



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 09:04 PM EDT

PDB ID : 5U0S  
EMDB ID : EMD-8480  
Title : Cryo-EM structure of the Mediator-RNAPII complex  
Authors : Tsai, K.-L.; Yu, X.; Gopalan, S.; Chao, T.-C.; Zhang, Y.; Florens, L.; Washburn, M.P.; Murakami, K.; Conaway, R.C.; Conaway, J.W.; Asturias, F.  
Deposited on : 2016-11-26  
Resolution : 7.80 Å(reported)

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

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

---

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

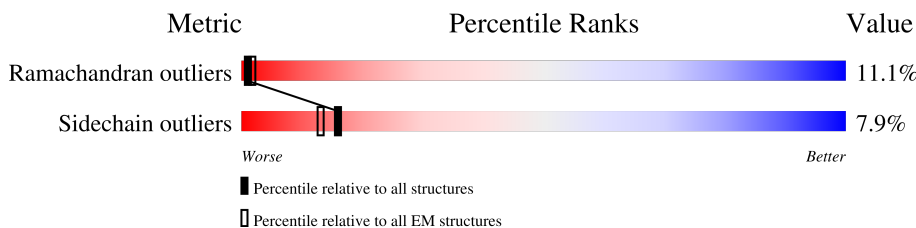
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 7.80 Å.

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



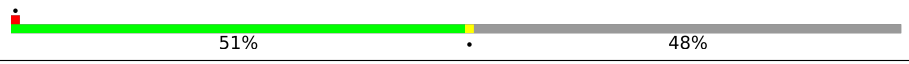





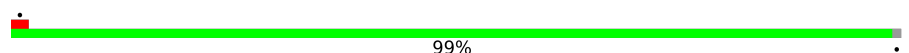
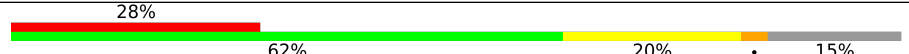
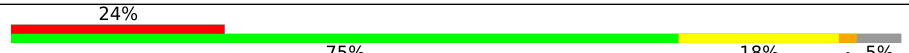
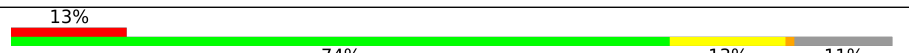

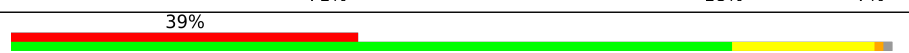


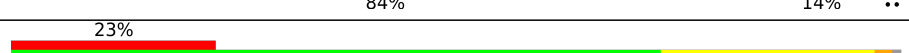

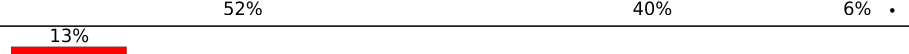
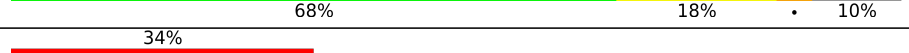

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	F	216	
2	H	200	
3	Q	545	
4	R	207	
5	T	193	
6	K	116	
7	V	136	
8	N	931	
9	D	239	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	G	376	
11	U	138	
12	3	139	
13	2	273	
14	I	121	
15	S	139	
16	J	132	
17	a	1752	
18	b	1210	
19	c	297	
20	d	135	
21	e	210	
22	f	142	
23	g	172	
24	h	125	
25	i	113	
26	j	71	
27	k	123	
28	l	63	

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 51548 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 Mediator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	188	1534	979	258	288	9	0	0

- Molecule 2 is a protein called Mediator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	182	1493	941	257	292	3	0	0

- Molecule 3 is a protein called Mediator complex subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	500	3787	2393	651	725	18	0	0

- Molecule 4 is a protein called Mediator complex subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	207	1694	1082	288	316	8	0	0

- Molecule 5 is a protein called Mediator complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	T	176	1435	938	234	258	5	0	0

- Molecule 6 is a protein called Mediator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	98	769	486	128	154	1	0	0

- Molecule 7 is a protein called Mediator complex subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	V	118	949	599	161	187	2	0	0

- Molecule 8 is a protein called Mediator complex subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	520	3887	2498	683	698	8	0	0

- Molecule 9 is a protein called Mediator complex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	D	96	480	288	96	96	0	0

- Molecule 10 is a protein called Mediator complex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	G	194	965	577	194	194	0	0

- Molecule 11 is a protein called Mediator complex subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	U	122	608	364	122	122	0	0

- Molecule 12 is a protein called Mediator complex subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	3	103	515	309	103	103	0	0

- Molecule 13 is a protein called Mediator complex subunit 27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	2	78	388	232	78	78	0	0

- Molecule 14 is a protein called Mediator complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	I	75	374	224	75	75	0	0

- Molecule 15 is a protein called Mediator complex subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	S	122	610	366	122	122	0	0

- Molecule 16 is a protein called Mediator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	J	131	655	393	131	131	0	0

- Molecule 17 is a protein called RNA polymerase II subunit Rpb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	a	1490	11761	7388	2065	2238	70	0	0

- Molecule 18 is a protein called RNA polymerase II subunit Rpb2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	b	1150	9180	5772	1630	1716	62	0	0

- Molecule 19 is a protein called RNA polymerase II subunit Rpb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	c	263	2088	1315	355	406	12	0	0

- Molecule 20 is a protein called RNA polymerase II subunit Rpb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	d	125	988	619	166	197	6	0	0

- Molecule 21 is a protein called RNA polymerase II subunit Rpb5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		

- Molecule 22 is a protein called RNA polymerase II subunit Rpb6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	83	Total	C	N	O	S	0	0
			656	416	112	125	3		

- Molecule 23 is a protein called RNA polymerase II subunit Rpb7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	170	Total	C	N	O	S	0	0
			1330	860	217	247	6		

- Molecule 24 is a protein called RNA polymerase II subunit Rpb8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	h	124	Total	C	N	O	S	0	0
			996	631	167	195	3		

- Molecule 25 is a protein called RNA polymerase II subunit Rpb9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	111	Total	C	N	O	S	0	0
			902	551	164	176	11		

- Molecule 26 is a protein called RNA polymerase II subunit Rpb10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	64	Total	C	N	O	S	0	0
			518	330	87	94	7		

- Molecule 27 is a protein called RNA polymerase II subunit Rpb11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	119	Total	C	N	O	S	0	0
			955	608	159	182	6		

- Molecule 28 is a protein called RNA polymerase II subunit Rpb12.

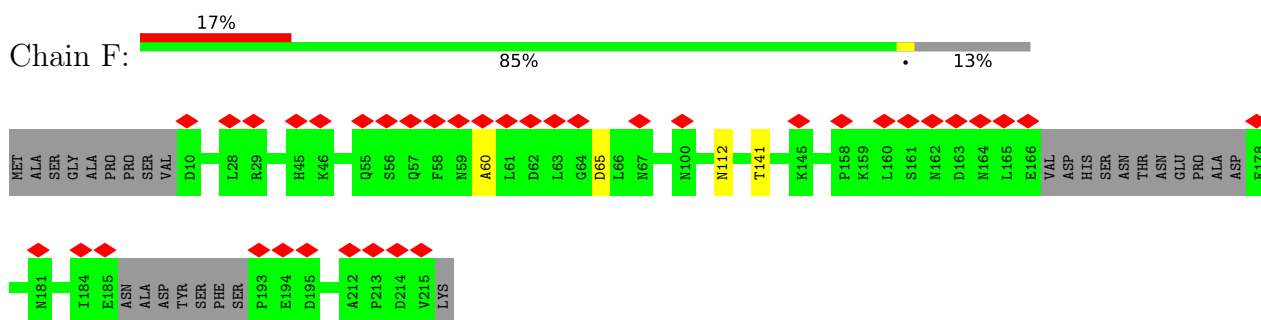
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	1	45	368	225	74	61	8	0	0



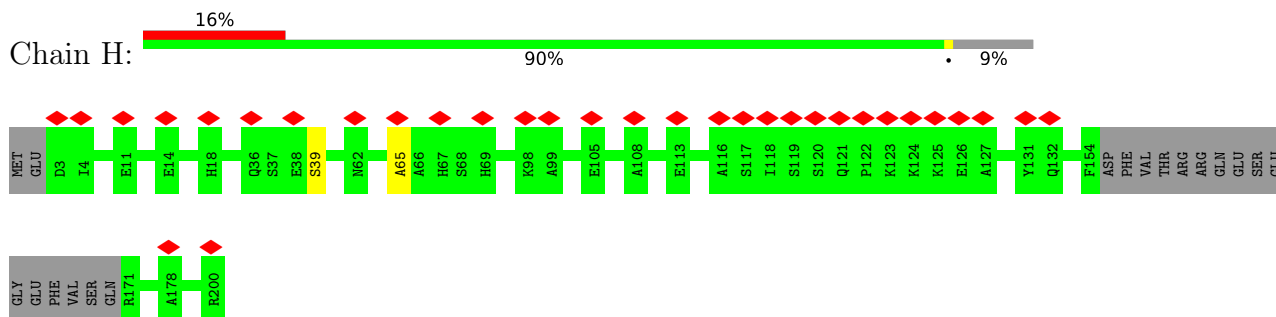
### 3 Residue-property plots [i](#)

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

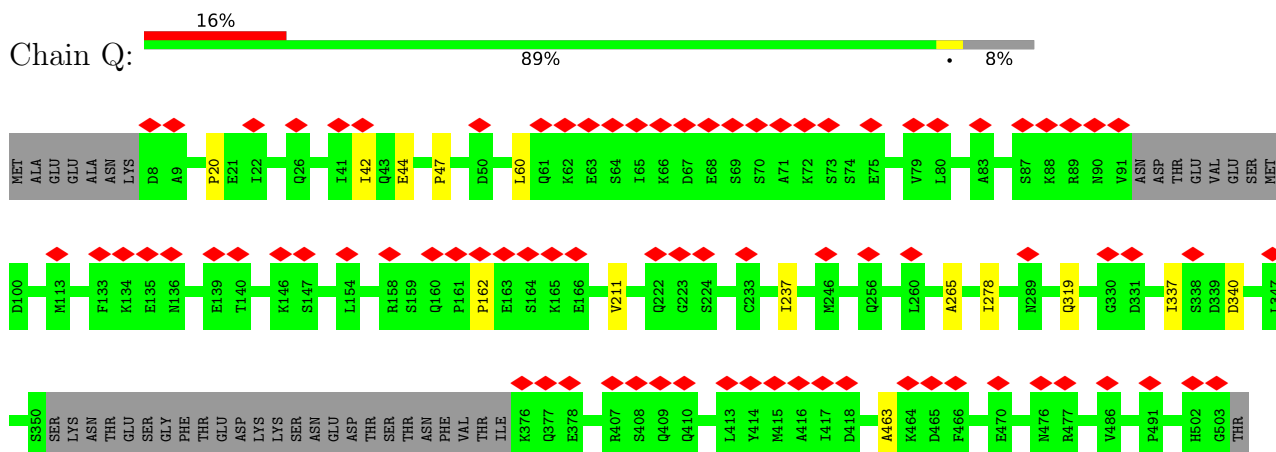
- Molecule 1: Mediator complex subunit 6

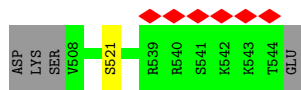


- Molecule 2: Mediator complex subunit 8

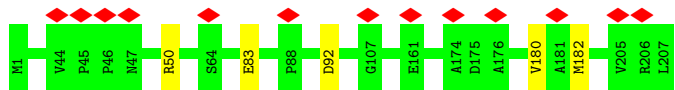


- Molecule 3: Mediator complex subunit 17

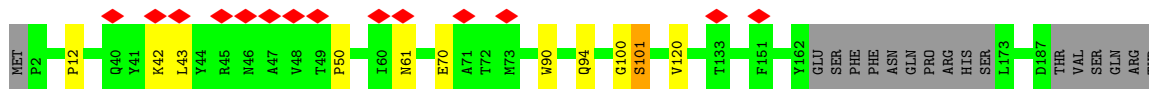
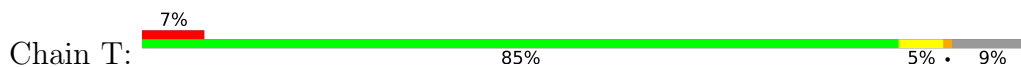




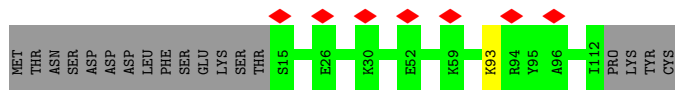
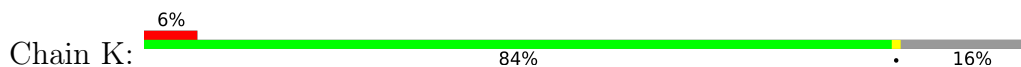
• Molecule 4: Mediator complex subunit 18



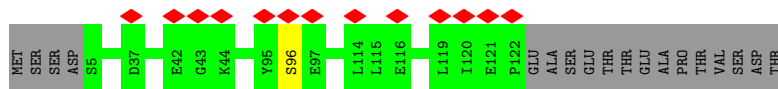
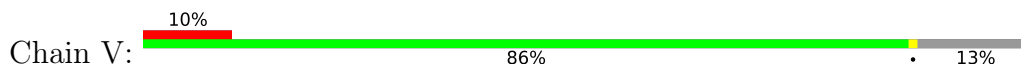
• Molecule 5: Mediator complex subunit 20



