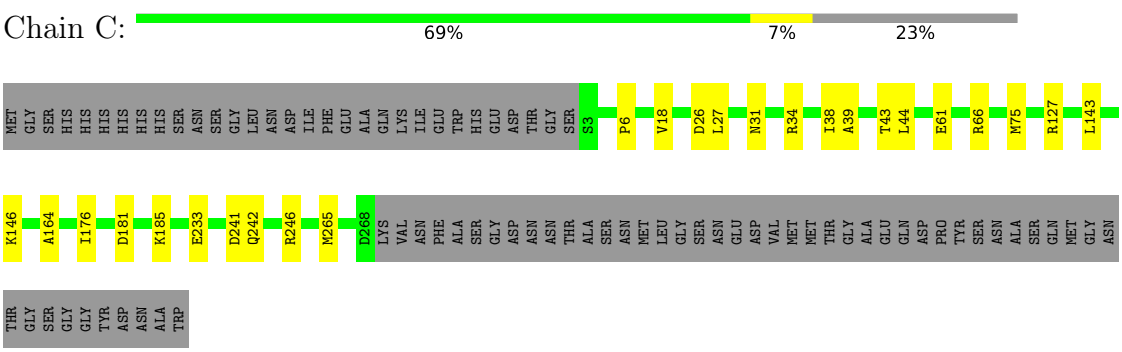
Chain A:

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

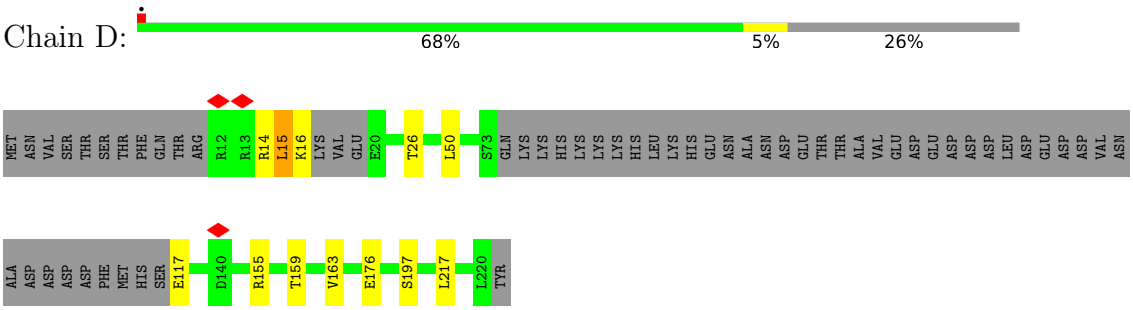
Chain B:



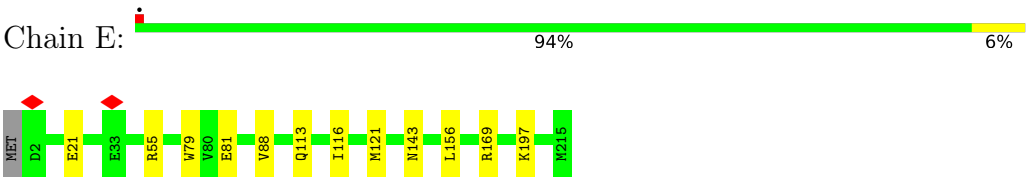
• Molecule 11: DNA-directed RNA polymerase II subunit RPB3



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

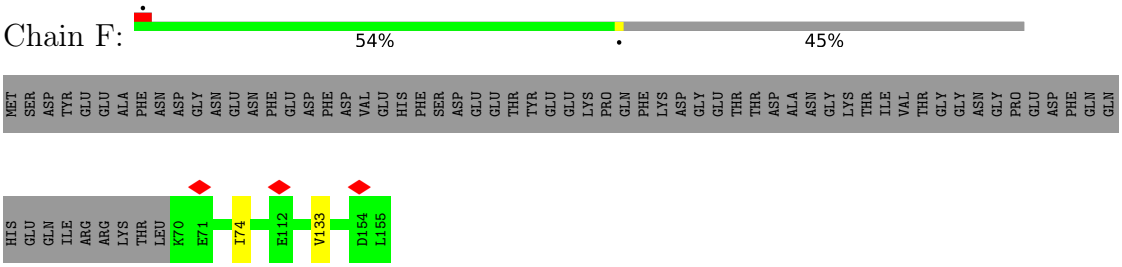


• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



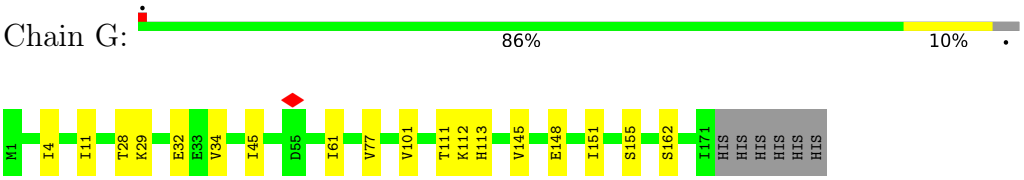
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



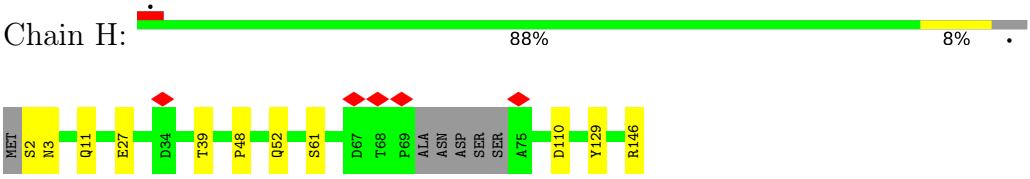
• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G:



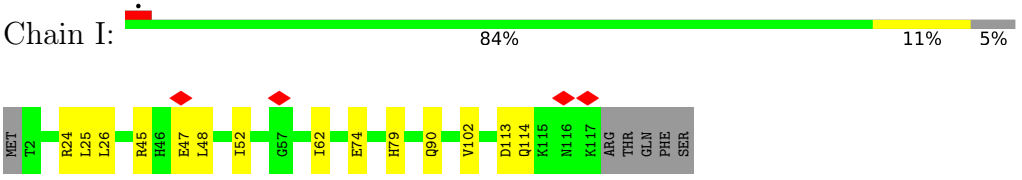
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



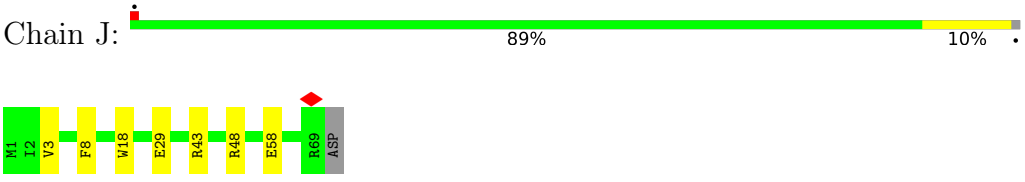
• Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:



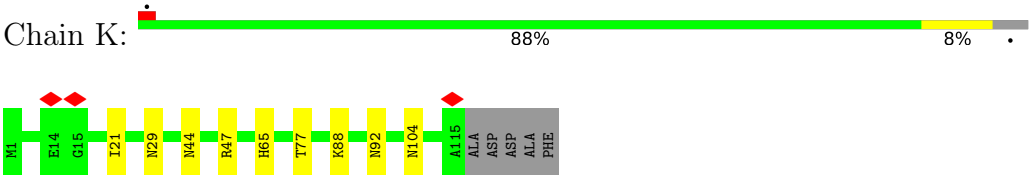
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



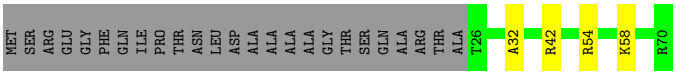
• Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K:



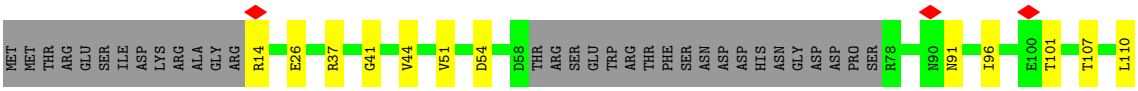
• Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

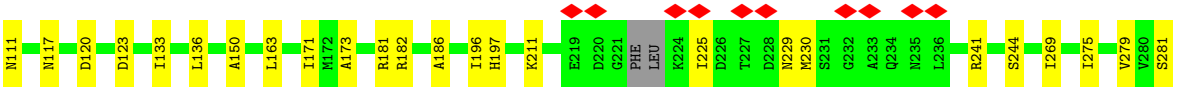
Chain L:

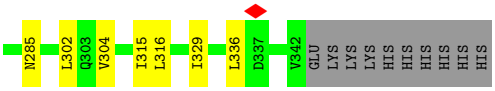


• Molecule 21: Transcription initiation factor IIB

Chain M:

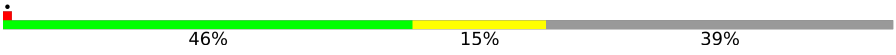


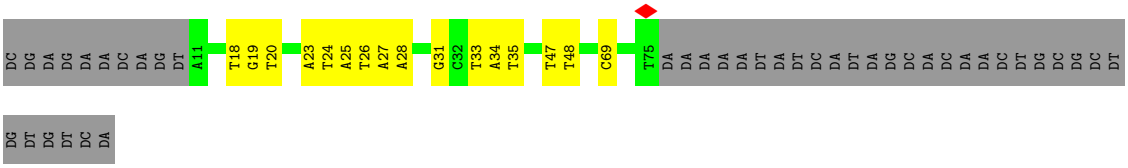




• Molecule 22: Non-template DNA

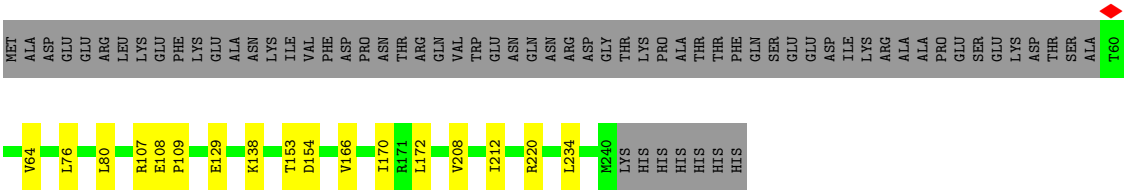
Chain N:





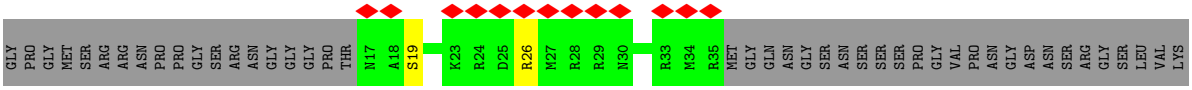
• Molecule 23: TATA-box-binding protein

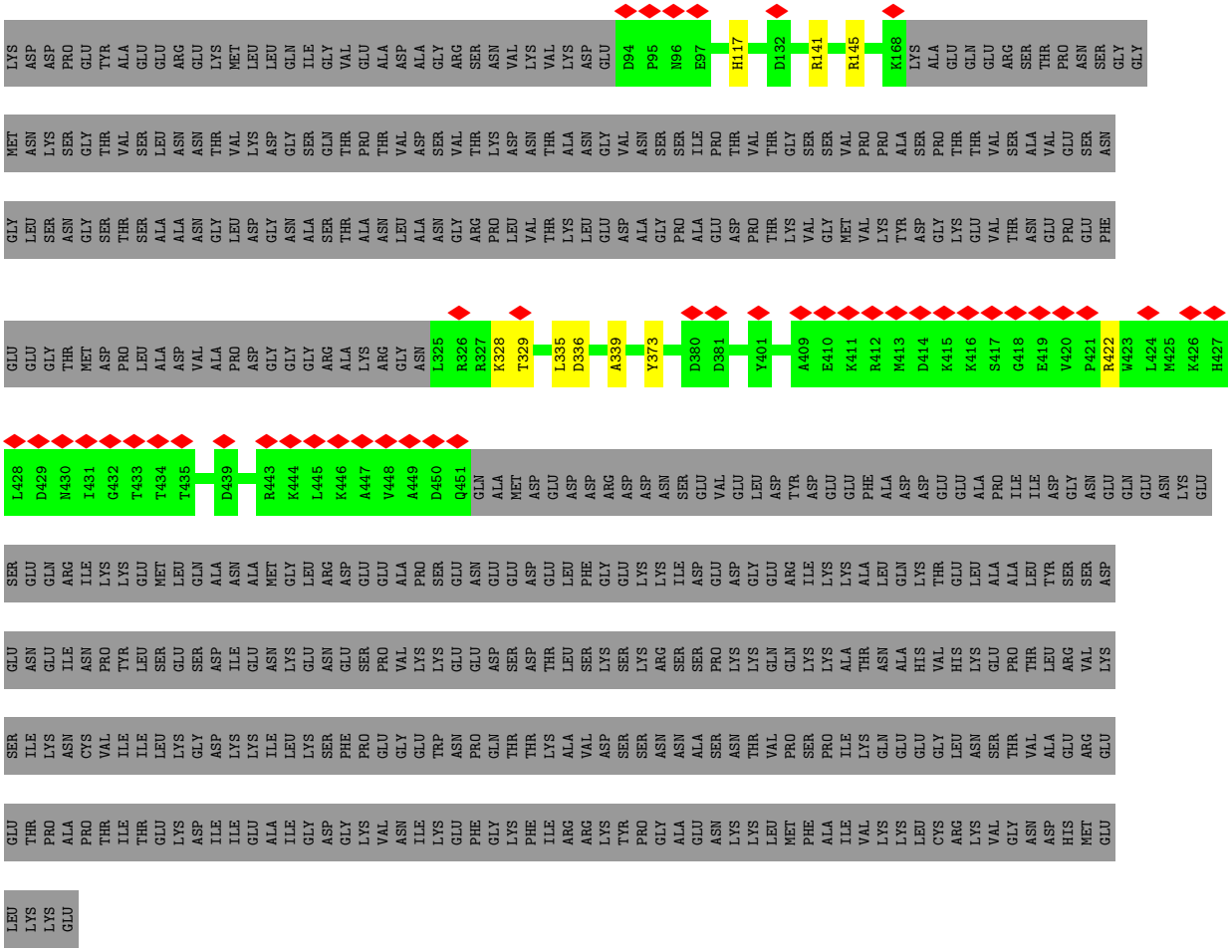
Chain O:



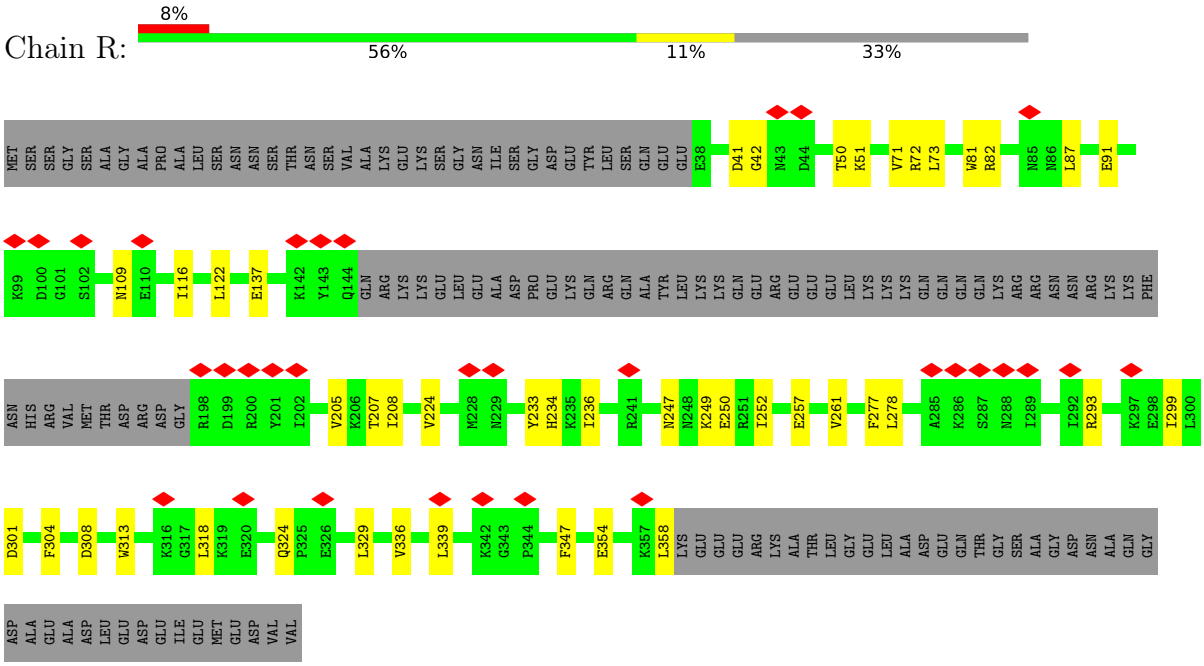
• Molecule 24: Transcription initiation factor IIF subunit alpha

