



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 05:21 PM JST

PDB ID : 7EDX
EMDB ID : EMD-31075
Title : p53-bound TFIID-based core PIC on HDM2 promoter
Authors : Chen, X.; Qi, Y.; Hou, H.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on : 2021-03-17
Resolution : 4.50 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

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.dev113
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

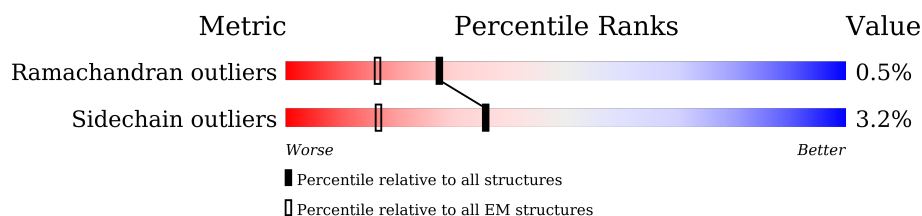
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.






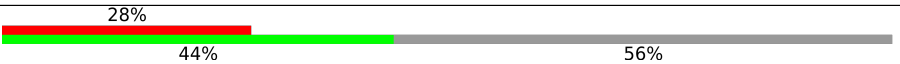


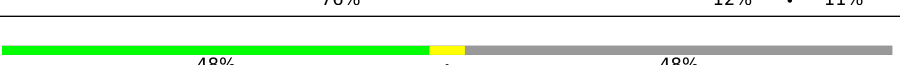

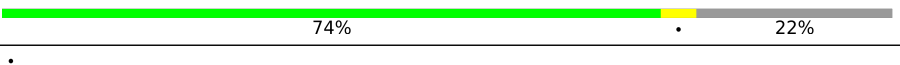

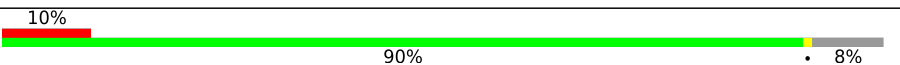
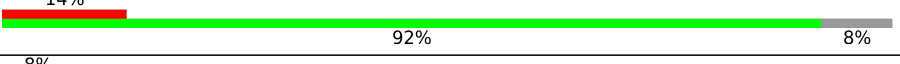



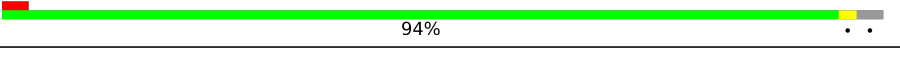
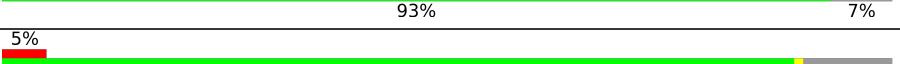
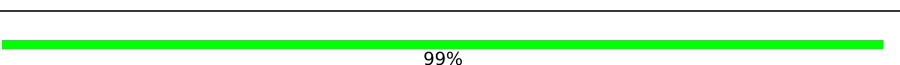

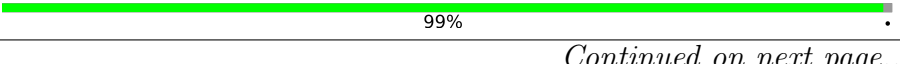



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	A	1872	
2	B	1199	
3	D	1085	
3	d	1085	
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	

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Mol	Chain	Length	Quality of chain
7	H	310	
8	I	264	
8	i	264	
9	J	218	
9	j	218	
10	L	161	
10	l	161	
11	O	109	
12	P	339	
13	Q	376	
14	R	316	
15	S	517	
16	T	249	
17	X	84	
18	Y	84	
19	c	929	
20	k	211	
21	m	124	
22	o	1970	
23	p	1174	
24	q	275	
25	r	142	
26	s	210	
27	t	127	
28	v	150	

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Mol	Chain	Length	Quality of chain
29	w	125	 90% 9%
30	x	67	 96%
31	y	117	 100%
32	z	58	 76% 24%
33	u	172	 98% ..

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81790 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4927	3142	858	899	28		

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

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

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	165	Total	C	N	O	S	0	0
			1377	858	257	258	4		
3	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	404	Total	C	N	O	S	0	0
			3081	1954	537	572	18		
5	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	89	Total	C	N	O	S	0	0
			709	457	114	134	4		
9	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
10	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 12 is a protein called TATA-box-binding protein.

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

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

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

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	248	Total	C	N	O	S	0	0
			1913	1200	338	358	17		

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	113	Total	C	N	O	S	0	0
			876	545	160	169	2		

- Molecule 17 is a DNA chain called DNA (84-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	77	Total	C	N	O	P	0	0
			1582	752	283	470	77		

- Molecule 18 is a DNA chain called DNA (84-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	77	Total	C	N	O	P	0	0
			1575	747	297	454	77		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 22 is a protein called RPB1.

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

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

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

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 29 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 30 is a protein called RPB10.

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

- Molecule 31 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 32 is a protein called RPB12.

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

- Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB7.

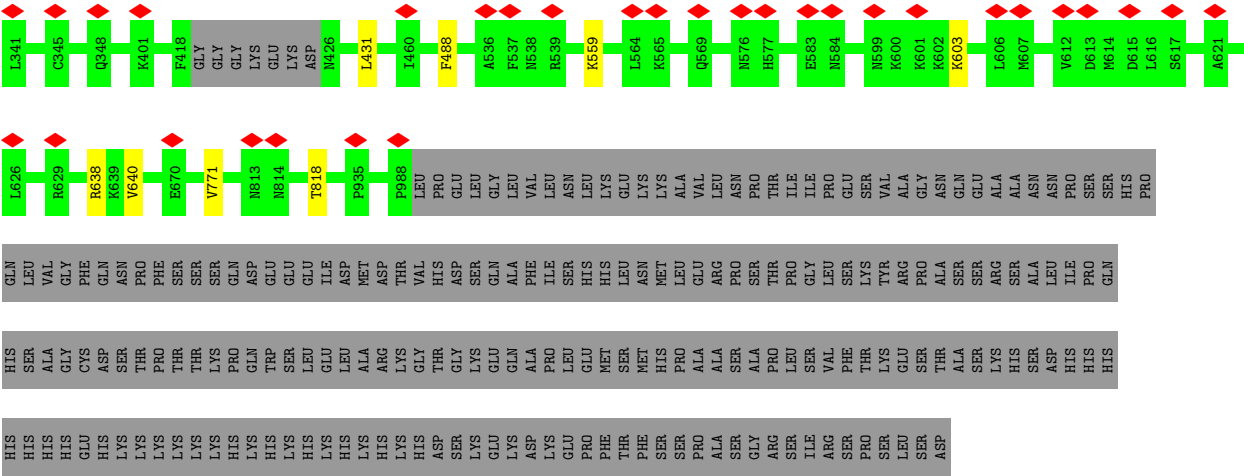
Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