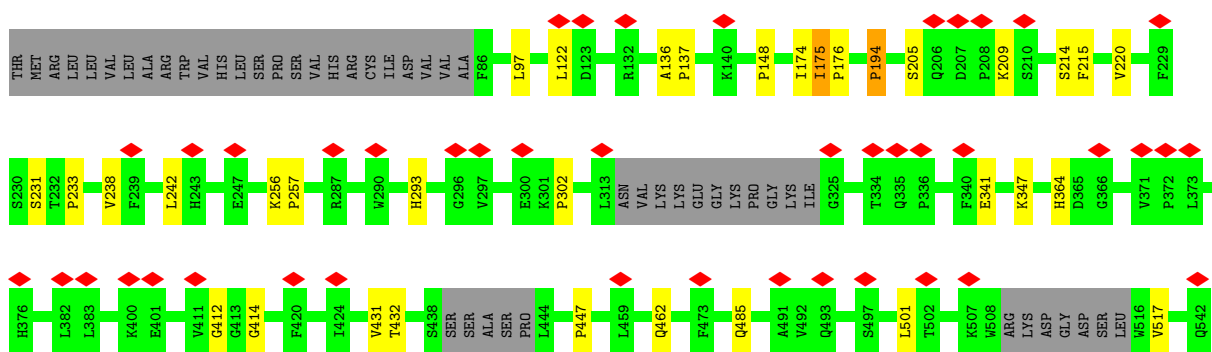
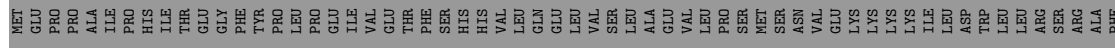
• Molecule 6: Mediator complex subunit 11



• Molecule 7: Mediator complex subunit 22

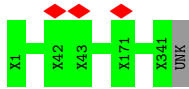


• Molecule 8: Mediator complex subunit 14

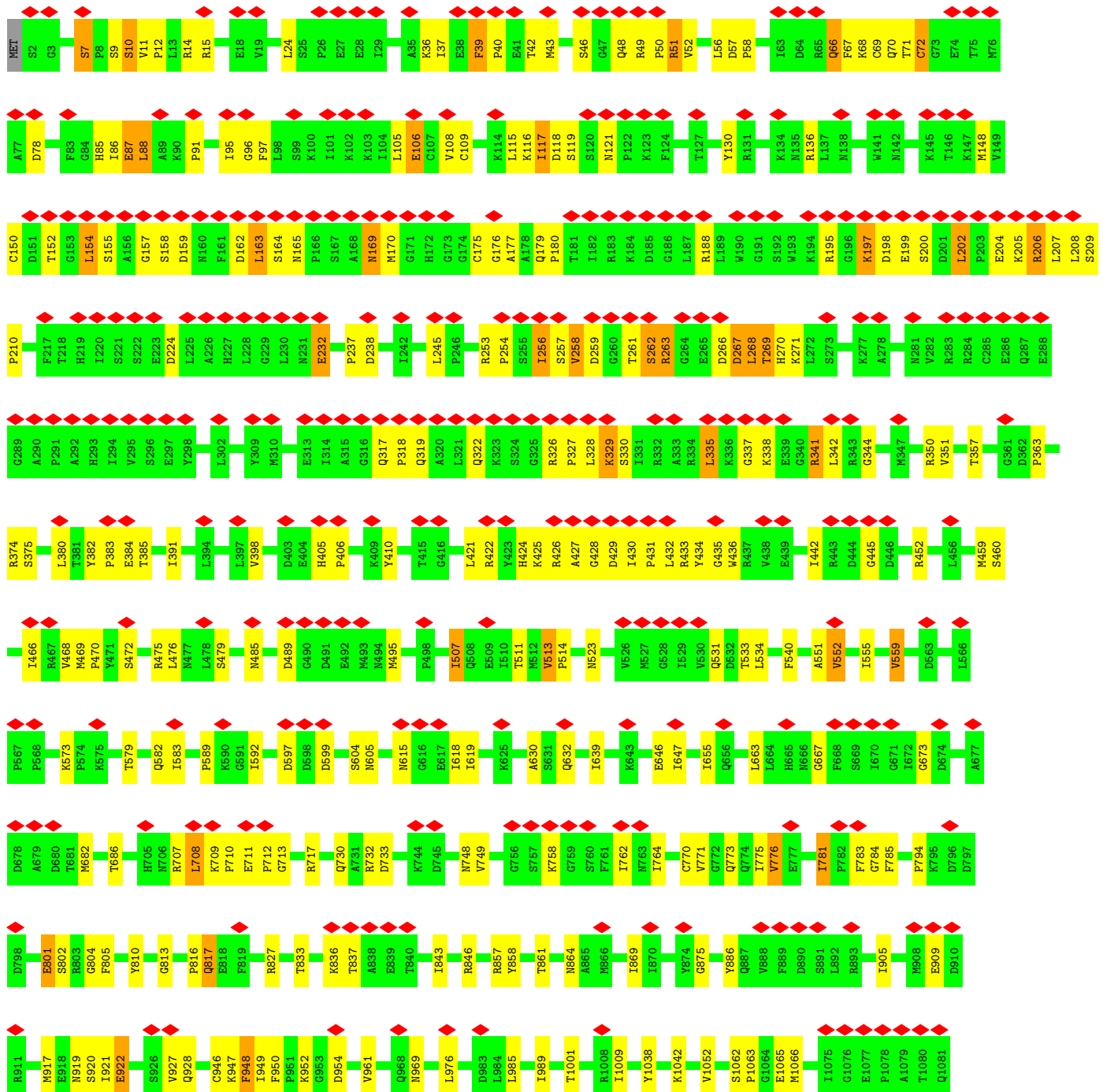


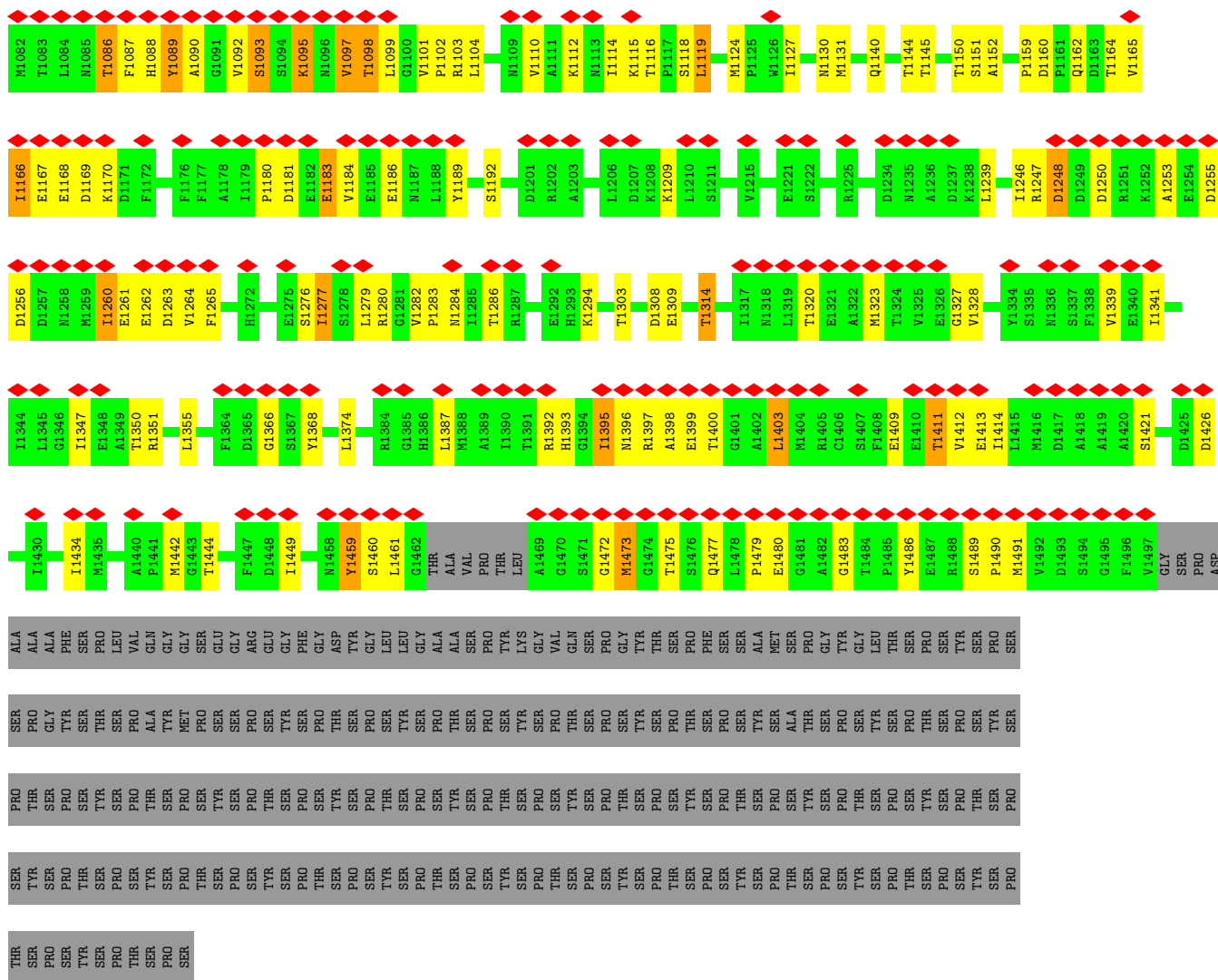




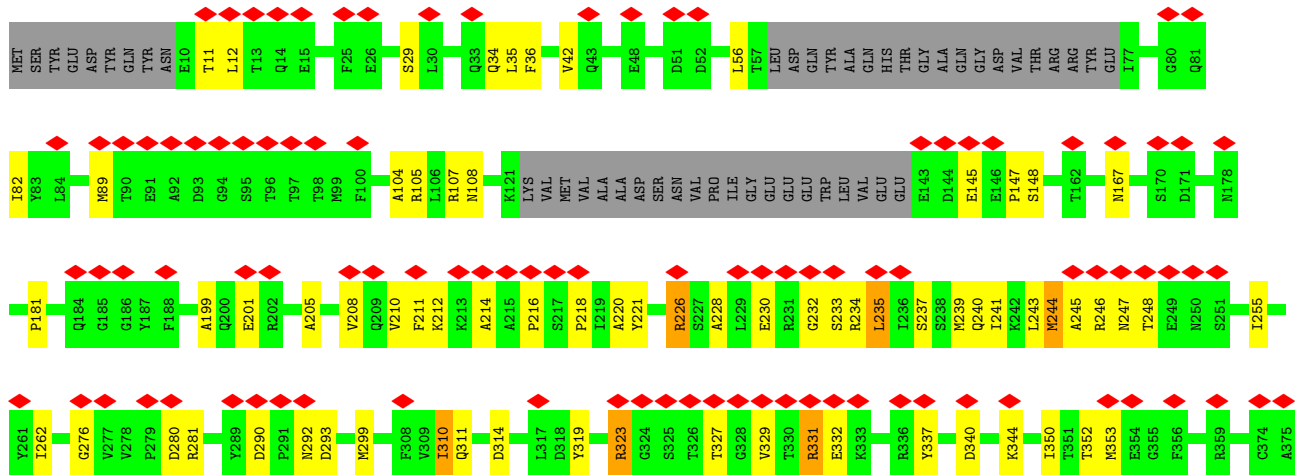
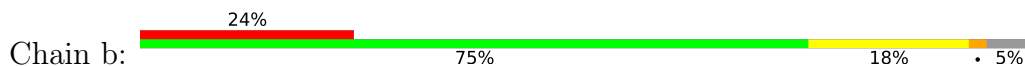