Chain Q:

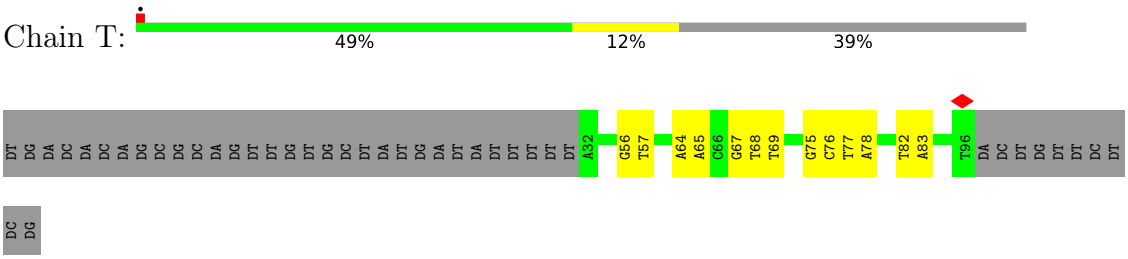




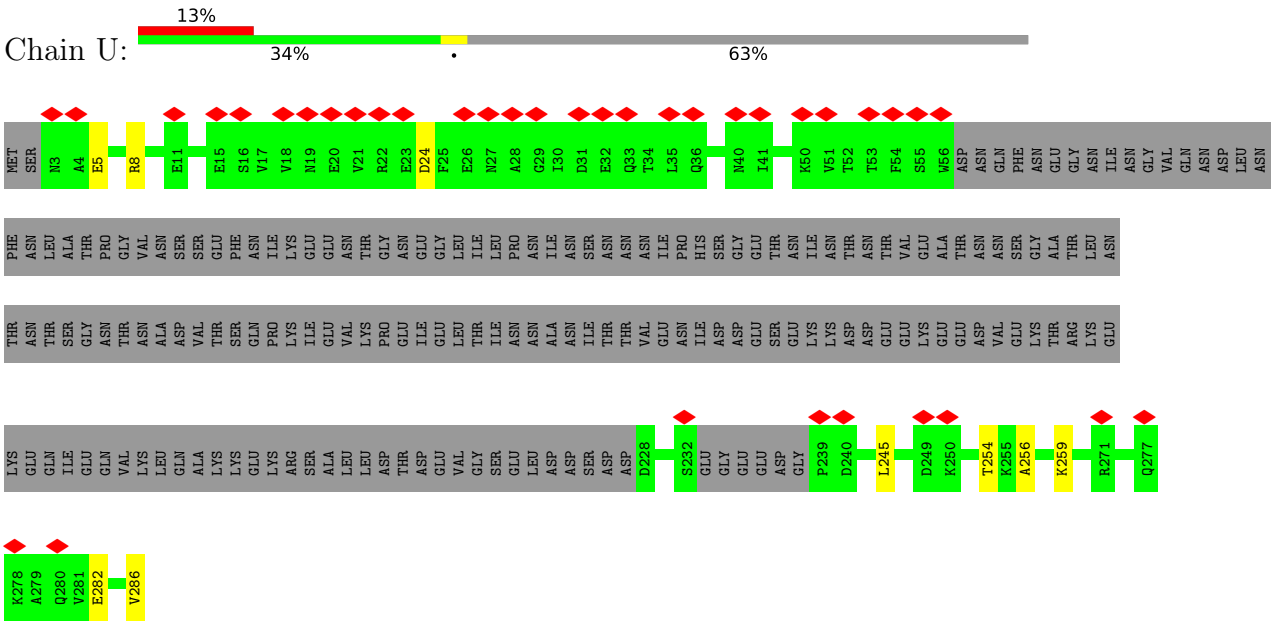
• Molecule 25: Transcription initiation factor IIF subunit beta



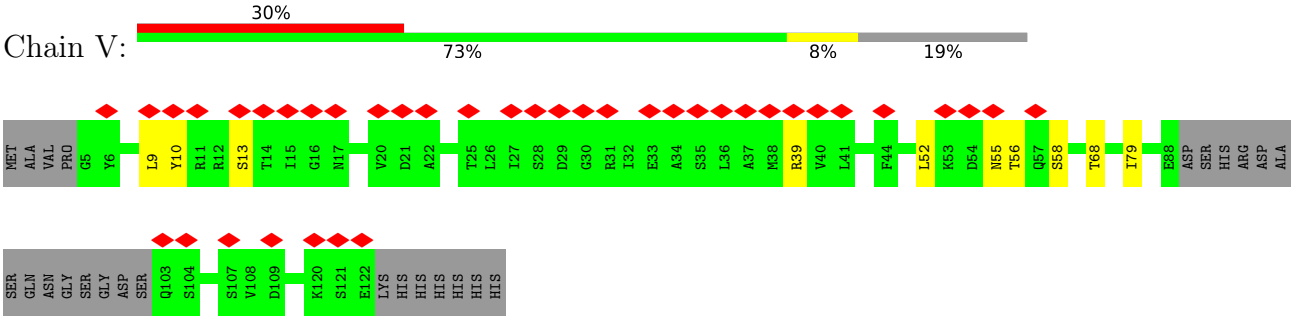
• Molecule 26: Template DNA



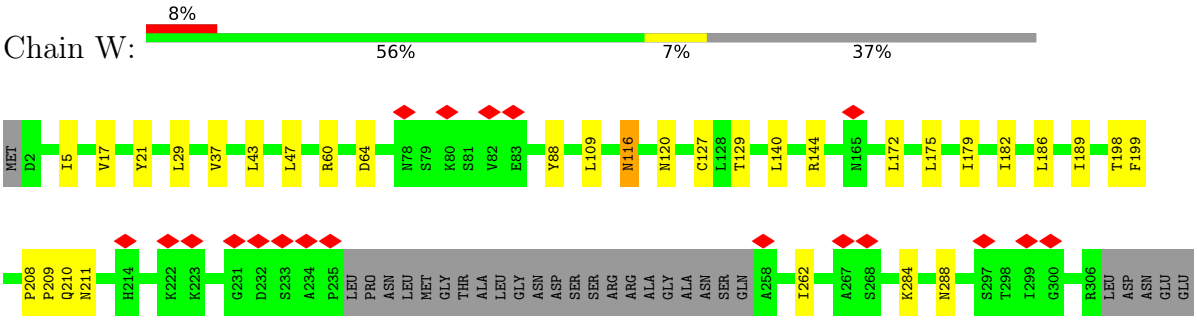
• Molecule 27: Transcription initiation factor IIA large subunit

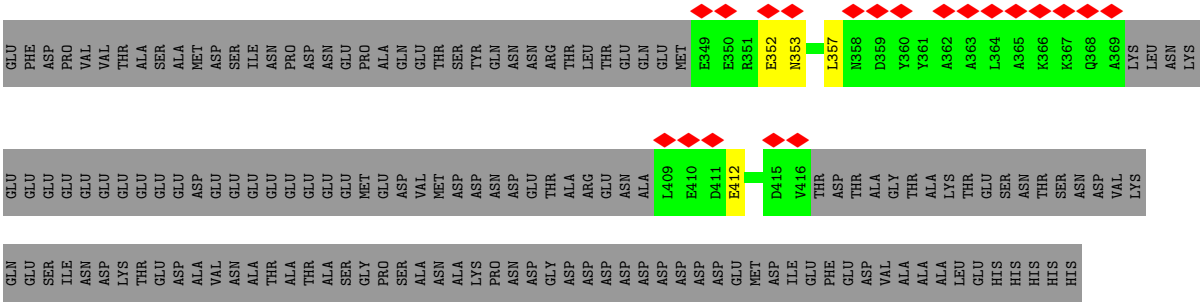


• Molecule 28: Transcription initiation factor IIA subunit 2

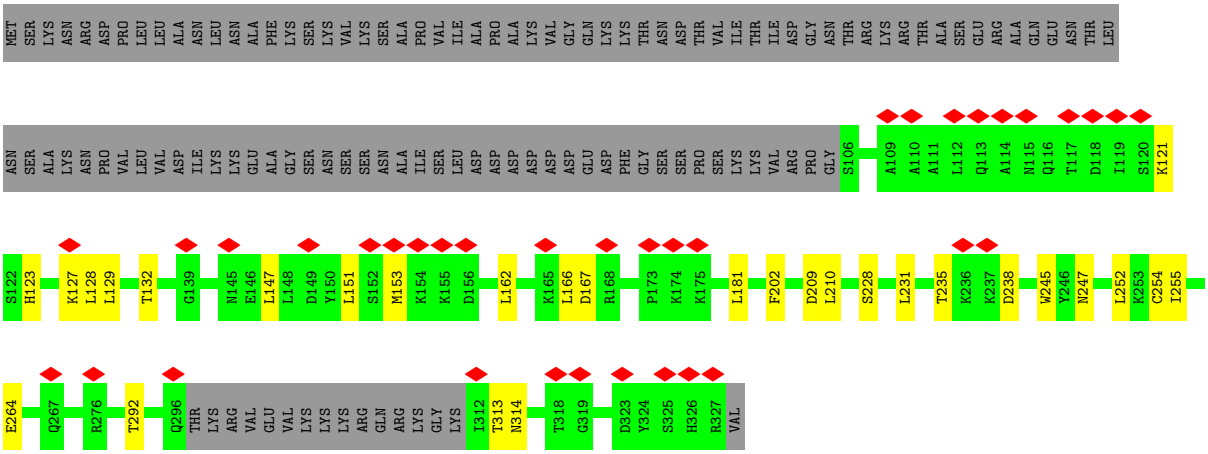


• Molecule 29: Transcription initiation factor IIE subunit alpha





• Molecule 30: Transcription initiation factor IIE subunit beta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10163	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	0.189	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	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: MG, ZN, BEF, SF4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.24	0/6209	0.39	0/8384
2	1	0.23	0/4277	0.37	0/5755
3	2	0.23	0/3664	0.37	0/4952
4	3	0.23	0/1109	0.36	0/1492
5	4	0.24	0/2312	0.39	0/3127
6	5	0.22	0/520	0.37	0/701
7	6	0.23	0/2851	0.39	0/3856
8	7	0.24	0/5059	0.39	0/6841
9	A	0.24	0/11439	0.40	0/15469
10	B	0.25	0/9589	0.41	0/12934
11	C	0.24	0/2130	0.40	0/2887
12	D	0.24	0/1314	0.40	0/1761
13	E	0.24	0/1788	0.38	0/2406
14	F	0.25	0/709	0.39	0/956
15	G	0.25	0/1367	0.41	0/1844
16	H	0.25	0/1139	0.43	0/1544
17	I	0.25	0/962	0.43	0/1295
18	J	0.25	0/578	0.39	0/775
19	K	0.25	0/942	0.40	0/1272
20	L	0.23	0/361	0.42	0/478
21	M	0.24	0/2387	0.39	0/3211
22	N	0.56	0/1492	0.98	0/2301
23	O	0.25	0/1449	0.43	0/1952
24	Q	0.24	0/1907	0.40	0/2556
25	R	0.23	0/2270	0.41	0/3052
26	T	0.56	0/1493	0.93	0/2302
27	U	0.22	0/898	0.39	0/1212
28	V	0.22	0/822	0.40	0/1109
29	W	0.23	0/2575	0.37	0/3473
30	X	0.23	0/1692	0.38	0/2280
All	All	0.26	0/75304	0.44	0/102177

There are no bond length outliers.

There are no bond angle outliers.

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	60	0
2	1	4214	0	4288	32	0
3	2	3597	0	3687	35	0
4	3	1089	0	1069	8	0
5	4	2274	0	2332	25	0
6	5	514	0	541	1	0
7	6	2794	0	2815	22	0
8	7	4954	0	4946	47	0
9	A	11238	0	11301	98	0
10	B	9404	0	9398	87	0
11	C	2092	0	2050	15	0
12	D	1307	0	1324	10	0
13	E	1752	0	1776	7	0
14	F	697	0	720	2	0
15	G	1339	0	1357	13	0
16	H	1120	0	1086	6	0
17	I	944	0	899	10	0
18	J	569	0	585	8	0
19	K	924	0	934	6	0
20	L	359	0	381	4	0
21	M	2360	0	2467	29	0
22	N	1332	0	737	13	0
23	O	1422	0	1500	12	0
24	Q	1871	0	1883	11	0
25	R	2230	0	2254	39	0
26	T	1330	0	734	9	0
27	U	885	0	866	7	0
28	V	815	0	822	7	0
29	W	2532	0	2529	27	0
30	X	1661	0	1694	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	0	8	0	0	0	0
32	3	2	0	0	0	0
32	4	1	0	0	0	0
32	6	4	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	W	1	0	0	0	0
33	7	4	0	0	1	0
34	7	1	0	0	0	0
34	A	1	0	0	0	0
35	7	27	0	12	1	0
All	All	73768	0	73142	583	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.