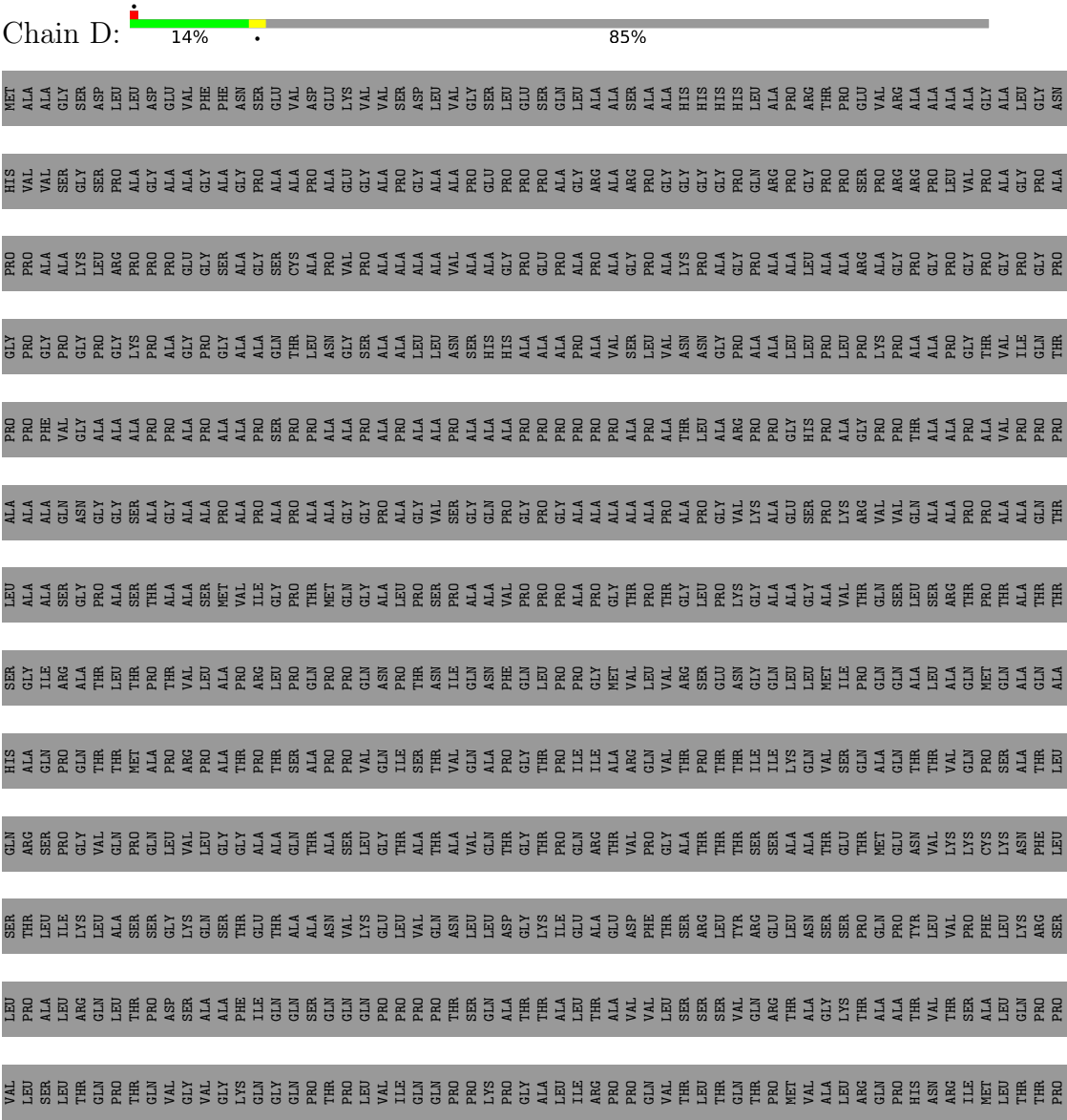
Mol	Chain	Residues	Atoms		AltConf
34	R	1	Total	Zn	0
			1	1	
34	o	2	Total	Zn	0
			2	2	
34	p	1	Total	Zn	0
			1	1	
34	q	1	Total	Zn	0
			1	1	
34	w	2	Total	Zn	0
			2	2	
34	x	1	Total	Zn	0
			1	1	
34	z	1	Total	Zn	0
			1	1	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



● Molecule 3: Transcription initiation factor TFIID subunit 4



LYS
GLU
ASP
ARG
GLY
GLU
GLU
GLN
LEU
SER
SER
GLN
GLU
GLU
GLU
GLU
GLU
LYS

• Molecule 7: Transcription initiation factor TFIID subunit 8



MET
ALA
ALA
ALA
ALA
THR
ALA
GLY
ALA
GLY
GLY
SER
GLN
THR
ASP
THR
GLN
LEU
SER
SER
THR
N24
I93
Q115
N126
Q127
P128
V129
T130
P131
K132
A133
L134
T135
A136
P141
Y159
T164
E167
P168
V169
S170
K205
D206
E231
L232
GLU
MET
GLN

GLN
MET
GLU
GLY
THR
ASP
SER
SER
GLN
GLY
THR
ASP
THR
GLN
ASN
GLY
SER
LEU
ALA
HIS
ILE
SER
MET
GLU
ASP
SER
GLY
ALA
GLY
LYS
GLU
ASN
THR
SER
VAL
LEU
GLN
GLN
ASN
PRO
SER
LEU
SER
GLY
SER
ASN
GLY
GLU
THR
ASN
ILE
ASP
ASN
TYR
LEU

ARG
PRO
VAL
LYS
LYS
PRO
LYS
ILE
ARG
GLY
LYS
LYS
SER
LEU
SER

• Molecule 8: Transcription initiation factor TFIID subunit 9



MET
GLU
SER
GLY
LYS
THR
ALA
SER
SER
PRO
LEU
GLY
SER
MET
P13
A64
P105
L132
GLN
LYS
LYS
SER
ALA
THR
SER
SER
GLY
ARG
ILE
THR
VAL
PRO
ARG
LEU
SER
VAL
GLN
SER
GLY
SER
ARG
PRO
SER
SER
THR
SER
THR
THR
PRO
THR
GLN
THR
MET
SER
VAL
SER

THR
LYS
VAL
GLY
THR
PRO
MET
SER
SER
SER
LEU
THR
GLY
GLN
PHE
THR
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MET
PRO
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ALA
VAL
LYS
SER
SER
SER
SER
TYR
ASN
LEU

GLN
ASN
THR
ALA
ASN
GLY
SER
SER
SER
SER
LEU
ALA
LYS
GLY
ARG
GLN
ASP
ASP
ASP
ASP
ASP
ASP
ASP
ASP
ASP
ASP
ASP
ASN
LEU

• Molecule 8: Transcription initiation factor TFIID subunit 9



MET
GLU
SER
GLY
LYS
THR
ALA
SER
SER
PRO
LEU
SER
M12
K14
D15
A16
Q17
M18
M19
A20
Q21
I22
L23
K24
D25
M26
G27
I28
T29
E30
Y31
E32
P33
R34
V35
I36
N37
Q38
M39
L40
E41
F42
A43
F44
R45
Y46
V47
T48
T49
I50
L51
D52
D53
A54
K55
I56
Y57
S58
S59
H60

A61
K62
K63
A64
T65
V66
D67
A68
D69
D70
V71
R72
L73
A74
I75
Q76
C77
R78
D90
L93
D94
R97
Q98
R99
M100
Q101
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L104
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I106
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P109
Y110
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G112
P113
R114
P117
D118
A124
P125
M126
Y127
R128
L129
K130
S131
L132
GLN
LYS
LYS
ALA
SER

THR
SER
ALA
GLY
ARG
ILE
THR
VAL
PRO
PRO
ARG
LEU
SER
VAL
VAL
GLY
VAL
THR
THR
SER
ARG
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SER
LEU
GLY
THR
PRO
PRO
GLN
THR
MET
SER
VAL
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GLN
ASN
THR
VAL
GLY
ALA
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PRO
ALA
THR
SER
SER
ALA
LEU
VAL
GLN
ASN
VAL
LEU
ILE
ASN
PRO
SER
SER
LEU
ILE
GLY
THR
LEU
LYS
ASN
GLY
THR
THR
ASN
MET
SER
SER
SER
GLN
ASN
THR
ALA
ALA
ASN
GLU
PRO
SER
SER
SER
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ARG
GLU
VAL
GLN
ASP
ASP
ASP
ASP
ASP
ASP
ASP