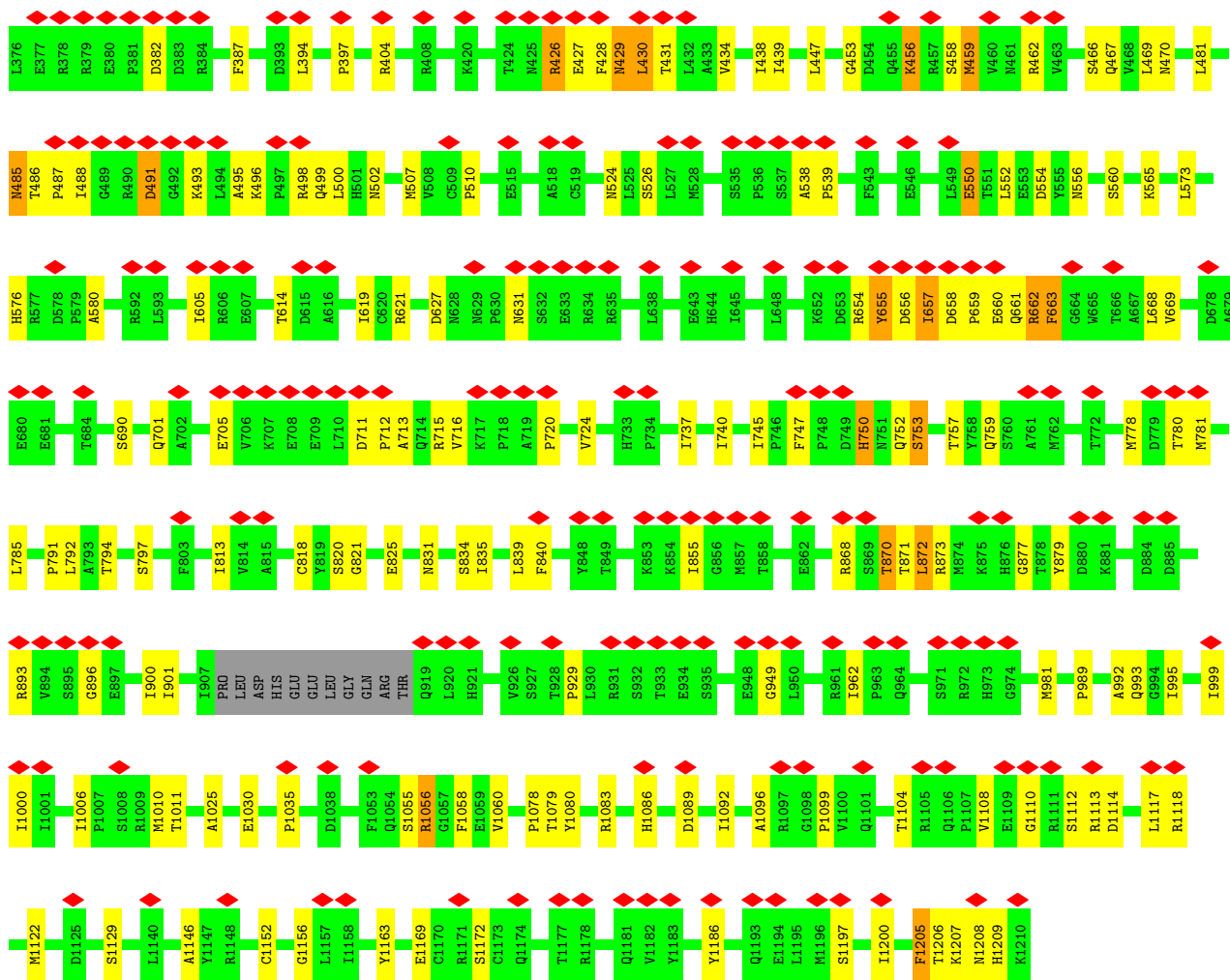
• Molecule 17: RNA polymerase II subunit Rpb1



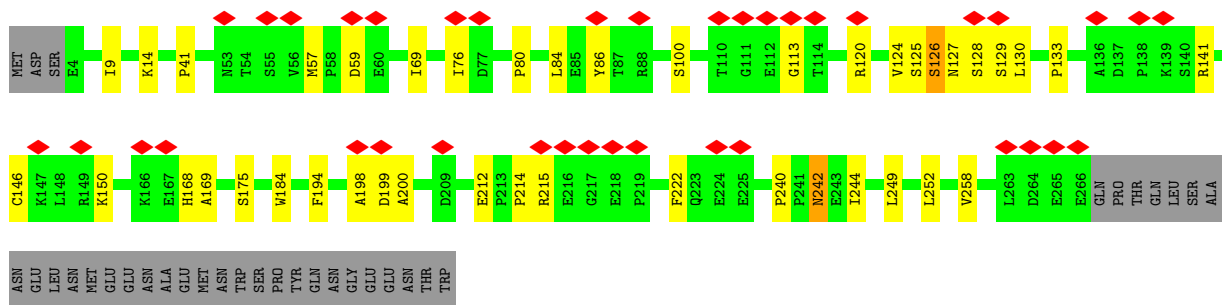
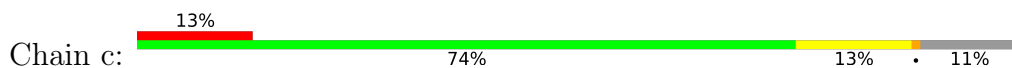


• Molecule 18: RNA polymerase II subunit Rpb2

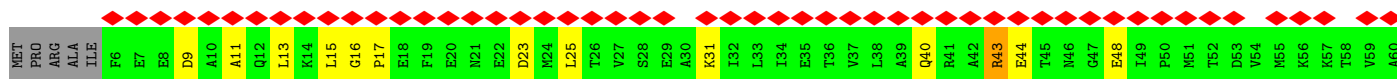
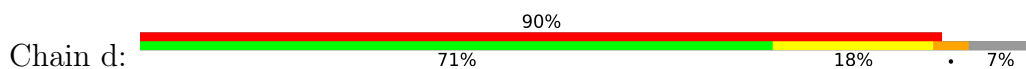




• Molecule 19: RNA polymerase II subunit Rpb3

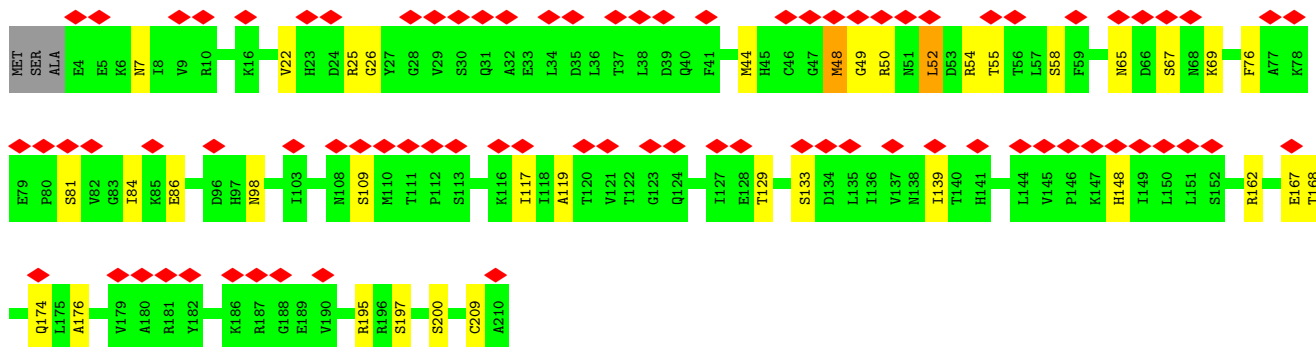
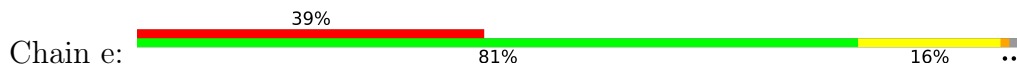


• Molecule 20: RNA polymerase II subunit Rpb4

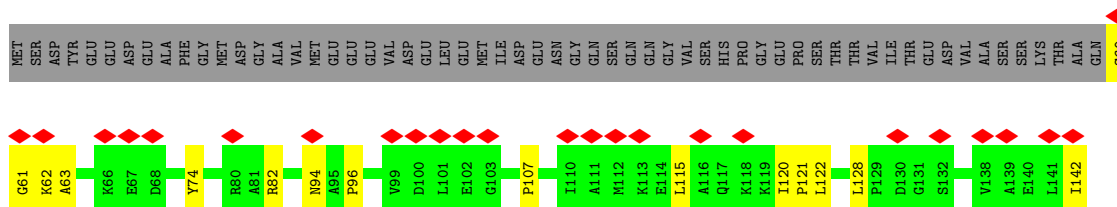




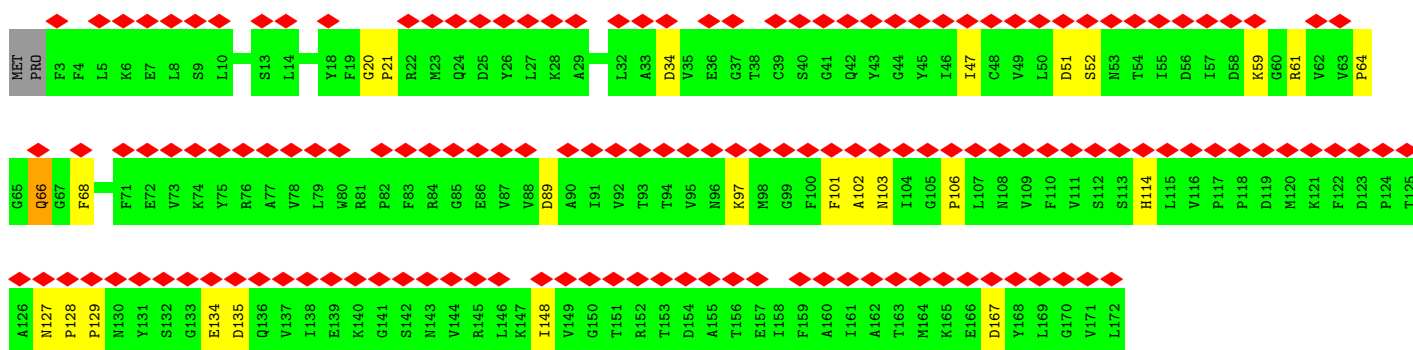
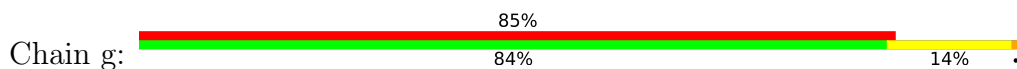
• Molecule 21: RNA polymerase II subunit Rpb5



• Molecule 22: RNA polymerase II subunit Rpb6

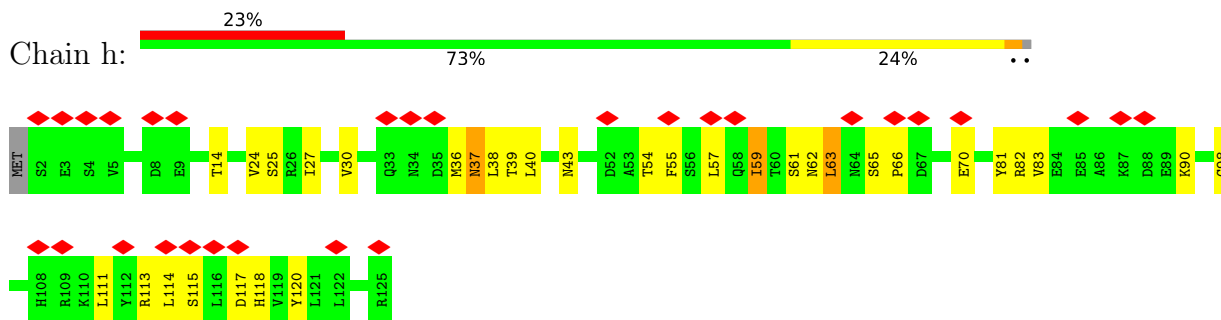


• Molecule 23: RNA polymerase II subunit Rpb7

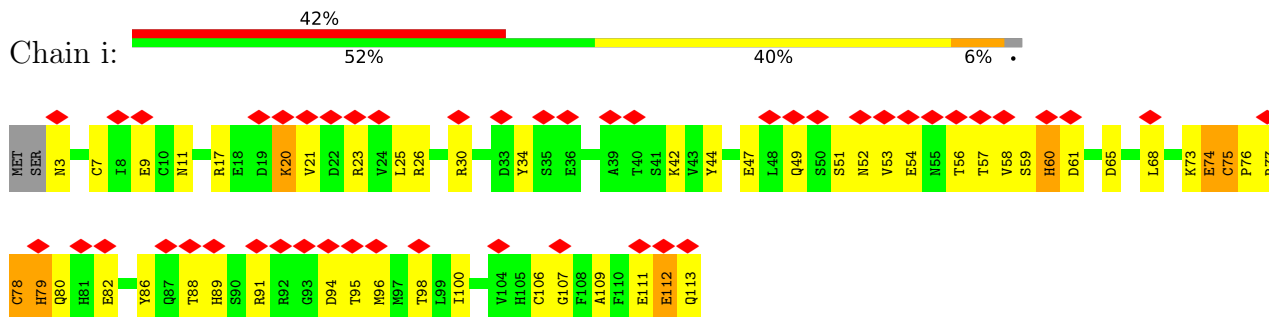


• Molecule 24: RNA polymerase II subunit Rpb8

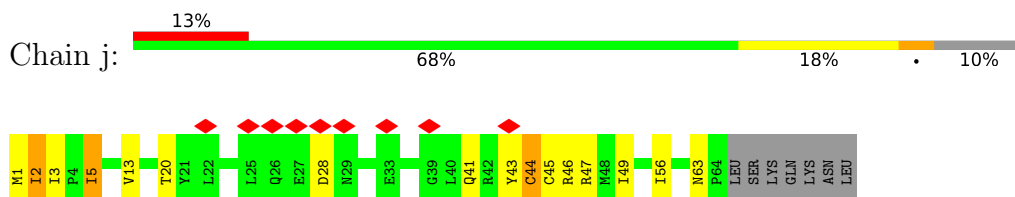




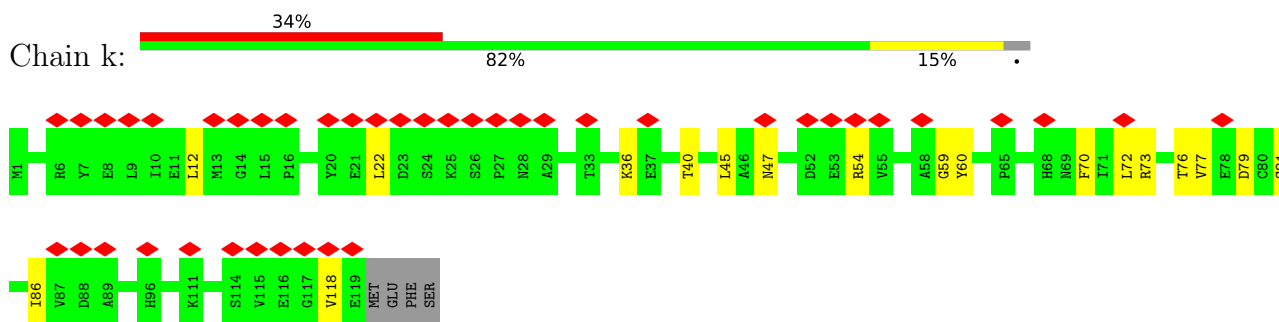
• Molecule 25: RNA polymerase II subunit Rpb9



