



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 04:58 AM JST

PDB ID : 7EGC  
EMDB ID : EMD-31112  
Title : p53-bound TFIID-based holo PIC on HDM2 promoter  
Authors : Chen, X.; Wu, Z.; Hou, H.; Qi, Y.; Wang, X.; Li, J.; Xu, Y.  
Deposited on : 2021-03-24  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

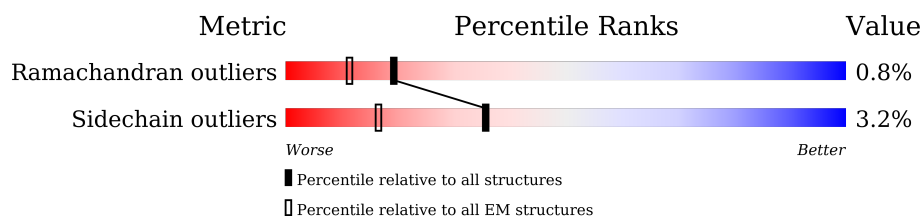


# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415


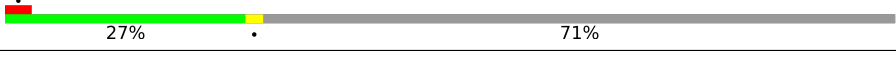
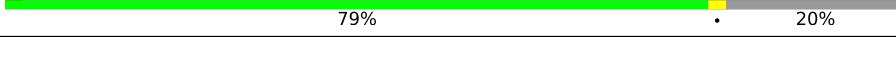

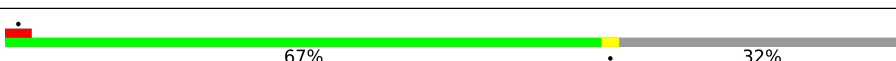


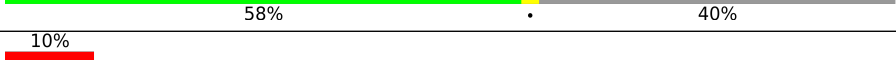
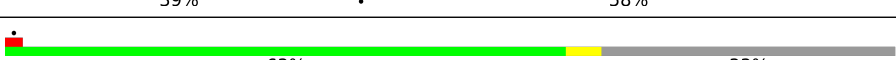




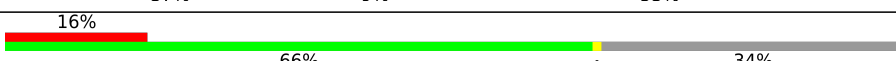

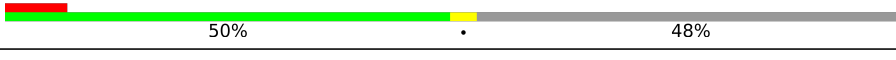








The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	309	<div> <div>20%</div> <div>75%</div> <div>24%</div> </div>
2	1	548	<div> <div>16%</div> <div>68%</div> <div>5%</div> <div>26%</div> </div>
3	2	395	<div> <div>5%</div> <div>81%</div> <div>16%</div> </div>
4	3	308	<div> <div>6%</div> <div>83%</div> <div>15%</div> </div>
5	4	462	<div> <div>9%</div> <div>93%</div> </div>
6	5	71	<div> <div>72%</div> <div>24%</div> </div>
7	6	782	<div> <div>70%</div> <div>8%</div> <div>23%</div> </div>
8	7	760	<div> <div>9%</div> <div>93%</div> </div>
9	8	346	<div> <div>17%</div> <div>84%</div> <div>14%</div> </div>

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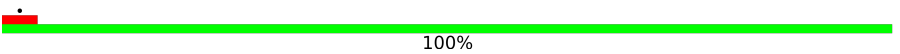
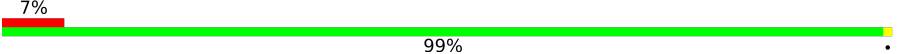

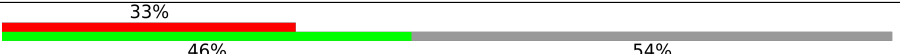
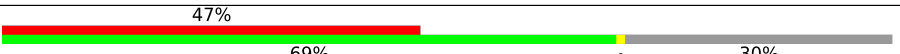
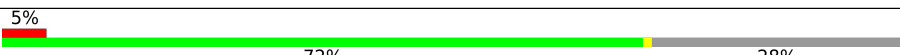
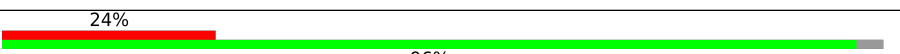
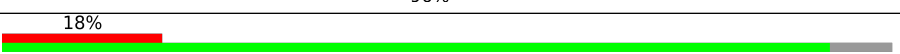
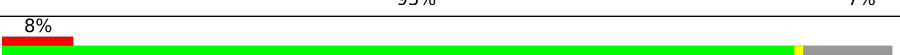
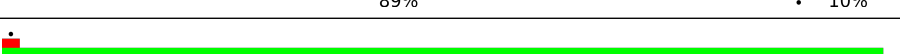
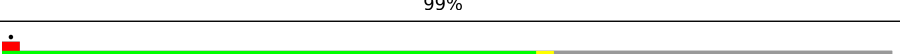
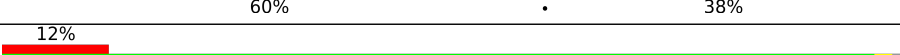
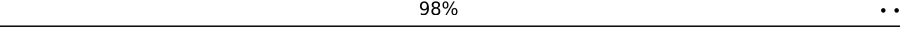
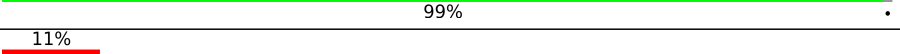
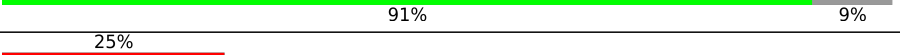
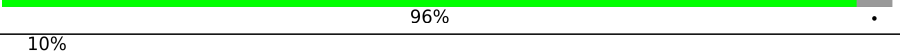
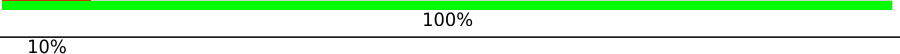
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Mol	Chain	Length	Quality of chain
10	9	323	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	

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Mol	Chain	Length	Quality of chain
29	X	71	 100%
30	Y	71	 99%
31	c	929	 86%
32	k	211	 54%
33	m	124	 69%
34	o	1970	 72%
35	p	1174	 96%
36	q	275	 93%
37	r	142	 89%
38	s	210	 99%
39	t	127	 60%
40	u	172	 98%
41	v	150	 99%
42	w	125	 91%
43	x	67	 96%
44	y	117	 100%
45	z	58	 76%



## 2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 113129 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	234	Total	C	N	O	S	0	0
			1774	1108	309	347	10		

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	405	Total	C	N	O	S	0	0
			2634	1640	486	501	7		

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	331	Total	C	N	O	S	0	0
			2534	1597	441	470	26		

- Molecule 4 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	449	Total	C	N	O	S	0	0
			3579	2303	624	638	14		

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	606	Total	C	N	O	S	0	0
			4880	3117	849	884	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	734	Total	C	N	O	S	0	0
			5833	3727	1022	1055	29		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2370	1531	404	424	11		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	287	Total	C	N	O	S	0	0
			2334	1493	402	422	17		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	550	Total	C	N	O	S	0	0
			4511	2882	782	820	27		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	158	Total	C	N	O	S	0	0
			1322	824	247	248	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
18	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.



Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	75	Total	C	N	O	S	0	0
			614	384	107	120	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 23 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	122	Total	C	N	O	S	0	0
			996	623	162	207	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	250	Total	C	N	O	S	0	0
			1929	1209	343	360	17		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	108	Total	C	N	O	S	0	0
			872	558	153	159	2		



- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	179	Total	C	N	O	S	0	0
			1476	932	261	272	11		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	172	Total	C	N	O	S	0	0
			1404	893	243	264	4		

- Molecule 29 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	71	Total	C	N	O	P	0	0
			1464	695	265	433	71		

- Molecule 30 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	71	Total	C	N	O	P	0	0
			1447	687	270	419	71		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.



Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1427	Total	C	N	O	S	0	0
			11308	7114	2023	2099	72		

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.



Mol	Chain	Residues	Atoms					AltConf	Trace
40	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 43 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 44 is a protein called RNA\_pol\_L\_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	y	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	1	Total	Zn	0
			1	1	

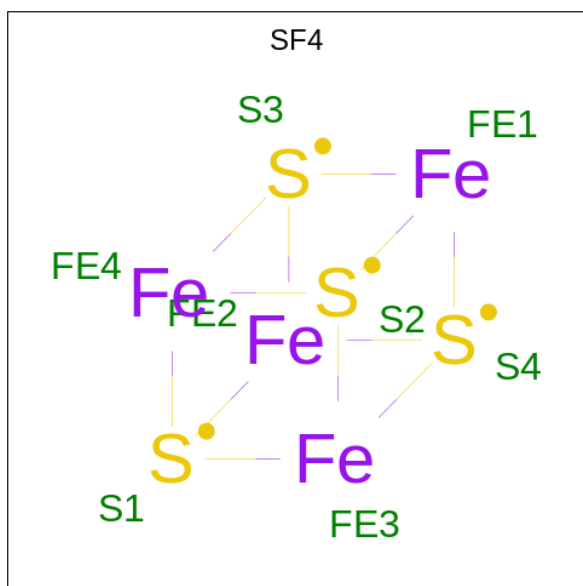
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Mol	Chain	Residues	Atoms		AltConf
46	R	1	Total 1	Zn 1	0
46	U	1	Total 1	Zn 1	0
46	o	2	Total 2	Zn 2	0
46	p	1	Total 1	Zn 1	0
46	q	1	Total 1	Zn 1	0
46	w	2	Total 2	Zn 2	0
46	x	1	Total 1	Zn 1	0
46	z	1	Total 1	Zn 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total 8	Fe 4	S 4	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



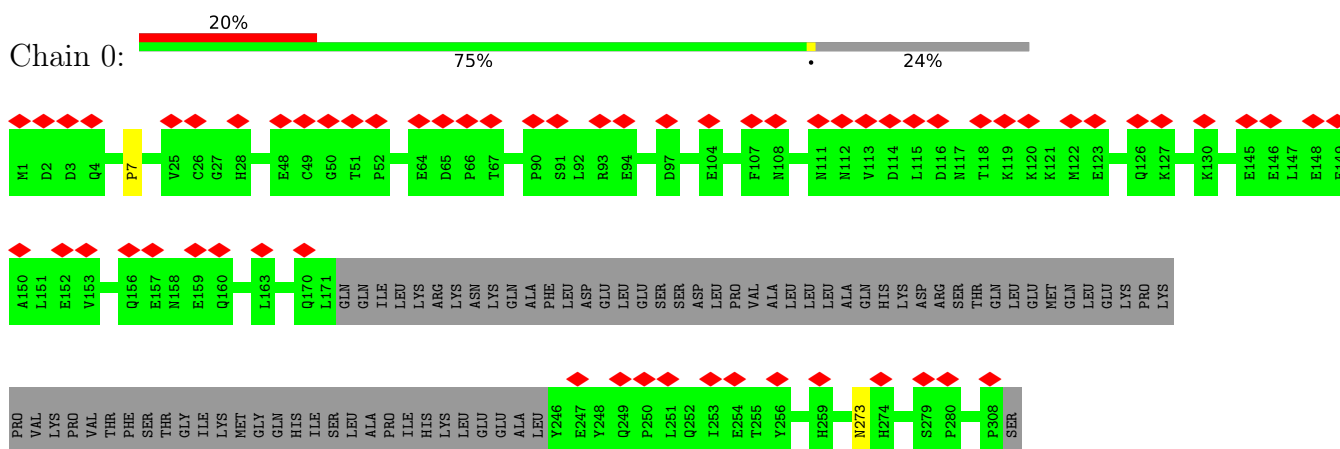
Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	Mg	0
			1	1	



