



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 07:45 AM EST

PDB ID : 6OUL
EMDB ID : EMD-20203
Title : Cryo-EM structure of Escherichia coli RNAP polymerase bound to rpsTP2 promoter DNA
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-05-04
Resolution : 3.40 Å(reported)

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

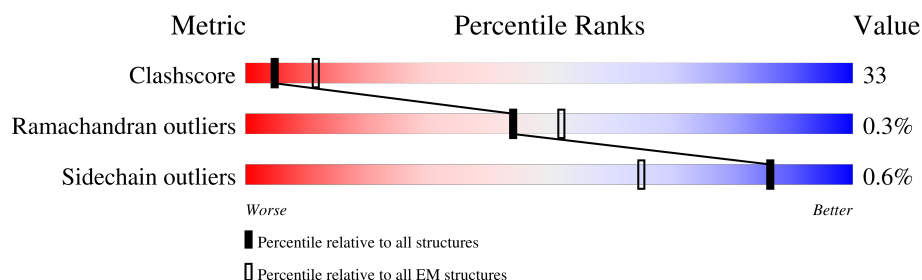
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	G	329	
1	H	329	
1	R	329	
2	I	1342	
3	J	1430	
4	K	91	
5	L	616	
6	P	85	

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Mol	Chain	Length	Quality of chain
7	Q	85	<div><div><div></div><div></div><div></div></div><div>24%15%51%34%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32044 atoms, of which 117 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	231	Total	C	N	O	S	0	0
			1785	1112	318	349	6		
1	H	219	Total	C	N	O	S	0	0
			1681	1050	295	330	6		
1	R	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1341	Total	C	N	O	S	0	0
			10575	6634	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1337	Total	C	N	O	S	0	0
			10386	6525	1851	1961	49		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP U9YPW3
J	1408	LEU	-	expression tag	UNP U9YPW3
J	1409	GLU	-	expression tag	UNP U9YPW3
J	1410	LEU	-	expression tag	UNP U9YPW3
J	1411	GLU	-	expression tag	UNP U9YPW3
J	1412	VAL	-	expression tag	UNP U9YPW3
J	1413	LEU	-	expression tag	UNP U9YPW3
J	1414	PHE	-	expression tag	UNP U9YPW3
J	1415	GLN	-	expression tag	UNP U9YPW3
J	1416	GLY	-	expression tag	UNP U9YPW3
J	1417	PRO	-	expression tag	UNP U9YPW3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1418	SER	-	expression tag	UNP U9YPW3
J	1419	SER	-	expression tag	UNP U9YPW3
J	1420	GLY	-	expression tag	UNP U9YPW3
J	1421	HIS	-	expression tag	UNP U9YPW3
J	1422	HIS	-	expression tag	UNP U9YPW3
J	1423	HIS	-	expression tag	UNP U9YPW3
J	1424	HIS	-	expression tag	UNP U9YPW3
J	1425	HIS	-	expression tag	UNP U9YPW3
J	1426	HIS	-	expression tag	UNP U9YPW3
J	1427	HIS	-	expression tag	UNP U9YPW3
J	1428	HIS	-	expression tag	UNP U9YPW3
J	1429	HIS	-	expression tag	UNP U9YPW3
J	1430	HIS	-	expression tag	UNP U9YPW3

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	471	Total	C	N	O	S	0	0
			3821	2397	681	720	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

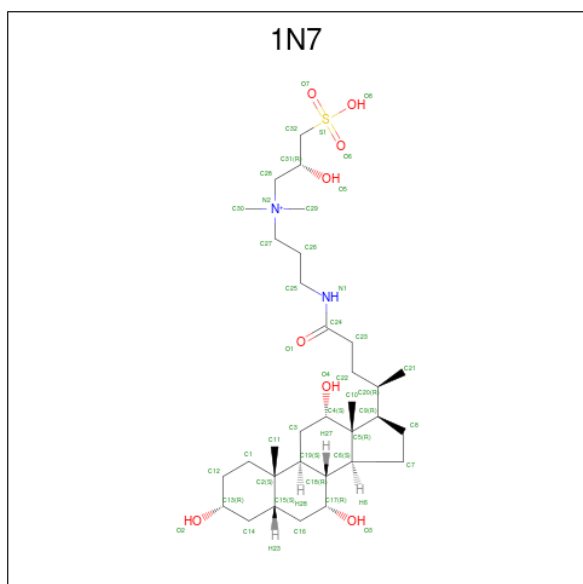
- Molecule 6 is a DNA chain called Non-template strand of rpsTP2 DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	61	Total	C	N	O	P	0	0
			1253	599	235	358	61		