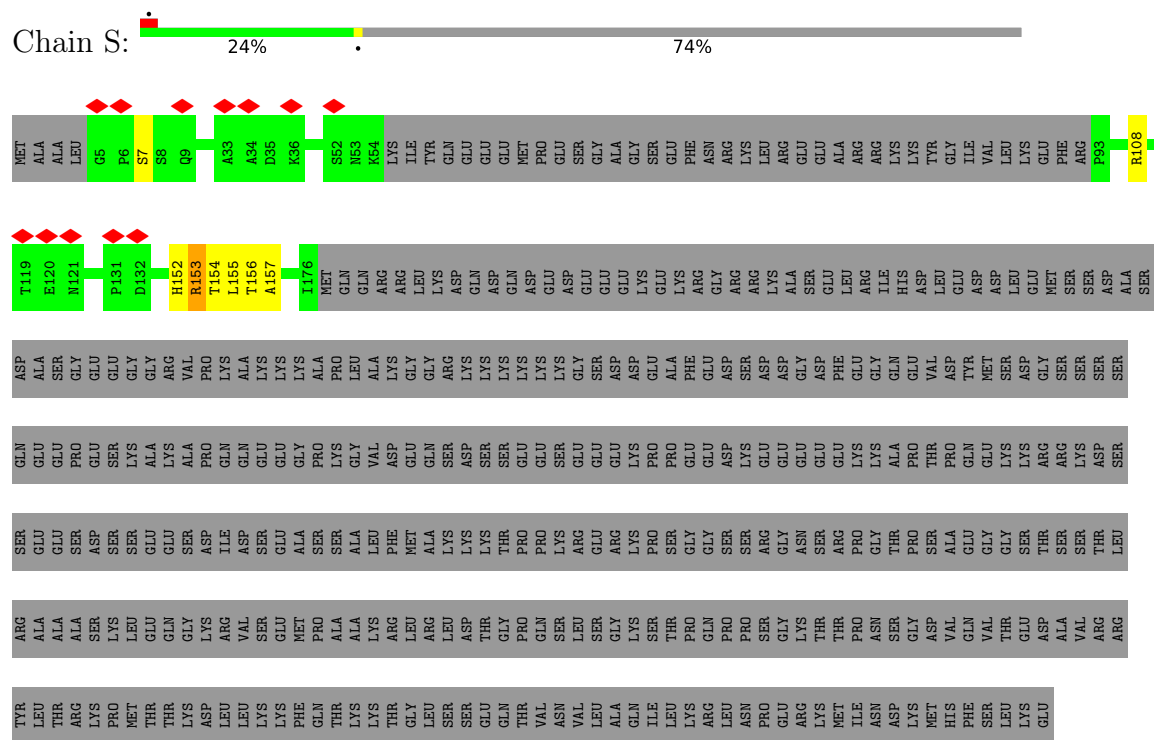
ASP
ASP
TYR
ASP
ASN
ASN
LEU

• Molecule 9: Transcription initiation factor TFIID subunit 10

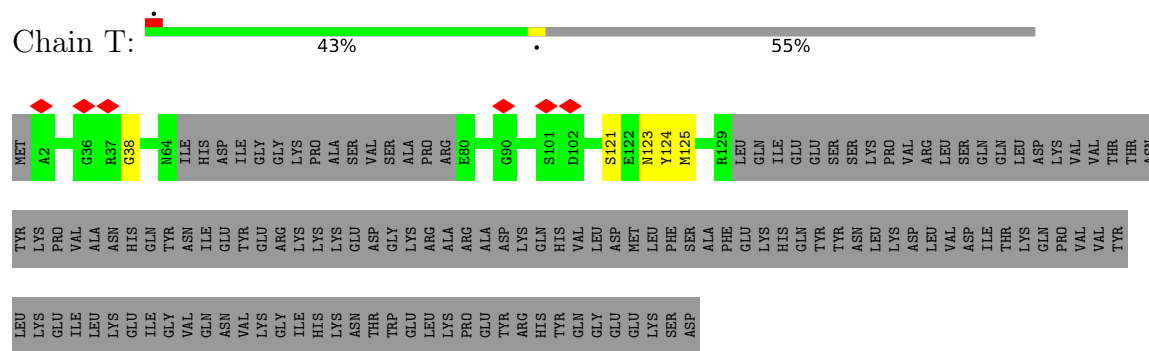


- [illegible]

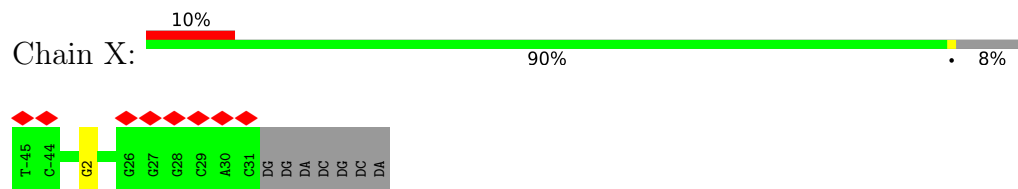
- Molecule 15: General transcription factor IIF subunit 1



- Molecule 16: General transcription factor IIF subunit 2

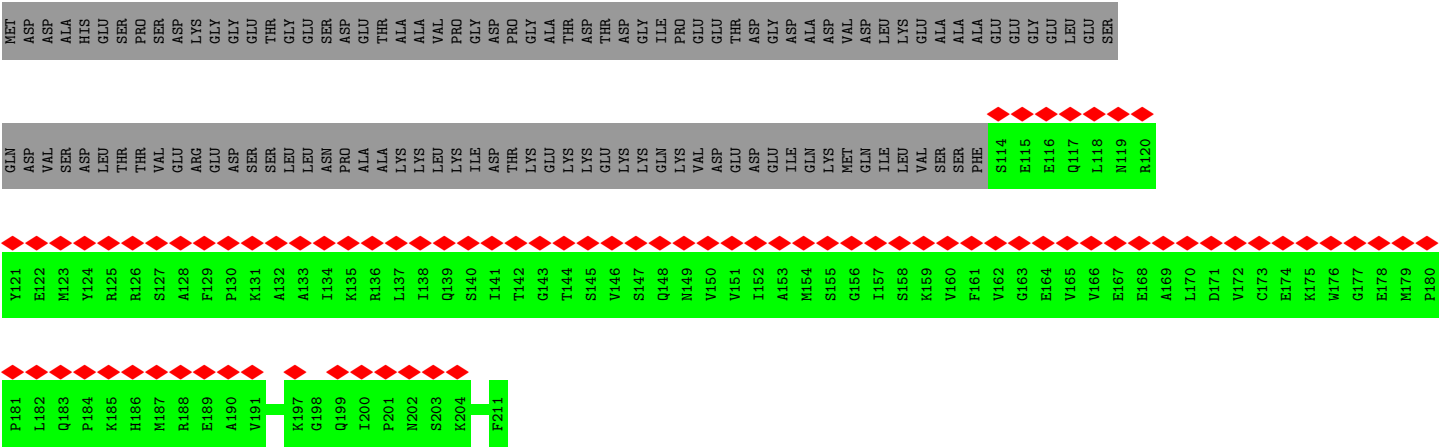


- Molecule 17: DNA (84-mer)

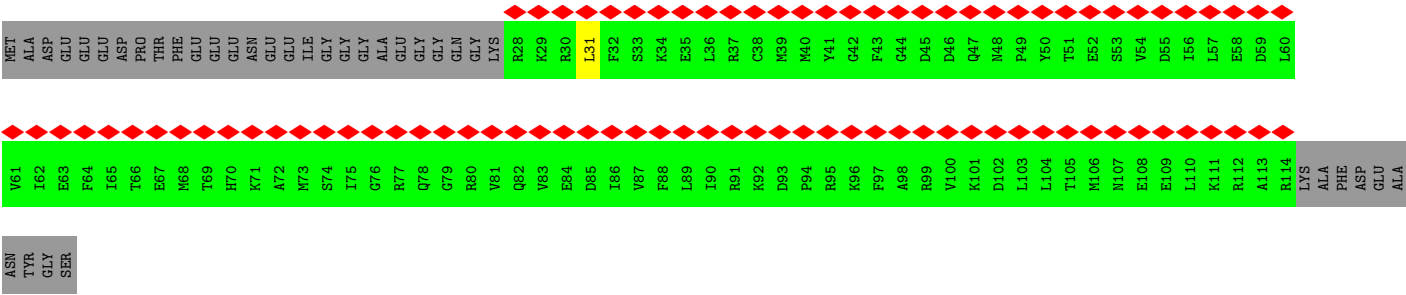


- Molecule 18: DNA (84-mer)