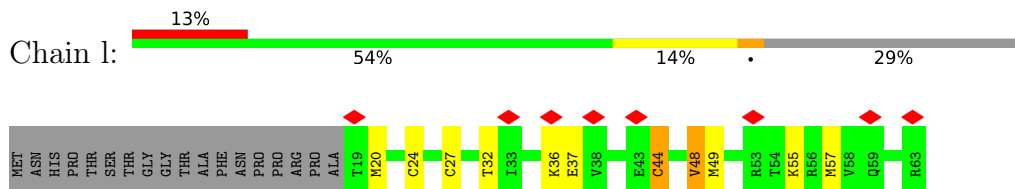
• Molecule 26: RNA polymerase II subunit Rpb10



• Molecule 27: RNA polymerase II subunit Rpb11



• Molecule 28: RNA polymerase II subunit Rpb12



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	9.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.229	Depositor
Minimum map value	-0.114	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	461.12, 461.12, 461.12	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.62, 2.62, 2.62	Depositor

## 5 Model quality [i](#)

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

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	F	0.28	0/1570	0.49	0/2126
2	H	0.27	0/1523	0.48	0/2063
3	Q	0.29	0/3856	0.49	2/5223 (0.0%)
4	R	0.28	0/1739	0.51	0/2362
5	T	0.31	0/1469	0.74	5/1992 (0.3%)
6	K	0.30	0/778	0.50	0/1049
7	V	0.27	0/963	0.46	0/1309
8	N	0.30	0/3865	0.61	6/5275 (0.1%)
10	G	0.30	0/961	0.50	0/1336
11	U	0.27	0/606	0.47	0/844
12	3	0.26	0/514	0.52	1/718 (0.1%)
13	2	0.23	0/382	0.40	0/524
14	I	0.25	0/373	0.45	0/520
17	a	0.42	0/11983	0.57	1/16197 (0.0%)
18	b	0.44	0/9360	0.60	5/12643 (0.0%)
19	c	0.45	0/2135	0.60	0/2904
20	d	0.25	0/1000	0.38	0/1348
21	e	0.39	0/1695	0.60	0/2287
22	f	0.50	0/666	0.67	0/901
23	g	0.27	0/1361	0.57	3/1847 (0.2%)
24	h	0.42	0/1010	0.65	0/1363
25	i	0.23	0/921	0.37	0/1246
26	j	0.57	0/526	0.77	0/709
27	k	0.47	0/972	0.62	0/1317
28	l	0.37	0/371	0.57	0/491
All	All	0.37	0/50599	0.57	23/68594 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
-----	-------	---------------------	---------------------

Mol	Chain	#Chirality outliers	#Planarity outliers
8	N	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	100	GLY	C-N-CA	12.78	153.64	121.70
5	T	101	SER	O-C-N	-9.55	107.42	122.70
8	N	175	ILE	C-N-CD	-9.20	100.37	120.60
8	N	194	PRO	CA-N-CD	-8.83	99.14	111.50
5	T	100	GLY	CA-C-N	7.08	132.76	117.20
3	Q	20	PRO	N-CA-CB	6.43	111.02	103.30
5	T	101	SER	CA-C-N	6.34	131.14	117.20
8	N	148	PRO	N-CA-CB	6.08	110.59	103.30
3	Q	47	PRO	N-CA-CB	6.01	110.51	103.30
8	N	175	ILE	C-N-CA	5.96	147.05	122.00
8	N	137	PRO	N-CA-CB	5.82	110.28	103.30
18	b	992	ALA	N-CA-C	-5.71	95.58	111.00
5	T	100	GLY	CA-C-O	-5.68	110.37	120.60
12	3	11	PRO	N-CA-CB	5.59	110.00	103.30
8	N	852	PRO	N-CA-CB	5.57	109.99	103.30
23	g	167	ASP	CB-CG-OD2	5.42	123.18	118.30
18	b	314	ASP	CB-CG-OD2	5.29	123.06	118.30
18	b	711	ASP	CB-CG-OD2	5.27	123.05	118.30
17	a	224	ASP	CB-CG-OD2	5.27	123.04	118.30
23	g	34	ASP	CB-CG-OD2	5.24	123.02	118.30
18	b	491	ASP	CB-CG-OD2	5.19	122.97	118.30
18	b	340	ASP	CB-CG-OD2	5.17	122.96	118.30
23	g	89	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	N	256	LYS	Peptide
8	N	302	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	182/216 (84%)	154 (85%)	24 (13%)	4 (2%)	6	35
2	H	178/200 (89%)	161 (90%)	15 (8%)	2 (1%)	14	52
3	Q	492/545 (90%)	424 (86%)	55 (11%)	13 (3%)	5	31
4	R	205/207 (99%)	177 (86%)	23 (11%)	5 (2%)	6	33
5	T	172/193 (89%)	141 (82%)	21 (12%)	10 (6%)	1	18
6	K	96/116 (83%)	88 (92%)	7 (7%)	1 (1%)	15	55
7	V	116/136 (85%)	107 (92%)	8 (7%)	1 (1%)	17	57
8	N	489/931 (52%)	382 (78%)	72 (15%)	35 (7%)	1	14
10	G	186/376 (50%)	166 (89%)	18 (10%)	2 (1%)	14	52
11	U	118/138 (86%)	110 (93%)	5 (4%)	3 (2%)	5	32
12	3	101/139 (73%)	76 (75%)	9 (9%)	16 (16%)	0	3
13	2	66/273 (24%)	62 (94%)	3 (4%)	1 (2%)	10	46
14	I	73/121 (60%)	67 (92%)	3 (4%)	3 (4%)	3	23
17	a	1486/1752 (85%)	937 (63%)	276 (19%)	273 (18%)	0	2
18	b	1142/1210 (94%)	735 (64%)	244 (21%)	163 (14%)	0	4
19	c	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	0	8
20	d	123/135 (91%)	85 (69%)	20 (16%)	18 (15%)	0	4
21	e	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0	6
22	f	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	0	9
23	g	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	0	10
24	h	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	i	109/113 (96%)	46 (42%)	27 (25%)	36 (33%)	0	0
26	j	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	0	10
27	k	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0	7
28	l	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	2
All	All	6393/8004 (80%)	4635 (72%)	1047 (16%)	711 (11%)	1	7

All (711) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	319	GLN
4	R	50	ARG
5	T	101	SER
8	N	175	ILE
8	N	194	PRO
8	N	209	LYS
8	N	214	SER
8	N	233	PRO
8	N	293	HIS
8	N	431	VAL
8	N	852	PRO
8	N	875	ILE
11	U	28	SER
12	3	11	PRO
12	3	60	PRO
12	3	80	ASN
13	2	134	ASP
14	I	94	ALA
17	a	10	SER
17	a	12	PRO
17	a	37	ILE
17	a	42	THR
17	a	50	PRO
17	a	52	VAL
17	a	57	ASP
17	a	58	PRO
17	a	66	GLN
17	a	69	CYS
17	a	87	GLU
17	a	88	LEU
17	a	91	PRO
17	a	95	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	105	LEU
17	a	106	GLU
17	a	117	ILE
17	a	148	MET
17	a	152	THR
17	a	154	LEU
17	a	169	ASN
17	a	175	CYS
17	a	177	ALA
17	a	179	GLN
17	a	197	LYS
17	a	199	GLU
17	a	202	LEU
17	a	256	ILE
17	a	258	VAL
17	a	261	THR
17	a	262	SER
17	a	263	ARG
17	a	267	ASP
17	a	269	THR
17	a	270	HIS
17	a	319	GLN
17	a	338	LYS
17	a	341	ARG
17	a	342	LEU
17	a	350	ARG
17	a	351	VAL
17	a	383	PRO
17	a	405	HIS
17	a	410	TYR
17	a	422	ARG
17	a	424	HIS
17	a	425	LYS
17	a	431	PRO
17	a	432	LEU
17	a	433	ARG
17	a	466	ILE
17	a	468	VAL
17	a	469	MET
17	a	507	ILE
17	a	540	PHE
17	a	551	ALA

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	559	VAL
17	a	573	LYS
17	a	582	GLN
17	a	599	ASP
17	a	630	ALA
17	a	632	GLN
17	a	709	LYS
17	a	771	VAL
17	a	776	VAL
17	a	794	PRO
17	a	804	GLY
17	a	922	GLU
17	a	948	PHE
17	a	952	LYS
17	a	1088	HIS
17	a	1089	TYR
17	a	1101	VAL
17	a	1115	LYS
17	a	1118	SER
17	a	1151	SER
17	a	1152	ALA
17	a	1159	PRO
17	a	1165	VAL
17	a	1168	GLU
17	a	1181	ASP
17	a	1183	GLU
17	a	1184	VAL
17	a	1189	TYR
17	a	1192	SER
17	a	1256	ASP
17	a	1277	ILE
17	a	1282	VAL
17	a	1283	PRO
17	a	1284	ASN
17	a	1314	THR
17	a	1320	THR
17	a	1368	TYR
17	a	1392	ARG
17	a	1393	HIS
17	a	1395	ILE
17	a	1396	ASN
17	a	1398	ALA

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	1403	LEU
17	a	1411	THR
17	a	1413	GLU
17	a	1459	TYR
17	a	1460	SER
17	a	1461	LEU
17	a	1486	TYR
17	a	1489	SER
17	a	1490	PRO
17	a	1491	MET
18	b	147	PRO
18	b	199	ALA
18	b	210	VAL
18	b	218	PRO
18	b	221	TYR
18	b	233	SER
18	b	234	ARG
18	b	235	LEU
18	b	244	MET
18	b	310	ILE
18	b	329	VAL
18	b	344	LYS
18	b	353	MET
18	b	426	ARG
18	b	428	PHE
18	b	430	LEU
18	b	456	LYS
18	b	458	SER
18	b	462	ARG
18	b	466	SER
18	b	485	ASN
18	b	486	THR
18	b	498	ARG
18	b	526	SER
18	b	554	ASP
18	b	576	HIS
18	b	580	ALA
18	b	656	ASP
18	b	657	ILE
18	b	659	PRO
18	b	661	GLN
18	b	662	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	663	PHE
18	b	716	VAL
18	b	720	PRO
18	b	750	HIS
18	b	753	SER
18	b	791	PRO
18	b	820	SER
18	b	870	THR
18	b	1010	MET
18	b	1058	PHE
18	b	1096	ALA
18	b	1113	ARG
18	b	1146	ALA
18	b	1207	LYS
18	b	1208	ASN
19	c	124	VAL
19	c	126	SER
19	c	133	PRO
19	c	194	PHE
19	c	198	ALA
19	c	212	GLU
19	c	215	ARG
20	d	15	LEU
20	d	43	ARG
20	d	44	GLU
20	d	48	GLU
20	d	69	LYS
20	d	87	LYS
20	d	112	ALA
21	e	52	LEU
21	e	55	THR
21	e	58	SER
21	e	76	PHE
21	e	81	SER
21	e	197	SER
22	f	121	PRO
22	f	122	LEU
23	g	47	ILE
23	g	97	LYS
23	g	127	ASN
23	g	135	ASP
24	h	24	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	h	37	ASN
24	h	66	PRO
24	h	82	ARG
24	h	114	LEU
24	h	117	ASP
24	h	118	HIS
25	i	7	CYS
25	i	20	LYS
25	i	21	VAL
25	i	23	ARG
25	i	49	GLN
25	i	51	SER
25	i	52	ASN
25	i	54	GLU
25	i	58	VAL
25	i	59	SER
25	i	74	GLU
25	i	79	HIS
25	i	80	GLN
25	i	96	MET
25	i	111	GLU
25	i	112	GLU
26	j	2	ILE
26	j	28	ASP
27	k	79	ASP
28	l	44	CYS
28	l	49	MET
2	H	65	ALA
4	R	92	ASP
4	R	182	MET
5	T	42	LYS
5	T	43	LEU
5	T	70	GLU
8	N	341	GLU
8	N	414	GLY
8	N	447	PRO
8	N	544	VAL
11	U	104	GLN
12	3	12	ASP
12	3	15	SER
12	3	16	ARG
12	3	18	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	3	44	ASP
12	3	68	TYR
12	3	82	GLN
12	3	83	PHE
12	3	87	ILE
17	a	14	ARG
17	a	24	LEU
17	a	51	ARG
17	a	71	THR
17	a	72	CYS
17	a	78	ASP
17	a	96	GLY
17	a	108	VAL
17	a	115	LEU
17	a	136	ARG
17	a	157	GLY
17	a	162	ASP
17	a	163	LEU
17	a	180	PRO
17	a	198	ASP
17	a	232	GLU
17	a	327	PRO
17	a	329	LYS
17	a	335	LEU
17	a	337	GLY
17	a	428	GLY
17	a	445	GLY
17	a	485	ASN
17	a	552	VAL
17	a	604	SER
17	a	615	ASN
17	a	647	ILE
17	a	710	PRO
17	a	748	ASN
17	a	749	VAL
17	a	784	GLY
17	a	801	GLU
17	a	805	PHE
17	a	810	TYR
17	a	817	GLN
17	a	836	LYS
17	a	909	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	917	MET
17	a	920	SER
17	a	927	VAL
17	a	928	GLN
17	a	949	ILE
17	a	976	LEU
17	a	1062	SER
17	a	1066	MET
17	a	1086	THR
17	a	1092	VAL
17	a	1095	LYS
17	a	1097	VAL
17	a	1119	LEU
17	a	1131	MET
17	a	1150	THR
17	a	1166	ILE
17	a	1170	LYS
17	a	1209	LYS
17	a	1247	ARG
17	a	1248	ASP
17	a	1253	ALA
17	a	1255	ASP
17	a	1262	GLU
17	a	1276	SER
17	a	1280	ARG
17	a	1366	GLY
17	a	1412	VAL
17	a	1475	THR
17	a	1477	GLN
17	a	1480	GLU
17	a	1483	GLY
18	b	105	ARG
18	b	108	ASN
18	b	148	SER
18	b	181	PRO
18	b	214	ALA
18	b	226	ARG
18	b	237	SER
18	b	280	ASP
18	b	293	ASP
18	b	299	MET
18	b	319	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	323	ARG
18	b	331	ARG
18	b	350	ILE
18	b	431	THR
18	b	470	ASN
18	b	481	LEU
18	b	491	ASP
18	b	495	ALA
18	b	499	GLN
18	b	510	PRO
18	b	655	TYR
18	b	701	GLN
18	b	705	GLU
18	b	713	ALA
18	b	781	MET
18	b	792	LEU
18	b	813	ILE
18	b	825	GLU
18	b	868	ARG
18	b	871	THR
18	b	877	GLY
18	b	896	GLY
18	b	1006	ILE
18	b	1055	SER
18	b	1056	ARG
18	b	1086	HIS
18	b	1089	ASP
18	b	1110	GLY
18	b	1118	ARG
18	b	1172	SER
18	b	1205	PHE
19	c	128	SER
19	c	141	ARG
19	c	150	LYS
19	c	199	ASP
19	c	200	ALA
19	c	244	ILE
20	d	66	ALA
20	d	81	LEU
20	d	118	GLN
21	e	22	VAL
21	e	25	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	e	48	MET
21	e	50	ARG
21	e	67	SER
21	e	69	LYS
21	e	98	ASN
21	e	119	ALA
21	e	129	THR
21	e	176	ALA
22	f	61	GLY
22	f	62	LYS
22	f	63	ALA
22	f	94	ASN
23	g	20	GLY
23	g	128	PRO
23	g	134	GLU
24	h	55	PHE
24	h	63	LEU
24	h	90	LYS
24	h	111	LEU
25	i	34	TYR
25	i	56	THR
25	i	60	HIS
25	i	73	LYS
25	i	76	PRO
25	i	86	TYR
25	i	98	THR
25	i	106	CYS
25	i	109	ALA
26	j	43	TYR
26	j	44	CYS
27	k	59	GLY
27	k	76	THR
28	l	36	LYS
28	l	48	VAL
28	l	57	MET
1	F	60	ALA
1	F	65	ASP
2	H	39	SER
3	Q	44	GLU
3	Q	265	ALA
3	Q	521	SER
5	T	61	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	T	90	TRP
5	T	94	GLN
8	N	122	LEU
8	N	205	SER
8	N	215	PHE
8	N	242	LEU
8	N	364	HIS
8	N	412	GLY
8	N	501	LEU
8	N	517	VAL
8	N	873	LEU
10	G	221	ILE
12	3	20	GLU
12	3	41	TYR
12	3	42	PHE
14	I	67	GLU
17	a	39	PHE
17	a	40	PRO
17	a	109	CYS
17	a	130	TYR
17	a	165	ASN
17	a	210	PRO
17	a	254	PRO
17	a	259	ASP
17	a	382	TYR
17	a	384	GLU
17	a	391	ILE
17	a	427	ALA
17	a	429	ASP
17	a	489	ASP
17	a	513	VAL
17	a	708	LEU
17	a	713	GLY
17	a	875	GLY
17	a	950	PHE
17	a	954	ASP
17	a	1042	LYS
17	a	1065	GLU
17	a	1090	ALA
17	a	1093	SER
17	a	1098	THR
17	a	1099	LEU