- Molecule 7 is a DNA chain called Template strand of rpsTP2 DNA promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	56	Total	C	N	O	P	0	0
			1143	549	192	346	56		

- Molecule 8 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms				AltConf
8	I	1	Total	C	H	O	0
			66	24	39	3	
8	J	1	Total	C	H	O	0
			66	24	39	3	
8	L	1	Total	C	H	O	0
			66	24	39	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total	Zn	0
			2	2	

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain R: 21%
6% 16% 78%

MET
GLN
GLY
SER
VAL
THR
GLU
PHE
LEU
LYS
PRO
ARG
LEU
VAL
ASP
GLN
ILE
GLU
ASP
GLN
ILE
GLN
VAL
SER
VAL
SER
ILE
THR
THR
HIS
ALA
LYS
VAL
THR
GLY
LEU
SER
GLN
ASP
GLY
CYS
ASP
VAL
THR
HIS
ASP
GLY
VAL
PRO
GLU
ASP

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

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

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ALA
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ALA
ARG
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VAL
HIS
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GLN
THR
ARG
THR
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THR
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ASN
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ASP
LEU
ASP
ARG
VAL
ARG
GLN
PRO

GLU
VAL
LYS
GLU
GLY
LYS
PRO
PHE
D250
P251
L252
L253
L254
R255
R256
P257
D258
D259
L260
E261
L262
L263
V264
R265
S266
A267
N268
C269
L270
K271
A272
E273
A274
L275
H276
Y277
L278
G279
D280
L281
V282
Q283
R284
T285
E286
V287
E288
L289
K291
T292
P293
N294
L295
G296
K297
K298
S299
L300

T301
E302
I303
K304
D305
V306
L307
A308
S309
R310
G311
L312
S313
L314
G315
M316
R317
L318
E319
N320
W321
P322
PRO
ALA
SER
ILE
ALA
ASP
GLU

• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 10%
50% 50%

MET
Y2
Y3
S4
Y5
Y6
E7
R8
K9
I11
R12
K13
D14
F15
G16
K17
R18
V21
L22
D23
V24
P25
Y26
L27
L28
S29
I30
Q31
L32
D33
K37
F38
I39
E44
Q45
Q46
L49
E50
A51
A52
F53
V56
F57
Q60
S61
Y62
S63
E67
L68
Q69
Y70
V71