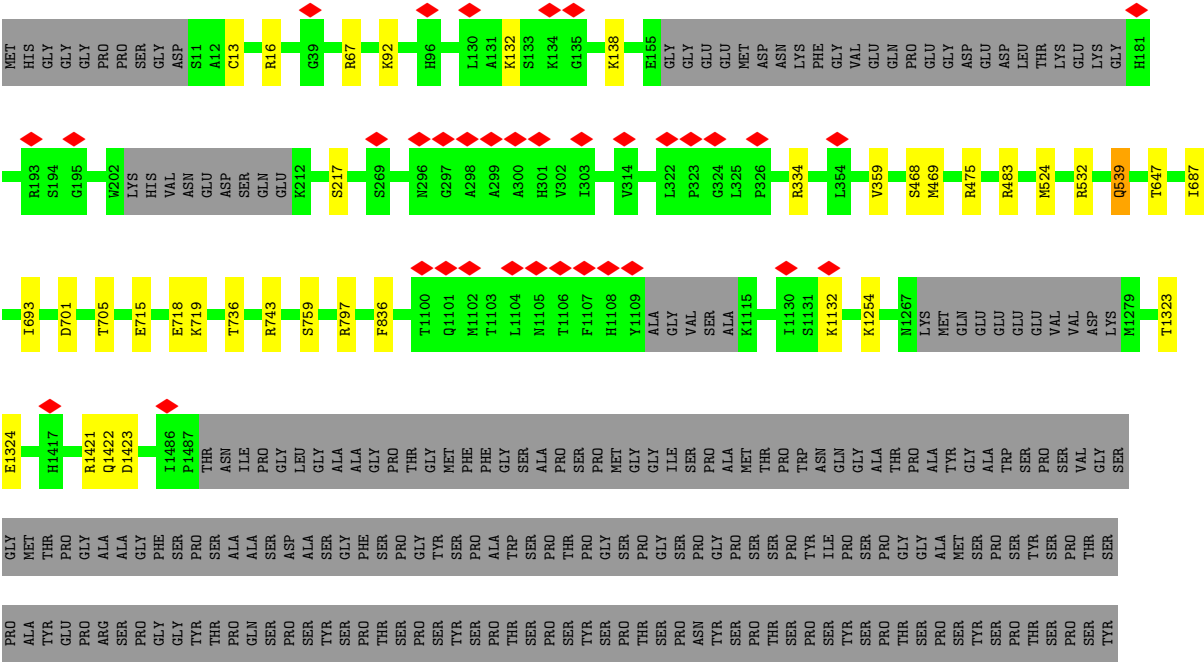


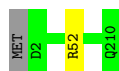


• Molecule 21: Transcription initiation factor TFIID subunit 13



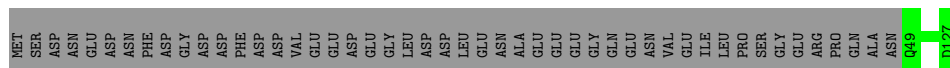
• Molecule 22: RPB1





- Molecule 27: DNA-directed RNA polymerase II subunit F

Chain t: 62% 38%



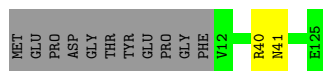
- Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 99%



- Molecule 29: DNA-directed RNA polymerase II subunit RPB9

Chain w: 90% 9%



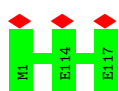
- Molecule 30: RPB10

Chain x: 96%



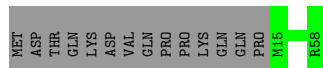
- Molecule 31: RNA_pol_L_2 domain-containing protein

Chain y: 100%



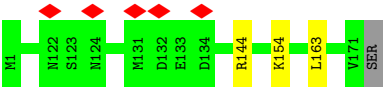
- Molecule 32: RPB12

Chain z: 76% 24%



- Molecule 33: DNA-directed RNA polymerase II subunit RPB7

Chain u: 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99580	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	1.612	Depositor
Minimum map value	-0.877	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/5046	0.66	1/6810 (0.0%)
2	B	0.46	0/7993	0.60	0/10836
3	D	0.51	0/1391	0.62	0/1859
3	d	0.29	0/1321	0.50	0/1772
4	E	0.34	0/4469	0.54	0/6050
4	e	0.32	0/4433	0.55	0/6004
5	F	0.51	0/3139	0.71	0/4264
5	f	0.41	0/3140	0.63	0/4268
6	G	0.53	0/1199	0.66	0/1612
7	H	0.39	0/1673	0.59	0/2285
8	I	0.28	0/981	0.47	0/1332
8	i	0.29	0/989	0.46	0/1343
9	J	0.31	0/724	0.50	0/982
9	j	0.30	0/775	0.52	0/1049
10	L	0.32	0/630	0.58	1/852 (0.1%)
10	l	0.29	0/888	0.56	3/1194 (0.3%)
11	O	0.52	0/781	0.73	0/1061
12	P	0.62	0/1438	0.80	2/1935 (0.1%)
13	Q	0.43	0/1013	0.67	0/1366
14	R	0.31	0/1941	0.54	0/2622
15	S	0.35	0/1130	0.53	0/1528
16	T	0.26	0/887	0.52	0/1193
17	X	0.66	1/1772 (0.1%)	1.11	0/2735
18	Y	0.66	0/1768	1.14	0/2724
19	c	0.39	0/1035	0.54	0/1406
20	k	0.30	0/799	0.47	0/1070
21	m	0.31	0/733	0.51	0/977
22	o	0.40	0/11516	0.54	0/15548
23	p	0.40	0/9243	0.50	0/12475
24	q	0.38	0/2102	0.46	0/2857
25	r	0.27	0/1019	0.47	0/1374
26	s	0.30	0/1751	0.45	0/2366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	t	0.37	0/645	0.46	0/871
28	v	0.37	0/1207	0.49	0/1628
29	w	0.31	0/948	0.47	0/1284
30	x	0.42	0/516	0.45	0/696
31	y	0.35	0/956	0.44	0/1294
32	z	0.38	0/377	0.45	0/500
33	u	0.33	0/1382	0.53	0/1874
All	All	0.42	1/83750 (0.0%)	0.60	7/113896 (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.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
23	p	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X	2	DG	O3'-P	5.29	1.67	1.61

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	203	ARG	CB-CA-C	10.12	130.65	110.40
1	A	498	PRO	N-CA-CB	6.71	111.36	103.30
12	P	202	MET	C-N-CA	-5.74	107.34	121.70
10	l	90	ASP	CB-CG-OD2	5.24	123.02	118.30
10	l	79	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	821	ARG	Peptide
23	p	1000	THR	Mainchain

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	A	584/1872 (31%)	543 (93%)	32 (6%)	9 (2%)	8	39
2	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
3	D	159/1085 (15%)	147 (92%)	9 (6%)	3 (2%)	6	33
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	540/800 (68%)	505 (94%)	33 (6%)	2 (0%)	30	68
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
5	F	400/677 (59%)	374 (94%)	18 (4%)	8 (2%)	6	32
5	f	399/677 (59%)	378 (95%)	21 (5%)	0	100	100
6	G	139/349 (40%)	132 (95%)	5 (4%)	2 (1%)	9	40
7	H	207/310 (67%)	189 (91%)	15 (7%)	3 (1%)	9	40
8	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100	100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
10	L	74/161 (46%)	69 (93%)	5 (7%)	0	100	100
10	l	105/161 (65%)	101 (96%)	4 (4%)	0	100	100
11	O	95/109 (87%)	81 (85%)	10 (10%)	4 (4%)	2	18
12	P	175/339 (52%)	169 (97%)	4 (2%)	2 (1%)	12	46
13	Q	118/376 (31%)	108 (92%)	9 (8%)	1 (1%)	16	54
14	R	244/316 (77%)	235 (96%)	8 (3%)	1 (0%)	30	68
15	S	130/517 (25%)	124 (95%)	4 (3%)	2 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	T	109/249 (44%)	102 (94%)	4 (4%)	3 (3%)	4	24
19	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
20	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
21	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
22	o	1417/1970 (72%)	1305 (92%)	110 (8%)	2 (0%)	48	83
23	p	1128/1174 (96%)	1051 (93%)	75 (7%)	2 (0%)	44	78
24	q	253/275 (92%)	226 (89%)	27 (11%)	0	100	100
25	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
26	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
27	t	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
28	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
29	w	112/125 (90%)	102 (91%)	9 (8%)	1 (1%)	14	51
30	x	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
31	y	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
32	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
33	u	169/172 (98%)	157 (93%)	11 (6%)	1 (1%)	22	60
All	All	9695/17897 (54%)	9057 (93%)	592 (6%)	46 (0%)	27	64