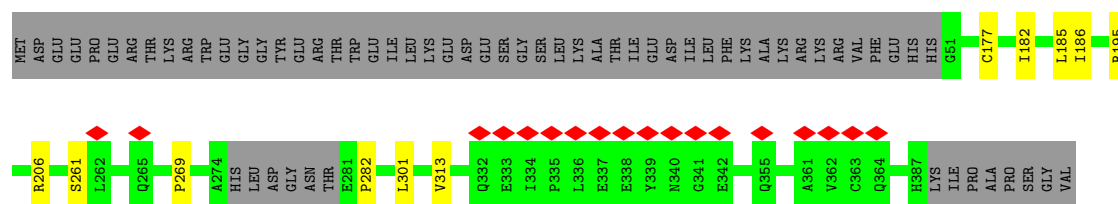
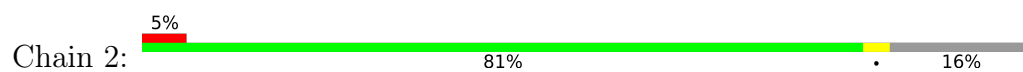
### 3 Residue-property plots

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

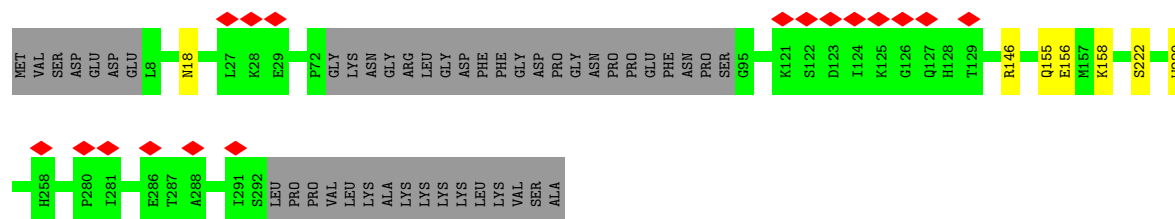
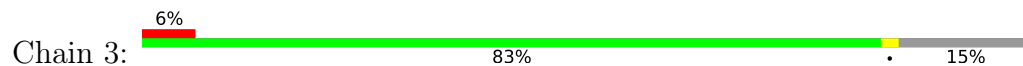
- Molecule 1: CDK-activating kinase assembly factor MAT1



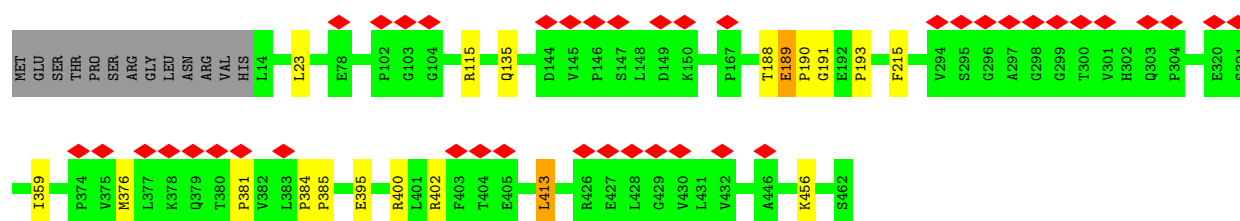




• Molecule 4: General transcription factor IIH subunit 3



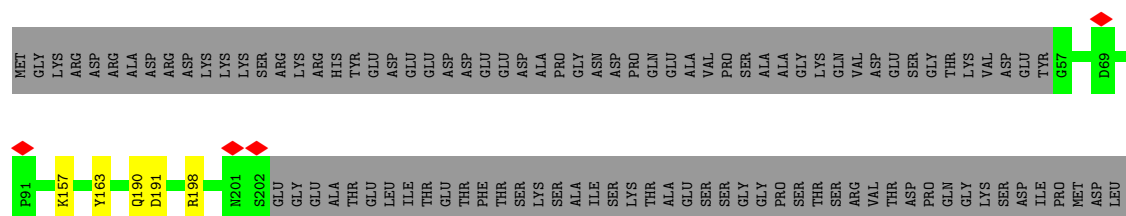
• Molecule 5: General transcription factor IIH subunit 4



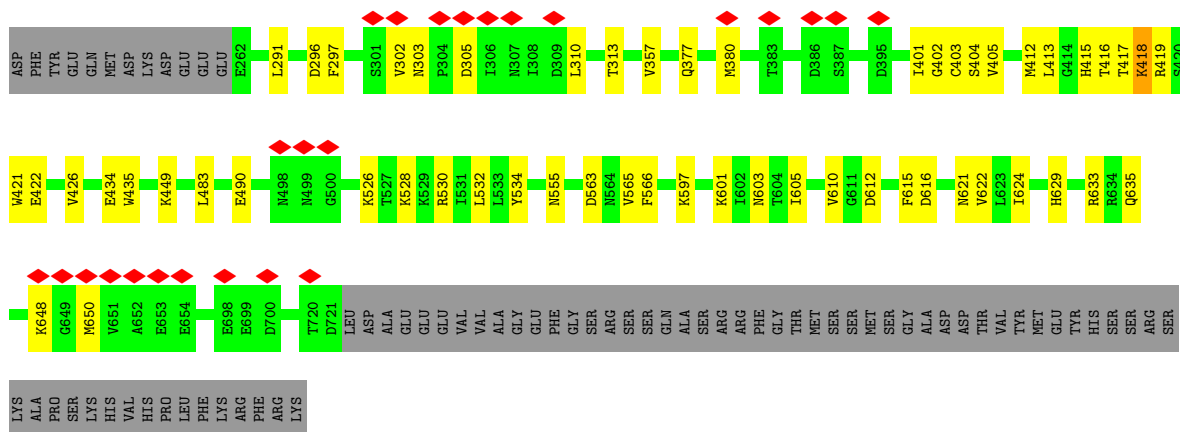
• Molecule 6: General transcription factor IIH subunit 5



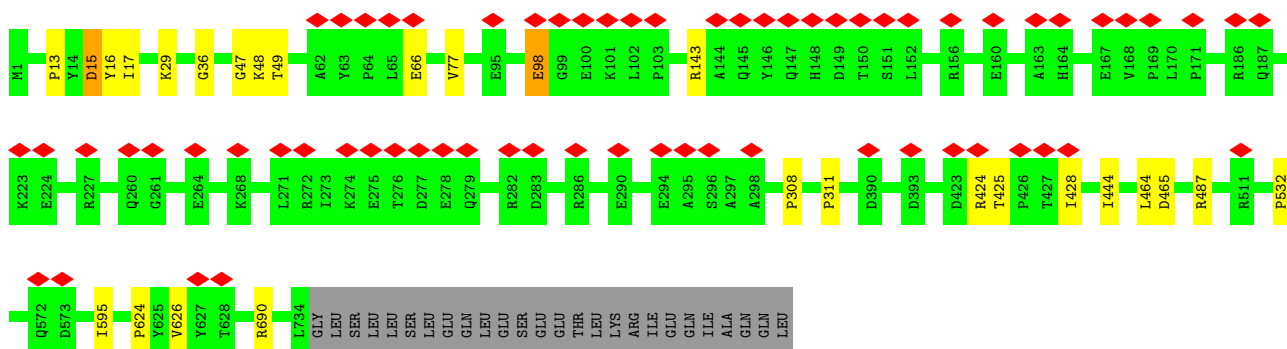
• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB



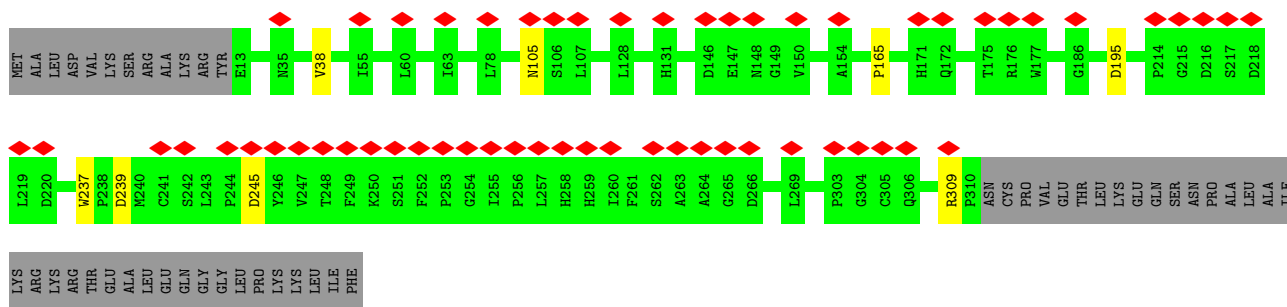
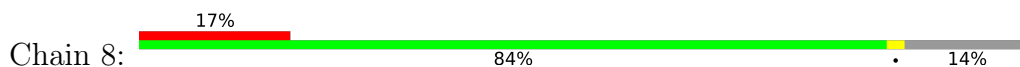




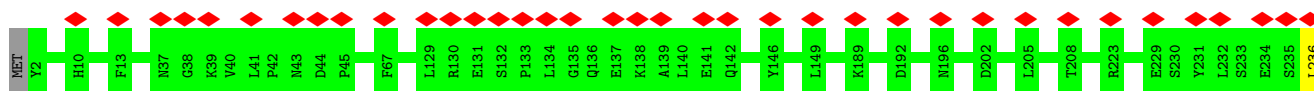
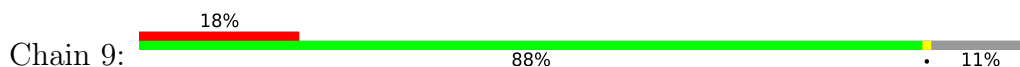
• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPD



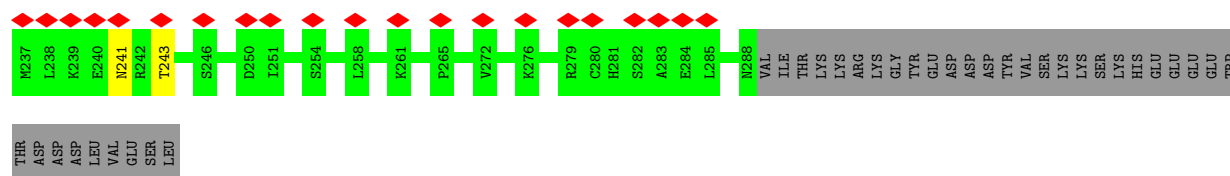
• Molecule 9: Cyclin-dependent kinase 7



• Molecule 10: Cyclin-H

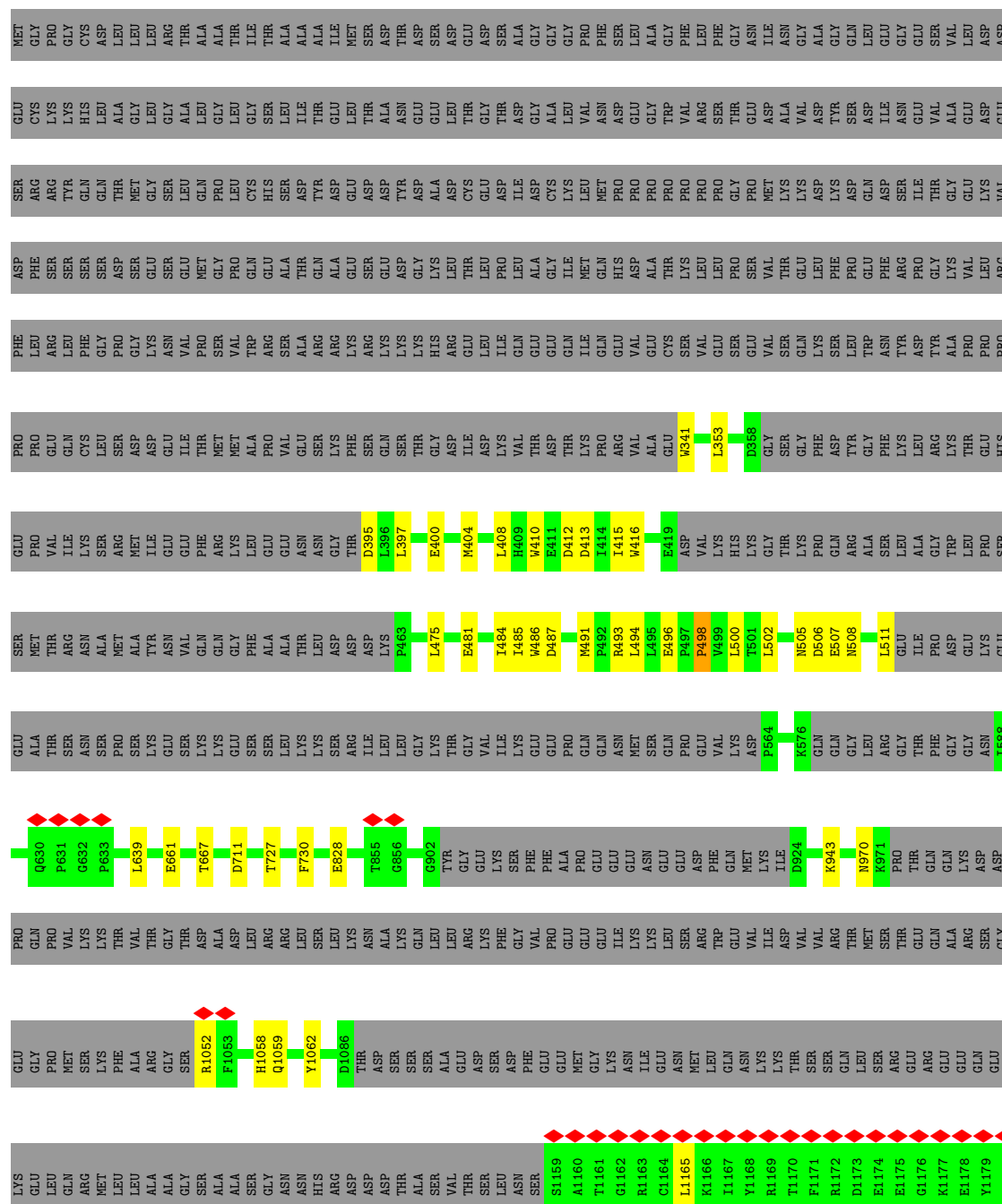






• Molecule 11: Transcription initiation factor TFIID subunit 1

Chain A: 27% 71%



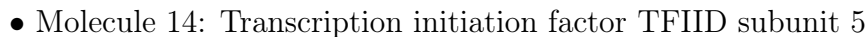






- Molecule 13: Transcription initiation factor TFIID subunit 4





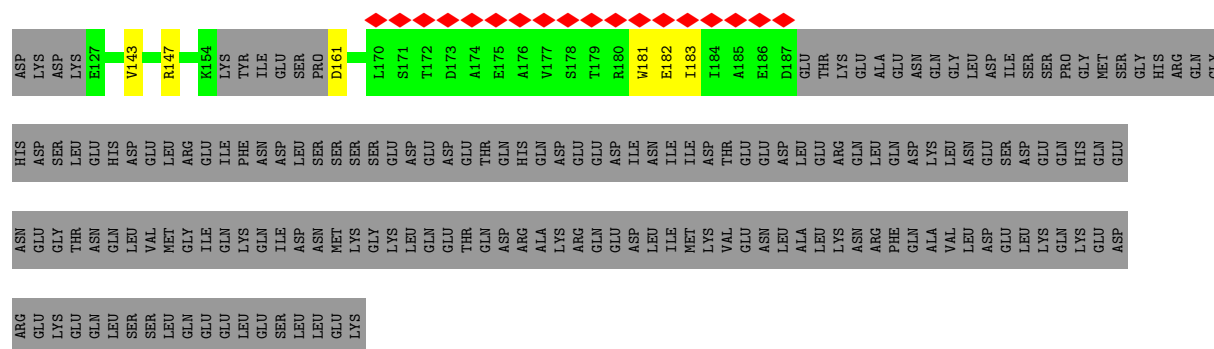






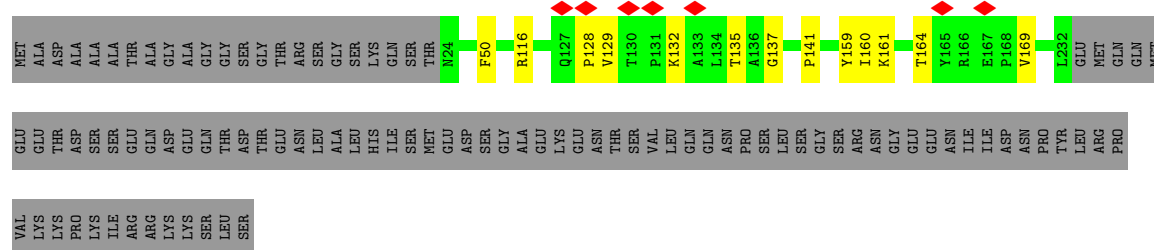






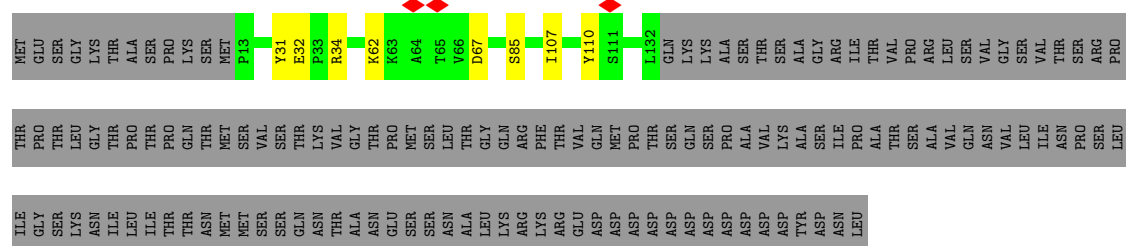
- Molecule 17: Transcription initiation factor TFIID subunit 8

Chain H: 63% 33%



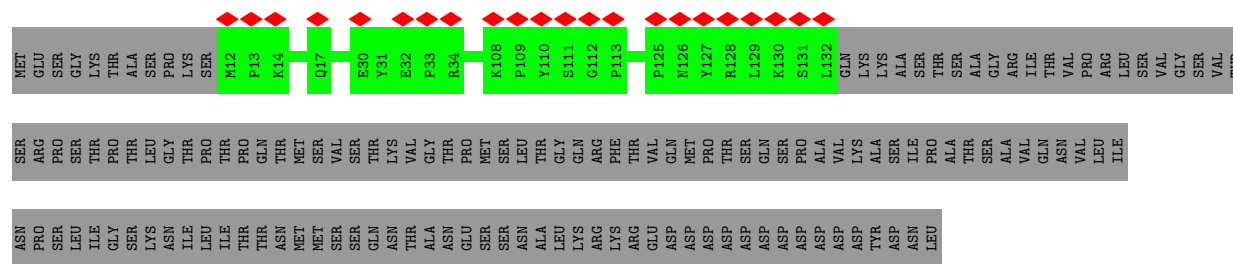
- Molecule 18: Transcription initiation factor TFIID subunit 9

Chain I: 42% 55%



- Molecule 18: Transcription initiation factor TFIID subunit 9

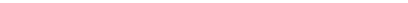
Chain i: 8% 46% 54%

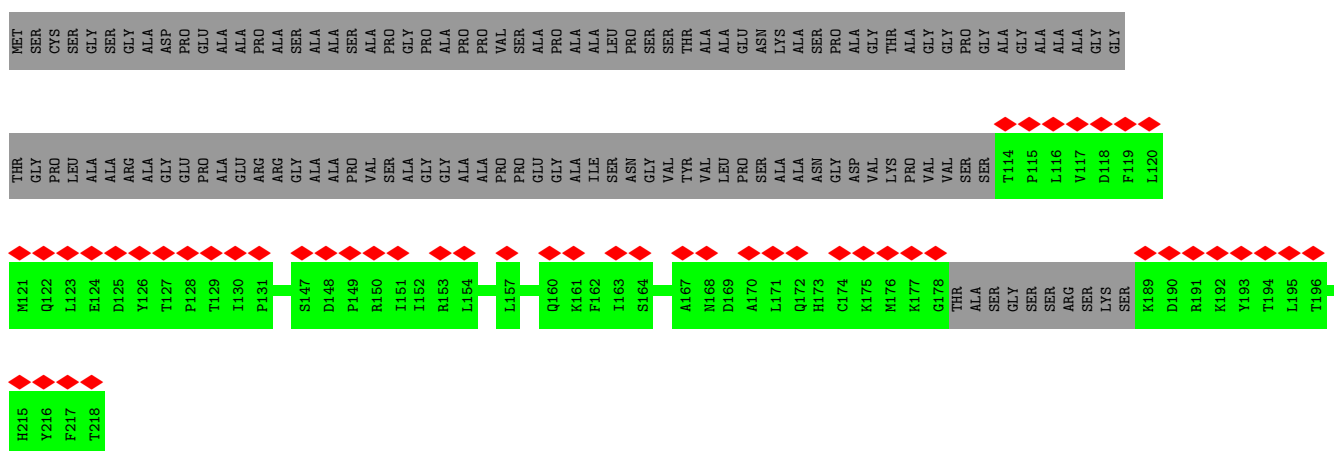


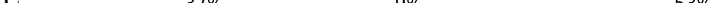
- Molecule 19: Transcription initiation factor TFIID subunit 10

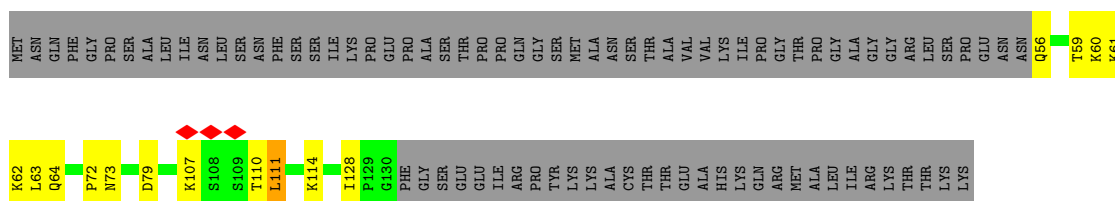


[illegible]

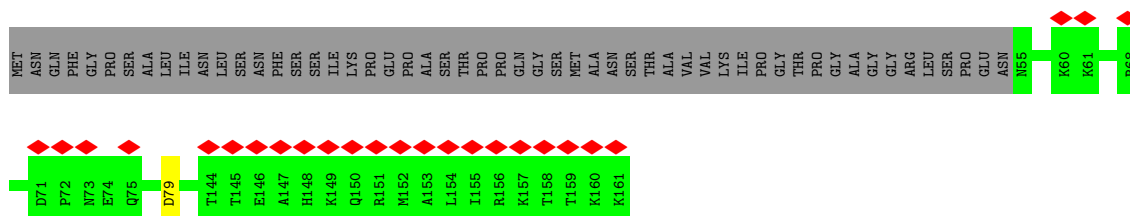
- Chain j: 