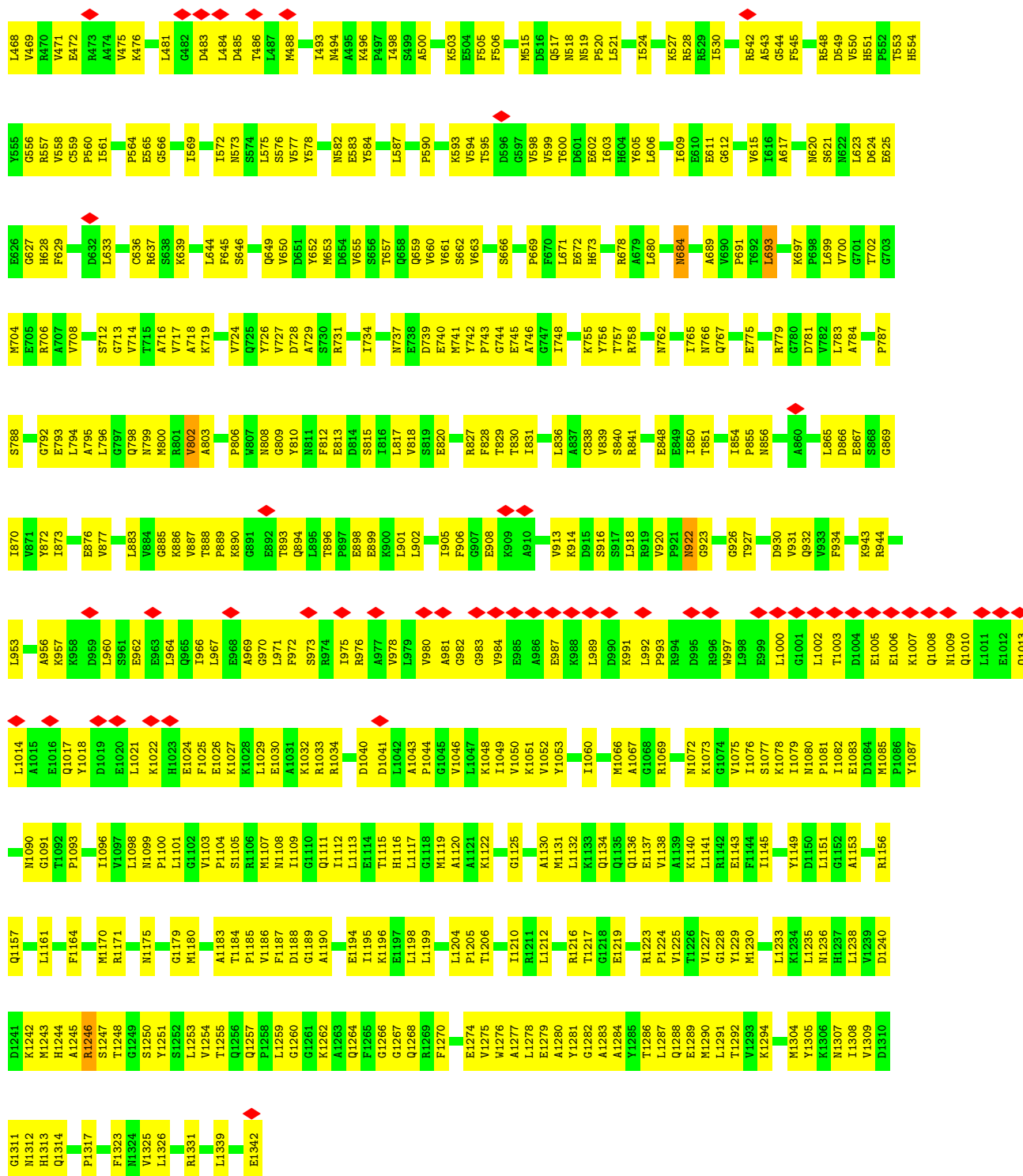
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R107
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A109
P110
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M124
G125
E126
I127
P128
L129
M130
T131
D132
N133
G134
T135
F136
V137
I138
T141
E142
R143
V144
I145
Q148

L149
H150
R151
V155
F156
F157
D158
S159
D160
K161
R162
K163
T164
H165
S166
S167
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R175
I176
L184
D185
F186
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F188
D189
D192
N193
F195
L204
T207
I208
N214
Y215
T216
T217
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L220
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F230
E231
I232
R233
D234
N235
K236
L237

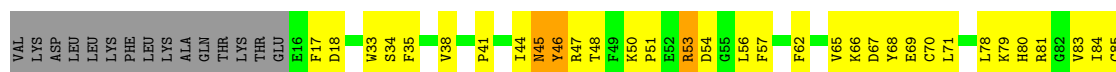
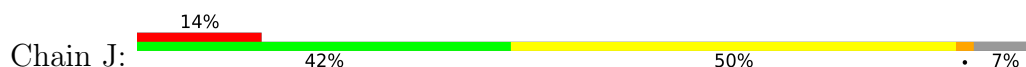
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I255
A257
N258
G259
K260
V261
Y262
V263
E264
K265
G266
R267
R268
I269
T270
A271
R272
H273
L274
R275
Q276
L277
E278
K279
D280
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A298
K299