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
1	A	1158	SER
3	D	958	LYS
5	F	323	VAL
5	F	396	LEU

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	A	536/1665 (32%)	473 (88%)	63 (12%)	4	17
2	B	876/1083 (81%)	859 (98%)	17 (2%)	52	69
3	D	149/815 (18%)	133 (89%)	16 (11%)	5	20
3	d	146/815 (18%)	144 (99%)	2 (1%)	62	75
4	E	478/657 (73%)	474 (99%)	4 (1%)	79	84
4	e	475/657 (72%)	473 (100%)	2 (0%)	89	90
5	F	320/574 (56%)	297 (93%)	23 (7%)	12	32
5	f	322/574 (56%)	313 (97%)	9 (3%)	38	59
6	G	133/322 (41%)	118 (89%)	15 (11%)	4	18
7	H	181/270 (67%)	176 (97%)	5 (3%)	38	59
8	I	106/235 (45%)	106 (100%)	0	100	100
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	71 (100%)	0	100	100
10	l	98/141 (70%)	98 (100%)	0	100	100
11	O	84/98 (86%)	73 (87%)	11 (13%)	3	15
12	P	153/293 (52%)	143 (94%)	10 (6%)	14	35
13	Q	111/324 (34%)	103 (93%)	8 (7%)	12	32
14	R	211/268 (79%)	198 (94%)	13 (6%)	15	37
15	S	117/448 (26%)	110 (94%)	7 (6%)	16	38
16	T	94/218 (43%)	92 (98%)	2 (2%)	48	67
19	c	113/833 (14%)	111 (98%)	2 (2%)	54	71
20	k	87/182 (48%)	87 (100%)	0	100	100
21	m	80/106 (76%)	79 (99%)	1 (1%)	65	77
22	o	1257/1748 (72%)	1222 (97%)	35 (3%)	38	59
23	p	993/1027 (97%)	970 (98%)	23 (2%)	45	64
24	q	234/252 (93%)	234 (100%)	0	100	100
25	r	106/126 (84%)	105 (99%)	1 (1%)	75	83
26	s	191/192 (100%)	190 (100%)	1 (0%)	86	89
27	t	69/111 (62%)	69 (100%)	0	100	100
28	v	129/131 (98%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	w	103/112 (92%)	102 (99%)	1 (1%)	73	81
30	x	53/56 (95%)	53 (100%)	0	100	100
31	y	106/106 (100%)	106 (100%)	0	100	100
32	z	41/55 (74%)	41 (100%)	0	100	100
33	u	152/153 (99%)	150 (99%)	2 (1%)	65	77
All	All	8643/15331 (56%)	8370 (97%)	273 (3%)	36	55

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	o	718	GLU
22	o	1132	LYS
23	p	1001	PRO
4	E	745	GLU
3	D	1055	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
10	L	117	GLN
23	p	1009	GLN
8	i	60	HIS
23	p	790	GLN
28	v	131	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

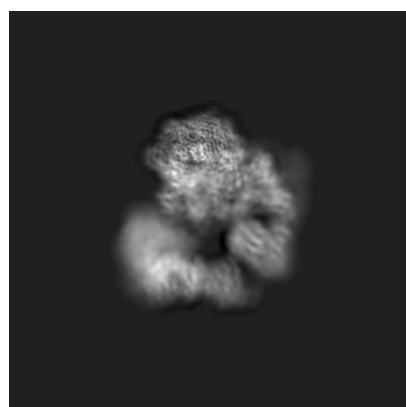
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31075. These allow visual inspection of the internal detail of the map and identification of artifacts.

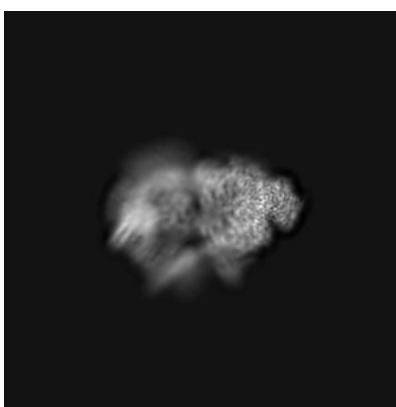
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

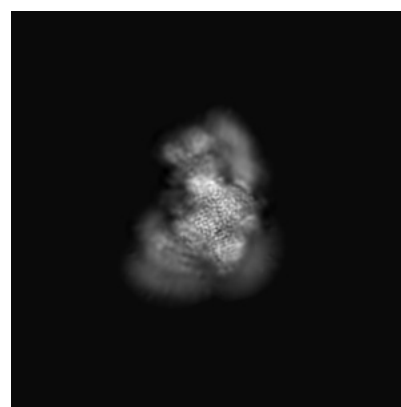
6.1.1 Primary map



X



Y

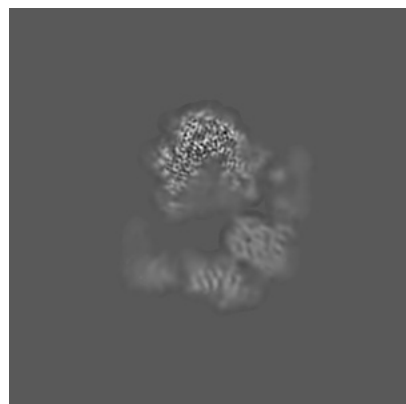


Z

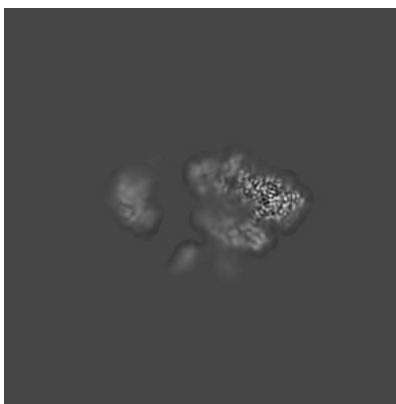
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

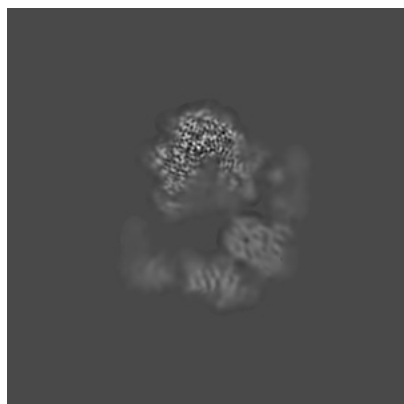


Z Index: 240

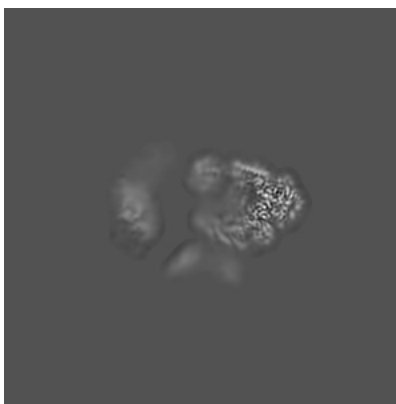
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

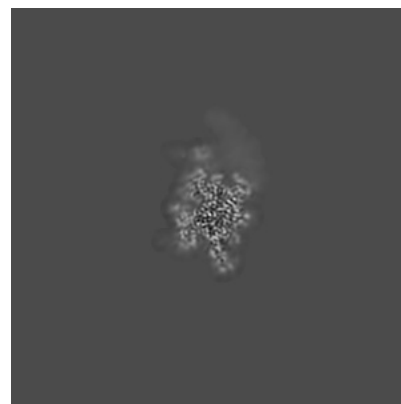
6.3.1 Primary map



X Index: 241



Y Index: 230

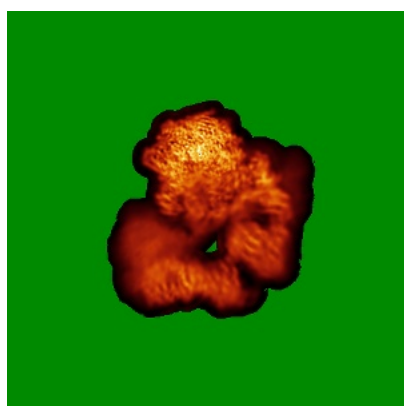


Z Index: 307

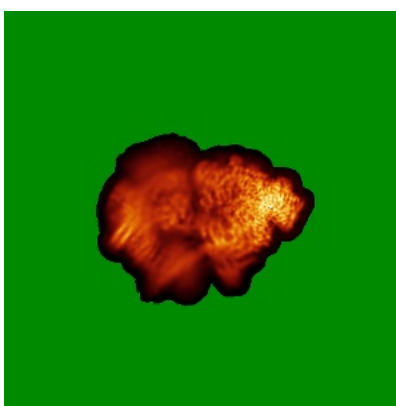
The images above show the largest variance slices of the map in three orthogonal directions.