All (583) 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)
30:X:235:THR:OG1	30:X:238:ASP:O	1.89	0.91
10:B:276:ILE:HG21	10:B:280:ILE:HD11	1.61	0.82
21:M:91:ASN:ND2	21:M:123:ASP:OD2	2.11	0.82
8:7:662:ILE:O	8:7:689:ARG:NH1	2.13	0.82
10:B:151:LEU:HD23	10:B:153:ALA:H	1.44	0.82
9:A:846:GLU:OE2	9:A:1425:SER:OG	1.99	0.81
18:J:29:GLU:OE1	24:Q:26:ARG:NH1	2.15	0.80
10:B:272:THR:HG22	10:B:279:ASP:OD1	1.82	0.80
9:A:500:GLU:OE1	10:B:1145:SER:OG	2.01	0.79
21:M:181:ARG:O	21:M:229:ASN:ND2	2.15	0.79
1:0:335:LEU:HD21	1:0:399:LEU:HD12	1.64	0.78
9:A:407:ARG:NH2	21:M:26:GLU:OE2	2.17	0.78
23:O:153:THR:HG22	23:O:154:ASP:H	1.49	0.77
8:7:683:GLU:OE1	8:7:722:ARG:NH1	2.17	0.77
16:H:48:PRO:O	16:H:146:ARG:NH2	2.17	0.77
5:4:85:TYR:OH	7:6:405:SER:O	2.02	0.77
9:A:882:SER:O	9:A:1025:ARG:NH2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:175:ARG:NH1	10:B:198:ASP:O	2.18	0.77
9:A:894:GLU:OE1	9:A:933:TYR:OH	2.02	0.76
10:B:667:GLN:NE2	10:B:668:ASP:OD1	2.18	0.76
10:B:895:ASP:O	20:L:42:ARG:NH2	2.18	0.76
1:0:552:SER:OG	2:1:371:THR:OG1	2.03	0.76
9:A:5:GLN:O	10:B:1159:ARG:NH2	2.18	0.76
25:R:233:TYR:O	25:R:234:HIS:ND1	2.20	0.74
10:B:118:ARG:NH2	10:B:202:TYR:OH	2.20	0.74
21:M:133:ILE:HD11	21:M:150:ALA:HB1	1.69	0.74
11:C:31:ASN:OD1	11:C:34:ARG:NH2	2.20	0.74
1:0:366:LEU:HD11	4:3:72:ILE:HG21	1.70	0.74
21:M:281:SER:O	21:M:285:ASN:ND2	2.21	0.73
7:6:338:CYS:SG	7:6:339:HIS:CE1	2.81	0.73
10:B:995:ARG:NH1	10:B:997:GLU:OE2	2.22	0.73
1:0:270:ARG:NH2	1:0:389:GLU:O	2.21	0.73
21:M:211:LYS:NZ	21:M:230:MET:SD	2.62	0.72
29:W:37:VAL:HG12	29:W:88:TYR:HB3	1.72	0.71
5:4:31:GLU:OE1	5:4:180:THR:OG1	2.06	0.71
25:R:358:LEU:HD22	30:X:162:LEU:HD13	1.70	0.71
2:1:13:SER:OG	29:W:210:GLN:O	2.09	0.71
3:2:11:THR:HG23	3:2:84:LEU:HD11	1.73	0.71
9:A:107:CYS:SG	9:A:171:GLN:NE2	2.63	0.70
1:0:620:VAL:HG21	1:0:669:VAL:HG21	1.73	0.70
10:B:193:LYS:NZ	20:L:32:ALA:O	2.24	0.70
27:U:5:GLU:OE1	28:V:58:SER:OG	2.09	0.70
1:0:140:GLN:OE1	1:0:143:ARG:NH2	2.26	0.69
1:0:385:VAL:HG13	1:0:390:VAL:HG21	1.75	0.69
9:A:860:LEU:HD11	9:A:1393:ASN:O	1.93	0.69
12:D:217:LEU:HD12	12:D:217:LEU:O	1.93	0.68
3:2:11:THR:CG2	3:2:84:LEU:HD11	2.24	0.68
10:B:928:ARG:NH1	10:B:929:THR:O	2.27	0.68
25:R:116:ILE:HG22	25:R:236:ILE:HD11	1.75	0.68
5:4:220:GLU:N	5:4:220:GLU:OE1	2.27	0.68
9:A:1198:ASP:OD2	9:A:1201:ALA:N	2.27	0.68
10:B:390:LEU:HD23	10:B:390:LEU:O	1.94	0.68
9:A:663:SER:OG	10:B:1084:GLN:O	2.12	0.67
10:B:287:ARG:NH1	10:B:292:ILE:O	2.27	0.67
3:2:272:THR:HG22	3:2:273:LYS:H	1.60	0.67
7:6:128:LEU:HD13	7:6:233:LEU:HD23	1.77	0.67
13:E:88:VAL:HB	13:E:116:ILE:HG22	1.77	0.67
1:0:620:VAL:CG2	1:0:669:VAL:HG21	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:496:ARG:NH2	10:B:540:SER:O	2.29	0.66
3:2:139:SER:CB	3:2:272:THR:HG21	2.26	0.65
10:B:898:LEU:O	20:L:58:LYS:NZ	2.29	0.65
23:O:129:GLU:OE1	23:O:220:ARG:NH2	2.28	0.65
9:A:555:ASP:OD2	9:A:648:ASN:ND2	2.29	0.65
17:I:74:GLU:OE2	17:I:79:HIS:ND1	2.28	0.65
23:O:107:ARG:NH1	27:U:286:VAL:O	2.29	0.65
3:2:200:LEU:HD11	3:2:258:LEU:HD11	1.78	0.65
8:7:467:SER:O	8:7:471:GLN:N	2.29	0.65
11:C:146:LYS:NZ	18:J:58:GLU:OE2	2.29	0.65
9:A:888:GLY:O	9:A:940:ARG:NH2	2.29	0.65
13:E:156:LEU:HD11	13:E:197:LYS:HB2	1.79	0.64
10:B:976:ILE:HG22	10:B:976:ILE:O	1.97	0.64
10:B:975:GLN:N	10:B:978:ASP:OD2	2.30	0.64
25:R:137:GLU:N	25:R:137:GLU:OE1	2.31	0.64
9:A:159:THR:OG1	9:A:160:GLN:OE1	2.16	0.64
9:A:1009:ASN:OD1	9:A:1012:ARG:NH2	2.31	0.64
23:O:129:GLU:OE1	23:O:129:GLU:N	2.31	0.64
1:0:295:SER:OG	1:0:379:GLU:OE1	2.09	0.63
2:1:602:ASN:OD1	2:1:603:GLY:N	2.30	0.63
8:7:190:THR:HG21	8:7:214:LYS:HD3	1.80	0.63
9:A:445:ASN:OD1	9:A:446:ARG:N	2.31	0.63
1:0:594:ARG:NH2	2:1:230:PRO:O	2.30	0.63
7:6:173:ILE:HD11	7:6:199:ILE:HD13	1.81	0.63
7:6:155:ASP:OD2	7:6:298:LYS:NZ	2.31	0.63
1:0:438:THR:HG22	2:1:352:ASN:ND2	2.14	0.63
9:A:120:GLU:OE1	9:A:123:ARG:NH2	2.32	0.63
15:G:4:ILE:CD1	15:G:77:VAL:HG22	2.28	0.63
8:7:351:ASP:OD1	8:7:405:LYS:NZ	2.27	0.63
10:B:957:ASN:OD1	10:B:961:LEU:N	2.32	0.63
4:3:44:ASP:O	4:3:48:SER:OG	2.14	0.62
3:2:436:THR:HG21	8:7:732:ALA:HB1	1.80	0.62
10:B:104:GLU:OE2	10:B:110:HIS:NE2	2.31	0.62
25:R:250:GLU:OE1	25:R:250:GLU:N	2.31	0.62
1:0:586:TYR:OH	1:0:616:TYR:O	2.13	0.62
1:0:241:ASP:OD1	1:0:242:ASN:N	2.32	0.62
1:0:615:GLN:NE2	1:0:616:TYR:CE1	2.67	0.61
10:B:604:ARG:NH1	10:B:691:GLU:OE2	2.33	0.61
29:W:284:LYS:O	29:W:288:ASN:ND2	2.33	0.61
3:2:250:LEU:HD12	3:2:259:VAL:HG11	1.81	0.61
5:4:58:ILE:HD13	5:4:125:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:450:LEU:HD13	9:A:1077:THR:HG21	1.83	0.61
9:A:590:ARG:NH2	9:A:621:THR:OG1	2.32	0.61
5:4:30:ILE:HG22	5:4:32:ILE:HG23	1.82	0.61
21:M:182:ARG:NH1	21:M:225:ILE:O	2.34	0.61
18:J:3:VAL:HG21	18:J:18:TRP:CG	2.36	0.61
10:B:810:GLU:OE1	10:B:815:ARG:NH1	2.33	0.61
22:N:27:DA:H2'	22:N:28:DA:C8	2.36	0.61
9:A:767:GLN:NE2	9:A:768:GLN:O	2.34	0.60
8:7:393:THR:HG23	8:7:420:TRP:NE1	2.16	0.60
3:2:35:ILE:O	3:2:38:ILE:HG22	2.02	0.60
2:1:346:ASP:O	2:1:349:VAL:HG23	2.01	0.60
9:A:493:GLN:N	10:B:1149:GLU:OE2	2.35	0.60
23:O:172:LEU:HD13	23:O:208:VAL:HG22	1.84	0.60
17:I:45:ARG:NH1	17:I:47:GLU:OE1	2.33	0.60
5:4:224:LEU:O	5:4:227:THR:OG1	2.19	0.59
8:7:491:HIS:CD2	8:7:492:VAL:HG13	2.37	0.59
4:3:18:THR:HG23	4:3:18:THR:O	2.03	0.59
9:A:132:LYS:NZ	9:A:1417:GLU:OE2	2.29	0.59
10:B:269:ILE:HD11	10:B:386:LEU:HD21	1.85	0.59
25:R:122:LEU:CD2	25:R:224:VAL:HG22	2.33	0.59
9:A:1420:ASP:OD2	9:A:1422:ARG:NH2	2.35	0.59
25:R:87:LEU:O	25:R:87:LEU:HD23	2.03	0.59
1:0:335:LEU:HD21	1:0:399:LEU:CD1	2.32	0.59
3:2:151:VAL:HG11	3:2:358:ALA:HB1	1.84	0.59
26:T:64:DA:H2"	26:T:65:DA:H5"	1.83	0.59
9:A:2:VAL:N	21:M:54:ASP:OD2	2.35	0.59
2:1:469:MET:HA	5:4:38:THR:HG21	1.85	0.58
5:4:179:LEU:HD23	5:4:213:VAL:HB	1.85	0.58
5:4:58:ILE:CD1	5:4:125:LEU:HD23	2.33	0.58
1:0:690:ARG:HG3	1:0:701:LEU:HD23	1.86	0.58
11:C:241:ASP:OD1	11:C:242:GLN:N	2.36	0.58
8:7:420:TRP:CZ3	8:7:424:PHE:CD1	2.92	0.58
4:3:23:SER:O	4:3:26:VAL:HG12	2.04	0.58
8:7:510:LYS:HB3	8:7:531:ILE:HG22	1.84	0.58
23:O:108:GLU:OE1	23:O:138:LYS:NZ	2.37	0.58
2:1:231:TYR:O	2:1:262:ASN:ND2	2.37	0.58
5:4:210:ILE:HG22	5:4:231:THR:OG1	2.04	0.57
24:Q:117:HIS:NE2	25:R:137:GLU:OE2	2.37	0.57
9:A:1257:ASP:OD2	24:Q:422:ARG:NH2	2.35	0.57
10:B:512:ARG:NH1	10:B:533:CYS:O	2.37	0.57
10:B:278:GLN:OE1	10:B:337:ARG:NE	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:5:ILE:HG22	1:0:6:ASP:H	1.69	0.57
2:1:320:GLU:OE2	2:1:323:ARG:NH2	2.37	0.57
3:2:63:ASP:OD1	3:2:71:LYS:NZ	2.36	0.57
9:A:228:PHE:CE1	12:D:15:LEU:HD23	2.40	0.57
9:A:736:ASN:O	9:A:736:ASN:ND2	2.36	0.57
9:A:465:TYR:CD2	10:B:976:ILE:HD12	2.40	0.57
9:A:469:ARG:NH2	10:B:991:GLY:O	2.34	0.57
10:B:63:ILE:HD11	10:B:95:ILE:HD12	1.86	0.57
2:1:192:MET:SD	29:W:357:LEU:HD13	2.45	0.56
25:R:205:VAL:HG13	25:R:207:THR:HG23	1.86	0.56
1:0:54:SER:HA	1:0:89:LEU:HD11	1.87	0.56
11:C:233:GLU:OE1	18:J:43:ARG:NH2	2.35	0.56
8:7:498:PHE:CG	22:N:69:DC:OP1	2.58	0.56
8:7:589:GLN:HB3	8:7:748:LEU:HD22	1.87	0.56
3:2:139:SER:HB2	3:2:272:THR:HG21	1.88	0.56
7:6:336:CYS:SG	7:6:340:SER:N	2.79	0.56
1:0:463:ILE:HG23	1:0:463:ILE:O	2.06	0.56
21:M:107:THR:O	21:M:111:ASN:ND2	2.37	0.56
2:1:31:SER:OG	29:W:211:ASN:OD1	2.22	0.56
8:7:498:PHE:O	8:7:501:VAL:HG22	2.06	0.56
2:1:270:TYR:O	2:1:274:VAL:HG23	2.06	0.56
9:A:951:GLU:OE2	9:A:952:ALA:N	2.38	0.56
26:T:77:DT:H2"	26:T:78:DA:H8	1.70	0.56
1:0:711:ASP:OD1	1:0:712:MET:N	2.39	0.55
21:M:133:ILE:HD11	21:M:150:ALA:CB	2.36	0.55
21:M:186:ALA:O	21:M:241:ARG:NH2	2.39	0.55
30:X:147:LEU:O	30:X:151:LEU:HD23	2.07	0.55
3:2:450:ARG:NH2	8:7:712:ASP:OD2	2.39	0.55
8:7:427:TRP:CZ2	35:7:903:ADP:C2	2.95	0.55
3:2:139:SER:HB3	3:2:272:THR:HG21	1.88	0.55
10:B:216:GLU:OE1	10:B:500:THR:OG1	2.24	0.55
11:C:181:ASP:OD2	11:C:185:LYS:N	2.39	0.55
1:0:413:GLU:N	1:0:413:GLU:OE1	2.40	0.55
8:7:438:PHE:CZ	8:7:473:VAL:HG11	2.42	0.55
1:0:615:GLN:HG2	1:0:616:TYR:CD1	2.41	0.55
9:A:1279:ILE:HG23	9:A:1308:THR:CG2	2.37	0.55
25:R:41:ASP:OD1	25:R:42:GLY:N	2.41	0.54
10:B:63:ILE:CD1	10:B:95:ILE:HD12	2.37	0.54
25:R:318:LEU:CD2	25:R:329:LEU:HD21	2.37	0.54
8:7:564:GLU:HG3	8:7:760:LEU:HD22	1.89	0.54
3:2:116:GLU:N	3:2:116:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:336:VAL:HG12	30:X:129:LEU:HD21	1.89	0.54
9:A:544:ASP:OD1	9:A:545:GLN:N	2.39	0.54
10:B:346:GLU:OE1	24:Q:145:ARG:NH1	2.41	0.54
8:7:577:ARG:NH2	8:7:714:GLN:OE1	2.41	0.53
9:A:63:ARG:CZ	10:B:925:LEU:HD11	2.38	0.53
15:G:11:ILE:HD11	15:G:29:LYS:HG3	1.90	0.53
21:M:117:ASN:ND2	21:M:120:ASP:OD2	2.40	0.53
4:3:19:ASP:OD1	4:3:20:ARG:N	2.42	0.53
9:A:443:LEU:HD13	9:A:501:LEU:HD11	1.91	0.53
9:A:562:THR:O	9:A:576:GLN:NE2	2.42	0.53
16:H:110:ASP:O	16:H:129:TYR:N	2.41	0.53
2:1:249:VAL:CG1	29:W:262:ILE:HG22	2.38	0.53
8:7:833:ILE:O	8:7:833:ILE:HG22	2.09	0.53
25:R:91:GLU:O	25:R:109:ASN:ND2	2.41	0.53
5:4:69:SER:O	5:4:117:ARG:NH1	2.40	0.53
8:7:493:VAL:N	8:7:494:PRO:CD	2.72	0.53
9:A:465:TYR:CG	10:B:976:ILE:HD12	2.44	0.53
24:Q:373:TYR:OH	25:R:72:ARG:NH2	2.41	0.53
13:E:55:ARG:NH1	13:E:113:GLN:OE1	2.41	0.53
19:K:44:ASN:OD1	19:K:47:ARG:NH2	2.41	0.53
21:M:163:LEU:HD23	21:M:171:ILE:HD12	1.90	0.53
7:6:338:CYS:SG	7:6:339:HIS:N	2.82	0.53
22:N:26:DT:H2'	22:N:27:DA:C8	2.43	0.53
1:0:592:ASN:OD1	1:0:593:GLY:N	2.42	0.53
9:A:1382:THR:HG23	9:A:1382:THR:O	2.09	0.53
10:B:848:ARG:NH1	18:J:8:PHE:O	2.42	0.53
12:D:117:GLU:O	12:D:155:ARG:NH2	2.42	0.53
24:Q:373:TYR:O	25:R:82:ARG:NH1	2.41	0.53
1:0:333:SER:OG	1:0:337:ARG:NH1	2.42	0.52
3:2:347:ILE:HD11	3:2:378:ILE:HD11	1.90	0.52
8:7:186:VAL:HG13	8:7:186:VAL:O	2.08	0.52
7:6:109:ARG:NH1	7:6:441:ASP:OD2	2.42	0.52
9:A:1136:SER:O	9:A:1274:ARG:NE	2.42	0.52
10:B:136:THR:HG23	10:B:152:ILE:HG22	1.91	0.52
2:1:462:LEU:HD12	2:1:462:LEU:O	2.10	0.52
29:W:109:LEU:HD12	29:W:175:LEU:HD22	1.92	0.52
22:N:33:DT:H2"	22:N:34:DA:C8	2.44	0.52
29:W:17:VAL:HG21	29:W:29:LEU:HD13	1.92	0.52
29:W:21:TYR:OH	29:W:64:ASP:OD2	2.22	0.52
2:1:233:VAL:HG11	2:1:259:ILE:HA	1.92	0.52
3:2:272:THR:HG22	3:2:273:LYS:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:J:3:VAL:HG21	18:J:18:TRP:CB	2.40	0.52
29:W:179:ILE:HG22	29:W:179:ILE:O	2.09	0.52
29:W:352:GLU:N	29:W:352:GLU:OE1	2.43	0.52
18:J:3:VAL:HG21	18:J:18:TRP:HB2	1.92	0.52
8:7:424:PHE:CZ	8:7:452:LEU:HD13	2.45	0.51
10:B:1115:THR:O	10:B:1115:THR:HG22	2.11	0.51
1:0:134:ARG:O	1:0:138:ASN:N	2.41	0.51
9:A:500:GLU:OE2	9:A:1438:THR:OG1	2.23	0.51
25:R:358:LEU:HD22	30:X:162:LEU:CD1	2.41	0.51
30:X:209:ASP:OD1	30:X:210:LEU:N	2.44	0.51
9:A:935:GLN:NE2	9:A:939:ASP:OD1	2.44	0.51
3:2:356:GLN:O	3:2:360:LEU:HD23	2.11	0.51
8:7:510:LYS:CB	8:7:531:ILE:HG22	2.40	0.51
17:I:24:ARG:HH12	17:I:26:LEU:HD11	1.75	0.51
21:M:173:ALA:HB2	21:M:196:ILE:HG21	1.92	0.51
5:4:34:PRO:O	5:4:38:THR:HG23	2.10	0.51
5:4:194:ILE:HG21	7:6:384:MET:SD	2.51	0.51
9:A:1148:ILE:HD11	9:A:1198:ASP:HB2	1.92	0.51
21:M:279:VAL:HG21	21:M:304:VAL:HG21	1.93	0.51
1:0:109:THR:OG1	1:0:113:ASN:OD1	2.29	0.51
9:A:690:VAL:O	9:A:694:THR:HG23	2.11	0.51
16:H:2:SER:OG	16:H:3:ASN:N	2.40	0.51
9:A:1147:THR:HG23	17:I:48:LEU:CD1	2.41	0.51
8:7:393:THR:HG23	8:7:420:TRP:CE2	2.46	0.51
21:M:37:ARG:O	21:M:41:GLY:N	2.44	0.51
23:O:153:THR:HG22	23:O:154:ASP:N	2.22	0.51
2:1:16:ILE:CG1	2:1:27:LEU:HD21	2.42	0.50
10:B:128:LEU:HD11	10:B:170:LEU:HB2	1.93	0.50
1:0:135:ARG:NH1	1:0:391:THR:OG1	2.44	0.50
23:O:170:ILE:HD11	23:O:234:LEU:HD21	1.93	0.50
25:R:339:LEU:H	25:R:339:LEU:HD23	1.76	0.50
1:0:438:THR:HG22	2:1:352:ASN:HD21	1.75	0.50
5:4:258:LEU:H	5:4:258:LEU:HD23	1.77	0.50
26:T:82:DT:H2'	26:T:83:DA:C8	2.46	0.50
10:B:1221:SER:HB3	12:D:14:ARG:NH2	2.27	0.50
25:R:304:PHE:HE2	30:X:129:LEU:HD22	1.77	0.50
7:6:429:CYS:O	7:6:433:LYS:N	2.43	0.49
2:1:196:GLN:NE2	29:W:353:ASN:OD1	2.45	0.49
10:B:861:ASP:OD2	10:B:939:THR:OG1	2.24	0.49
3:2:130:VAL:CG2	3:2:134:LEU:HD13	2.42	0.49
7:6:120:ARG:NH1	7:6:307:PRO:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:601:ARG:NH1	8:7:603:ASP:OD2	2.42	0.49
10:B:244:LEU:HD23	10:B:244:LEU:H	1.76	0.49
26:T:77:DT:H2"	26:T:78:DA:C8	2.47	0.49
3:2:256:TYR:HB2	3:2:258:LEU:HD13	1.94	0.49
3:2:145:THR:HG22	3:2:155:LEU:HD21	1.94	0.49
10:B:679:TYR:OH	10:B:687:GLU:OE1	2.30	0.49
1:0:64:PRO:O	1:0:66:HIS:ND1	2.45	0.49
17:I:24:ARG:NH1	17:I:26:LEU:HD11	2.27	0.49
1:0:5:ILE:HG22	1:0:6:ASP:N	2.28	0.49
5:4:153:MET:O	5:4:157:LEU:HD23	2.12	0.49
10:B:806:THR:HG23	10:B:1045:SER:HA	1.95	0.49
28:V:10:TYR:O	28:V:13:SER:OG	2.32	0.48
9:A:394:ASN:ND2	9:A:398:GLU:OE1	2.46	0.48
22:N:31:DG:OP1	25:R:293:ARG:NE	2.46	0.48
25:R:301:ASP:OD1	30:X:121:LYS:NZ	2.45	0.48
8:7:419:GLN:NE2	8:7:661:SER:O	2.46	0.48
10:B:302:CYS:SG	10:B:311:LEU:HD21	2.53	0.48
10:B:737:THR:HG22	10:B:737:THR:O	2.13	0.48
27:U:8:ARG:NH1	28:V:55:ASN:OD1	2.46	0.48
9:A:216:VAL:O	9:A:220:THR:HG23	2.14	0.48
16:H:11:GLN:NE2	16:H:52:GLN:OE1	2.47	0.48
1:0:20:GLU:OE2	1:0:486:THR:N	2.43	0.48
21:M:275:ILE:O	21:M:279:VAL:HG23	2.14	0.48
9:A:254:GLU:OE1	10:B:935:ARG:NH2	2.45	0.48
9:A:1038:THR:HG22	9:A:1039:LYS:N	2.29	0.48
21:M:101:THR:O	21:M:101:THR:HG23	2.14	0.48
21:M:315:ILE:H	21:M:315:ILE:HD12	1.79	0.48
26:T:67:DG:H2"	26:T:68:DT:H5'	1.95	0.48
10:B:104:GLU:OE1	20:L:54:ARG:NE	2.46	0.48
3:2:250:LEU:CD1	3:2:259:VAL:HG11	2.43	0.48
13:E:79:TRP:NE1	13:E:81:GLU:OE1	2.46	0.48
10:B:61:ASP:OD2	25:R:249:LYS:NZ	2.47	0.47
10:B:661:LEU:HD11	10:B:684:LEU:HD11	1.96	0.47
25:R:233:TYR:O	25:R:234:HIS:CG	2.67	0.47
25:R:299:ILE:HD13	25:R:324:GLN:OE1	2.14	0.47
9:A:514:PRO:HG2	9:A:1067:LEU:HD11	1.94	0.47
25:R:347:PHE:CG	26:T:69:DT:H4'	2.49	0.47
9:A:1209:MET:HA	9:A:1212:VAL:HG22	1.97	0.47
11:C:26:ASP:OD1	11:C:27:LEU:N	2.48	0.47
2:1:437:LEU:HD11	5:4:307:ALA:HB1	1.96	0.47
1:0:83:LEU:HD13	1:0:177:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:29:ILE:HD11	5:4:176:LEU:HD12	1.97	0.47
8:7:742:MET:O	8:7:745:ILE:HG22	2.15	0.47
9:A:315:LEU:HD23	9:A:321:PRO:HA	1.96	0.47
9:A:362:ASP:OD2	9:A:459:ARG:NE	2.41	0.47
9:A:1223:ASP:O	9:A:1243:VAL:HG12	2.14	0.47
9:A:1230:GLU:N	9:A:1230:GLU:OE1	2.47	0.47
9:A:1348:LEU:HD21	9:A:1375:MET:CE	2.44	0.47
10:B:599:THR:O	10:B:603:LEU:HD23	2.15	0.47
21:M:279:VAL:HG22	21:M:302:LEU:HD13	1.96	0.47
1:0:289:LEU:HD21	1:0:383:LEU:HD13	1.96	0.47
9:A:335:ARG:HE	10:B:1202:LEU:HD23	1.79	0.47
9:A:512:VAL:CG2	9:A:634:THR:HG21	2.44	0.47
9:A:871:ASP:OD1	9:A:872:GLY:N	2.47	0.47
11:C:6:PRO:O	19:K:104:ASN:ND2	2.48	0.47
23:O:108:GLU:HB3	23:O:109:PRO:HD3	1.96	0.47
8:7:160:ILE:HG22	8:7:183:ALA:CB	2.45	0.47
9:A:254:GLU:CD	10:B:935:ARG:HH22	2.18	0.47
10:B:60:GLN:OE1	10:B:95:ILE:HG22	2.15	0.47
10:B:886:LYS:NZ	10:B:938:SER:O	2.38	0.47
9:A:228:PHE:CE1	12:D:15:LEU:CD2	2.99	0.46
9:A:474:VAL:HG22	9:A:474:VAL:O	2.15	0.46
1:0:30:LYS:O	1:0:34:VAL:HG12	2.15	0.46
7:6:173:ILE:CD1	7:6:199:ILE:HD13	2.44	0.46
9:A:542:GLU:OE2	9:A:569:LYS:NZ	2.35	0.46
19:K:29:ASN:OD1	19:K:77:THR:OG1	2.26	0.46
25:R:50:THR:HG23	25:R:51:LYS:HG2	1.98	0.46
25:R:122:LEU:HD23	25:R:224:VAL:HG22	1.97	0.46
25:R:318:LEU:HD21	25:R:329:LEU:HD11	1.98	0.46
3:2:433:LEU:HD11	3:2:438:VAL:CG2	2.46	0.46
5:4:287:PHE:O	5:4:296:LEU:N	2.48	0.46
7:6:334:THR:OG1	7:6:355:LYS:NZ	2.35	0.46
27:U:254:THR:O	27:U:256:ALA:N	2.43	0.46
10:B:235:SER:OG	10:B:267:ARG:NH2	2.49	0.46
3:2:433:LEU:HD11	3:2:438:VAL:HG23	1.97	0.46
9:A:346:ASP:OD1	10:B:1106:ARG:NE	2.47	0.46
9:A:440:ASP:OD1	9:A:498:ARG:NH2	2.40	0.46
10:B:1002:THR:HG21	10:B:1070:GLU:OE1	2.16	0.46
13:E:21:GLU:OE1	13:E:143:ASN:ND2	2.47	0.46
15:G:101:VAL:HG21	15:G:145:VAL:HG21	1.98	0.46
30:X:292:THR:HG22	30:X:292:THR:O	2.16	0.46
9:A:997:LEU:O	9:A:1011:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1257:ASP:OD1	9:A:1258:HIS:N	2.49	0.46
30:X:202:PHE:O	30:X:245:TRP:NE1	2.49	0.46
1:0:303:GLU:OE2	1:0:386:ARG:NE	2.48	0.46
3:2:375:LEU:HD23	3:2:375:LEU:H	1.81	0.46
24:Q:336:ASP:OD1	24:Q:339:ALA:HB3	2.16	0.46
25:R:277:PHE:CE2	25:R:278:LEU:HD23	2.51	0.46
3:2:7:LYS:HA	3:2:38:ILE:HD11	1.98	0.46
7:6:427:TYR:O	7:6:436:PHE:N	2.46	0.46
15:G:28:THR:O	15:G:32:GLU:OE1	2.33	0.46
29:W:412:GLU:OE1	29:W:412:GLU:N	2.41	0.46
2:1:445:THR:N	5:4:280:GLY:O	2.48	0.46
7:6:251:ILE:HD11	7:6:272:ILE:HD11	1.97	0.46
8:7:330:CYS:HA	8:7:333:ILE:HG22	1.98	0.46
30:X:127:LYS:NZ	30:X:153:MET:SD	2.70	0.46
1:0:5:ILE:HG21	1:0:29:LYS:HD3	1.98	0.45
2:1:184:LEU:HD13	2:1:220:PHE:CD1	2.52	0.45
12:D:26:THR:HG22	12:D:26:THR:O	2.15	0.45
19:K:88:LYS:O	19:K:92:ASN:ND2	2.49	0.45
7:6:114:ASN:O	7:6:114:ASN:ND2	2.49	0.45
9:A:1311:VAL:HG13	9:A:1311:VAL:O	2.17	0.45
10:B:315:LYS:O	10:B:318:VAL:HG22	2.16	0.45
23:O:76:LEU:CD1	23:O:80:LEU:HD11	2.46	0.45
10:B:136:THR:HG23	10:B:152:ILE:CG2	2.46	0.45
10:B:441:ASP:OD2	21:M:197:HIS:NE2	2.49	0.45
21:M:269:ILE:HD13	21:M:316:LEU:HD11	1.97	0.45
9:A:994:GLN:OE1	9:A:1023:ARG:NH1	2.49	0.45
1:0:381:LEU:O	1:0:385:VAL:HG23	2.16	0.45
3:2:140:ALA:O	3:2:144:GLU:N	2.44	0.45
5:4:289:CYS:O	5:4:293:LEU:N	2.47	0.45
8:7:487:LEU:HD12	8:7:531:ILE:HG21	1.98	0.45
10:B:95:ILE:HG23	25:R:252:ILE:HD12	1.97	0.45
3:2:239:ILE:HD11	3:2:247:ARG:HG2	1.98	0.45
9:A:928:LEU:HD21	9:A:987:VAL:HG21	1.99	0.45
10:B:292:ILE:N	10:B:293:PRO:CD	2.80	0.45
10:B:558:LEU:HD21	10:B:600:LEU:HD11	1.98	0.45
29:W:60:ARG:NH2	30:X:264:GLU:OE2	2.50	0.45
3:2:466:GLN:OE1	3:2:466:GLN:N	2.49	0.45
9:A:672:ASP:OD1	9:A:675:THR:HG22	2.17	0.45
11:C:43:THR:HG22	11:C:44:LEU:N	2.31	0.45
13:E:116:ILE:HD11	13:E:121:MET:SD	2.56	0.45
15:G:155:SER:O	15:G:155:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:277:PHE:CZ	25:R:278:LEU:HD23	2.52	0.45
1:0:722:ARG:NH1	7:6:266:LEU:O	2.48	0.45
2:1:270:TYR:CZ	2:1:274:VAL:HG21	2.52	0.45
2:1:559:GLU:OE2	2:1:563:HIS:NE2	2.49	0.45
9:A:312:PRO:HG3	21:M:110:LEU:HD12	1.99	0.45
9:A:932:GLU:OE1	9:A:1028:THR:OG1	2.31	0.45
28:V:52:LEU:O	28:V:56:THR:HG22	2.17	0.45
1:0:56:THR:HG21	1:0:233:ILE:HD11	1.99	0.44
6:5:43:ASN:OD1	6:5:45:SER:N	2.47	0.44
11:C:75:MET:O	11:C:246:ARG:NH2	2.50	0.44
17:I:113:ASP:OD1	17:I:114:GLN:N	2.50	0.44
22:N:47:DT:H2'	22:N:48:DT:H72	1.99	0.44
27:U:259:LYS:NZ	27:U:282:GLU:OE1	2.50	0.44
10:B:90:ILE:HD12	10:B:432:MET:SD	2.57	0.44
11:C:39:ALA:HA	11:C:164:ALA:HB3	1.99	0.44
26:T:82:DT:C2'	26:T:83:DA:C8	3.00	0.44
9:A:1224:LEU:HD23	9:A:1224:LEU:H	1.82	0.44
12:D:176:GLU:OE1	12:D:197:SER:OG	2.30	0.44
15:G:113:HIS:NE2	29:W:120:ASN:OD1	2.50	0.44
2:1:263:TYR:CD1	2:1:296:LEU:HD22	2.52	0.44
9:A:709:THR:HG22	9:A:710:LEU:N	2.33	0.44
10:B:361:LEU:HB3	10:B:364:ILE:HD12	1.98	0.44
23:O:166:VAL:HG13	23:O:212:ILE:HD13	1.98	0.44
29:W:140:LEU:HD11	29:W:144:ARG:HD3	1.99	0.44
1:0:334:PHE:CE1	1:0:369:ILE:HG23	2.52	0.44
1:0:497:ILE:HG21	1:0:525:MET:HE1	1.99	0.44
29:W:127:CYS:SG	29:W:129:THR:OG1	2.62	0.44
1:0:614:HIS:N	1:0:675:ASP:OD2	2.50	0.44
3:2:369:ARG:HG3	3:2:374:VAL:HG22	2.00	0.44
9:A:96:ILE:HG21	9:A:176:LYS:HE2	2.00	0.44
9:A:691:LEU:O	9:A:694:THR:OG1	2.31	0.44
10:B:867:GLY:O	10:B:868:MET:CG	2.66	0.44
15:G:148:GLU:OE2	15:G:162:SER:OG	2.33	0.44
21:M:329:ILE:HD12	21:M:336:LEU:HD13	1.99	0.44
5:4:276:CYS:SG	5:4:277:TYR:N	2.91	0.44
9:A:1384:VAL:HG12	9:A:1384:VAL:O	2.17	0.44
13:E:169:ARG:HH12	14:F:74:ILE:HD11	1.83	0.44
1:0:495:MET:CG	1:0:680:VAL:HG12	2.48	0.44
9:A:174:ILE:CG2	9:A:181:LEU:HD22	2.48	0.44
1:0:443:SER:HA	1:0:446:ILE:HG22	1.99	0.43
2:1:249:VAL:HG12	29:W:262:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:105:VAL:HG23	8:7:105:VAL:O	2.18	0.43
10:B:979:LYS:HD2	10:B:1095:LEU:HD12	2.00	0.43
5:4:64:HIS:O	5:4:71:ASN:ND2	2.49	0.43
7:6:214:LEU:HD12	7:6:254:LEU:HD11	2.00	0.43
1:0:551:VAL:HG11	2:1:375:LEU:HD21	2.00	0.43
1:0:68:LYS:O	1:0:231:ILE:N	2.43	0.43
9:A:1260:LEU:HD23	9:A:1263:ILE:HD11	2.01	0.43
22:N:18:DT:H2"	22:N:19:DG:C8	2.53	0.43
30:X:202:PHE:O	30:X:245:TRP:CD1	2.71	0.43
1:0:108:LEU:HD23	1:0:109:THR:N	2.33	0.43
3:2:146:ILE:HD11	3:2:167:LEU:HD11	2.01	0.43
4:3:106:TYR:CZ	4:3:110:LEU:HD11	2.53	0.43
9:A:335:ARG:NH2	10:B:1114:LEU:HD21	2.33	0.43
15:G:11:ILE:HD11	15:G:29:LYS:CG	2.48	0.43
25:R:313:TRP:HE1	25:R:318:LEU:HA	1.84	0.43
8:7:416:SER:CB	8:7:661:SER:HG	2.31	0.43
4:3:16:CYS:O	29:W:172:LEU:HD21	2.19	0.43
8:7:663:ASP:O	8:7:664:LEU:HD22	2.19	0.43
10:B:590:HIS:CD2	10:B:596:LEU:HD22	2.54	0.43
10:B:976:ILE:O	10:B:976:ILE:CG2	2.64	0.43
24:Q:19:SER:O	24:Q:19:SER:OG	2.33	0.43
8:7:224:LYS:HG2	8:7:338:LEU:HD21	2.00	0.43
9:A:1443:VAL:HG13	15:G:61:ILE:HB	2.01	0.43
22:N:33:DT:H2"	22:N:34:DA:H8	1.83	0.43
29:W:182:ILE:O	29:W:186:LEU:HD23	2.18	0.43
30:X:167:ASP:O	30:X:181:LEU:HD23	2.18	0.43
2:1:286:ARG:NH1	2:1:310:ILE:HD12	2.33	0.43
8:7:564:GLU:CG	8:7:760:LEU:HD22	2.49	0.43
9:A:1348:LEU:HD21	9:A:1375:MET:HE2	2.00	0.43
1:0:666:LEU:HD22	1:0:679:MET:HB3	2.00	0.43
8:7:619:ALA:O	8:7:623:GLY:N	2.52	0.43
9:A:1206:ASP:C	9:A:1207:LEU:HD12	2.40	0.43
25:R:71:VAL:CG1	25:R:224:VAL:HG23	2.49	0.43
8:7:241:ILE:HD12	8:7:241:ILE:H	1.84	0.42
10:B:240:ILE:HG23	10:B:240:ILE:O	2.19	0.42
10:B:322:PHE:O	10:B:325:GLN:NE2	2.52	0.42
2:1:30:ARG:HD2	2:1:31:SER:O	2.19	0.42
9:A:512:VAL:HG23	9:A:634:THR:HG21	2.02	0.42
25:R:73:LEU:HD21	25:R:81:TRP:CE3	2.54	0.42
8:7:338:LEU:HD23	8:7:338:LEU:H	1.84	0.42
9:A:1293:SER:N	9:A:1297:GLU:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:2:SER:OG	16:H:61:SER:OG	2.35	0.42
17:I:62:ILE:HG21	17:I:102:VAL:HG11	2.01	0.42
29:W:116:ASN:O	29:W:116:ASN:ND2	2.50	0.42
8:7:551:ASN:O	8:7:703:ALA:N	2.43	0.42
9:A:1428:VAL:HG13	10:B:1151:LEU:HD13	2.01	0.42
10:B:1009:ASP:OD2	18:J:48:ARG:NH2	2.52	0.42
27:U:24:ASP:OD2	28:V:39:ARG:NH1	2.52	0.42
30:X:231:LEU:HD23	30:X:252:LEU:HD21	2.00	0.42
2:1:16:ILE:HG13	2:1:27:LEU:HD21	2.01	0.42
24:Q:141:ARG:O	25:R:208:ILE:N	2.44	0.42
26:T:56:DG:H2'	26:T:57:DT:H72	2.01	0.42
22:N:23:DA:H2"	22:N:24:DT:H5'	2.01	0.42
1:0:634:ILE:HD12	1:0:634:ILE:H	1.84	0.42
8:7:493:VAL:HG12	8:7:494:PRO:HD3	2.01	0.42
8:7:631:THR:O	8:7:636:ARG:NH2	2.50	0.42
9:A:298:PHE:HE2	21:M:96:ILE:HD12	1.85	0.42
9:A:350:ARG:NH1	9:A:488:ASN:OD1	2.45	0.42
9:A:471:ASN:O	9:A:474:VAL:HG12	2.20	0.42
12:D:15:LEU:HB3	12:D:16:LYS:H	1.52	0.42
25:R:318:LEU:HD22	25:R:329:LEU:HD21	2.01	0.42
1:0:232:VAL:HG21	1:0:453:PHE:CG	2.55	0.42
10:B:628:THR:O	10:B:628:THR:HG22	2.20	0.42
22:N:24:DT:H2'	22:N:25:DA:C8	2.55	0.42
7:6:336:CYS:SG	7:6:339:HIS:N	2.88	0.42
21:M:136:LEU:HD13	21:M:196:ILE:HD11	2.00	0.42
1:0:625:ILE:HD12	1:0:685:ARG:HB2	2.02	0.42
3:2:224:PHE:O	3:2:228:LEU:N	2.49	0.42
8:7:459:MET:O	8:7:466:ARG:NH2	2.53	0.42
22:N:26:DT:H2'	22:N:27:DA:N7	2.34	0.42
25:R:257:GLU:OE2	25:R:261:VAL:HG11	2.20	0.42
29:W:198:THR:HG22	29:W:199:PHE:N	2.35	0.42
7:6:450:ASN:OD1	7:6:450:ASN:N	2.52	0.41
8:7:114:ARG:HG3	8:7:114:ARG:O	2.20	0.41
8:7:324:GLU:OE2	8:7:499:ARG:NH2	2.53	0.41
9:A:123:ARG:NH2	9:A:155:GLU:OE2	2.49	0.41
9:A:1147:THR:HG23	17:I:48:LEU:HD13	2.02	0.41
15:G:34:VAL:HG12	15:G:45:ILE:HG21	2.02	0.41
29:W:179:ILE:O	29:W:179:ILE:CG2	2.67	0.41
30:X:228:SER:O	30:X:247:ASN:ND2	2.50	0.41
30:X:313:THR:O	30:X:314:ASN:OD1	2.37	0.41
3:2:67:ASN:OD1	3:2:68:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:179:CYS:SG	10:B:180:TYR:N	2.93	0.41
15:G:111:THR:HG22	15:G:112:LYS:N	2.36	0.41
15:G:151:ILE:HG23	15:G:151:ILE:O	2.21	0.41
22:N:19:DG:C8	22:N:20:DT:H72	2.55	0.41
28:V:68:THR:O	28:V:79:ILE:N	2.50	0.41
2:1:180:LEU:HD21	2:1:221:ALA:HB2	2.03	0.41
3:2:217:ASP:OD1	3:2:218:LEU:N	2.54	0.41
5:4:210:ILE:HG23	5:4:210:ILE:O	2.21	0.41
9:A:1163:ILE:H	9:A:1163:ILE:HD12	1.85	0.41
10:B:540:SER:OG	10:B:748:ILE:O	2.31	0.41
29:W:5:ILE:HD11	29:W:189:ILE:HA	2.02	0.41
7:6:140:ASP:OD1	7:6:141:LEU:N	2.53	0.41
9:A:356:ASP:OD2	19:K:65:HIS:NE2	2.49	0.41
9:A:1446:ASP:HB2	14:F:133:VAL:HG23	2.01	0.41
11:C:265:MET:HE1	19:K:21:ILE:HD11	2.02	0.41
16:H:27:GLU:OE2	16:H:39:THR:HG23	2.20	0.41
3:2:125:VAL:HG12	3:2:125:VAL:O	2.21	0.41
11:C:66:ARG:NH2	11:C:143:LEU:O	2.47	0.41
12:D:50:LEU:HD11	15:G:4:ILE:CG1	2.50	0.41
24:Q:335:LEU:H	24:Q:335:LEU:HD23	1.85	0.41
5:4:288:ILE:HG22	5:4:295:VAL:HA	2.02	0.41
9:A:683:ILE:HG21	9:A:801:GLU:HG3	2.01	0.41
10:B:298:LEU:HD13	10:B:314:LEU:HD13	2.03	0.41
17:I:52:ILE:O	17:I:90:GLN:NE2	2.51	0.41
21:M:14:ARG:O	21:M:14:ARG:NE	2.52	0.41
27:U:245:LEU:HD13	28:V:9:LEU:O	2.21	0.41
29:W:208:PRO:HA	29:W:209:PRO:HD3	1.97	0.41
30:X:254:CYS:O	30:X:255:ILE:HD13	2.20	0.41
1:0:497:ILE:HG21	1:0:525:MET:CE	2.51	0.41
9:A:1002:GLY:HA3	9:A:1007:ILE:HG21	2.03	0.41
3:2:141:ASN:O	3:2:145:THR:HG23	2.21	0.41
10:B:893:LEU:HD22	10:B:897:GLY:C	2.40	0.41
17:I:25:LEU:C	17:I:26:LEU:HD12	2.40	0.41
23:O:64:VAL:O	23:O:64:VAL:HG13	2.20	0.41
24:Q:328:LYS:O	24:Q:329:THR:HG23	2.20	0.41
25:R:308:ASP:OD2	30:X:123:HIS:NE2	2.54	0.41
1:0:601:VAL:HG12	1:0:603:ARG:H	1.85	0.41
2:1:234:LEU:HD12	2:1:263:TYR:CZ	2.55	0.41
7:6:135:ALA:O	7:6:145:ARG:NH1	2.52	0.41
8:7:689:ARG:NH2	8:7:692:ARG:NH2	2.69	0.41
9:A:694:THR:HG22	9:A:714:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:86:ARG:NH1	10:B:138:GLU:OE1	2.53	0.41
22:N:34:DA:H2'	22:N:35:DT:H71	2.02	0.41
30:X:128:LEU:HD23	30:X:132:THR:HG23	2.03	0.41
1:0:678:VAL:HG11	1:0:717:THR:HG23	2.03	0.41
9:A:115:LEU:HD21	9:A:145:LYS:HD2	2.03	0.41
10:B:259:TYR:OH	10:B:279:ASP:OD2	2.36	0.41
11:C:18:VAL:HG13	11:C:18:VAL:O	2.21	0.41
8:7:115:SER:O	8:7:115:SER:OG	2.32	0.40
9:A:1279:ILE:HG23	9:A:1308:THR:HG21	2.03	0.40
21:M:44:VAL:HG12	21:M:51:VAL:HG22	2.03	0.40
25:R:247:ASN:OD1	25:R:247:ASN:N	2.54	0.40
25:R:354:GLU:HG2	30:X:166:LEU:HD22	2.04	0.40
29:W:140:LEU:HD11	29:W:144:ARG:CD	2.51	0.40
1:0:5:ILE:O	1:0:6:ASP:C	2.59	0.40
10:B:106:ASP:OD1	10:B:108:VAL:HG12	2.21	0.40
1:0:277:VAL:HG23	1:0:278:ASP:N	2.35	0.40
1:0:310:PRO:HB3	1:0:404:THR:HG23	2.02	0.40
1:0:619:THR:HG22	1:0:678:VAL:HG22	2.02	0.40
4:3:14:PRO:O	4:3:17:LYS:NZ	2.47	0.40
12:D:159:THR:O	12:D:163:VAL:HG23	2.21	0.40
26:T:75:DG:H2"	26:T:76:DC:C6	2.57	0.40
5:4:254:ILE:O	5:4:259:ARG:NH2	2.55	0.40
8:7:489:GLU:OE2	33:7:901:BEF:F1	2.29	0.40
9:A:1443:VAL:HG13	9:A:1443:VAL:O	2.20	0.40
10:B:108:VAL:HG23	21:M:244:SER:HB2	2.04	0.40
10:B:971:THR:OG1	11:C:61:GLU:CD	2.59	0.40
11:C:38:ILE:HG13	11:C:176:ILE:HD12	2.04	0.40
29:W:43:LEU:HD12	29:W:47:LEU:HD13	2.02	0.40
1:0:334:PHE:CZ	1:0:369:ILE:HG23	2.57	0.40
1:0:374:LEU:HD23	1:0:410:SER:HB3	2.03	0.40
2:1:184:LEU:HD13	2:1:220:PHE:CG	2.57	0.40
10:B:526:GLU:OE2	10:B:775:LYS:NZ	2.48	0.40
10:B:910:VAL:O	10:B:910:VAL:HG13	2.21	0.40