- Chain L:  37% 9% 53%



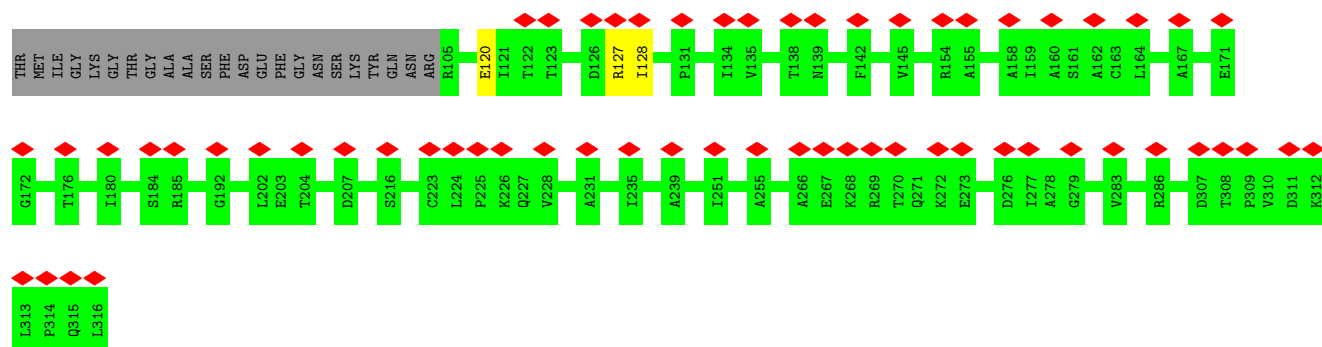
- Chain 1:  16% 66% 34%



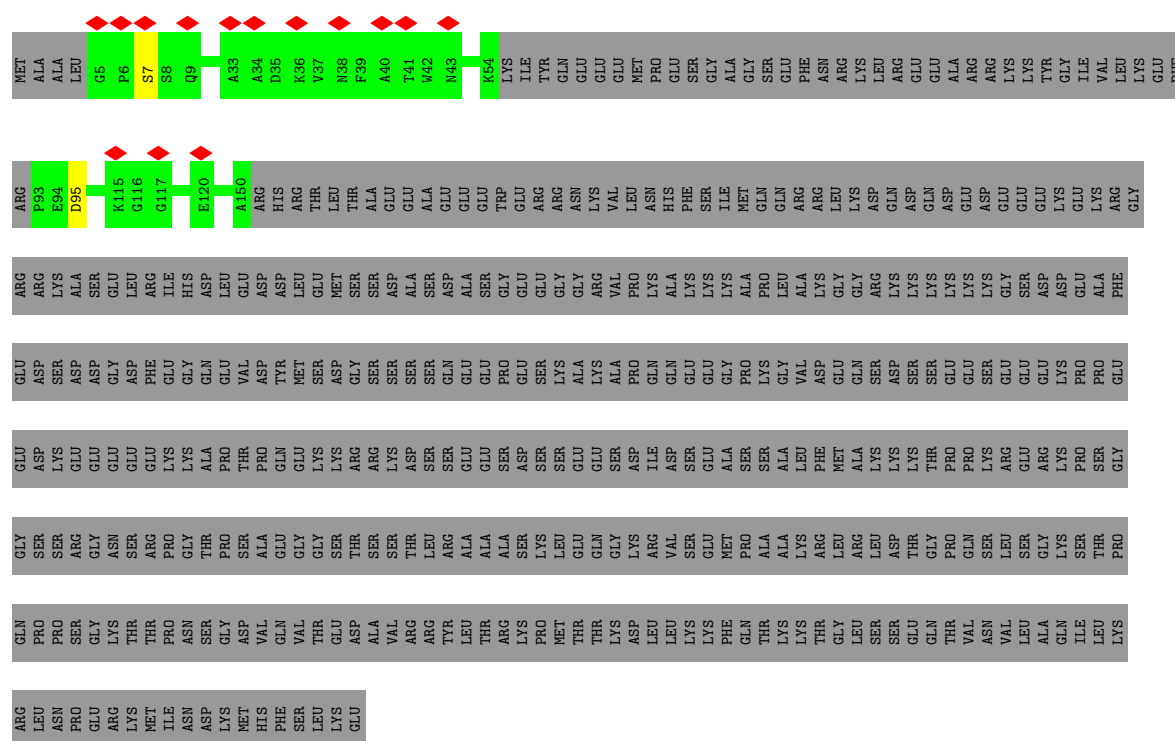


- Chain R:
- 
- | Amino Acid | Value |
|------------|-------|
| MET        |       |
| ALA        |       |
| SER        |       |
| THR        |       |
| SER        |       |
| ARG        |       |
| LEU        |       |
| ASP        |       |
| ALA        |       |
| LEU        |       |
| PRO        |       |
| ARG        |       |
| V13        | 20%   |
| I22        | 76%   |
| Y27        |       |
| R28        |       |
| L39        |       |
| V40        |       |
| V41        |       |
| V45        |       |
| I46        |       |
| D47        |       |
| V48        | 21%   |
| G49        |       |
| S50        |       |
| GLU        |       |
| TRP        |       |
| ARG        |       |
| THR        |       |
| PHE        |       |
| SER        |       |
| SER        |       |
| ASN        |       |
| ASP        |       |
| LYS        |       |
| ALA        |       |
| THR        |       |
| LYS        |       |
| ASP        |       |
| ASP        |       |
| PRO        |       |
| SER        |       |
| ARG        |       |
| VAL        |       |
| GLY        |       |
| ASP        |       |
| SER        |       |
| ASN        |       |
| PRO        |       |
| LEU        |       |
| LEU        |       |
| SER        |       |
| ASP        |       |
| GLY        |       |
| ASP        |       |
| LEU        |       |

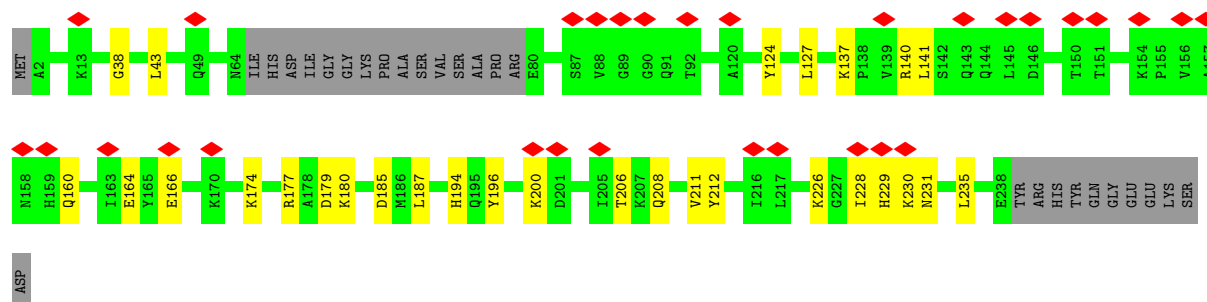
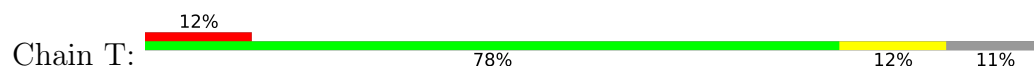