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	1102	PRO
17	a	1164	THR
17	a	1186	GLU
17	a	1239	LEU
17	a	1260	ILE
17	a	1264	VAL
17	a	1265	PHE
17	a	1286	THR
17	a	1294	LYS
17	a	1339	VAL
17	a	1409	GLU
17	a	1426	ASP
17	a	1472	GLY
17	a	1473	MET
18	b	11	THR
18	b	34	GLN
18	b	167	ASN
18	b	211	PHE
18	b	220	ALA
18	b	240	GLN
18	b	243	LEU
18	b	245	ALA
18	b	248	THR
18	b	276	GLY
18	b	292	ASN
18	b	387	PHE
18	b	394	LEU
18	b	467	GLN
18	b	496	LYS
18	b	539	PRO
18	b	556	ASN
18	b	614	THR
18	b	621	ARG
18	b	627	ASP
18	b	658	ASP
18	b	660	GLU
18	b	712	PRO
18	b	821	GLY
18	b	872	LEU
18	b	893	ARG
18	b	1025	ALA
18	b	1078	PRO

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	1163	TYR
18	b	1206	THR
19	c	41	PRO
19	c	113	GLY
19	c	175	SER
19	c	184	TRP
19	c	240	PRO
19	c	242	ASN
20	d	11	ALA
20	d	16	GLY
20	d	84	ARG
20	d	99	GLU
21	e	54	ARG
21	e	65	ASN
21	e	86	GLU
21	e	109	SER
21	e	117	ILE
21	e	167	GLU
22	f	107	PRO
23	g	66	GLN
23	g	102	ALA
23	g	103	ASN
23	g	106	PRO
24	h	81	TYR
24	h	115	SER
25	i	9	GLU
25	i	11	ASN
25	i	78	CYS
25	i	89	HIS
25	i	95	THR
26	j	5	ILE
27	k	47	ASN
27	k	81	SER
1	F	112	ASN
1	F	141	THR
3	Q	337	ILE
3	Q	340	ASP
5	T	50	PRO
5	T	120	VAL
6	K	93	LYS
8	N	136	ALA
8	N	220	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	N	238	VAL
8	N	257	PRO
8	N	347	LYS
17	a	9	SER
17	a	70	GLN
17	a	170	MET
17	a	206	ARG
17	a	238	ASP
17	a	245	LEU
17	a	318	PRO
17	a	380	LEU
17	a	435	GLY
17	a	531	GLN
17	a	597	ASP
17	a	619	ILE
17	a	646	GLU
17	a	781	ILE
17	a	858	TYR
17	a	1144	THR
17	a	1167	GLU
17	a	1263	ASP
17	a	1279	LEU
17	a	1303	THR
17	a	1327	GLY
17	a	1479	PRO
18	b	29	SER
18	b	36	PHE
18	b	104	ALA
18	b	205	ALA
18	b	216	PRO
18	b	230	GLU
18	b	239	MET
18	b	281	ARG
18	b	332	GLU
18	b	382	ASP
18	b	459	MET
18	b	631	ASN
18	b	724	VAL
18	b	1114	ASP
18	b	1156	GLY
18	b	1186	TYR
18	b	1209	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	c	100	SER
19	c	168	HIS
21	e	26	GLY
21	e	49	GLY
21	e	133	SER
23	g	21	PRO
23	g	52	SER
23	g	129	PRO
24	h	43	ASN
24	h	54	THR
24	h	59	ILE
25	i	82	GLU
25	i	91	ARG
25	i	107	GLY
27	k	22	LEU
27	k	36	LYS
27	k	40	THR
27	k	45	LEU
28	l	37	GLU
28	l	55	LYS
3	Q	60	LEU
4	R	83	GLU
4	R	180	VAL
5	T	12	PRO
7	V	96	SER
8	N	97	LEU
8	N	174	ILE
8	N	231	SER
8	N	432	THR
8	N	485	GLN
8	N	851	ALA
11	U	30	HIS
17	a	7	SER
17	a	11	VAL
17	a	97	PHE
17	a	268	LEU
17	a	317	GLN
17	a	344	GLY
17	a	667	GLY
17	a	673	GLY
17	a	711	GLU
17	a	783	PHE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	1038	TYR
17	a	1116	THR
17	a	1130	ASN
17	a	1145	THR
17	a	1308	ASP
17	a	1421	SER
18	b	12	LEU
18	b	56	LEU
18	b	107	ARG
18	b	228	ALA
18	b	429	ASN
18	b	487	PRO
18	b	538	ALA
18	b	737	ILE
18	b	929	PRO
18	b	949	GLY
18	b	989	PRO
18	b	1030	GLU
18	b	1169	GLU
19	c	86	TYR
19	c	169	ALA
19	c	214	PRO
19	c	222	PHE
20	d	68	PHE
20	d	116	ASP
23	g	64	PRO
24	h	30	VAL
24	h	113	ARG
24	h	120	TYR
25	i	75	CYS
26	j	63	ASN
27	k	60	TYR
27	k	70	PHE
27	k	77	VAL
3	Q	463	ALA
10	G	75	GLN
12	3	13	ASP
17	a	209	SER
17	a	813	GLY
17	a	816	PRO
17	a	961	VAL
17	a	1009	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	1434	ILE
18	b	145	GLU
18	b	247	ASN
18	b	550	GLU
18	b	605	ILE
20	d	98	CYS
24	h	61	SER
28	l	32	THR
3	Q	278	ILE
14	I	65	PRO
17	a	406	PRO
17	a	514	PRO
17	a	589	PRO
17	a	1052	VAL
17	a	1110	VAL
17	a	1124	MET
18	b	42	VAL
18	b	232	GLY
18	b	434	VAL
27	k	118	VAL
17	a	176	GLY
18	b	453	GLY
18	b	560	SER
18	b	855	ILE
18	b	1108	VAL
19	c	258	VAL
25	i	65	ASP
3	Q	42	ILE
3	Q	237	ILE
8	N	462	GLN
17	a	1414	ILE
18	b	397	PRO
17	a	470	PRO
17	a	1180	PRO
20	d	17	PRO
23	g	148	ILE
24	h	83	VAL
25	i	53	VAL
3	Q	211	VAL
17	a	237	PRO
18	b	208	VAL
18	b	1099	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	f	96	PRO
24	h	98	GLY
8	N	176	PRO
19	c	80	PRO
3	Q	162	PRO
17	a	712	PRO
17	a	1063	PRO

### 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	F	171/198 (86%)	171 (100%)	0	100	100
2	H	168/185 (91%)	168 (100%)	0	100	100
3	Q	389/509 (76%)	389 (100%)	0	100	100
4	R	191/191 (100%)	191 (100%)	0	100	100
5	T	161/178 (90%)	161 (100%)	0	100	100
6	K	88/108 (82%)	88 (100%)	0	100	100
7	V	112/129 (87%)	112 (100%)	0	100	100
8	N	369/799 (46%)	369 (100%)	0	100	100
17	a	1296/1536 (84%)	1109 (86%)	187 (14%)	3	16
18	b	1012/1064 (95%)	912 (90%)	100 (10%)	8	26
19	c	236/267 (88%)	219 (93%)	17 (7%)	14	39
20	d	106/115 (92%)	90 (85%)	16 (15%)	3	14
21	e	182/184 (99%)	169 (93%)	13 (7%)	14	39
22	f	71/121 (59%)	64 (90%)	7 (10%)	8	26
23	g	146/148 (99%)	139 (95%)	7 (5%)	25	51
24	h	113/114 (99%)	99 (88%)	14 (12%)	4	19
25	i	103/105 (98%)	80 (78%)	23 (22%)	1	5
26	j	59/66 (89%)	46 (78%)	13 (22%)	1	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	k	109/113 (96%)	104 (95%)	5 (5%)	27	52
28	l	39/53 (74%)	34 (87%)	5 (13%)	4	18
All	All	5121/6183 (83%)	4714 (92%)	407 (8%)	16	35

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	a	7	SER
17	a	10	SER
17	a	15	ARG
17	a	36	LYS
17	a	39	PHE
17	a	43	MET
17	a	46	SER
17	a	48	GLN
17	a	49	ARG
17	a	51	ARG
17	a	56	LEU
17	a	66	GLN
17	a	67	PHE
17	a	68	LYS
17	a	72	CYS
17	a	85	HIS
17	a	86	ILE
17	a	87	GLU
17	a	88	LEU
17	a	106	GLU
17	a	116	LYS
17	a	117	ILE
17	a	118	ASP
17	a	119	SER
17	a	121	ASN
17	a	150	CYS
17	a	154	LEU
17	a	155	SER
17	a	158	SER
17	a	159	ASP
17	a	163	LEU
17	a	164	SER
17	a	169	ASN
17	a	188	ARG