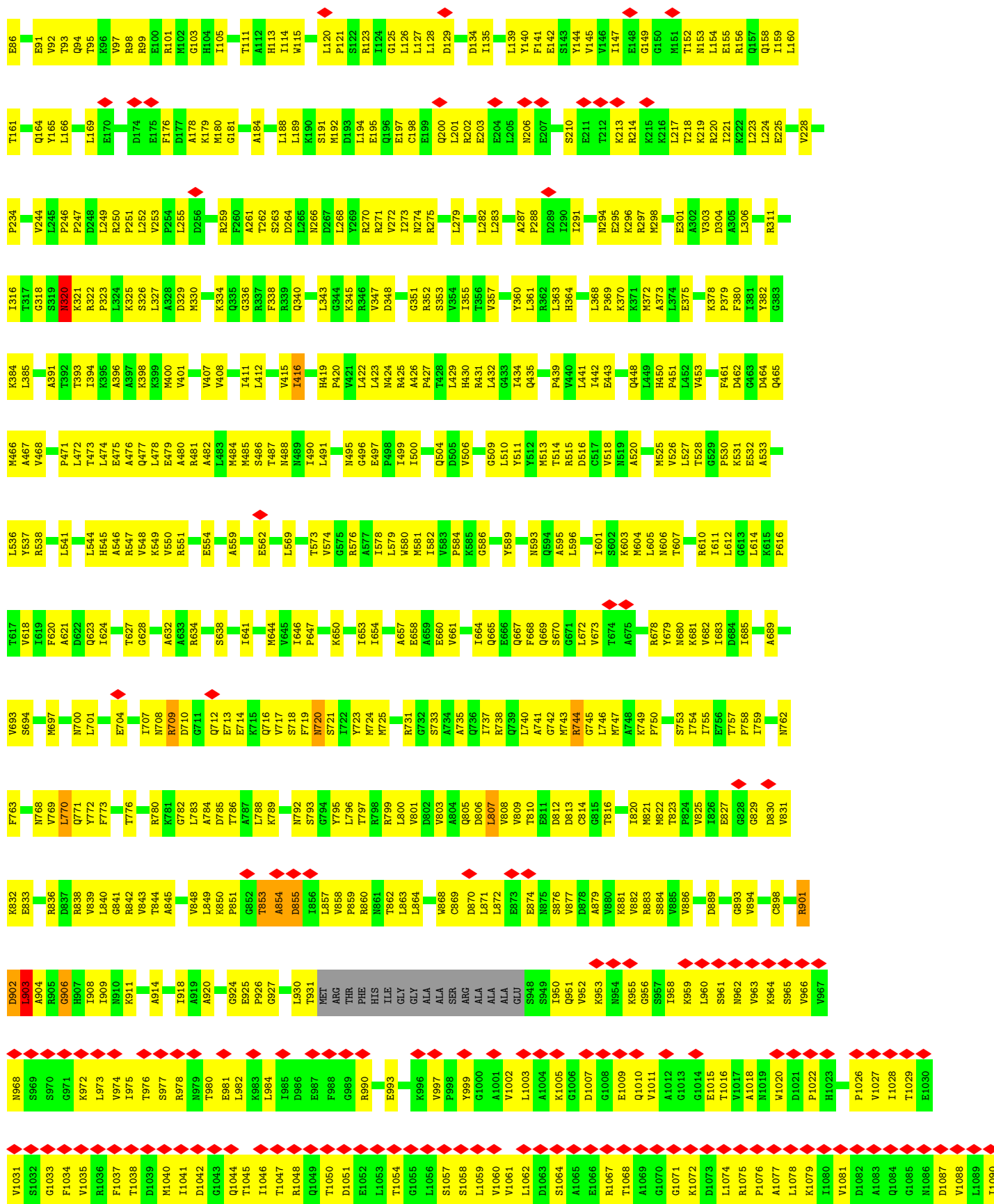
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L319
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L321
L322
A323
K324
L325
S326
Q327
S328
G329
H330
K331
R332
I333
E334
F337
T338
N339
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L360
L363
V364
E365
I366
Y367