- Molecule 25: General transcription factor IIF subunit 1



- Molecule 26: General transcription factor IIF subunit 2



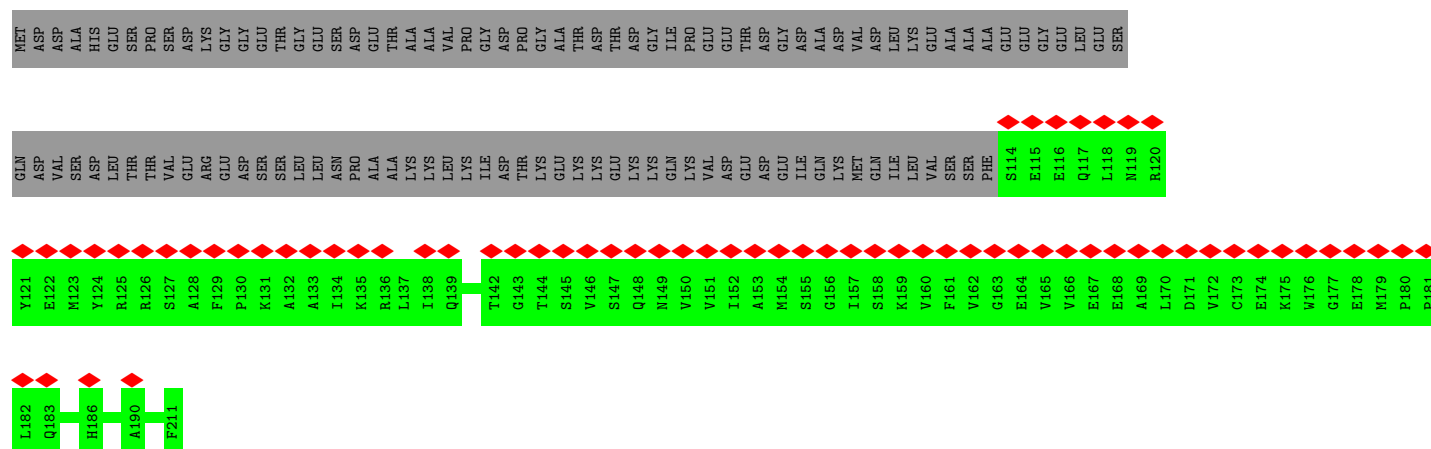




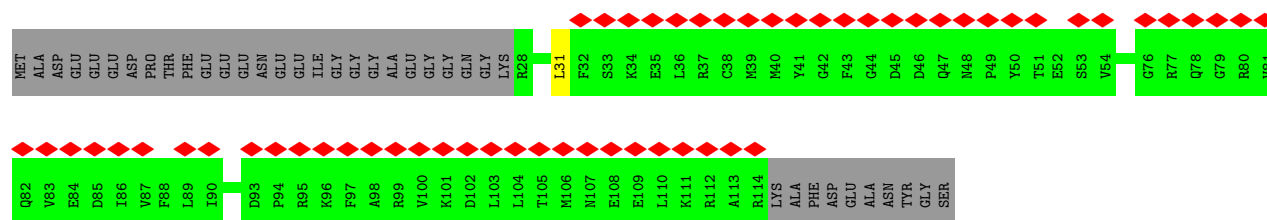




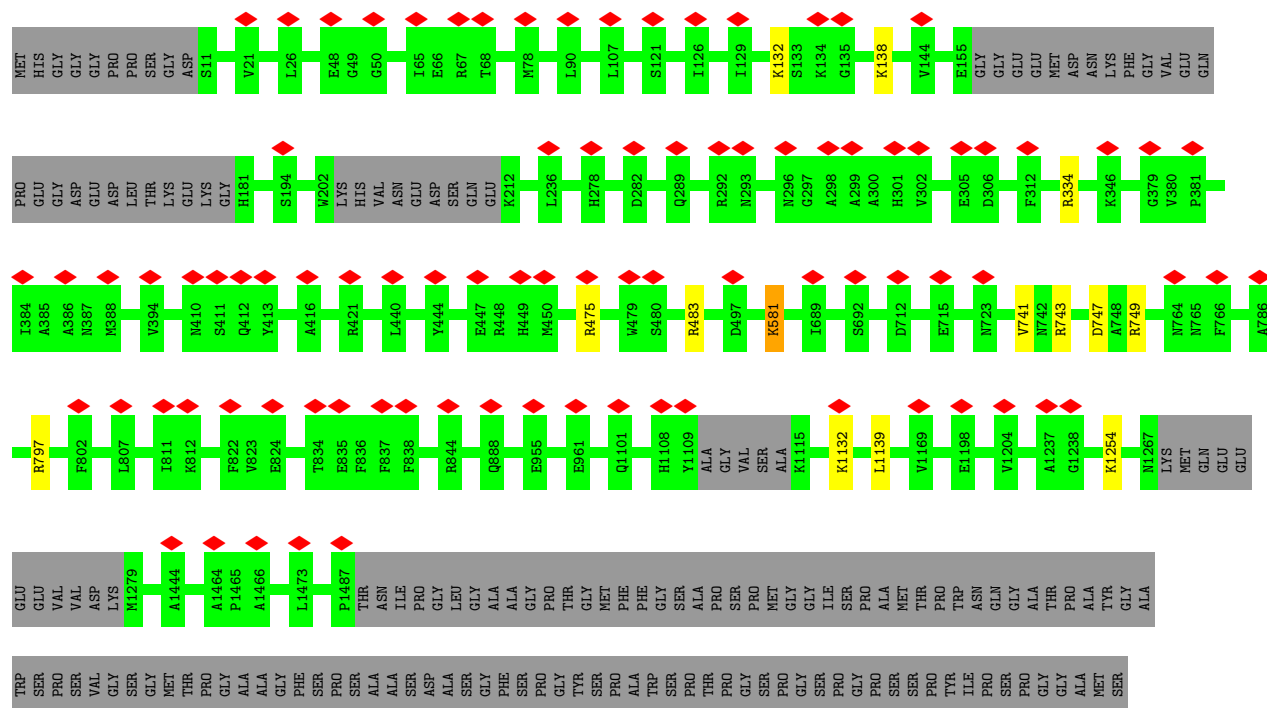




• Molecule 33: Transcription initiation factor TFIID subunit 13

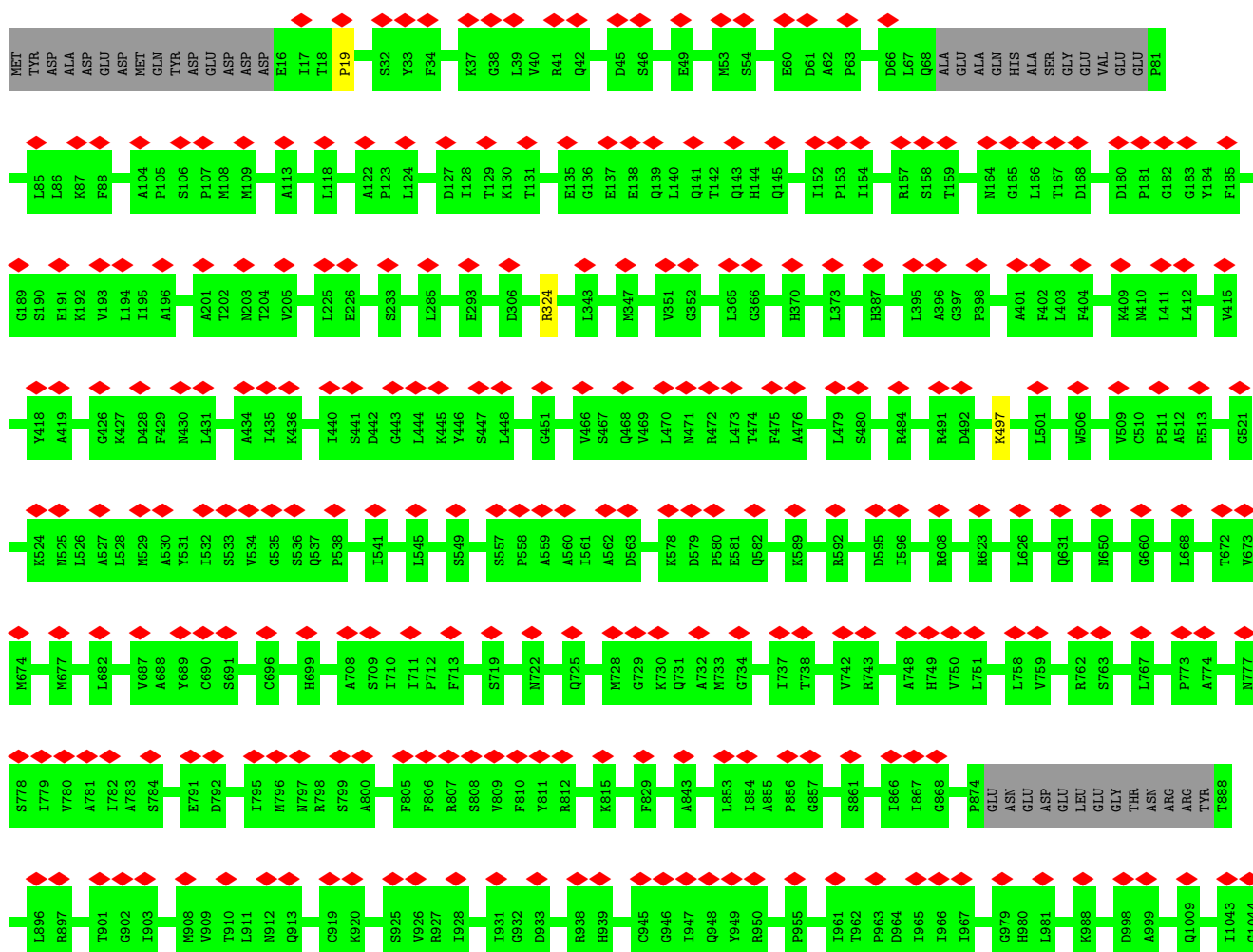


• Molecule 34: DNA-directed RNA polymerase II subunit RPB1

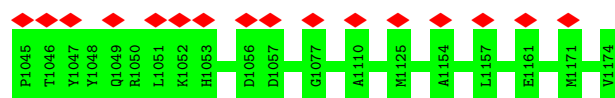




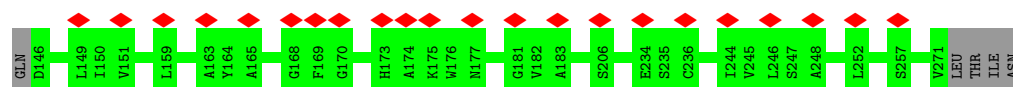
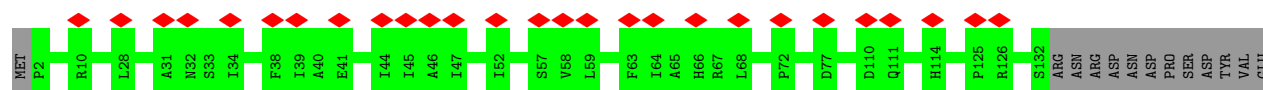
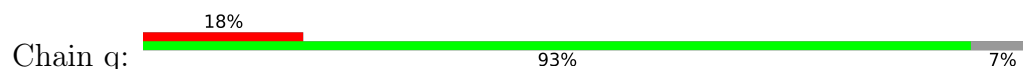
- Molecule 35: DNA-directed RNA polymerase subunit beta



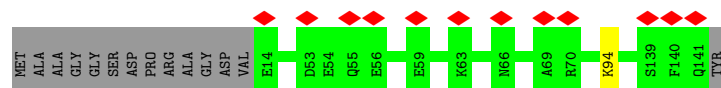
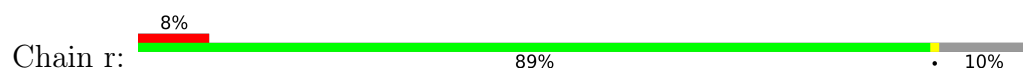




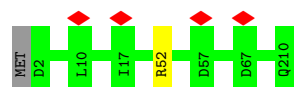
- Molecule 36: DNA-directed RNA polymerase II subunit RPB3



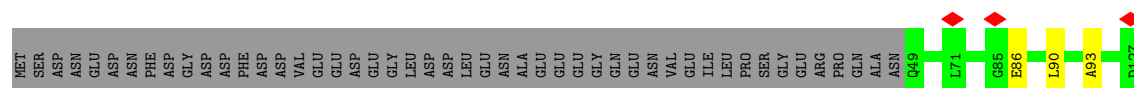
- Molecule 37: DNA-directed RNA polymerase II subunit RPB4



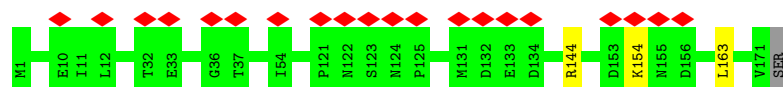
- Molecule 38: DNA-directed RNA polymerase II subunit E



- Molecule 39: DNA-directed RNA polymerase II subunit F



- Molecule 40: DNA-directed RNA polymerase II subunit RPB7



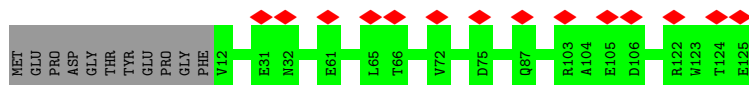
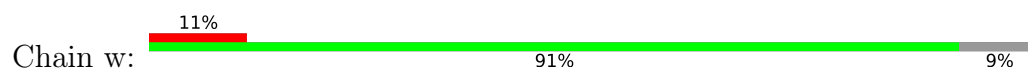
- Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3



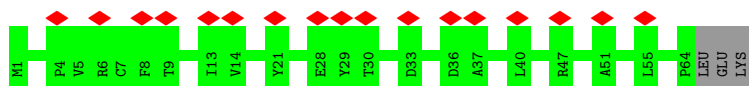




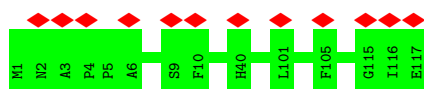
- Molecule 42: DNA-directed RNA polymerase II subunit RPB9



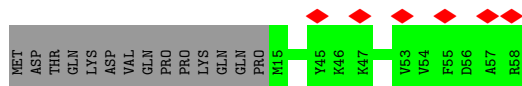
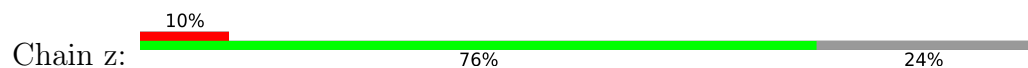
- Molecule 43: RPB10



- Molecule 44: RNA\_pol\_L\_2 domain-containing protein



- Molecule 45: RPB12





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42939	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.116	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0051	Depositor
Map size ( $\text{\AA}$ )	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0.36	0/1804	0.57	0/2443
2	1	0.44	0/2674	0.65	7/3660 (0.2%)
3	2	0.45	0/2588	0.66	2/3509 (0.1%)
4	3	0.43	0/2102	0.61	0/2844
5	4	0.44	0/3663	0.63	0/4965
6	5	0.37	0/433	0.54	0/585
7	6	0.45	0/4983	0.61	0/6731
8	7	0.46	0/5957	0.66	2/8071 (0.0%)
9	8	0.55	0/2429	0.69	0/3295
10	9	0.54	0/2384	0.61	0/3220
11	A	0.48	0/4627	0.65	1/6248 (0.0%)
12	B	0.47	0/7993	0.61	0/10836
13	D	0.39	0/1335	0.51	0/1784
13	d	0.28	0/1321	0.49	0/1772
14	E	0.37	0/4469	0.55	0/6050
14	e	0.33	0/4433	0.55	0/6004
15	F	0.50	0/3167	0.69	0/4303
15	f	0.42	0/3140	0.64	0/4268
16	G	0.52	0/1199	0.63	0/1612
17	H	0.36	0/1673	0.53	0/2285
18	I	0.50	0/981	0.59	0/1332
18	i	0.30	0/989	0.46	0/1343
19	J	0.29	0/736	0.46	0/998
19	j	0.30	0/775	0.52	0/1049
20	L	0.41	0/622	0.63	1/841 (0.1%)
20	l	0.35	0/888	0.52	1/1194 (0.1%)
21	O	0.53	0/781	0.71	0/1061
22	P	0.67	0/1438	0.79	0/1935
23	Q	0.43	0/1013	0.62	0/1366
24	R	0.35	0/1957	0.64	0/2643
25	S	0.32	0/896	0.49	0/1213
26	T	0.51	0/1817	0.73	0/2445



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	U	0.52	1/1499 (0.1%)	0.81	5/2012 (0.2%)
28	V	0.46	0/1428	0.61	0/1917
29	X	0.76	0/1641	0.96	0/2534
30	Y	0.79	1/1623 (0.1%)	0.98	0/2499
31	c	0.39	0/1035	0.54	0/1406
32	k	0.30	0/799	0.48	0/1070
33	m	0.31	0/733	0.51	0/977
34	o	0.35	0/11516	0.52	0/15548
35	p	0.38	0/9243	0.49	0/12475
36	q	0.38	0/2102	0.46	0/2857
37	r	0.27	0/1019	0.47	0/1374
38	s	0.31	0/1751	0.47	0/2366
39	t	0.49	0/645	0.65	0/871
40	u	0.32	0/1382	0.53	0/1874
41	v	0.37	0/1207	0.49	0/1628
42	w	0.30	0/948	0.46	0/1284
43	x	0.42	0/516	0.45	0/696
44	y	0.35	0/956	0.44	0/1294
45	z	0.38	0/377	0.44	0/500
All	All	0.43	2/115687 (0.0%)	0.60	19/157087 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	-24	DC	C1'-N1	5.96	1.56	1.49
27	U	183	GLN	C-O	5.40	1.33	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	U	186	PRO	CA-N-CD	-12.85	93.52	111.50
27	U	127	PHE	CB-CA-C	8.09	126.58	110.40
2	1	276	PRO	N-CA-CB	7.81	112.67	103.30
2	1	353	LYS	CB-CA-C	6.44	123.29	110.40
8	7	311	PRO	N-CA-CB	6.08	110.60	103.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	230/309 (74%)	199 (86%)	29 (13%)	2 (1%)	14	48
2	1	399/548 (73%)	311 (78%)	70 (18%)	18 (4%)	2	20
3	2	327/395 (83%)	288 (88%)	37 (11%)	2 (1%)	22	57
4	3	259/308 (84%)	243 (94%)	16 (6%)	0	100	100
5	4	447/462 (97%)	399 (89%)	38 (8%)	10 (2%)	5	32
6	5	52/71 (73%)	47 (90%)	4 (8%)	1 (2%)	6	34
7	6	602/782 (77%)	512 (85%)	79 (13%)	11 (2%)	7	35
8	7	732/760 (96%)	649 (89%)	74 (10%)	9 (1%)	11	43
9	8	296/346 (86%)	261 (88%)	33 (11%)	2 (1%)	19	54
10	9	285/323 (88%)	270 (95%)	14 (5%)	1 (0%)	30	65
11	A	534/1872 (28%)	505 (95%)	26 (5%)	3 (1%)	22	57
12	B	959/1199 (80%)	912 (95%)	47 (5%)	0	100	100
13	D	152/1085 (14%)	146 (96%)	5 (3%)	1 (1%)	19	54
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
14	E	540/800 (68%)	506 (94%)	33 (6%)	1 (0%)	44	75
14	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
15	F	404/677 (60%)	380 (94%)	17 (4%)	7 (2%)	7	36
15	f	399/677 (59%)	378 (95%)	20 (5%)	1 (0%)	37	70
16	G	139/349 (40%)	135 (97%)	4 (3%)	0	100	100
17	H	207/310 (67%)	190 (92%)	13 (6%)	4 (2%)	6	34
18	I	118/264 (45%)	111 (94%)	5 (4%)	2 (2%)	7	36