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%)	733 (98%)	17 (2%)	0	100	100
2	1	508/645 (79%)	505 (99%)	3 (1%)	0	100	100
3	2	435/517 (84%)	432 (99%)	3 (1%)	0	100	100
4	3	129/324 (40%)	126 (98%)	3 (2%)	0	100	100
5	4	287/341 (84%)	286 (100%)	1 (0%)	0	100	100
6	5	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
7	6	352/464 (76%)	348 (99%)	4 (1%)	0	100	100
8	7	609/843 (72%)	593 (97%)	16 (3%)	0	100	100
9	A	1420/1733 (82%)	1392 (98%)	27 (2%)	1 (0%)	51	82
10	B	1168/1224 (95%)	1129 (97%)	39 (3%)	0	100	100
11	C	264/347 (76%)	259 (98%)	5 (2%)	0	100	100
12	D	157/221 (71%)	154 (98%)	3 (2%)	0	100	100
13	E	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
14	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
15	G	169/177 (96%)	167 (99%)	2 (1%)	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%)	66 (98%)	1 (2%)	0	100	100
19	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
20	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
21	M	302/352 (86%)	296 (98%)	6 (2%)	0	100	100
23	O	179/247 (72%)	176 (98%)	3 (2%)	0	100	100
24	Q	215/738 (29%)	207 (96%)	8 (4%)	0	100	100
25	R	264/400 (66%)	255 (97%)	9 (3%)	0	100	100
27	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	V	100/129 (78%)	99 (99%)	1 (1%)	0	100	100
29	W	304/492 (62%)	294 (97%)	10 (3%)	0	100	100
30	X	203/328 (62%)	192 (95%)	11 (5%)	0	100	100
All	All	8748/11560 (76%)	8555 (98%)	192 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	465	TYR