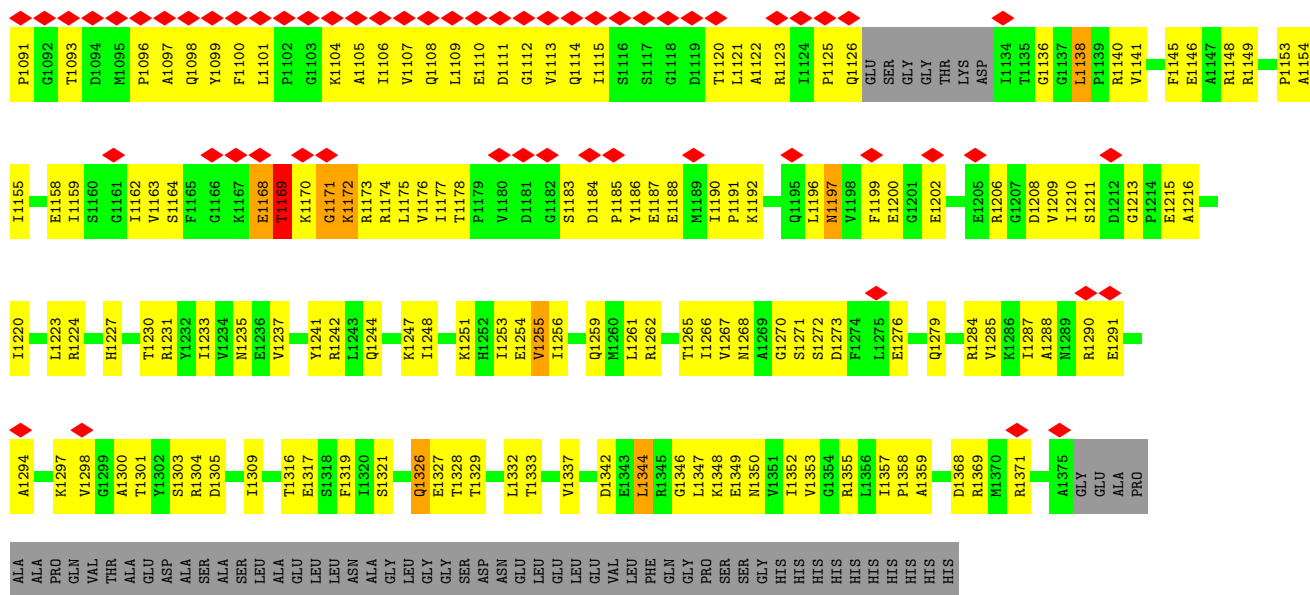
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G401
E412
E413
G418
K422
D423
D424
I425
V428
K431
L432
I435
V442
D443
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I453
R454
S455
V456
G457
E458
M459
Q463



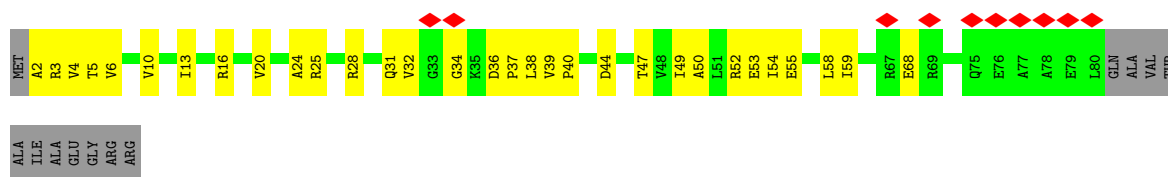
● Molecule 3: DNA-directed RNA polymerase subunit beta'