*Continued on next page...*



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
20	L	73/161 (45%)	64 (88%)	4 (6%)	5 (7%)	1	14
20	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
21	O	95/109 (87%)	82 (86%)	8 (8%)	5 (5%)	1	18
22	P	175/339 (52%)	168 (96%)	5 (3%)	2 (1%)	12	45
23	Q	118/376 (31%)	106 (90%)	9 (8%)	3 (2%)	4	30
24	R	246/316 (78%)	234 (95%)	10 (4%)	2 (1%)	16	51
25	S	104/517 (20%)	102 (98%)	2 (2%)	0	100	100
26	T	218/249 (88%)	204 (94%)	11 (5%)	3 (1%)	9	39
27	U	175/439 (40%)	165 (94%)	9 (5%)	1 (1%)	22	57
28	V	170/291 (58%)	144 (85%)	17 (10%)	9 (5%)	1	18
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
34	o	1417/1970 (72%)	1310 (92%)	106 (8%)	1 (0%)	48	80
35	p	1128/1174 (96%)	1054 (93%)	73 (6%)	1 (0%)	48	80
36	q	253/275 (92%)	225 (89%)	28 (11%)	0	100	100
37	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
38	s	207/210 (99%)	195 (94%)	12 (6%)	0	100	100
39	t	77/127 (61%)	73 (95%)	3 (4%)	1 (1%)	10	41
40	u	169/172 (98%)	156 (92%)	12 (7%)	1 (1%)	22	57
41	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
42	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
43	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
44	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
45	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	13701/22931 (60%)	12591 (92%)	1001 (7%)	109 (1%)	19	51

5 of 109 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	1	106	LYS
2	1	108	ASN
2	1	110	GLU
2	1	114	LYS
2	1	120	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	173/283 (61%)	173 (100%)	0	100	100
2	1	176/484 (36%)	167 (95%)	9 (5%)	20	45
3	2	279/352 (79%)	272 (98%)	7 (2%)	42	62
4	3	234/272 (86%)	227 (97%)	7 (3%)	36	58
5	4	387/399 (97%)	376 (97%)	11 (3%)	38	59
6	5	48/64 (75%)	46 (96%)	2 (4%)	25	49
7	6	533/688 (78%)	482 (90%)	51 (10%)	7	25
8	7	616/664 (93%)	598 (97%)	18 (3%)	37	59
9	8	258/299 (86%)	252 (98%)	6 (2%)	45	64
10	9	259/296 (88%)	257 (99%)	2 (1%)	79	84
11	A	488/1665 (29%)	446 (91%)	42 (9%)	8	31
12	B	876/1083 (81%)	856 (98%)	20 (2%)	45	64
13	D	143/815 (18%)	138 (96%)	5 (4%)	31	54
13	d	146/815 (18%)	146 (100%)	0	100	100
14	E	478/657 (73%)	466 (98%)	12 (2%)	42	62
14	e	475/657 (72%)	473 (100%)	2 (0%)	89	91
15	F	324/574 (56%)	298 (92%)	26 (8%)	10	33
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
16	G	133/322 (41%)	125 (94%)	8 (6%)	16	41
17	H	181/270 (67%)	172 (95%)	9 (5%)	20	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	I	106/235 (45%)	100 (94%)	6 (6%)	17	43
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	78 (99%)	1 (1%)	65	76
19	j	83/154 (54%)	83 (100%)	0	100	100
20	L	70/141 (50%)	60 (86%)	10 (14%)	2	16
20	l	98/141 (70%)	98 (100%)	0	100	100
21	O	84/98 (86%)	75 (89%)	9 (11%)	5	22
22	P	153/293 (52%)	146 (95%)	7 (5%)	23	47
23	Q	111/324 (34%)	107 (96%)	4 (4%)	30	54
24	R	212/268 (79%)	201 (95%)	11 (5%)	19	45
25	S	93/448 (21%)	91 (98%)	2 (2%)	47	65
26	T	196/218 (90%)	170 (87%)	26 (13%)	3	18
27	U	163/373 (44%)	145 (89%)	18 (11%)	5	21
28	V	155/261 (59%)	135 (87%)	20 (13%)	3	18
31	c	113/833 (14%)	111 (98%)	2 (2%)	54	71
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	79 (99%)	1 (1%)	65	76
34	o	1257/1748 (72%)	1243 (99%)	14 (1%)	70	79
35	p	993/1027 (97%)	991 (100%)	2 (0%)	92	94
36	q	234/252 (93%)	234 (100%)	0	100	100
37	r	106/126 (84%)	105 (99%)	1 (1%)	75	83
38	s	191/192 (100%)	190 (100%)	1 (0%)	86	90
39	t	69/111 (62%)	67 (97%)	2 (3%)	37	59
40	u	152/153 (99%)	150 (99%)	2 (1%)	65	76
41	v	129/131 (98%)	129 (100%)	0	100	100
42	w	103/112 (92%)	103 (100%)	0	100	100
43	x	53/56 (95%)	53 (100%)	0	100	100
44	y	106/106 (100%)	106 (100%)	0	100	100
45	z	41/55 (74%)	41 (100%)	0	100	100
All	All	11953/19766 (60%)	11567 (97%)	386 (3%)	36	56

5 of 386 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
17	H	160	ILE
26	T	124	TYR
18	I	67	ASP
21	O	90	VAL
26	T	196	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
26	T	158	ASN
34	o	372	ASN
27	U	123	ASN
15	f	325	ASN
34	o	780	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	SF4	7	1000	8	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	7	1000	8	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



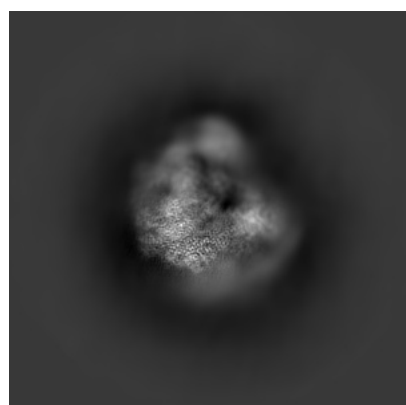
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31112. These allow visual inspection of the internal detail of the map and identification of artifacts.

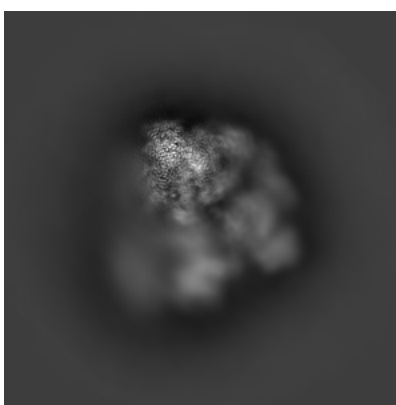
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

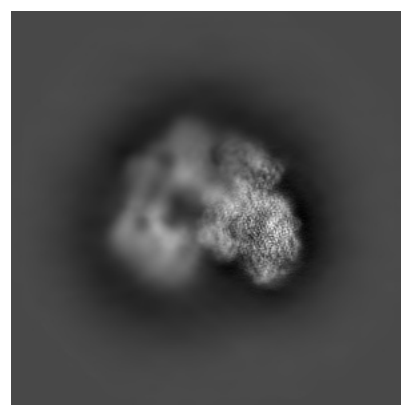
#### 6.1.1 Primary map



X



Y

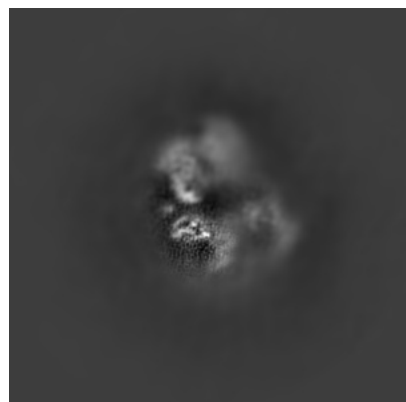


Z

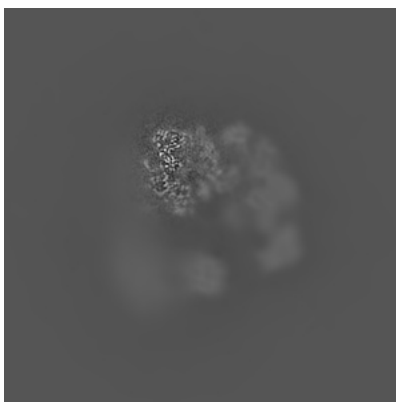
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

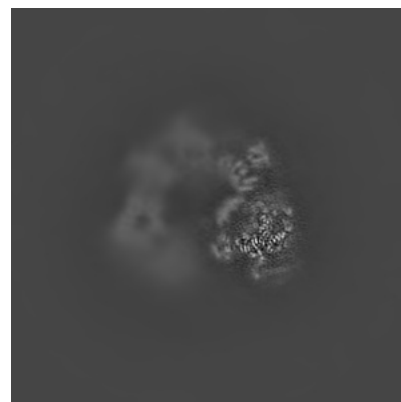
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



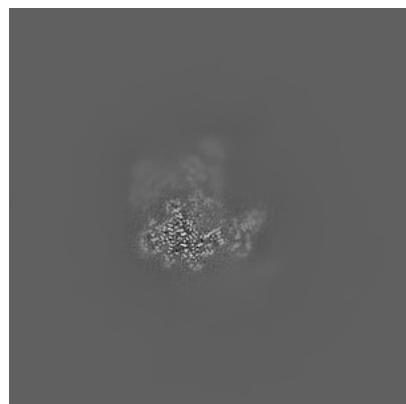
Z Index: 256



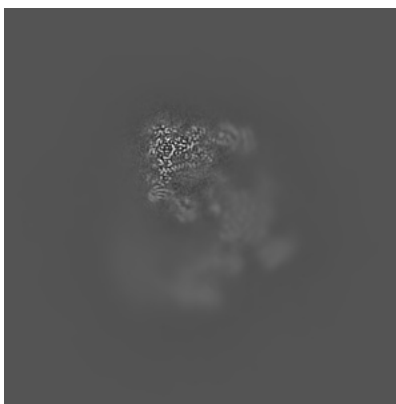
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

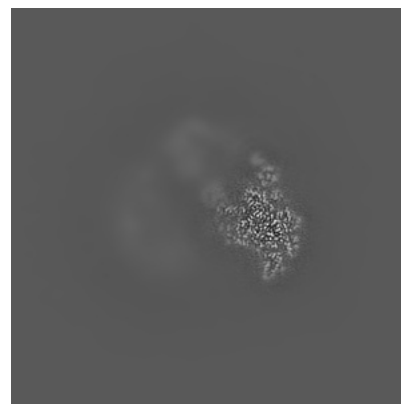
### 6.3.1 Primary map



X Index: 334



Y Index: 228

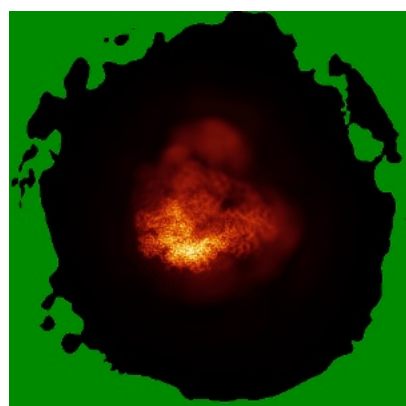


Z Index: 209

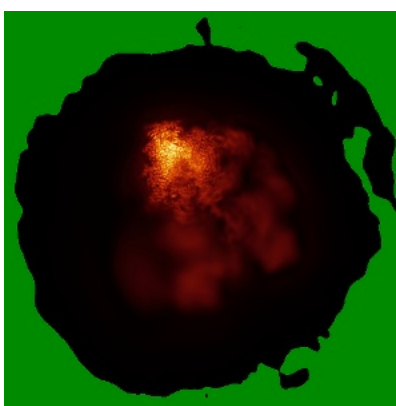
The images above show the largest variance slices of the map in three orthogonal directions.