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	195	ARG
17	a	197	LYS
17	a	200	SER
17	a	202	LEU
17	a	204	GLU
17	a	205	LYS
17	a	206	ARG
17	a	207	LEU
17	a	208	LEU
17	a	232	GLU
17	a	253	ARG
17	a	256	ILE
17	a	257	SER
17	a	258	VAL
17	a	262	SER
17	a	263	ARG
17	a	266	ASP
17	a	267	ASP
17	a	268	LEU
17	a	269	THR
17	a	271	LYS
17	a	322	GLN
17	a	326	ARG
17	a	328	LEU
17	a	329	LYS
17	a	330	SER
17	a	335	LEU
17	a	341	ARG
17	a	357	THR
17	a	363	PRO
17	a	374	ARG
17	a	375	SER
17	a	385	THR
17	a	398	VAL
17	a	421	LEU
17	a	426	ARG
17	a	430	ILE
17	a	434	TYR
17	a	436	TRP
17	a	442	ILE
17	a	452	ARG
17	a	459	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	460	SER
17	a	472	SER
17	a	475	ARG
17	a	476	LEU
17	a	479	SER
17	a	495	MET
17	a	507	ILE
17	a	511	THR
17	a	513	VAL
17	a	523	ASN
17	a	533	THR
17	a	534	LEU
17	a	552	VAL
17	a	555	ILE
17	a	559	VAL
17	a	579	THR
17	a	583	ILE
17	a	592	ILE
17	a	605	ASN
17	a	618	ILE
17	a	639	ILE
17	a	655	ILE
17	a	663	LEU
17	a	682	MET
17	a	686	THR
17	a	707	ARG
17	a	708	LEU
17	a	717	ARG
17	a	730	GLN
17	a	732	ARG
17	a	733	ASP
17	a	758	LYS
17	a	762	ILE
17	a	764	ILE
17	a	770	CYS
17	a	773	GLN
17	a	775	ILE
17	a	776	VAL
17	a	781	ILE
17	a	785	PHE
17	a	801	GLU
17	a	802	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	817	GLN
17	a	827	ARG
17	a	833	THR
17	a	837	THR
17	a	843	ILE
17	a	846	ARG
17	a	857	ARG
17	a	861	THR
17	a	864	ASN
17	a	869	ILE
17	a	886	TYR
17	a	905	ILE
17	a	919	ASN
17	a	921	ILE
17	a	922	GLU
17	a	946	CYS
17	a	947	LYS
17	a	948	PHE
17	a	969	ASN
17	a	985	LEU
17	a	989	ILE
17	a	1001	THR
17	a	1086	THR
17	a	1087	PHE
17	a	1089	TYR
17	a	1093	SER
17	a	1095	LYS
17	a	1097	VAL
17	a	1098	THR
17	a	1103	ARG
17	a	1104	LEU
17	a	1112	LYS
17	a	1114	ILE
17	a	1119	LEU
17	a	1127	ILE
17	a	1140	GLN
17	a	1160	ASP
17	a	1162	GLN
17	a	1166	ILE
17	a	1169	ASP
17	a	1183	GLU
17	a	1246	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	1248	ASP
17	a	1250	ASP
17	a	1260	ILE
17	a	1261	GLU
17	a	1277	ILE
17	a	1309	GLU
17	a	1314	THR
17	a	1323	MET
17	a	1328	VAL
17	a	1341	ILE
17	a	1347	ILE
17	a	1350	THR
17	a	1351	ARG
17	a	1355	LEU
17	a	1374	LEU
17	a	1387	LEU
17	a	1395	ILE
17	a	1397	ARG
17	a	1399	GLU
17	a	1400	THR
17	a	1403	LEU
17	a	1411	THR
17	a	1442	MET
17	a	1444	THR
17	a	1449	ILE
17	a	1459	TYR
17	a	1473	MET
18	b	35	LEU
18	b	82	ILE
18	b	89	MET
18	b	201	GLU
18	b	212	LYS
18	b	226	ARG
18	b	235	LEU
18	b	241	ILE
18	b	244	MET
18	b	246	ARG
18	b	255	ILE
18	b	262	ILE
18	b	290	ASP
18	b	310	ILE
18	b	311	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	323	ARG
18	b	327	THR
18	b	331	ARG
18	b	337	TYR
18	b	352	THR
18	b	404	ARG
18	b	426	ARG
18	b	427	GLU
18	b	429	ASN
18	b	430	LEU
18	b	438	ILE
18	b	439	ILE
18	b	447	LEU
18	b	456	LYS
18	b	459	MET
18	b	469	LEU
18	b	485	ASN
18	b	488	ILE
18	b	493	LYS
18	b	500	LEU
18	b	502	ASN
18	b	507	MET
18	b	524	ASN
18	b	550	GLU
18	b	552	LEU
18	b	565	LYS
18	b	573	LEU
18	b	619	ILE
18	b	654	ARG
18	b	655	TYR
18	b	657	ILE
18	b	662	ARG
18	b	663	PHE
18	b	668	LEU
18	b	669	VAL
18	b	690	SER
18	b	715	ARG
18	b	740	ILE
18	b	745	ILE
18	b	747	PHE
18	b	750	HIS
18	b	752	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	753	SER
18	b	757	THR
18	b	759	GLN
18	b	778	MET
18	b	780	THR
18	b	785	LEU
18	b	794	THR
18	b	797	SER
18	b	818	CYS
18	b	831	ASN
18	b	834	SER
18	b	835	ILE
18	b	839	LEU
18	b	840	PHE
18	b	870	THR
18	b	872	LEU
18	b	873	ARG
18	b	879	TYR
18	b	900	ILE
18	b	901	ILE
18	b	962	ILE
18	b	981	MET
18	b	993	GLN
18	b	995	ILE
18	b	999	ILE
18	b	1000	ILE
18	b	1011	THR
18	b	1035	PRO
18	b	1056	ARG
18	b	1060	VAL
18	b	1079	THR
18	b	1080	TYR
18	b	1083	ARG
18	b	1092	ILE
18	b	1104	THR
18	b	1112	SER
18	b	1117	LEU
18	b	1122	MET
18	b	1129	SER
18	b	1152	CYS
18	b	1197	SER
18	b	1200	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	1205	PHE
19	c	9	ILE
19	c	14	LYS
19	c	57	MET
19	c	59	ASP
19	c	69	ILE
19	c	76	ILE
19	c	84	LEU
19	c	120	ARG
19	c	125	SER
19	c	126	SER
19	c	127	ASN
19	c	129	SER
19	c	130	LEU
19	c	146	CYS
19	c	242	ASN
19	c	249	LEU
19	c	252	LEU
20	d	9	ASP
20	d	13	LEU
20	d	23	ASP
20	d	25	LEU
20	d	31	LYS
20	d	40	GLN
20	d	43	ARG
20	d	67	ARG
20	d	84	ARG
20	d	85	PHE
20	d	87	LYS
20	d	95	THR
20	d	96	LEU
20	d	97	CYS
20	d	98	CYS
20	d	99	GLU
21	e	7	ASN
21	e	44	MET
21	e	48	MET
21	e	52	LEU
21	e	84	ILE
21	e	139	ILE
21	e	148	HIS
21	e	162	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	e	168	THR
21	e	174	GLN
21	e	195	ARG
21	e	200	SER
21	e	209	CYS
22	f	60	SER
22	f	74	TYR
22	f	82	ARG
22	f	115	LEU
22	f	120	ILE
22	f	128	LEU
22	f	142	ILE
23	g	51	ASP
23	g	59	LYS
23	g	61	ARG
23	g	66	GLN
23	g	68	PHE
23	g	101	PHE
23	g	114	HIS
24	h	14	THR
24	h	25	SER
24	h	27	ILE
24	h	36	MET
24	h	37	ASN
24	h	38	LEU
24	h	39	THR
24	h	40	LEU
24	h	57	LEU
24	h	59	ILE
24	h	62	ASN
24	h	63	LEU
24	h	65	SER
24	h	70	GLU
25	i	3	ASN
25	i	17	ARG
25	i	20	LYS
25	i	25	LEU
25	i	26	ARG
25	i	30	ARG
25	i	42	LYS
25	i	44	TYR
25	i	47	GLU

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	i	57	THR
25	i	60	HIS
25	i	61	ASP
25	i	68	LEU
25	i	74	GLU
25	i	75	CYS
25	i	77	ARG
25	i	78	CYS
25	i	79	HIS
25	i	88	THR
25	i	94	ASP
25	i	100	ILE
25	i	112	GLU
25	i	113	GLN
26	j	1	MET
26	j	2	ILE
26	j	3	ILE
26	j	5	ILE
26	j	13	VAL
26	j	20	THR
26	j	41	GLN
26	j	44	CYS
26	j	45	CYS
26	j	46	ARG
26	j	47	ARG
26	j	49	ILE
26	j	56	ILE
27	k	12	LEU
27	k	54	ARG
27	k	72	LEU
27	k	73	ARG
27	k	86	ILE
28	l	20	MET
28	l	24	CYS
28	l	27	CYS
28	l	44	CYS
28	l	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	59	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	69	GLN
1	F	112	ASN
1	F	137	GLN
1	F	152	GLN
1	F	162	ASN
1	F	207	HIS
2	H	25	GLN
2	H	47	HIS
2	H	51	ASN
2	H	62	ASN
2	H	63	ASN
3	Q	116	GLN
3	Q	302	GLN
3	Q	442	GLN
3	Q	502	HIS
3	Q	518	ASN
3	Q	525	ASN
3	Q	528	GLN
3	Q	532	HIS
4	R	142	GLN
4	R	148	GLN
5	T	4	HIS
5	T	22	GLN
5	T	33	HIS
5	T	154	ASN
6	K	23	ASN
6	K	75	GLN
7	V	111	GLN
8	N	159	HIS
8	N	162	ASN
8	N	186	ASN
8	N	195	ASN
8	N	206	GLN
8	N	223	GLN
8	N	243	HIS
8	N	273	GLN
8	N	276	ASN
8	N	364	HIS
8	N	381	HIS
8	N	449	HIS
8	N	490	HIS
17	a	48	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	a	82	HIS
17	a	121	ASN
17	a	128	GLN
17	a	179	GLN
17	a	214	HIS
17	a	219	HIS
17	a	227	HIS
17	a	231	ASN
17	a	312	ASN
17	a	393	GLN
17	a	395	GLN
17	a	457	HIS
17	a	477	ASN
17	a	496	HIS
17	a	521	GLN
17	a	545	ASN
17	a	550	ASN
17	a	582	GLN
17	a	593	ASN
17	a	656	GLN
17	a	665	HIS
17	a	705	HIS
17	a	763	ASN
17	a	773	GLN
17	a	817	GLN
17	a	864	ASN
17	a	887	GLN
17	a	898	GLN
17	a	919	ASN
17	a	937	GLN
17	a	969	ASN
17	a	972	GLN
17	a	1014	GLN
17	a	1088	HIS
17	a	1109	ASN
17	a	1156	HIS
17	a	1162	GLN
17	a	1293	HIS
17	a	1373	HIS
17	a	1438	GLN
18	b	34	GLN
18	b	108	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	b	200	GLN
18	b	339	HIS
18	b	386	HIS
18	b	419	GLN
18	b	441	ASN
18	b	455	GLN
18	b	485	ASN
18	b	501	HIS
18	b	576	HIS
18	b	581	HIS
18	b	644	HIS
18	b	646	GLN
18	b	661	GLN
18	b	725	HIS
18	b	733	HIS
18	b	752	GLN
18	b	765	GLN
18	b	783	ASN
18	b	824	GLN
18	b	831	ASN
18	b	876	HIS
18	b	940	GLN
18	b	964	GLN
18	b	973	HIS
18	b	975	GLN
18	b	985	HIS
18	b	993	GLN
18	b	1051	HIS
18	b	1063	HIS
18	b	1086	HIS
18	b	1093	HIS
18	b	1106	GLN
18	b	1130	HIS
18	b	1181	GLN
18	b	1209	HIS
19	c	30	ASN
19	c	89	ASN
19	c	132	HIS
19	c	168	HIS
19	c	188	GLN
19	c	189	HIS
19	c	253	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	d	40	GLN
20	d	86	HIS
20	d	92	GLN
21	e	19	HIS
21	e	45	HIS
21	e	68	ASN
21	e	98	ASN
21	e	99	HIS
21	e	124	GLN
21	e	142	HIS
21	e	174	GLN
22	f	94	ASN
23	g	53	ASN
23	g	114	HIS
24	h	33	GLN
24	h	108	HIS
25	i	49	GLN
25	i	55	ASN
25	i	79	HIS
25	i	80	GLN
25	i	81	HIS
25	i	87	GLN
26	j	52	HIS
27	k	39	HIS
27	k	64	HIS
27	k	68	HIS
27	k	96	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	S	6
16	J	3
9	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	56:UNK	C	160:UNK	N	39.54
1	J	204:UNK	C	310:UNK	N	28.97
1	S	265:UNK	C	271:UNK	N	28.24
1	S	366:UNK	C	381:UNK	N	25.63
1	S	287:UNK	C	301:UNK	N	18.84
1	S	349:UNK	C	351:UNK	N	13.73
1	S	82:UNK	C	251:UNK	N	12.85
1	D	27:UNK	C	33:UNK	N	10.35
1	S	322:UNK	C	331:UNK	N	7.69
1	J	22:UNK	C	25:UNK	N	5.75

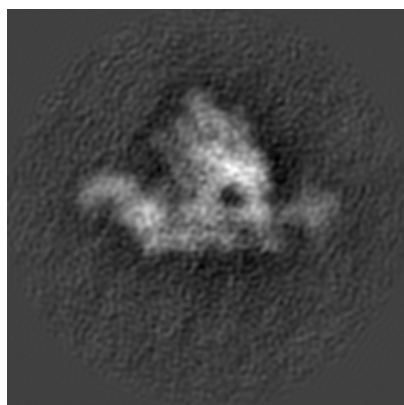
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8480. These allow visual inspection of the internal detail of the map and identification of artifacts.