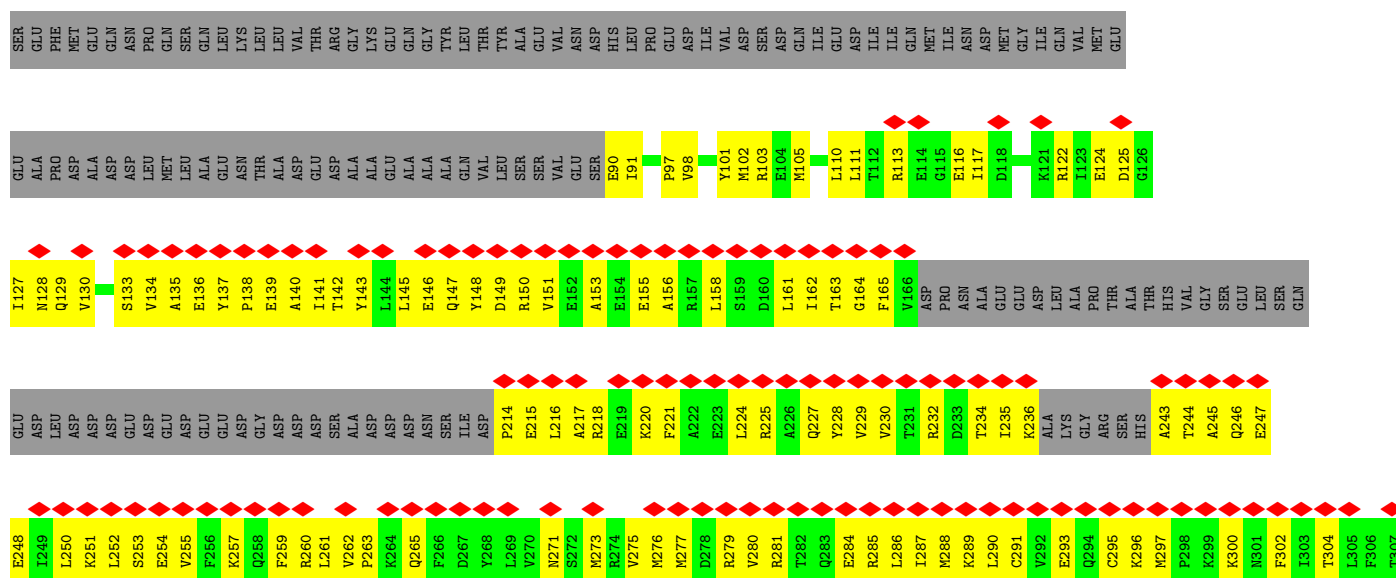




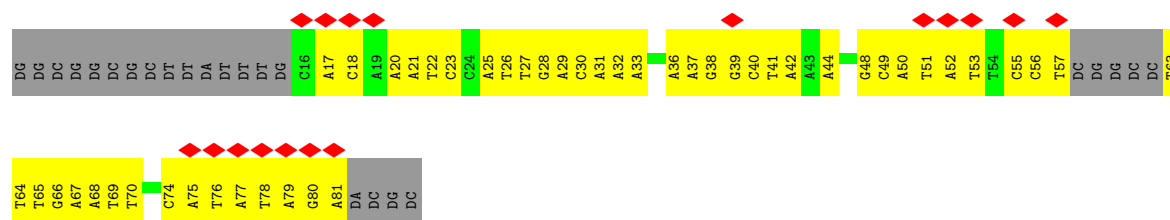
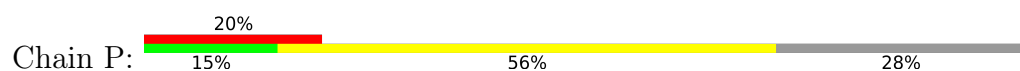
• Molecule 4: DNA-directed RNA polymerase subunit omega



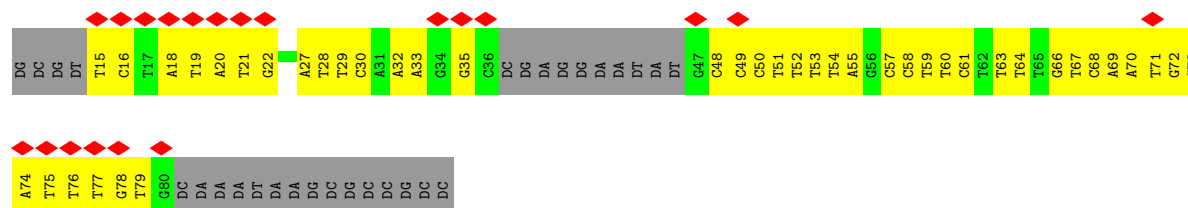
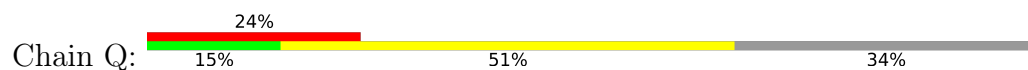
• Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 6: Non-template strand of rpsTP2 DNA promoter