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

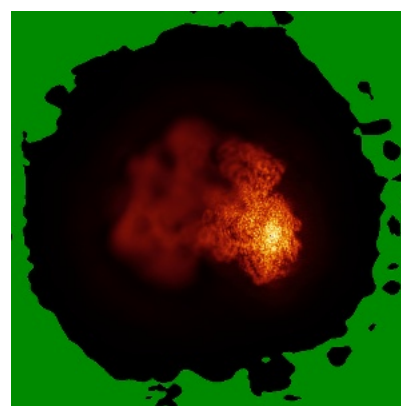
### 6.4.1 Primary map



X



Y



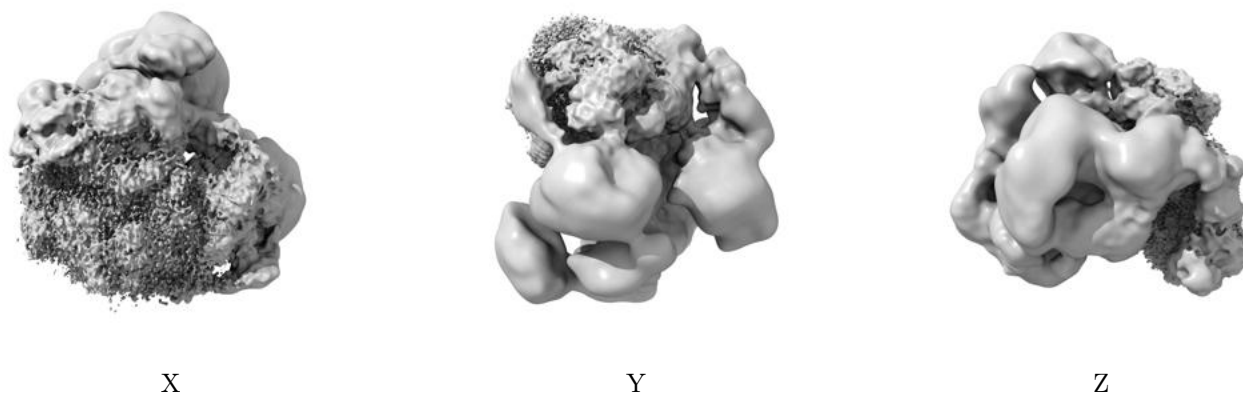
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0051. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

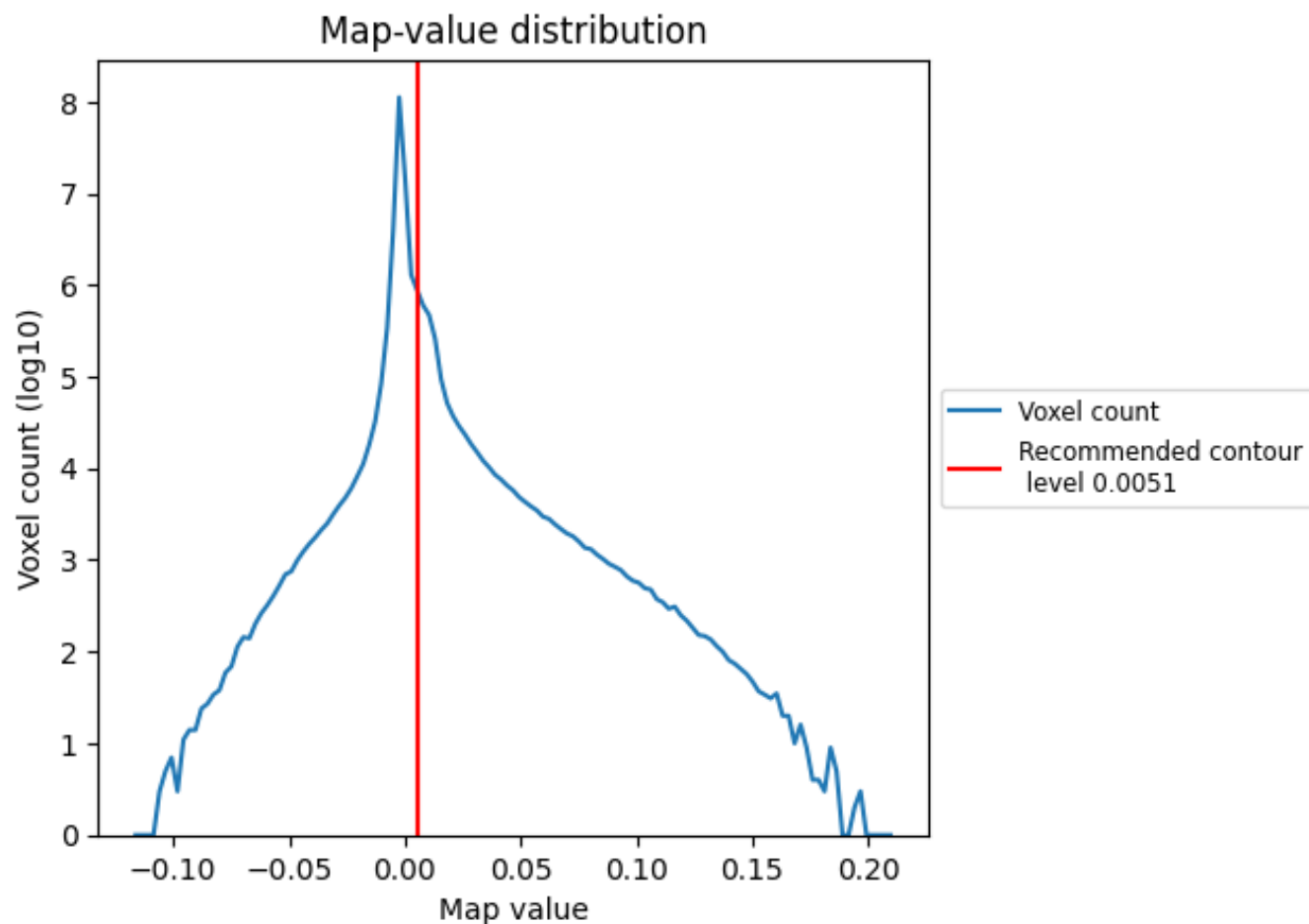
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

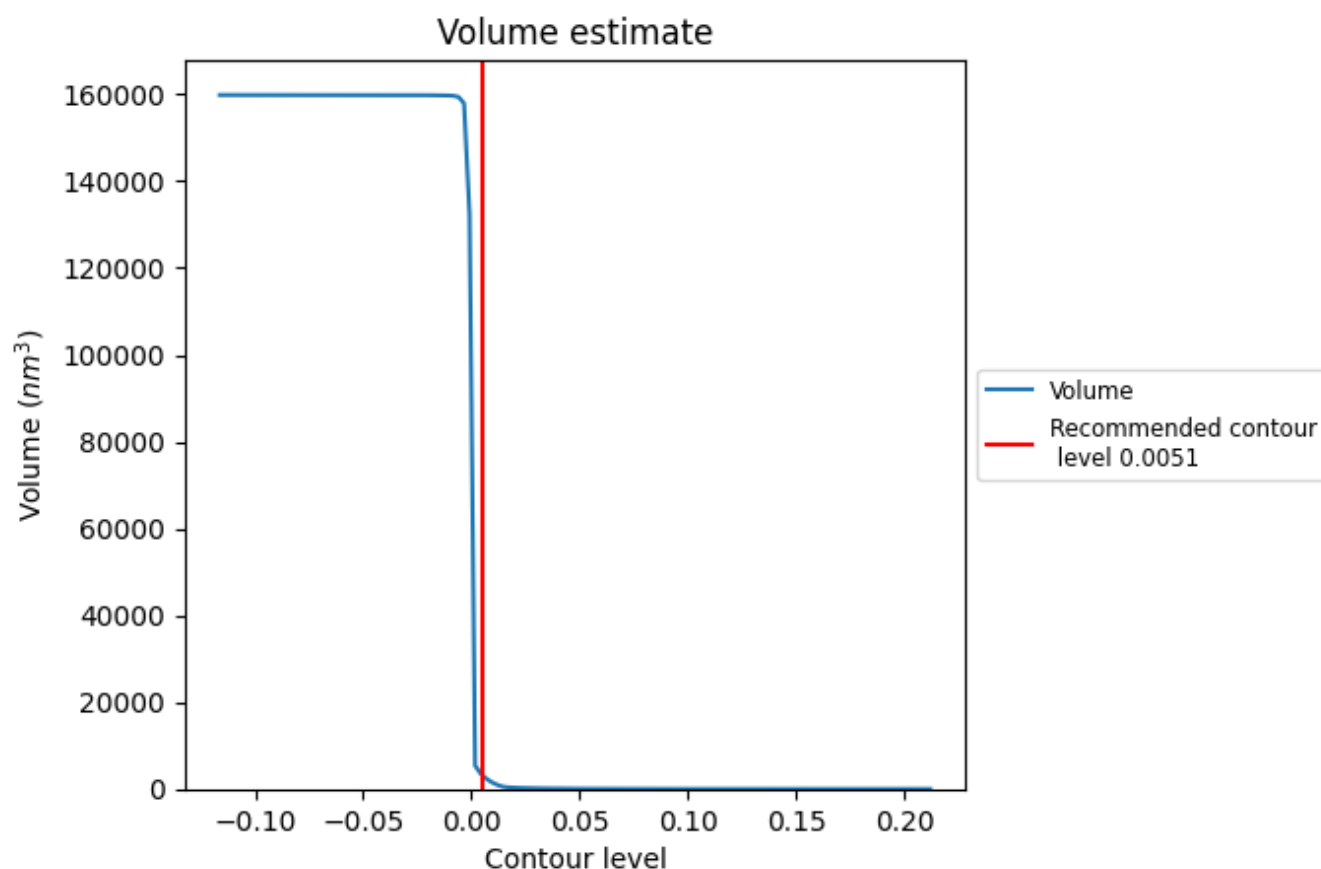
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

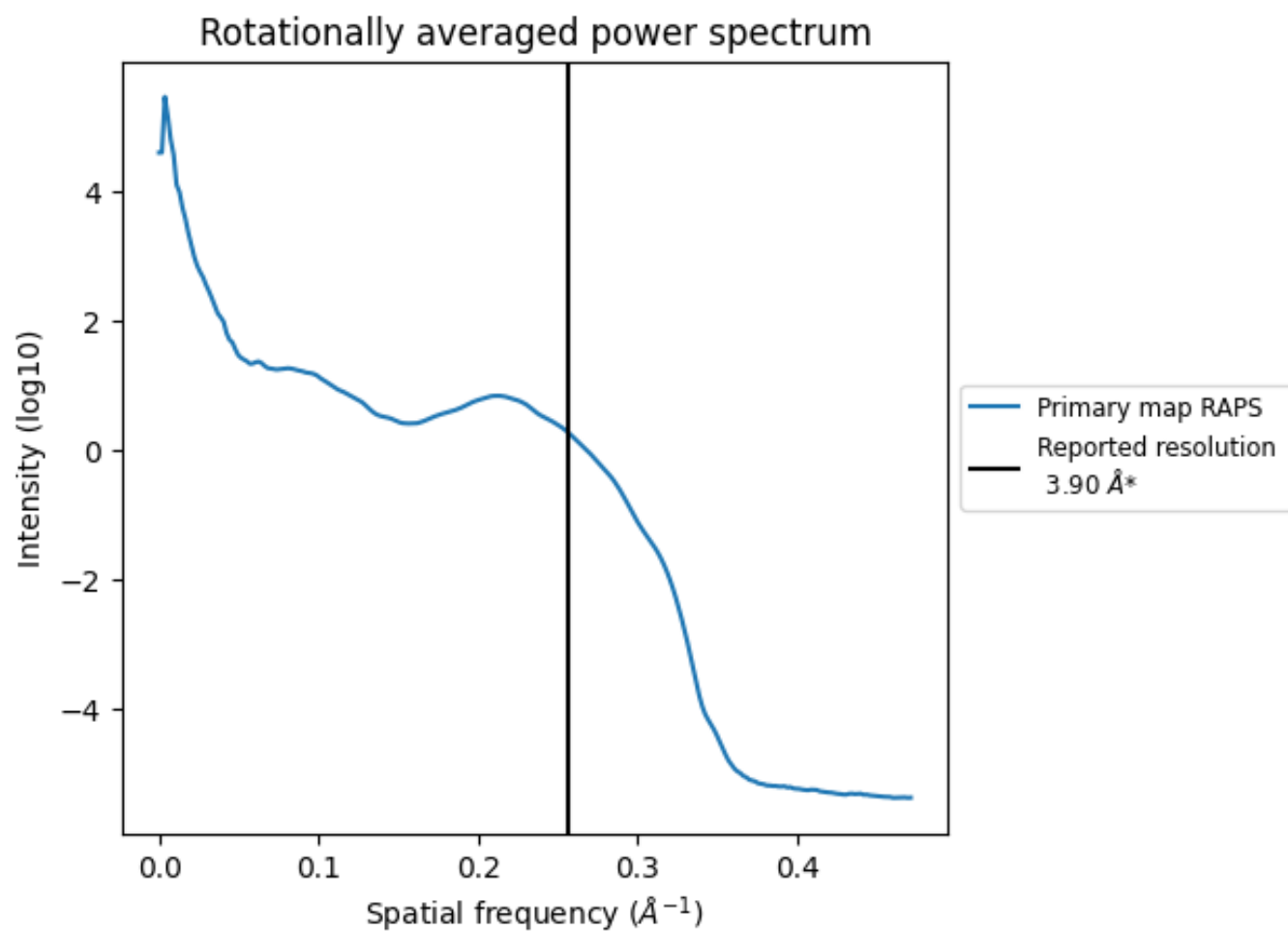


The volume at the recommended contour level is 3205  $\text{nm}^3$ ; this corresponds to an approximate mass of 2895 kDa.