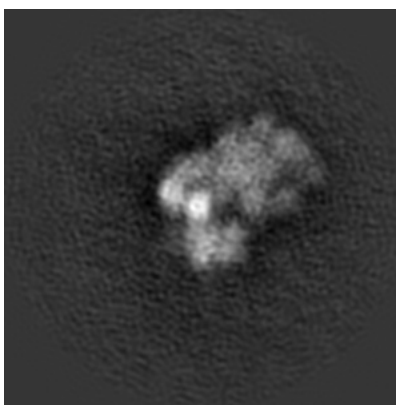
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

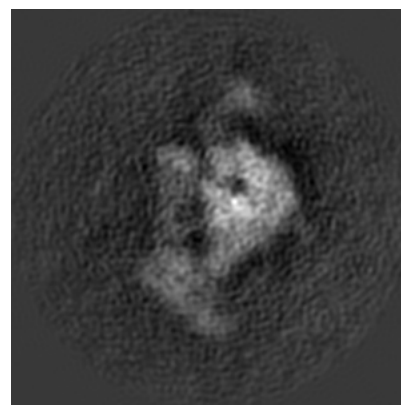
#### 6.1.1 Primary map



X



Y

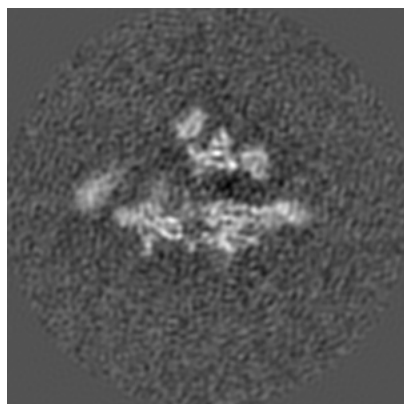


Z

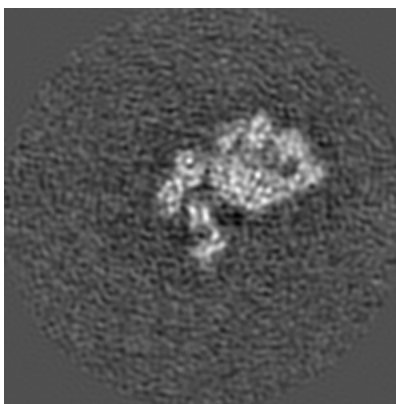
The images above show the map projected in three orthogonal directions.

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

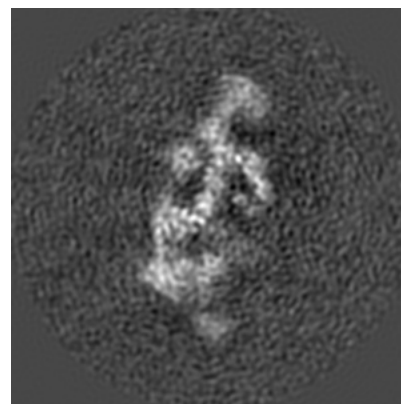
#### 6.2.1 Primary map



X Index: 88



Y Index: 88

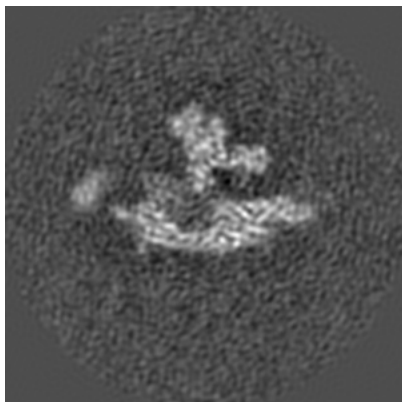


Z Index: 88

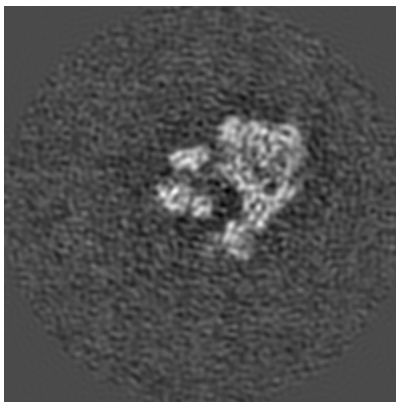
The images above show central slices of the map in three orthogonal directions.

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

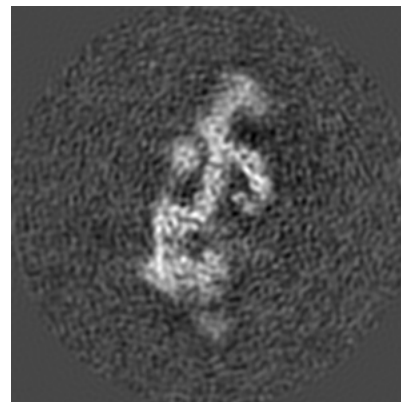
### 6.3.1 Primary map



X Index: 91



Y Index: 94

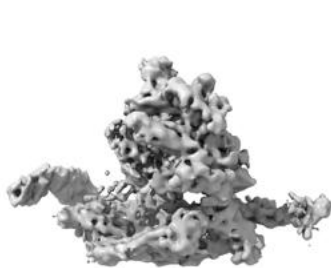


Z Index: 87

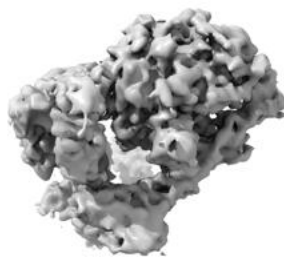
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



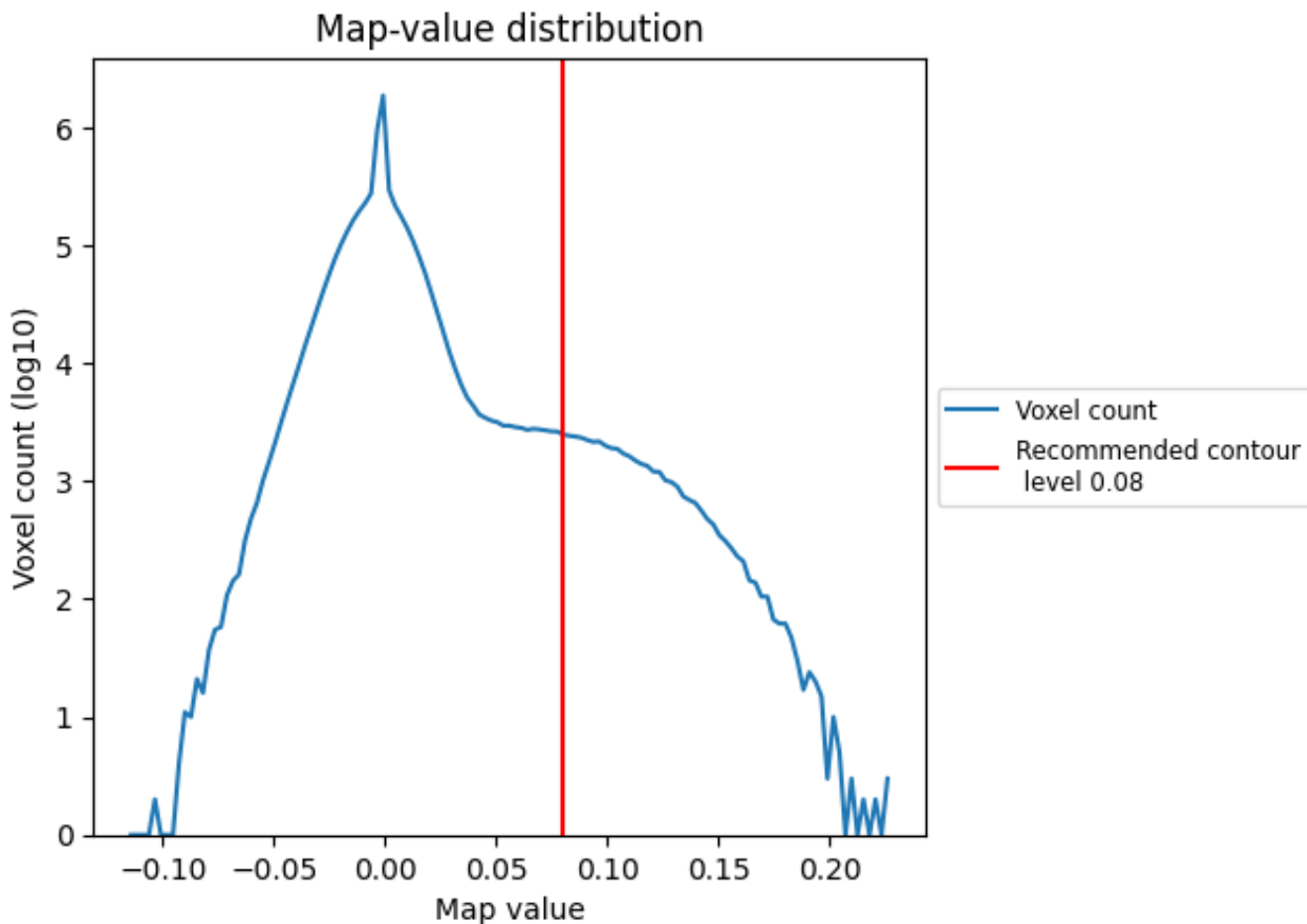
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

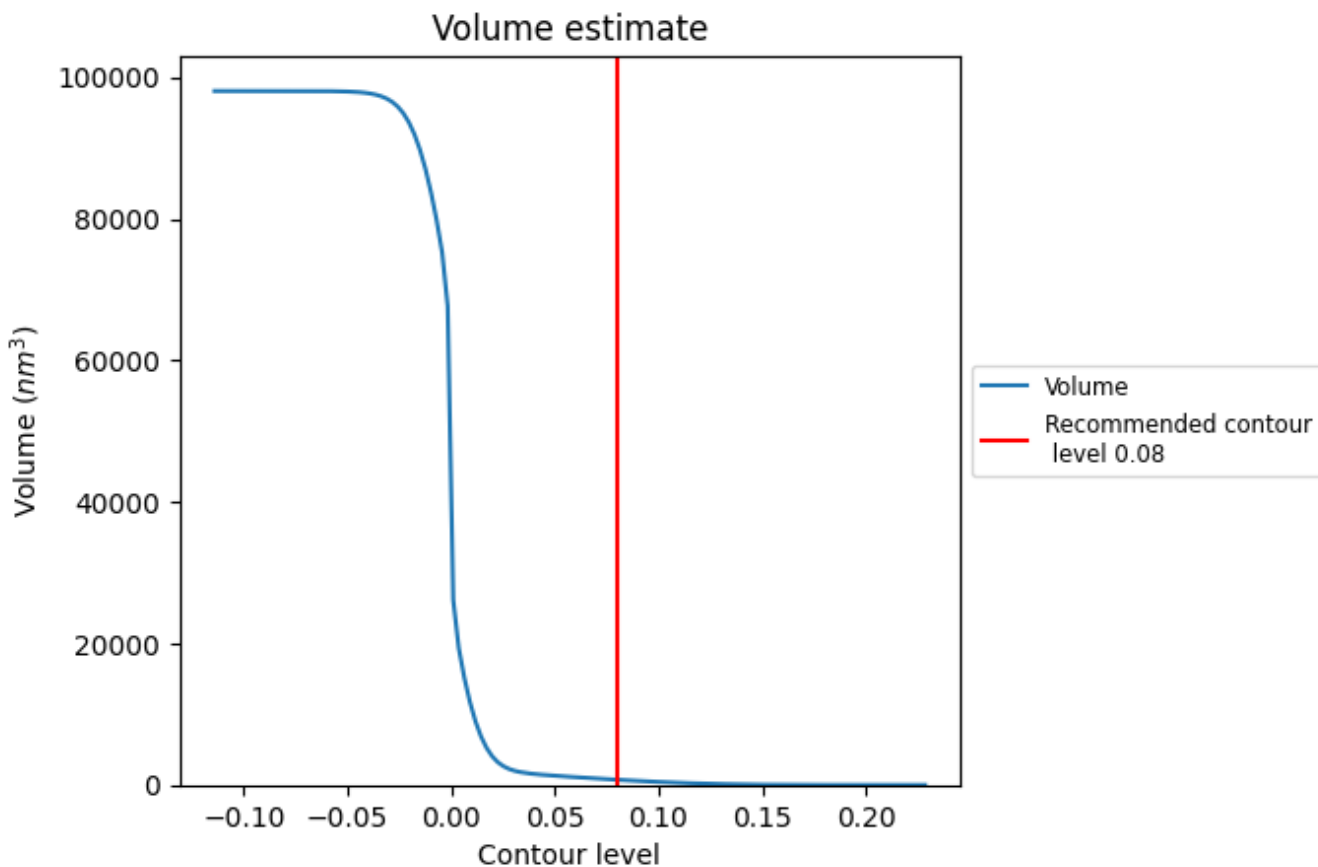
This section contains the results of statistical analysis of the map.