- Molecule 7: Template strand of rpsTP2 DNA promoter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	289670	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3, 1.3, 1.3	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: 1N7, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.71	0/1807	0.69	1/2449 (0.0%)
1	H	0.55	0/1700	0.65	1/2305 (0.0%)
1	R	0.26	0/579	0.51	0/784
2	I	0.75	0/10744	0.68	3/14496 (0.0%)
3	J	0.70	2/10543 (0.0%)	0.69	3/14239 (0.0%)
4	K	0.50	0/629	0.59	0/847
5	L	0.42	0/3872	0.55	0/5204
6	P	0.75	0/1407	0.97	0/2166
7	Q	0.73	0/1276	0.99	0/1965
All	All	0.68	2/32557 (0.0%)	0.70	8/44455 (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
2	I	0	1
3	J	0	10
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1255	VAL	CB-CG1	-5.31	1.41	1.52
3	J	453	VAL	CB-CG1	-5.03	1.42	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1344	LEU	CA-CB-CG	-6.66	99.97	115.30
3	J	903	LEU	CA-CB-CG	6.38	129.96	115.30
2	I	693	LEU	CA-CB-CG	5.57	128.10	115.30
3	J	807	LEU	CA-CB-CG	-5.45	102.77	115.30
2	I	28	LEU	CA-CB-CG	-5.36	102.98	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1185	PRO	Peptide
3	J	320	ASN	Peptide
3	J	416	ILE	Peptide
3	J	853	THR	Peptide
3	J	855	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1785	0	1806	120	0
1	H	1681	0	1708	148	0
1	R	572	0	602	84	0
2	I	10575	0	10584	682	0
3	J	10386	0	10594	791	0
4	K	627	0	634	39	0
5	L	3821	0	3891	312	0
6	P	1253	0	689	72	0
7	Q	1143	0	640	50	0
8	I	27	39	37	6	0
8	J	27	39	37	4	0
8	L	27	39	38	4	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31927	117	31260	2115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 2115 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.83	1.55
8:J:1504:1N7:C19	8:J:1504:1N7:C3	1.84	1.54
8:L:701:1N7:C19	8:L:701:1N7:C3	1.84	1.52
1:H:105:SER:HA	1:H:138:ALA:HB2	1.42	1.01
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.43	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	229/329 (70%)	194 (85%)	35 (15%)	0	100	100
1	H	215/329 (65%)	185 (86%)	30 (14%)	0	100	100
1	R	71/329 (22%)	62 (87%)	9 (13%)	0	100	100
2	I	1339/1342 (100%)	1161 (87%)	175 (13%)	3 (0%)	47	78
3	J	1331/1430 (93%)	1167 (88%)	157 (12%)	7 (0%)	29	61
4	K	77/91 (85%)	67 (87%)	10 (13%)	0	100	100
5	L	465/616 (76%)	428 (92%)	37 (8%)	0	100	100
All	All	3727/4466 (84%)	3264 (88%)	453 (12%)	10 (0%)	44	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	854	ALA
3	J	1169	THR
2	I	399	ALA
3	J	320	ASN
3	J	1172	LYS

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	G	196/286 (68%)	195 (100%)	1 (0%)	88	94
1	H	186/286 (65%)	186 (100%)	0	100	100
1	R	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1149 (100%)	6 (0%)	88	94
3	J	1118/1189 (94%)	1108 (99%)	10 (1%)	78	90
4	K	67/75 (89%)	67 (100%)	0	100	100
5	L	415/543 (76%)	414 (100%)	1 (0%)	93	98
All	All	3202/3822 (84%)	3184 (99%)	18 (1%)	86	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	901	ARG
5	L	476	ARG
3	J	1197	ASN
3	J	53	ARG
3	J	770	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	817	HIS
5	L	265	GLN
3	J	1010	GLN
3	J	1326	GLN
5	L	331	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	1N7	J	1504	-	30,30,46	5.12	15 (50%)	47,48,72	2.84	25 (53%)
8	1N7	I	1401	-	30,30,46	5.03	16 (53%)	47,48,72	2.59	17 (36%)
8	1N7	L	701	-	30,30,46	5.03	14 (46%)	47,48,72	2.67	16 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	1N7	J	1504	-	-	7/7/72/92	0/4/4/4
8	1N7	I	1401	-	-	1/7/72/92	0/4/4/4
8	1N7	L	701	-	-	0/7/72/92	0/4/4/4

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C3-C19	18.52	1.84	1.53
8	L	701	1N7	C3-C19	18.49	1.84	1.53
8	I	1401	1N7	C3-C19	17.99	1.83	1.53
8	I	1401	1N7	C3-C4	12.22	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	1N7	C3-C4	11.66	1.73	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	1504	1N7	C9-C5-C4	-8.57	109.84	117.67
8	L	701	1N7	C7-C6-C18	-7.10	108.40	118.33
8	L	701	1N7	C9-C5-C6	6.82	106.97	100.09
8	I	1401	1N7	C9-C5-C6	6.44	106.59	100.09
8	L	701	1N7	C9-C5-C4	-6.15	112.05	117.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1504	1N7	C21-C20-C9-C5
8	J	1504	1N7	C21-C20-C9-C8
8	J	1504	1N7	C22-C20-C9-C5
8	J	1504	1N7	C22-C20-C9-C8
8	J	1504	1N7	C9-C20-C22-C23

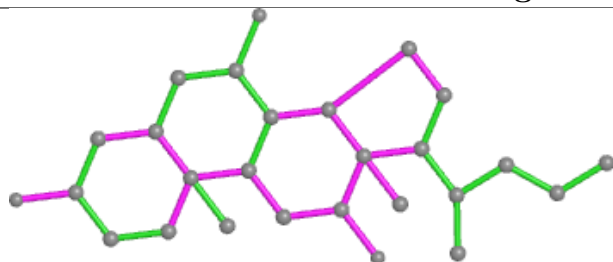
There are no ring outliers.