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	483/590 (82%)	483 (100%)	0	100	100
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	323/419 (77%)	323 (100%)	0	100	100
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1250/1520 (82%)	1249 (100%)	1 (0%)	93	98
10	B	1024/1061 (96%)	1023 (100%)	1 (0%)	93	98
11	C	234/299 (78%)	233 (100%)	1 (0%)	91	95
12	D	145/200 (72%)	144 (99%)	1 (1%)	84	92
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	76/137 (56%)	76 (100%)	0	100	100
15	G	152/158 (96%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	H	123/128 (96%)	123 (100%)	0	100 100
17	I	110/116 (95%)	110 (100%)	0	100 100
18	J	64/65 (98%)	64 (100%)	0	100 100
19	K	99/102 (97%)	99 (100%)	0	100 100
20	L	40/57 (70%)	40 (100%)	0	100 100
21	M	265/306 (87%)	265 (100%)	0	100 100
23	O	153/212 (72%)	153 (100%)	0	100 100
24	Q	204/642 (32%)	204 (100%)	0	100 100
25	R	252/363 (69%)	252 (100%)	0	100 100
27	U	99/260 (38%)	99 (100%)	0	100 100
28	V	94/115 (82%)	94 (100%)	0	100 100
29	W	281/436 (64%)	280 (100%)	1 (0%)	91 95
30	X	186/295 (63%)	186 (100%)	0	100 100
All	All	7936/10267 (77%)	7931 (100%)	5 (0%)	93 98