### 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.

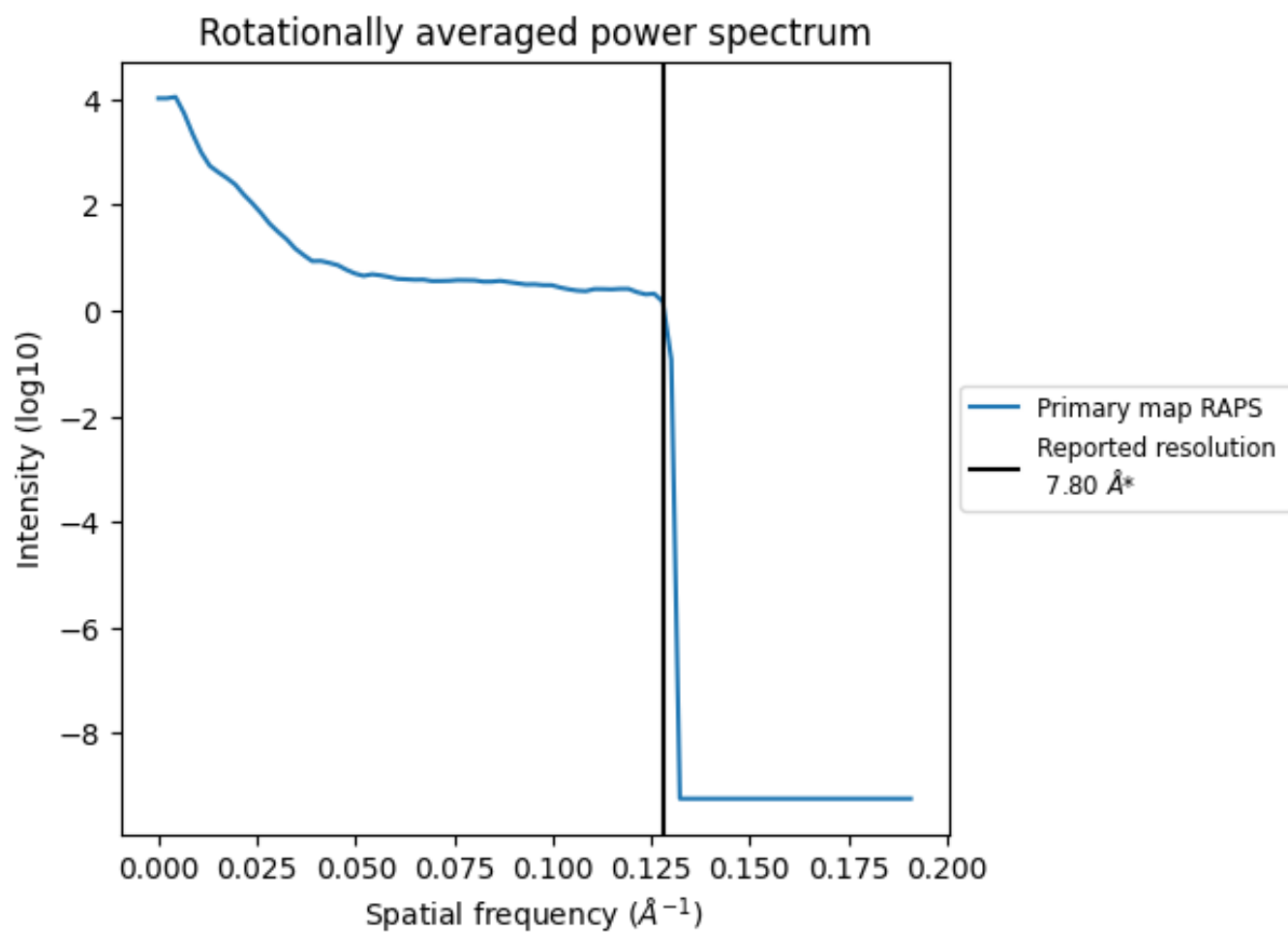
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 735  $\text{nm}^3$ ; this corresponds to an approximate mass of 664 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 0.128 Å<sup>-1</sup>

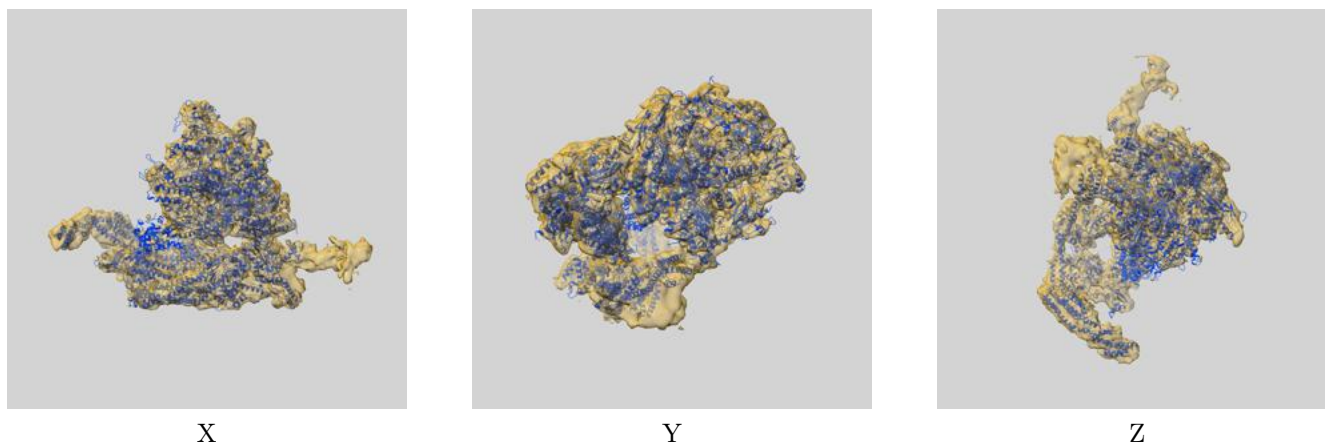
## 8 Fourier-Shell correlation

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

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

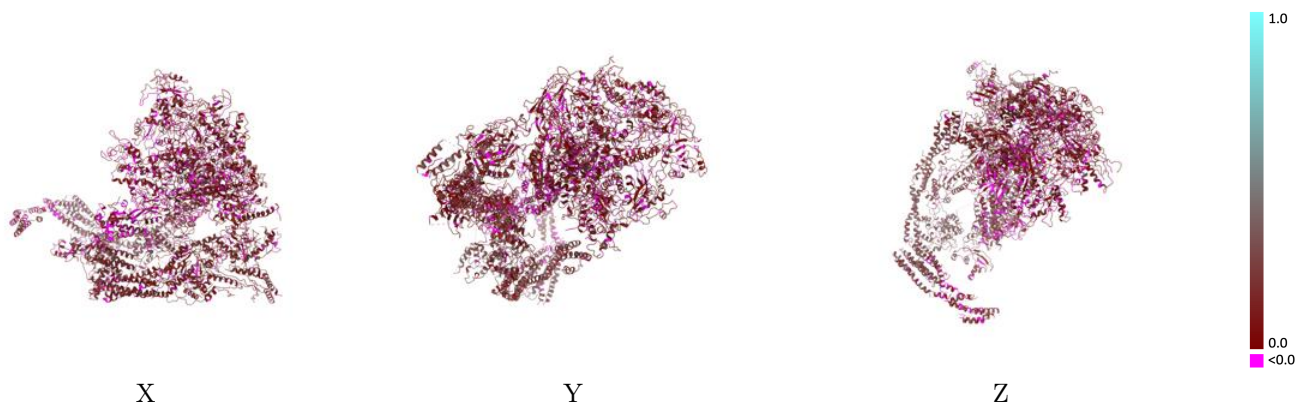
This section contains information regarding the fit between EMDB map EMD-8480 and PDB model 5U0S. Per-residue inclusion information can be found in section 3 on page 9.

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



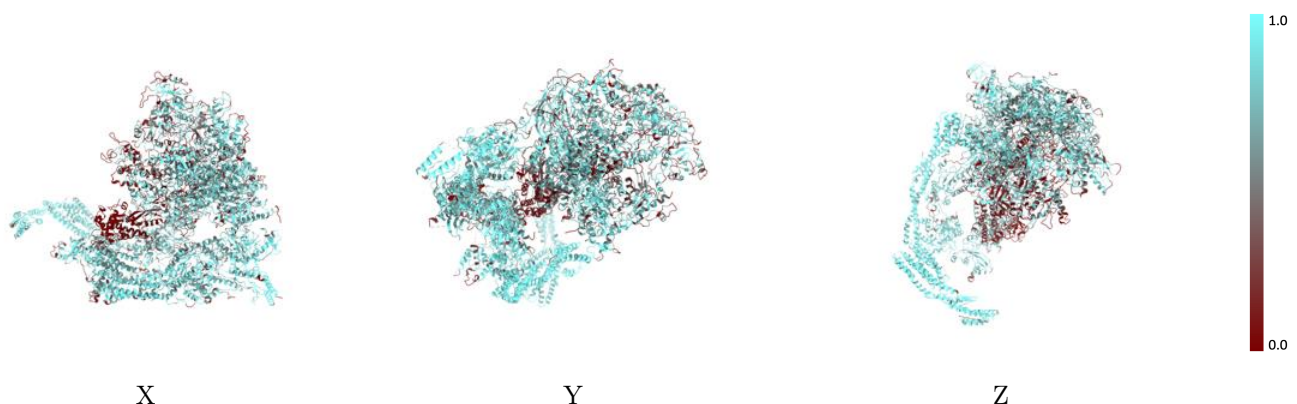
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



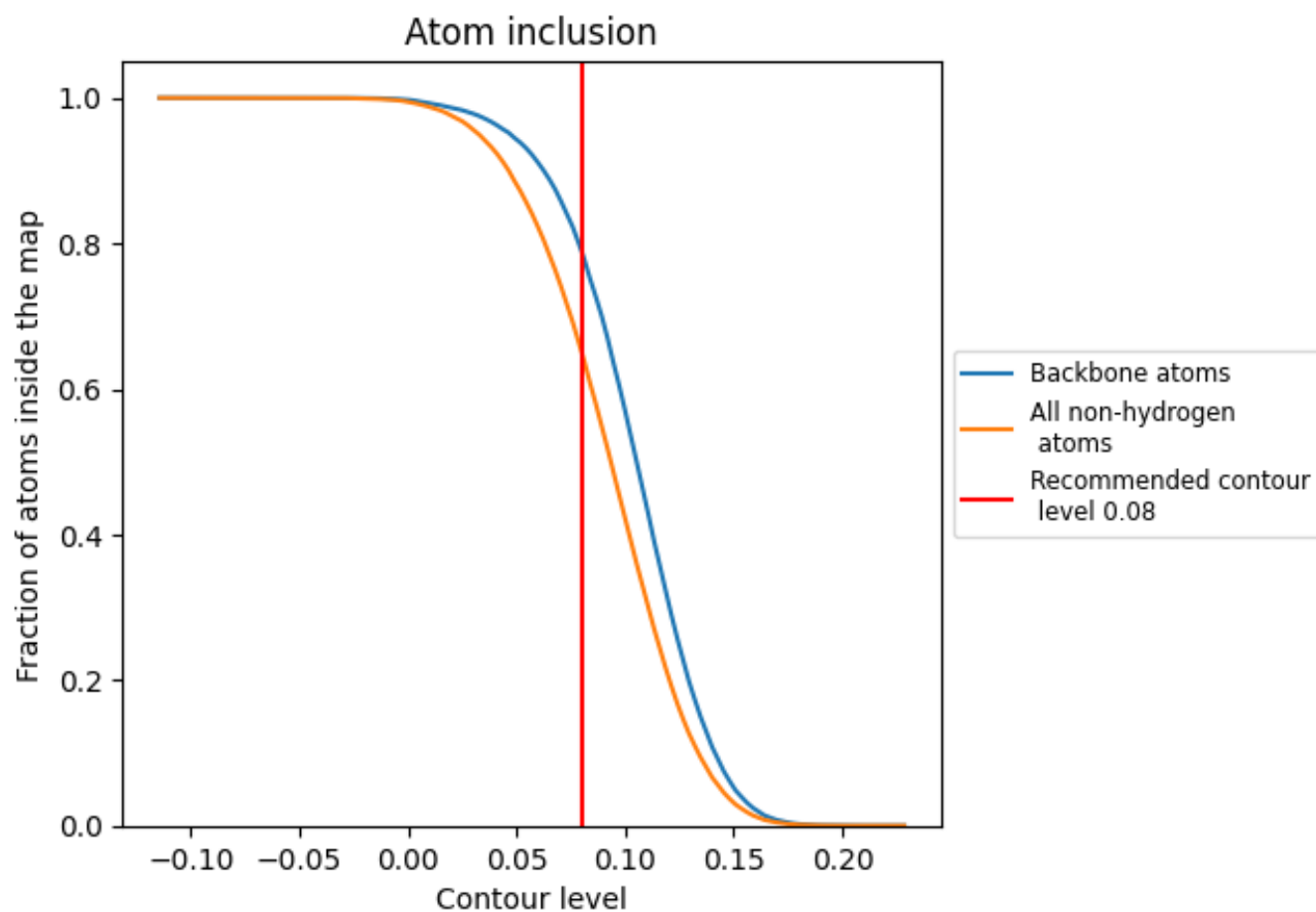
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

## 9.4 Atom inclusion [i](#)





























































At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.1230
2	 0.9433	 0.2260
3	 0.9437	 0.2070
D	 0.9042	 0.2350
F	 0.7215	 0.1270
G	 0.9513	 0.2160
H	 0.6984	 0.1620
I	 0.9465	 0.2090
J	 0.9649	 0.1540
K	 0.8314	 0.1410
N	 0.7832	 0.1550
Q	 0.7089	 0.1510
R	 0.7782	 0.1390
S	 0.8951	 0.1070
T	 0.8173	 0.1470
U	 0.9293	 0.1950
V	 0.7994	 0.1510
a	 0.5629	 0.1050
b	 0.6172	 0.1000
c	 0.7057	 0.1160
d	 0.0247	 0.0450
e	 0.5413	 0.1010
f	 0.5837	 0.1210
g	 0.1185	 0.0370
h	 0.6745	 0.1180
i	 0.4989	 0.0900
j	 0.7095	 0.0990
k	 0.5408	 0.1320
l	 0.6193	 0.0870