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

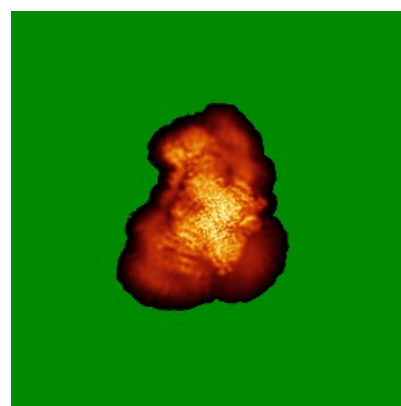
6.4.1 Primary map



X



Y

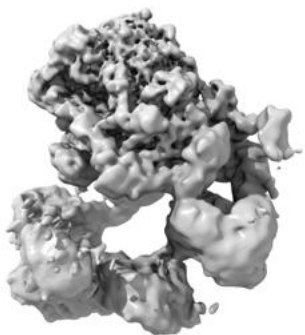


Z

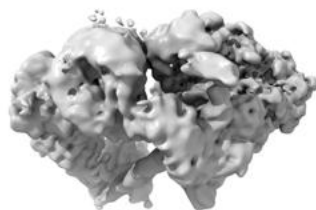
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

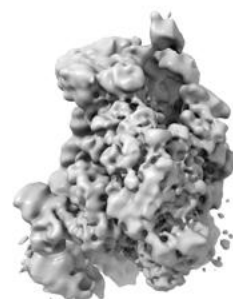
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

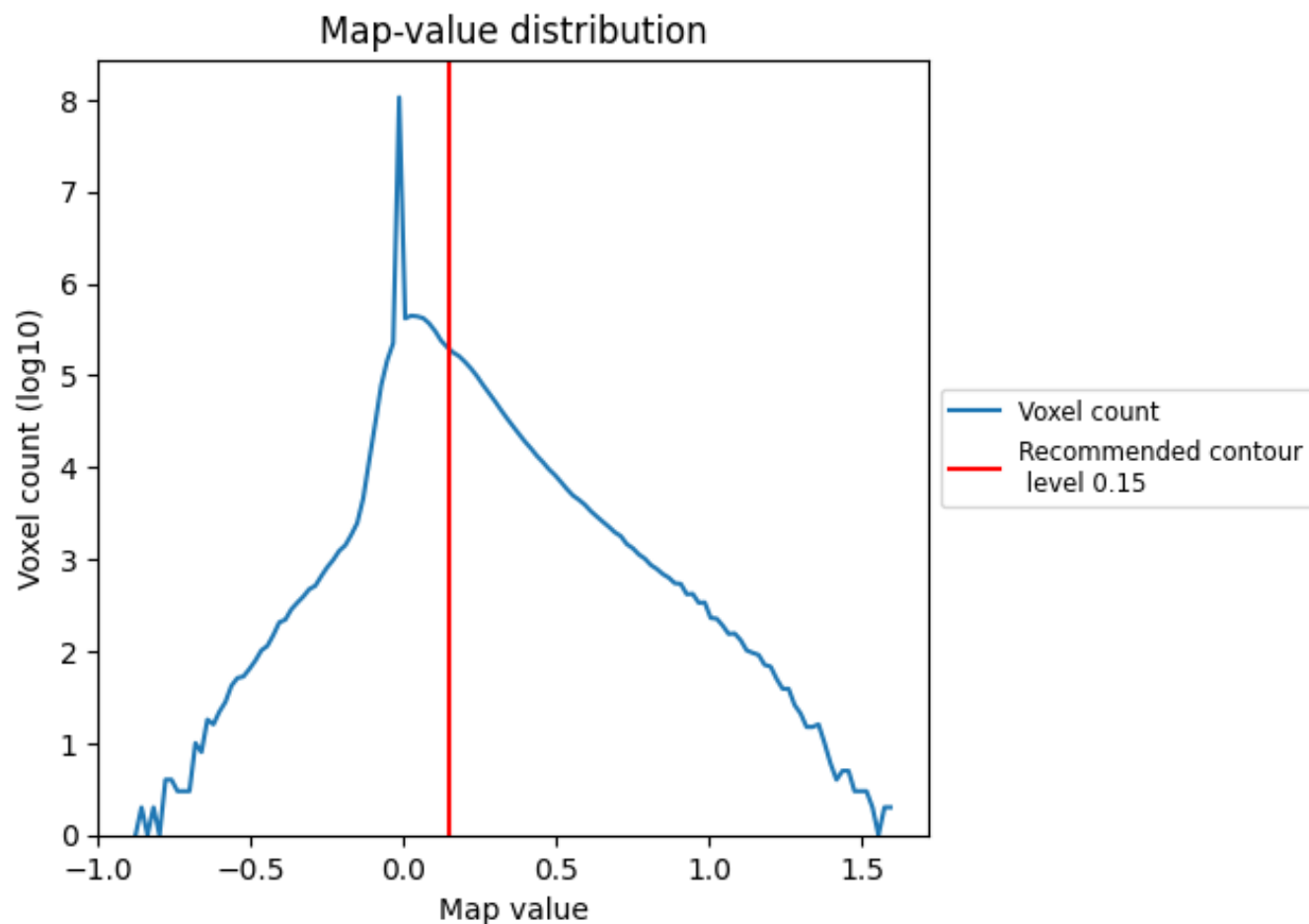
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

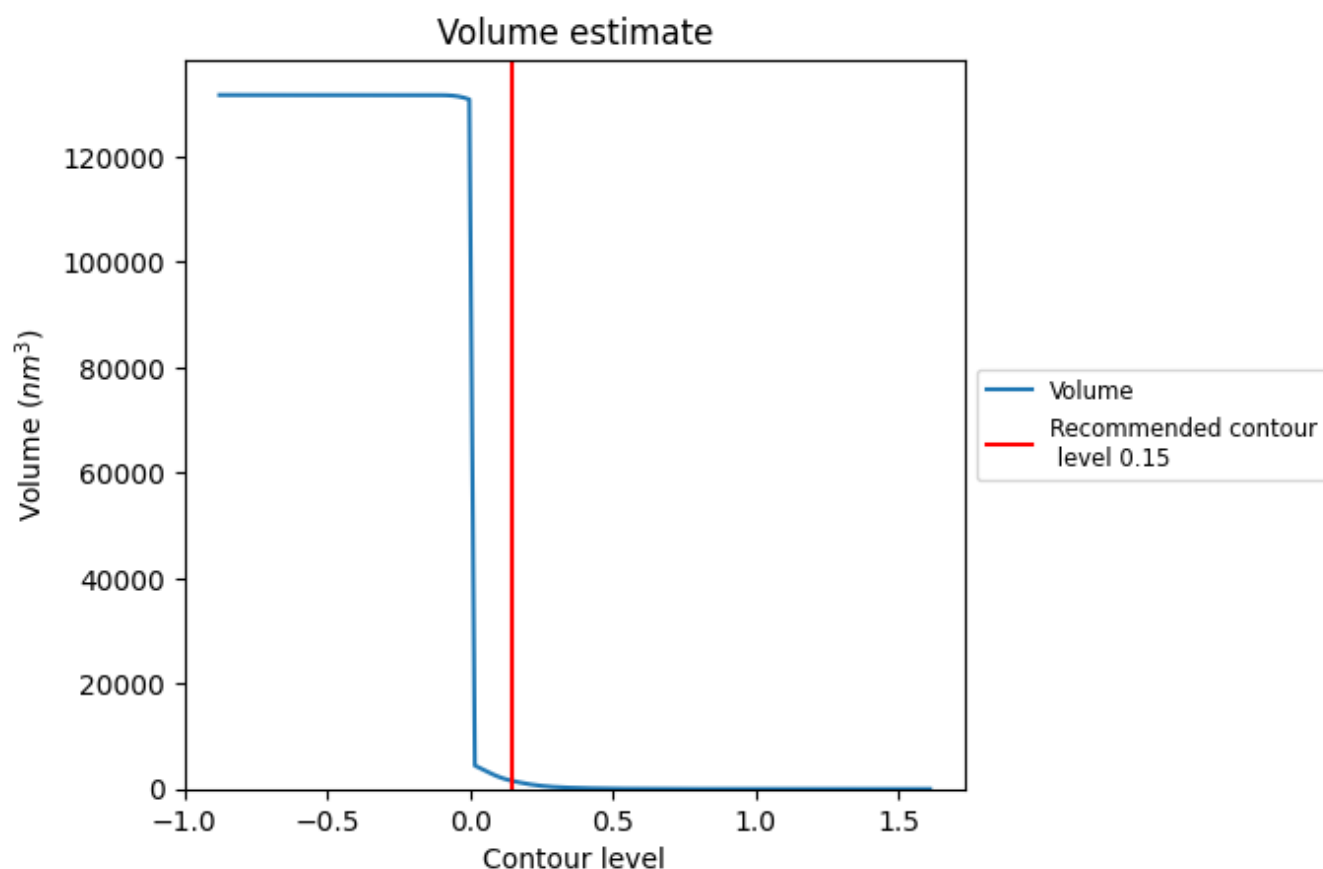
This section contains the results of statistical analysis of the map.