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

Mol	Chain	Res	Type
9	A	736	ASN
10	B	928	ARG
11	C	127	ARG
12	D	15	LEU
29	W	116	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	362	HIS
2	1	352	ASN
9	A	451	HIS
10	B	667	GLN
16	H	11	GLN

5.3.3 RNA

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 22 ligands modelled in this entry, 19 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	$\#\|Z\| > 2$
31	SF4	0	801	1	0,12,12	-	-	-		
33	BEF	7	901	35	0,3,3	-	-	-		
35	ADP	7	903	33,34	24,29,29	0.68	0	29,45,45	0.70	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
31	SF4	0	801	1	-	-	0/6/5/5
35	ADP	7	903	33,34	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	903	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
35	7	903	ADP	PA-O3A-PB-O3B

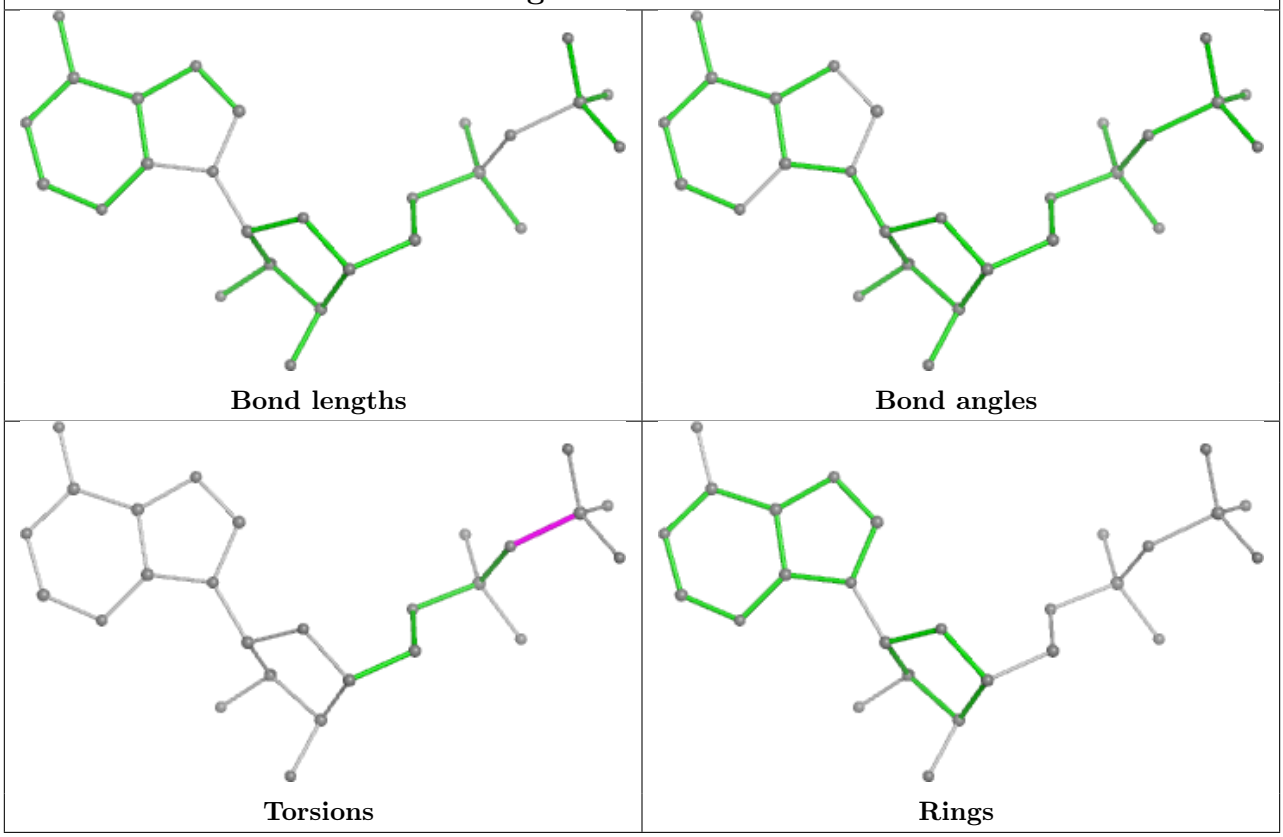
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	7	901	BEF	1	0
35	7	903	ADP	1	0

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.

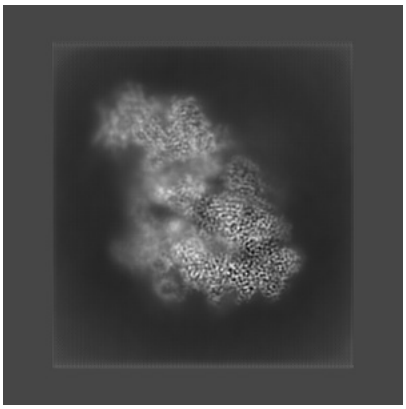
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12744. These allow visual inspection of the internal detail of the map and identification of artifacts.

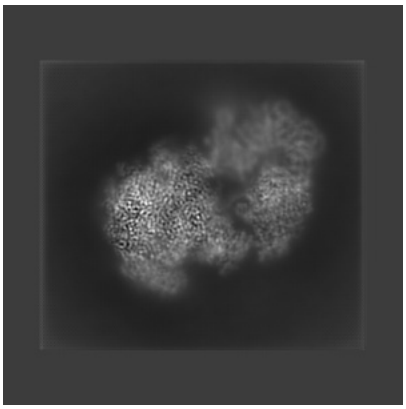
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

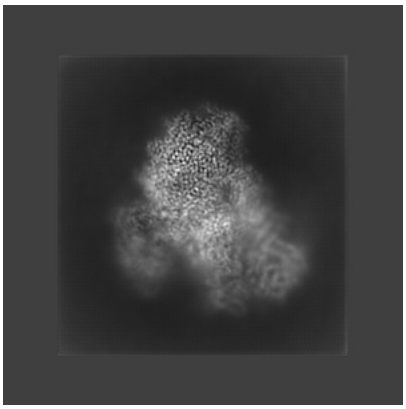
6.1.1 Primary map



X

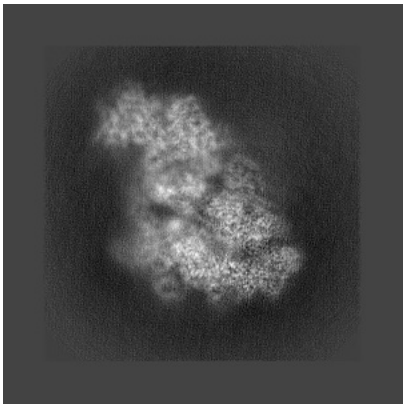


Y

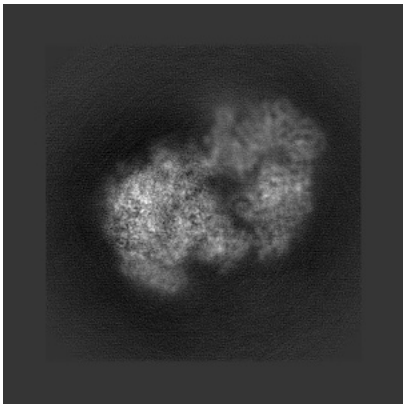


Z

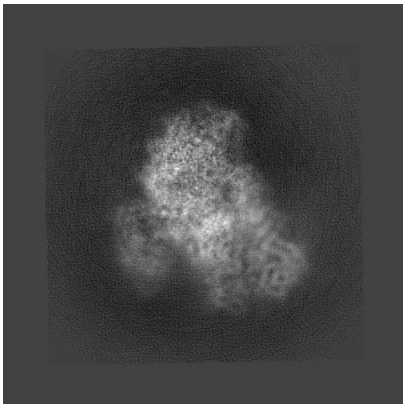
6.1.2 Raw map



X



Y

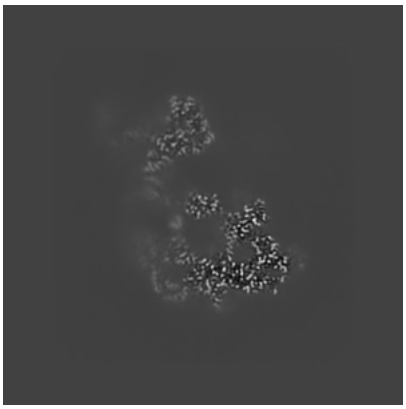


Z

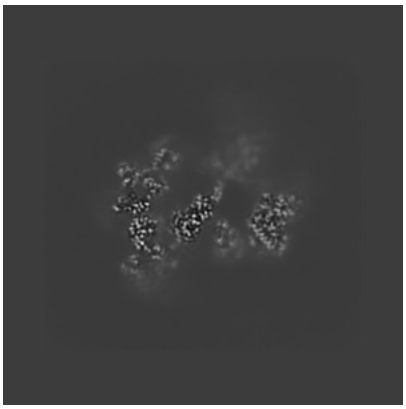
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



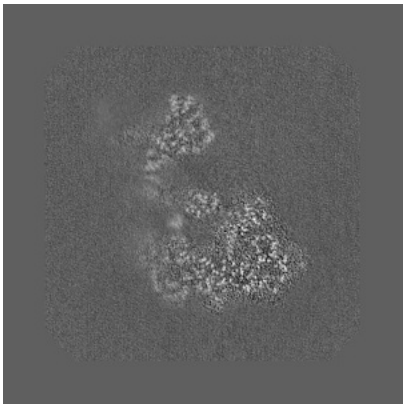
X Index: 190



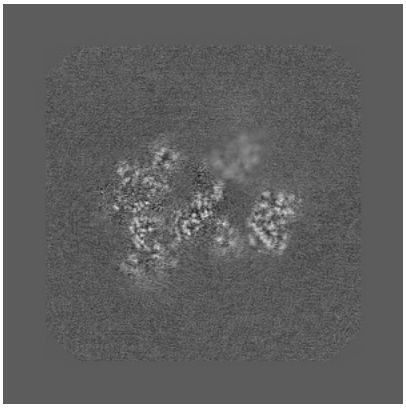
Y Index: 190

Z Index: 190

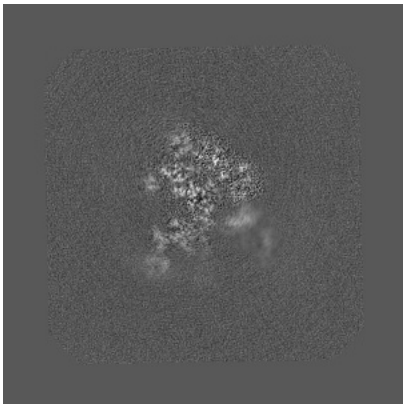
6.2.2 Raw map



X Index: 190



Y Index: 190

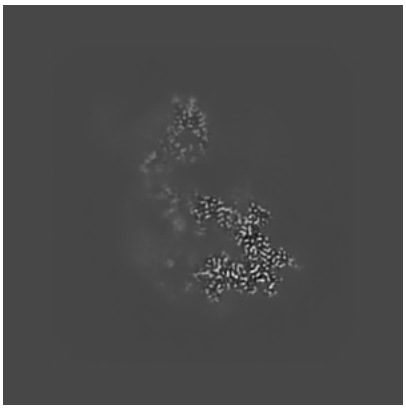


Z Index: 190

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

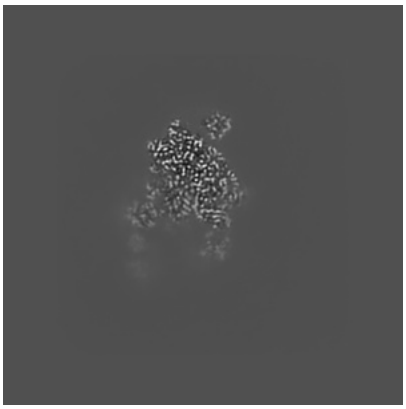
6.3 Largest variance slices (i)

6.3.1 Primary map



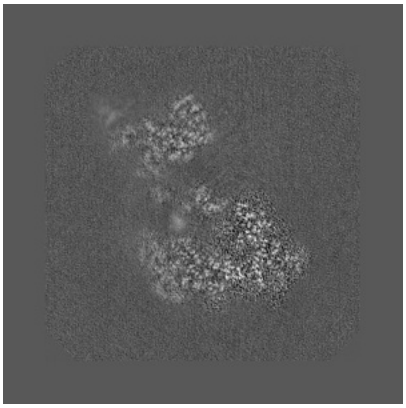
X Index: 183

Y Index: 234

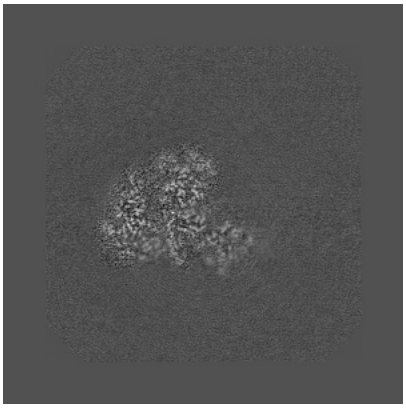


Z Index: 124

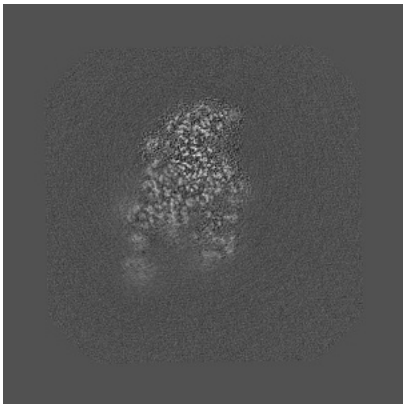
6.3.2 Raw map



X Index: 196



Y Index: 223

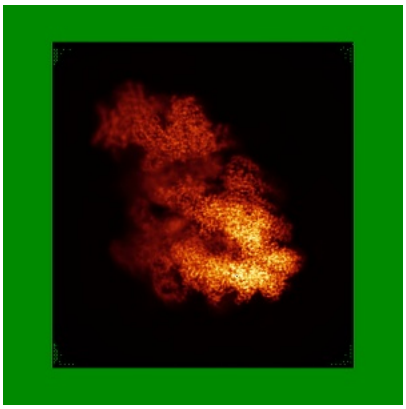


Z Index: 131

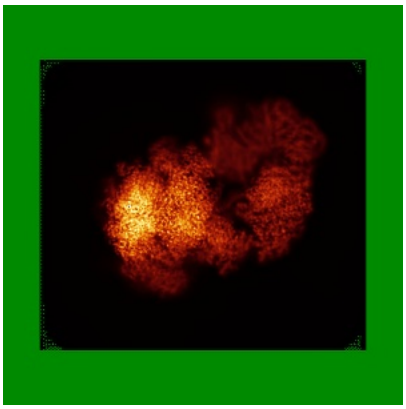
The images above show the largest variance slices of the map in three orthogonal directions.