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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

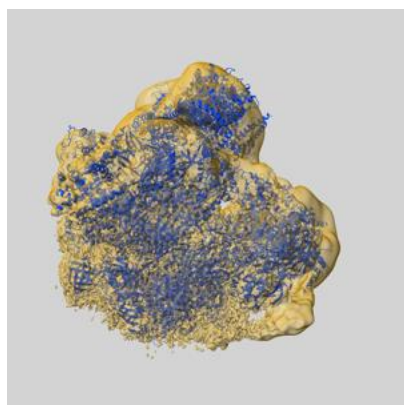
This section was not generated. No FSC curve or half-maps provided.



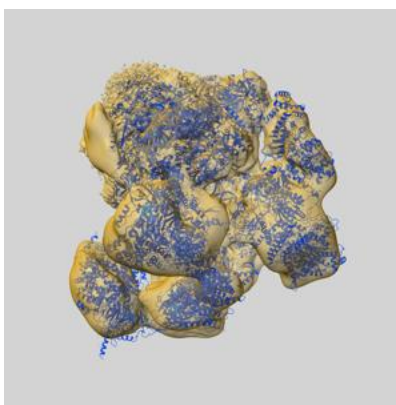
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31112 and PDB model 7EGC. Per-residue inclusion information can be found in section [3](#) on page [14](#).

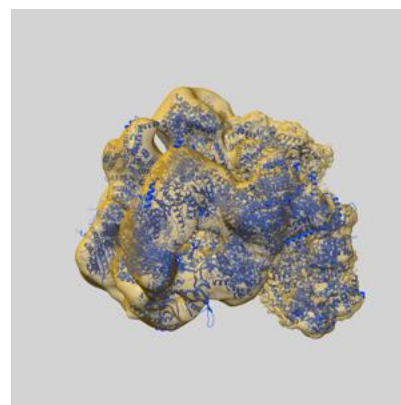
### 9.1 Map-model overlay [i](#)



X



Y

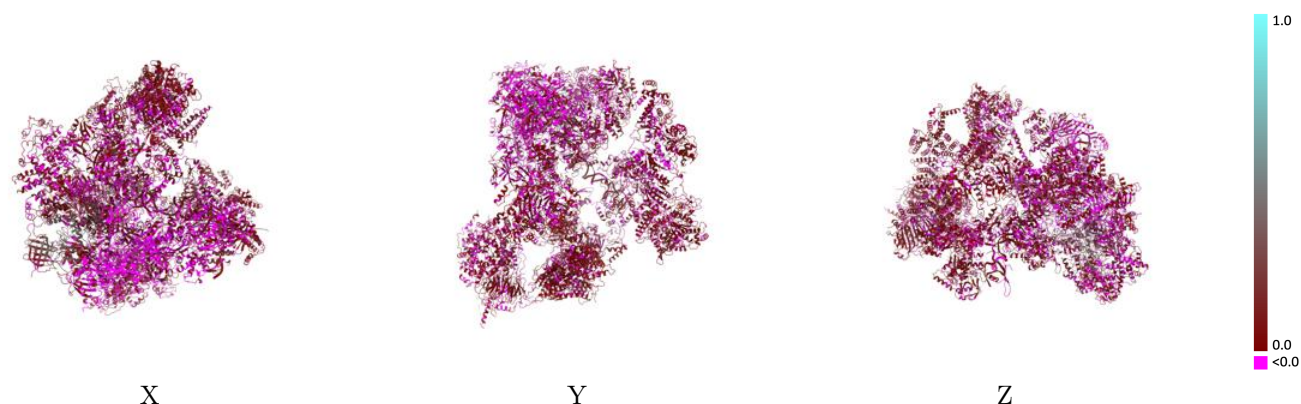


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

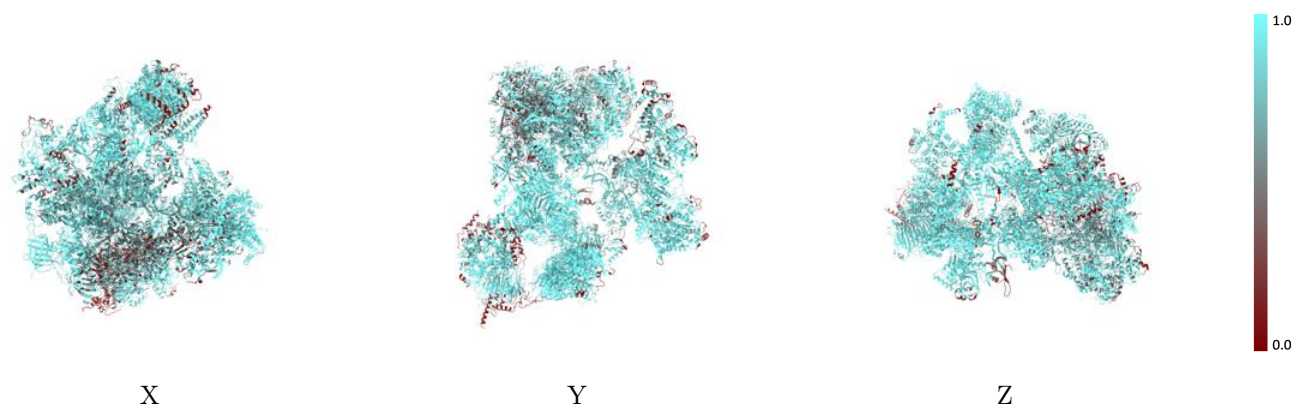


## 9.2 Q-score mapped to coordinate model [i](#)



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

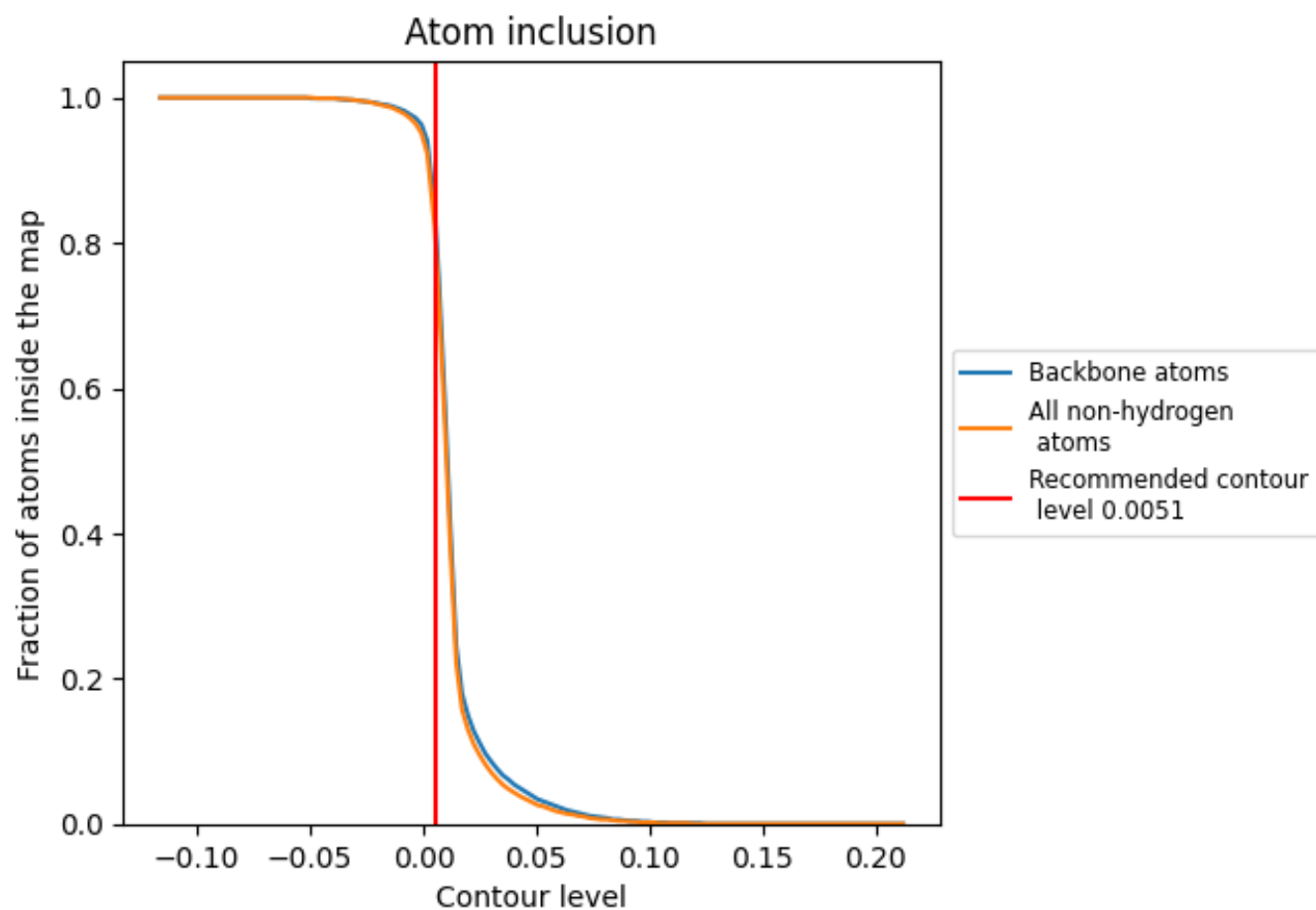
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0051).



## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.0051) and Q-score for the entire model and for each chain.



































Chain	Atom inclusion	Q-score
All	 0.8210	 0.0510
0	 0.6780	 0.0570
1	 0.7750	 0.0270
2	 0.9400	 0.0590
3	 0.9280	 0.0540
4	 0.8880	 0.0660
5	 0.9290	 0.0540
6	 0.9350	 0.0560
7	 0.8980	 0.0570
8	 0.7650	 0.0310
9	 0.7140	 0.0580
A	 0.9050	 0.0510
B	 0.9610	 0.0590
D	 0.9570	 0.0370
E	 0.9470	 0.0620
F	 0.9620	 0.0700
G	 0.7490	 0.0490
H	 0.9540	 0.0570
I	 0.9500	 0.0490
J	 1.0000	 0.0740
L	 0.9600	 0.0400
O	 0.8670	 0.0250
P	 0.7910	 -0.0350
Q	 0.8340	 0.0430
R	 0.6570	 -0.0250
S	 0.8680	 0.0190
T	 0.7950	 0.0260
U	 0.8710	 0.0620
V	 0.9120	 0.0630
X	 0.8320	 0.0580
Y	 0.8250	 0.0620
c	 0.5150	 0.0220
d	 0.5320	 0.0350
e	 0.8140	 0.0440
f	 0.8270	 0.0520



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Chain	Atom inclusion	Q-score
i	 0.7930	 0.0320
j	 0.4240	 0.0270
k	 0.2970	 0.0090
l	 0.7300	 0.0210
m	 0.3460	 0.0180
o	 0.8150	 0.1210
p	 0.6110	 -0.0170
q	 0.6790	 -0.0350
r	 0.8940	 0.0770
s	 0.8650	 0.1030
t	 0.7920	 0.1140
u	 0.8390	 0.0330
v	 0.9310	 0.2230
w	 0.7750	 0.0030
x	 0.5760	 -0.0350
y	 0.7790	 0.1080
z	 0.6400	 -0.0420