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.

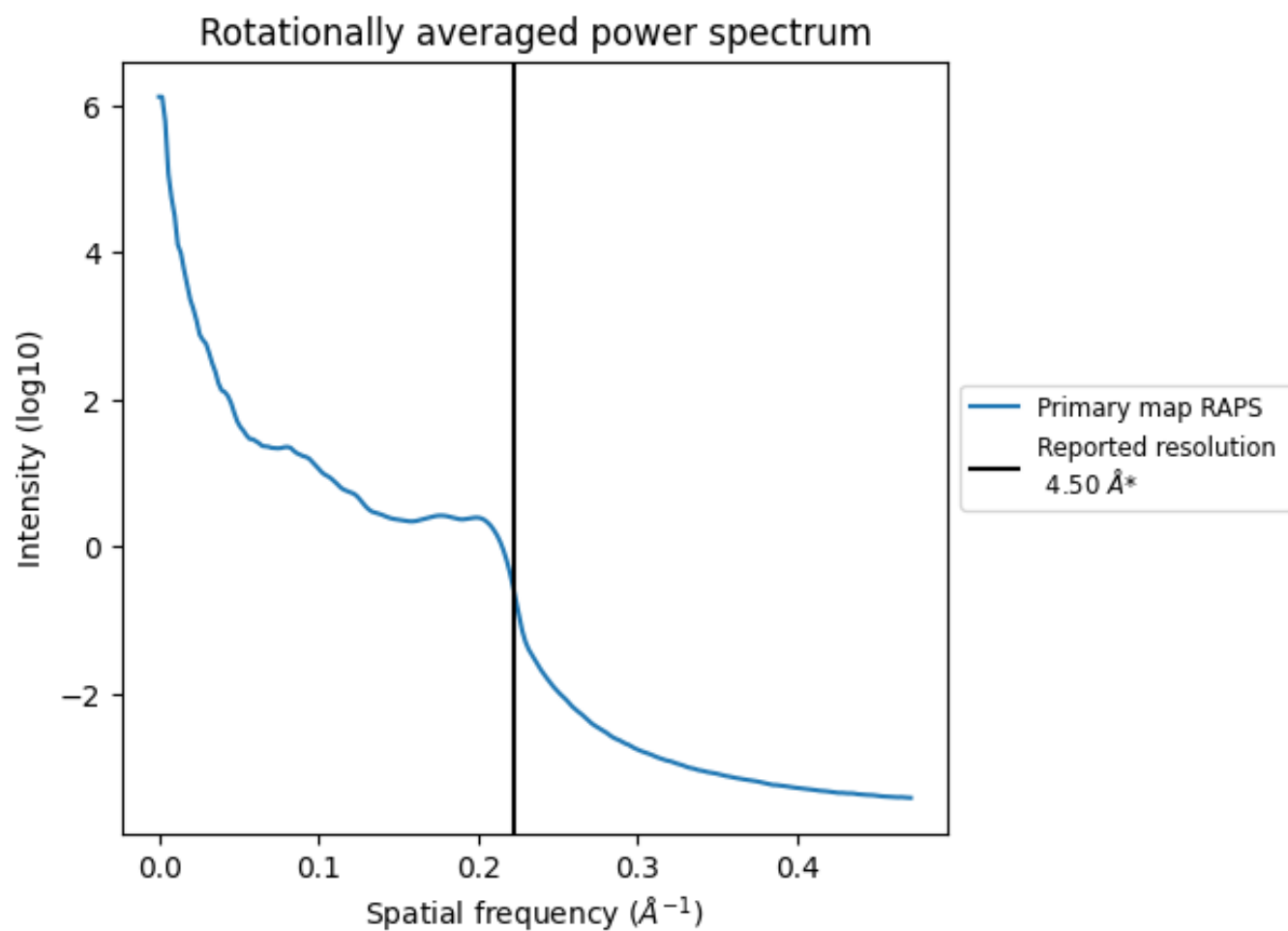
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1509 nm^3 ; this corresponds to an approximate mass of 1363 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 0.222 Å⁻¹

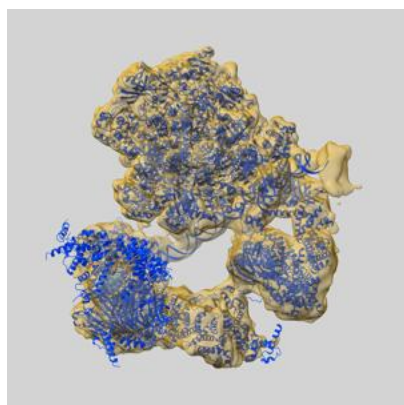
8 Fourier-Shell correlation

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

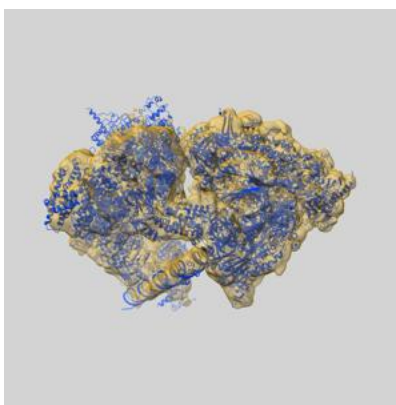
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31075 and PDB model 7EDX. Per-residue inclusion information can be found in section 3 on page 11.