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

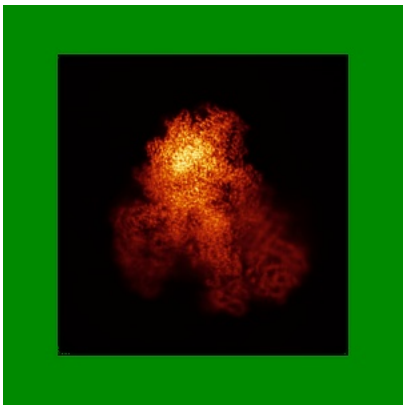
6.4.1 Primary map



X

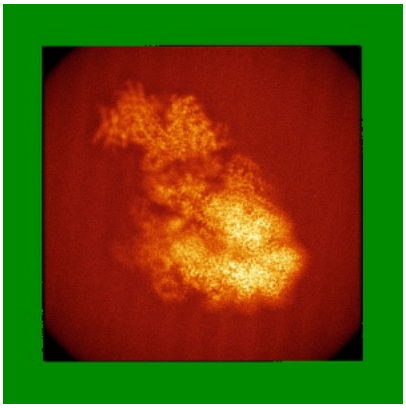


Y

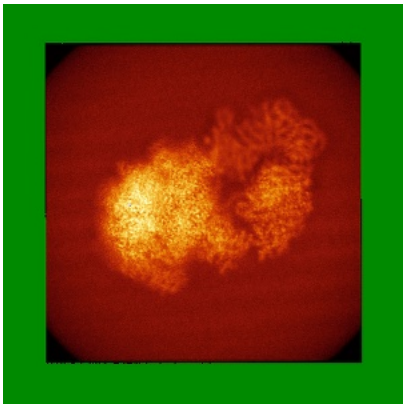


Z

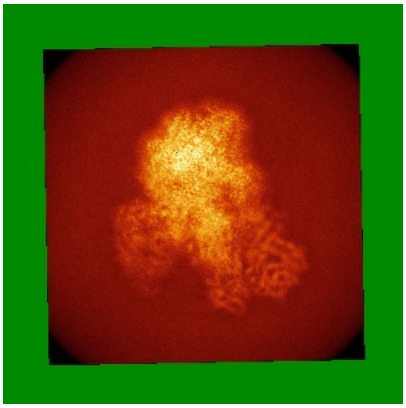
6.4.2 Raw map



X



Y

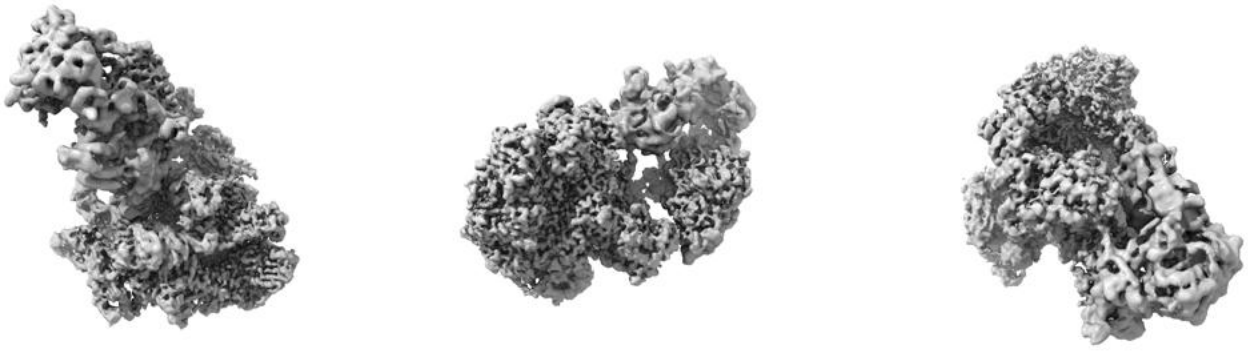


Z

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

6.5 Orthogonal surface views (i)

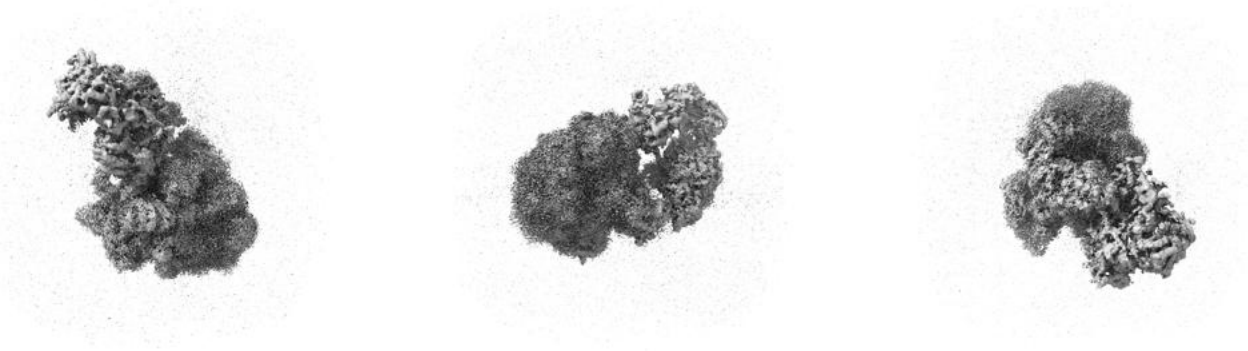
6.5.1 Primary map



X Y Z

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



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.

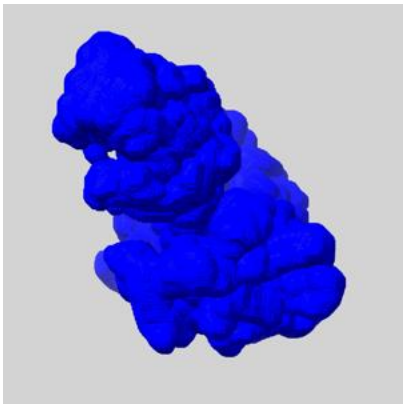
6.6 Mask visualisation

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

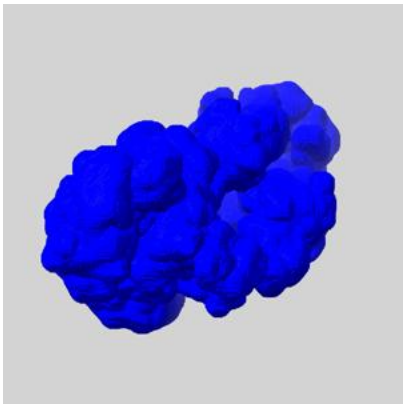
A mask typically either:

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

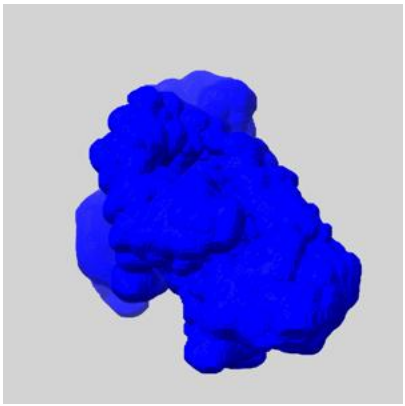
6.6.1 emd_12744_msk_1.map



X



Y

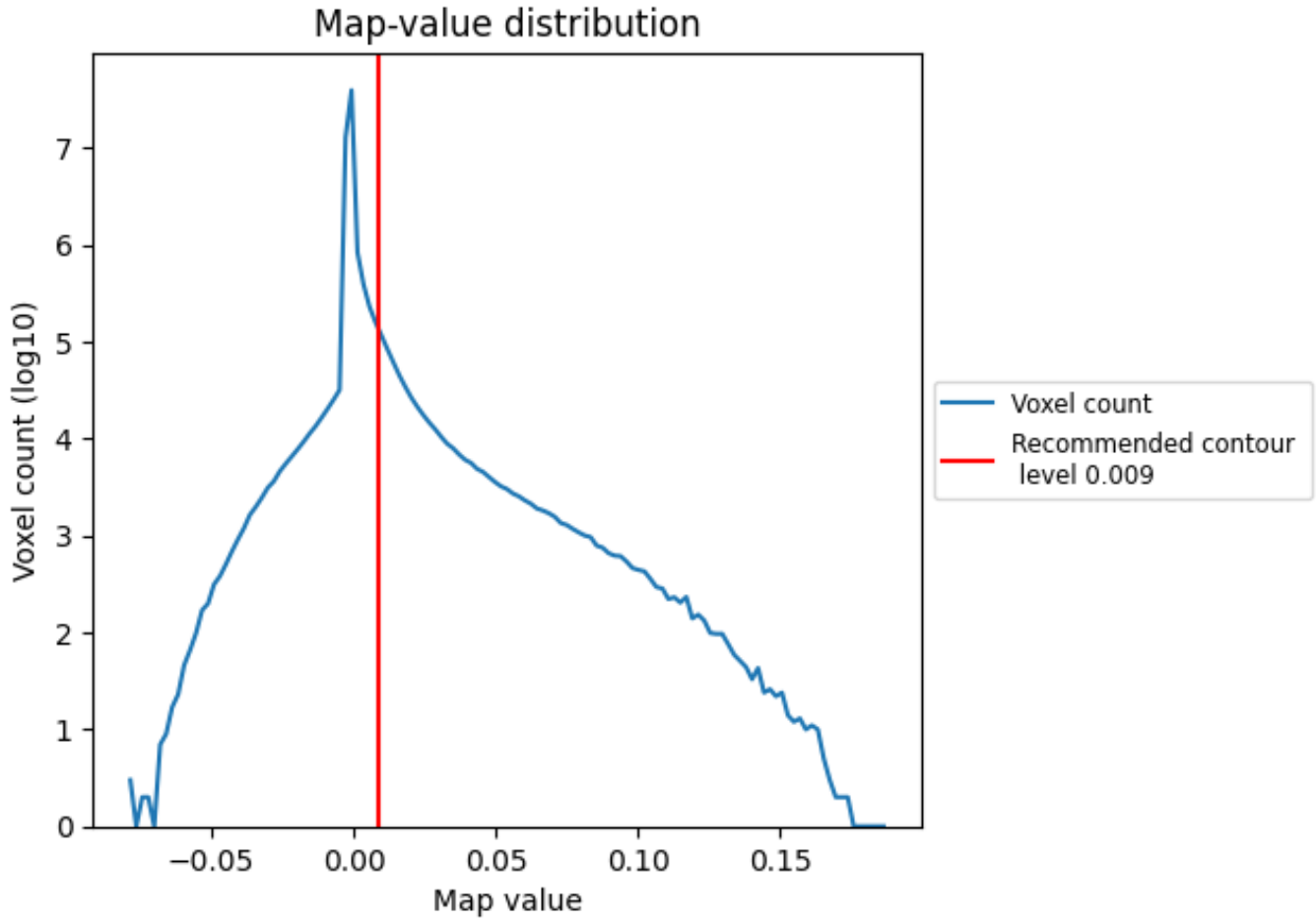


Z

7 Map analysis

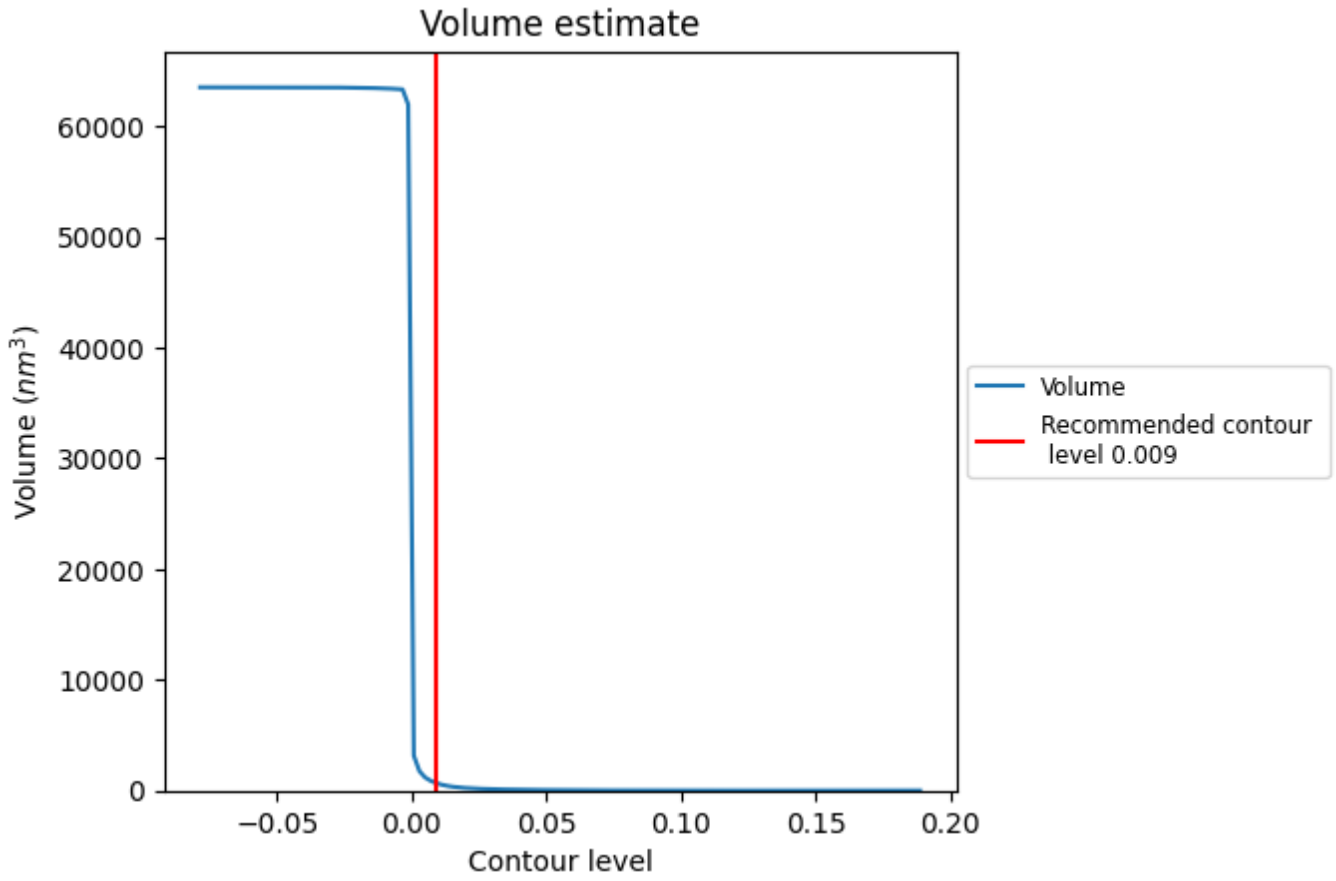
This section contains the results of statistical analysis of the map.

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.