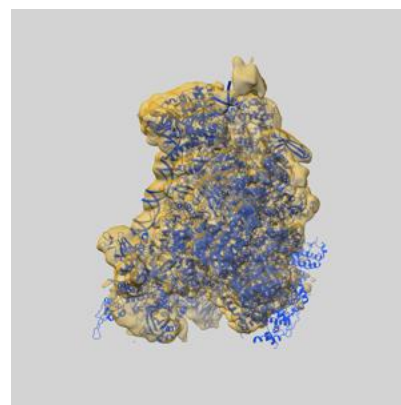
9.1 Map-model overlay [i](#)



X



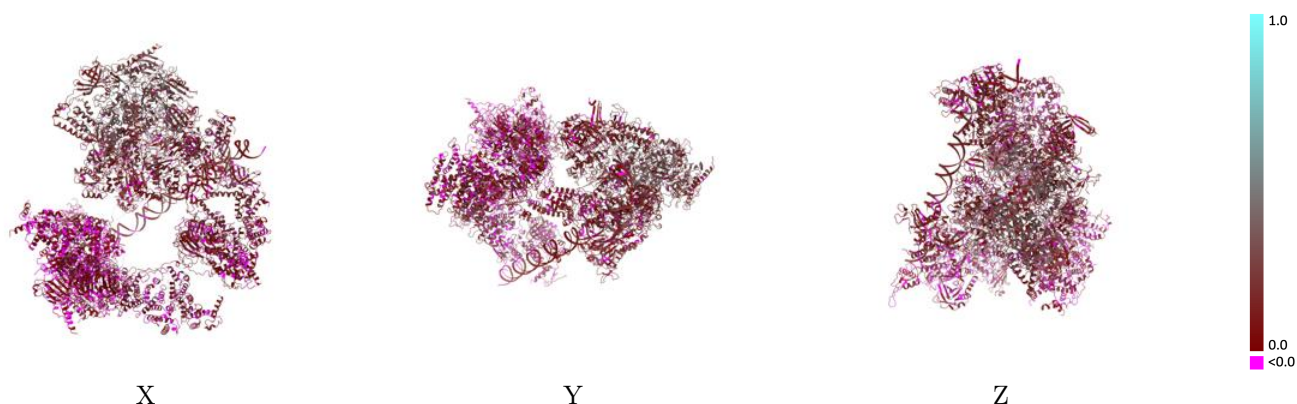
Y



Z

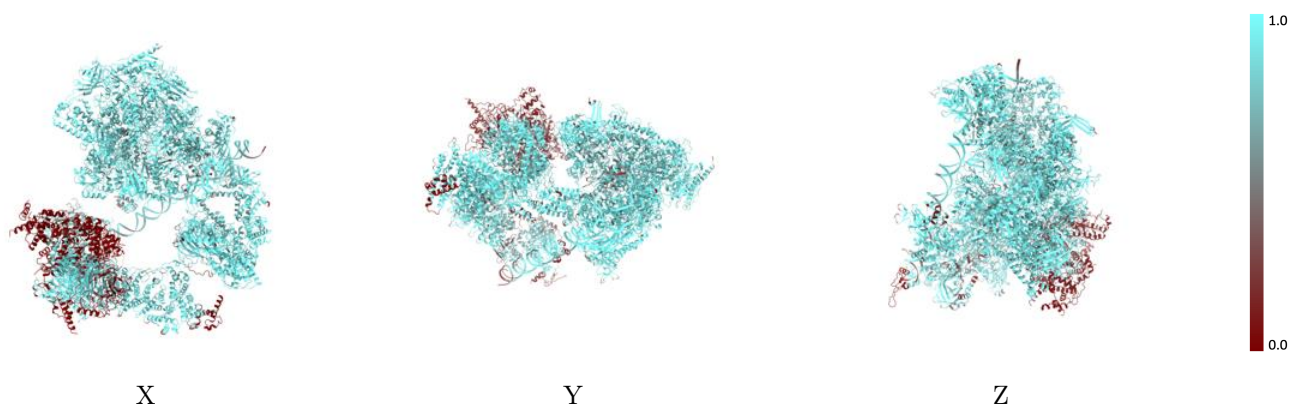
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



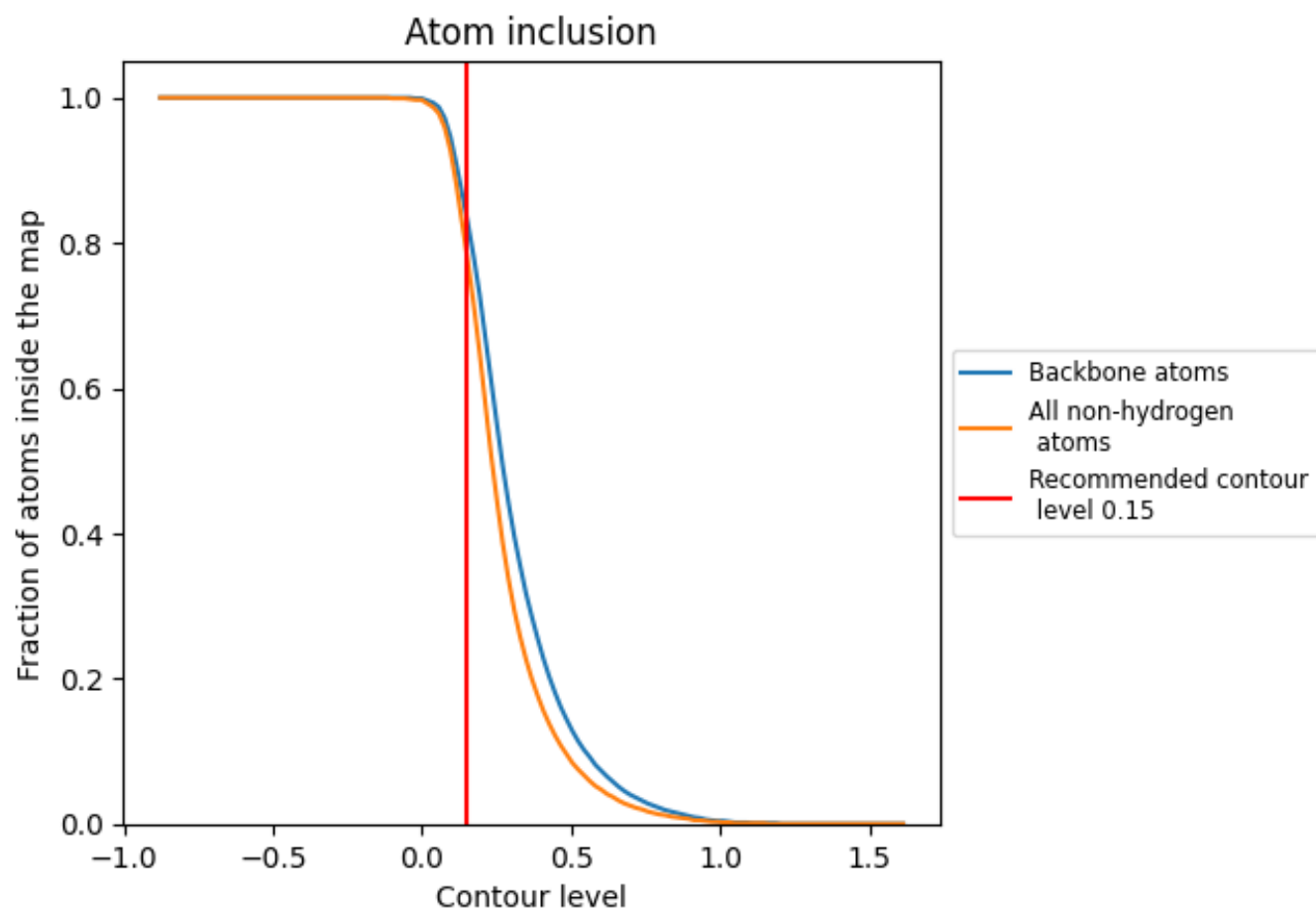
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.1300
A	 0.7320	 0.0490
B	 0.8960	 0.0780
D	 0.8660	 0.1150
E	 0.9060	 0.0940
F	 0.8200	 0.0910
G	 0.7500	 0.0360
H	 0.8650	 0.0890
I	 0.9400	 0.0780
J	 0.9680	 0.0620
L	 0.9200	 0.1140
O	 0.9290	 0.1400
P	 0.9700	 0.1270
Q	 0.9280	 0.0970
R	 0.9030	 0.1670
S	 0.8560	 0.0980
T	 0.8910	 0.1130
X	 0.7990	 0.1150
Y	 0.7750	 0.1120
c	 0.4460	 0.0240
d	 0.2820	 0.0290
e	 0.3020	 0.0310
f	 0.6410	 0.0430
i	 0.2250	 0.0250
j	 0.3380	 0.0260
k	 0.1280	 0.0230
l	 0.1280	 0.0200
m	 0.0060	 0.0120
o	 0.8920	 0.2240
p	 0.8560	 0.2220
q	 0.9420	 0.2680
r	 0.8690	 0.1400
s	 0.9300	 0.2020
t	 0.9290	 0.2630
u	 0.9350	 0.1370



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Chain	Atom inclusion	Q-score
v	 0.9080	 0.2410
w	 0.9410	 0.1850
x	 0.9460	 0.3130
y	 0.8930	 0.2800
z	 0.9550	 0.2230