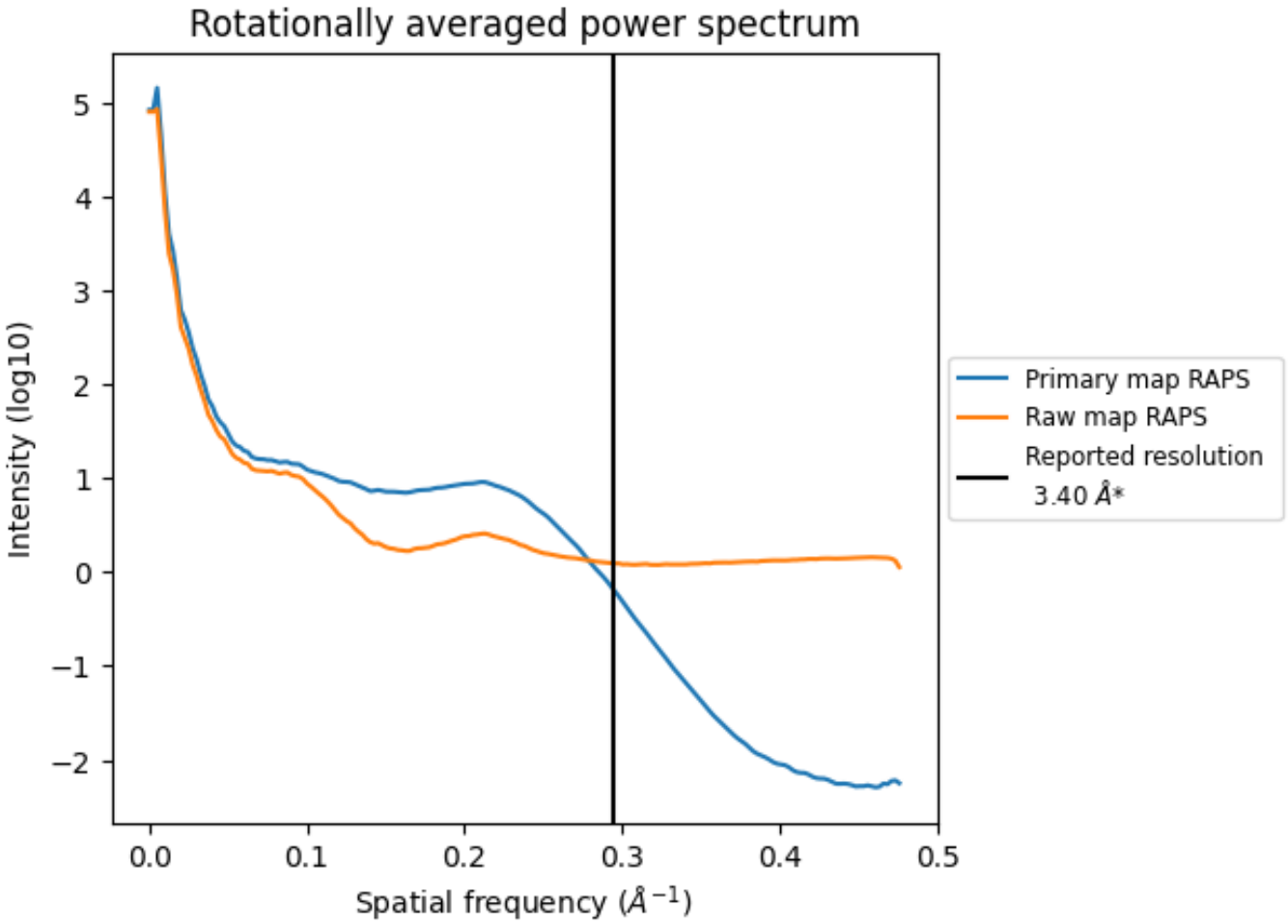
7.2 Volume estimate



The volume at the recommended contour level is 685 nm^3; this corresponds to an approximate mass of 619 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)

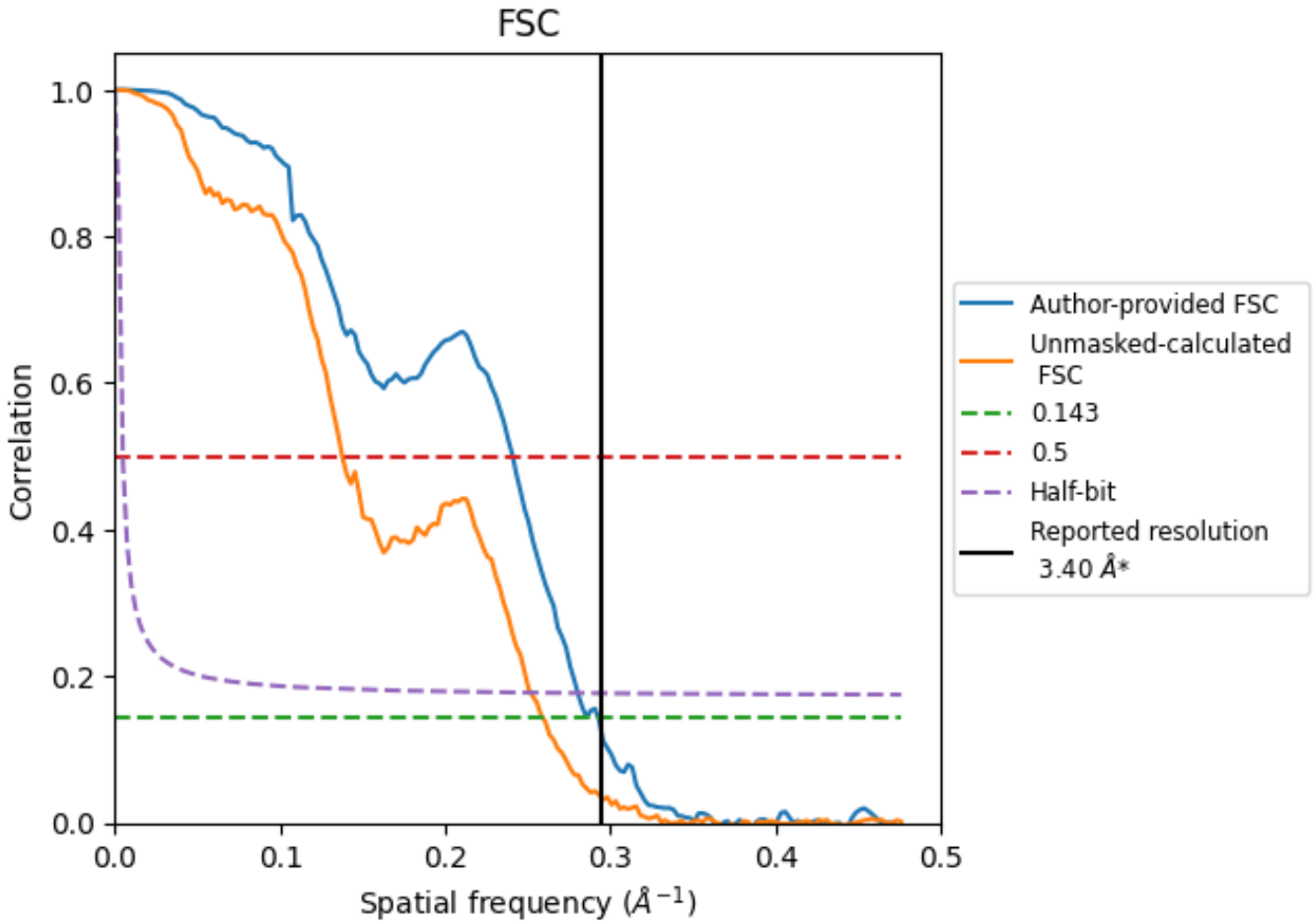


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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)

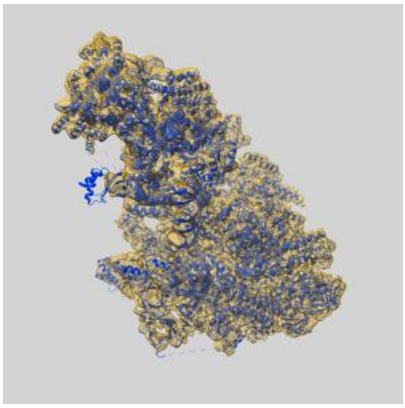
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.15	3.57
Unmasked-calculated*	3.86	7.26	3.97

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

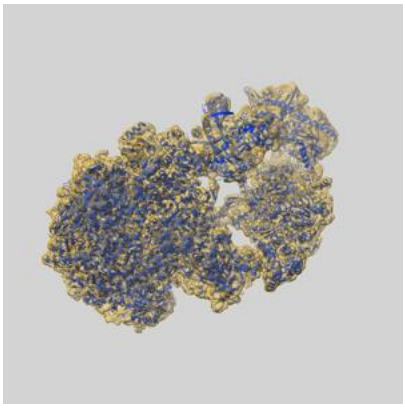
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12744 and PDB model 7O73. Per-residue inclusion information can be found in section 3 on page 15.

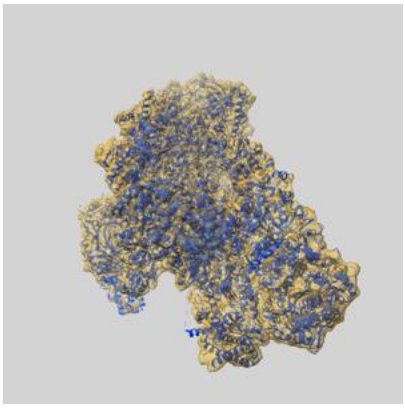
9.1 Map-model overlay



X



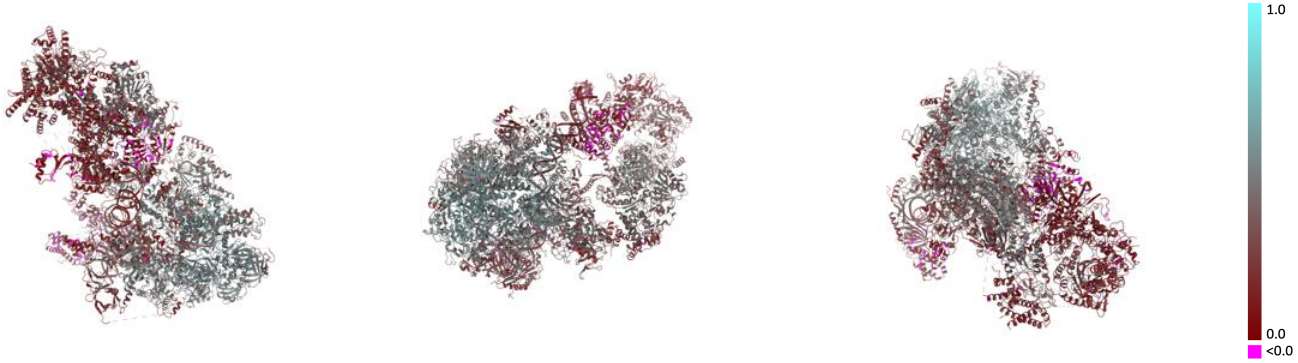
Y



Z

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

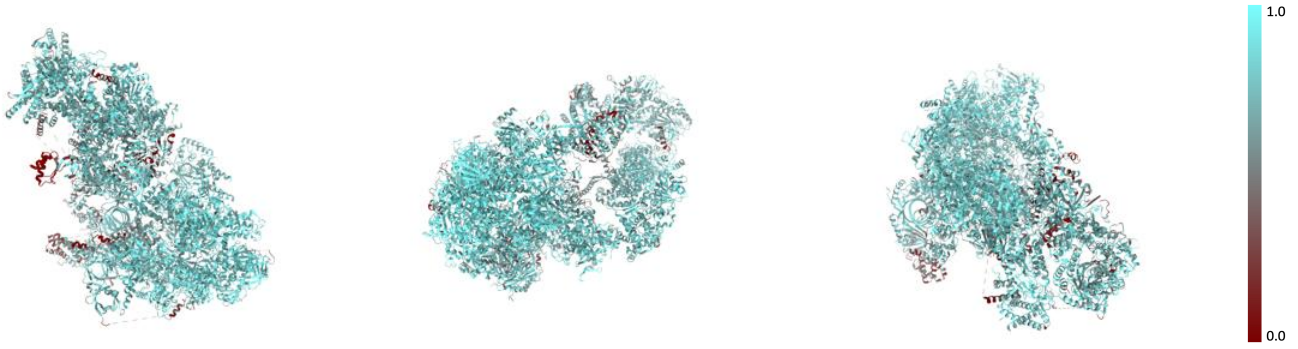
9.2 Q-score mapped to coordinate model (i)



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.

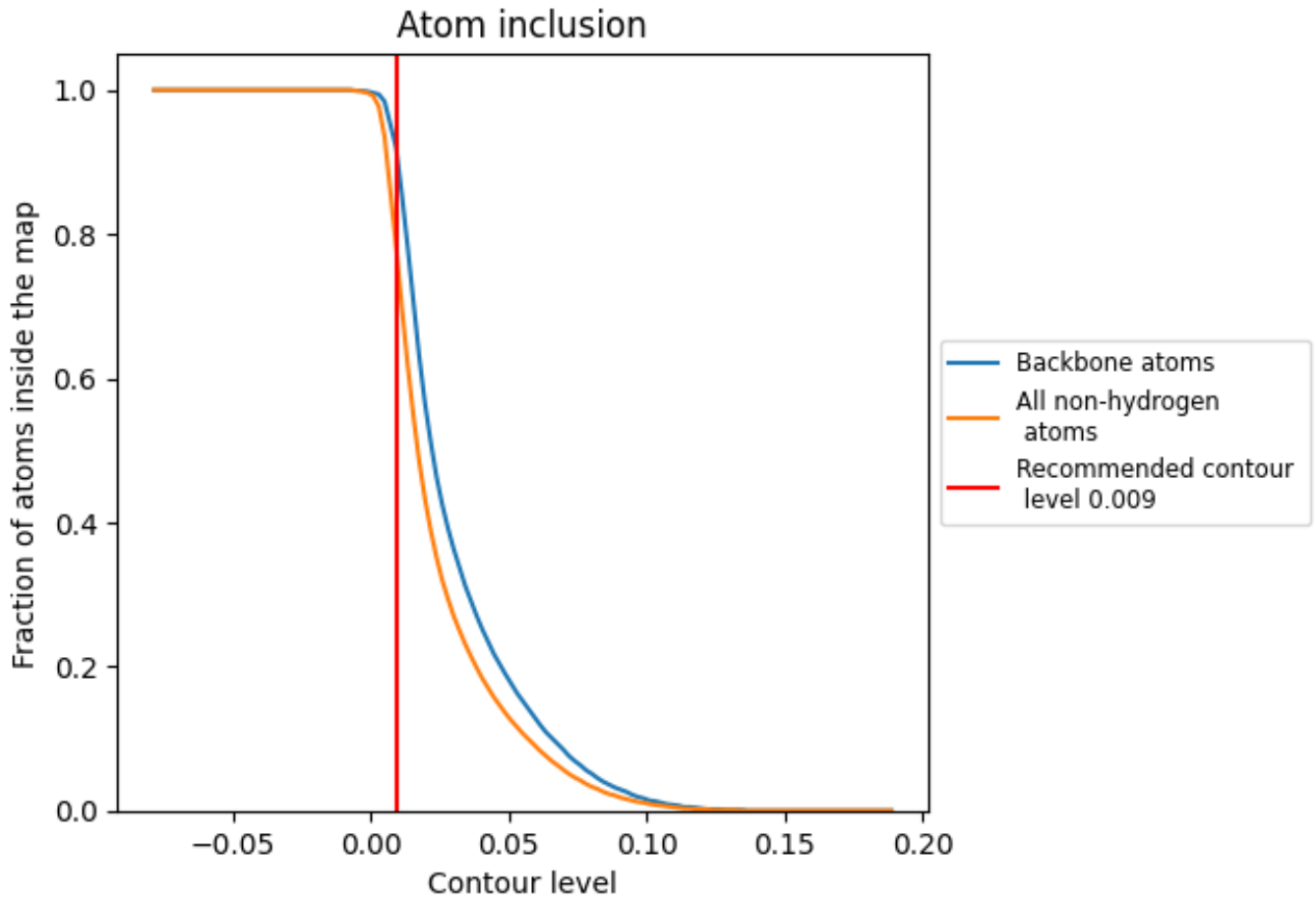
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 79% 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	0.7880	0.3500
0	0.8370	0.4110
1	0.7090	0.2560
2	0.6330	0.1690
3	0.7780	0.2650
4	0.7670	0.2700
5	0.6510	0.1550
6	0.7940	0.3470
7	0.6990	0.1200
A	0.8790	0.4740
B	0.8670	0.4810
C	0.8960	0.5160
D	0.7750	0.3360
E	0.8400	0.4220
F	0.8820	0.5120
G	0.8620	0.4250
H	0.8490	0.4660
I	0.8130	0.3700
J	0.8840	0.5140
K	0.8900	0.5210
L	0.8620	0.4580
M	0.7710	0.3690
N	0.8220	0.2010
O	0.7930	0.2620
Q	0.6050	0.2600
R	0.7010	0.2360
T	0.8410	0.2100
U	0.4830	0.1390
V	0.4700	0.1320
W	0.7120	0.3140
X	0.6690	0.2390