3 monomers are involved in 14 short contacts:

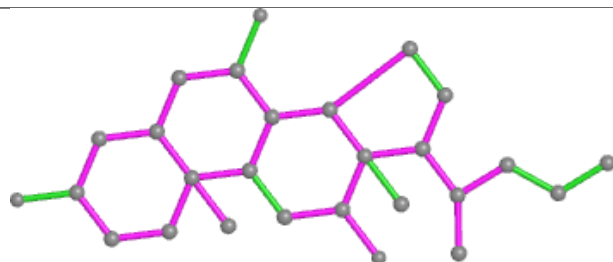
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1504	1N7	4	0
8	I	1401	1N7	6	0
8	L	701	1N7	4	0

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

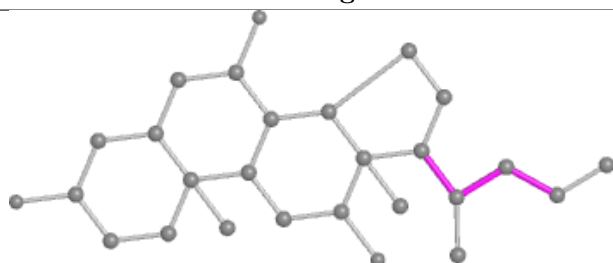
Ligand 1N7 J 1504



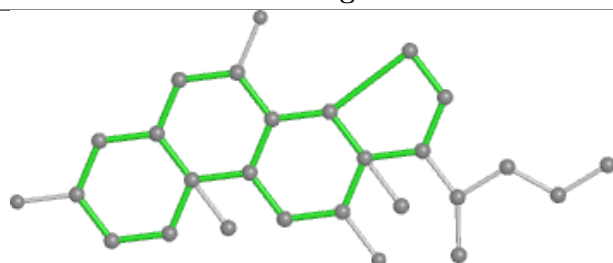
Bond lengths



Bond angles

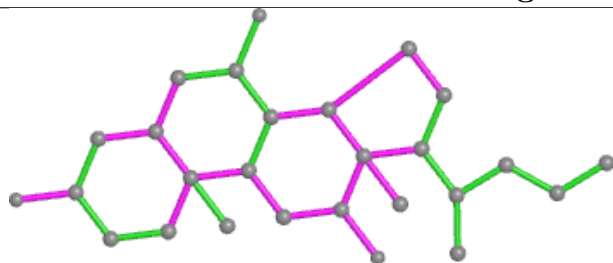


Torsions

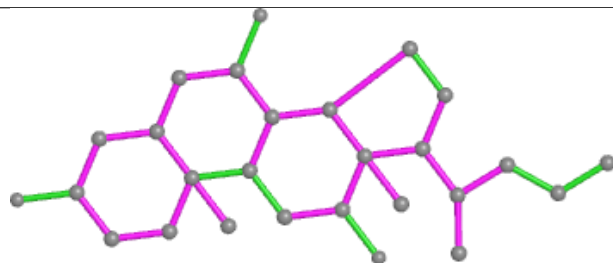


Rings

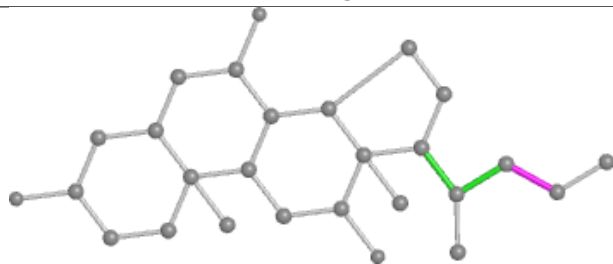
Ligand 1N7 I 1401



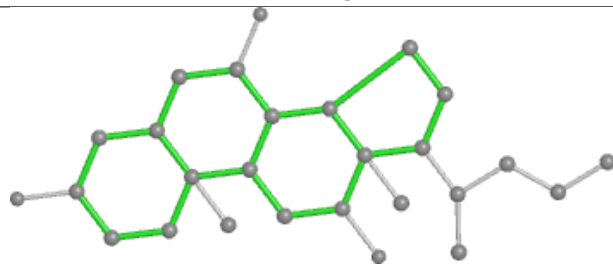
Bond lengths



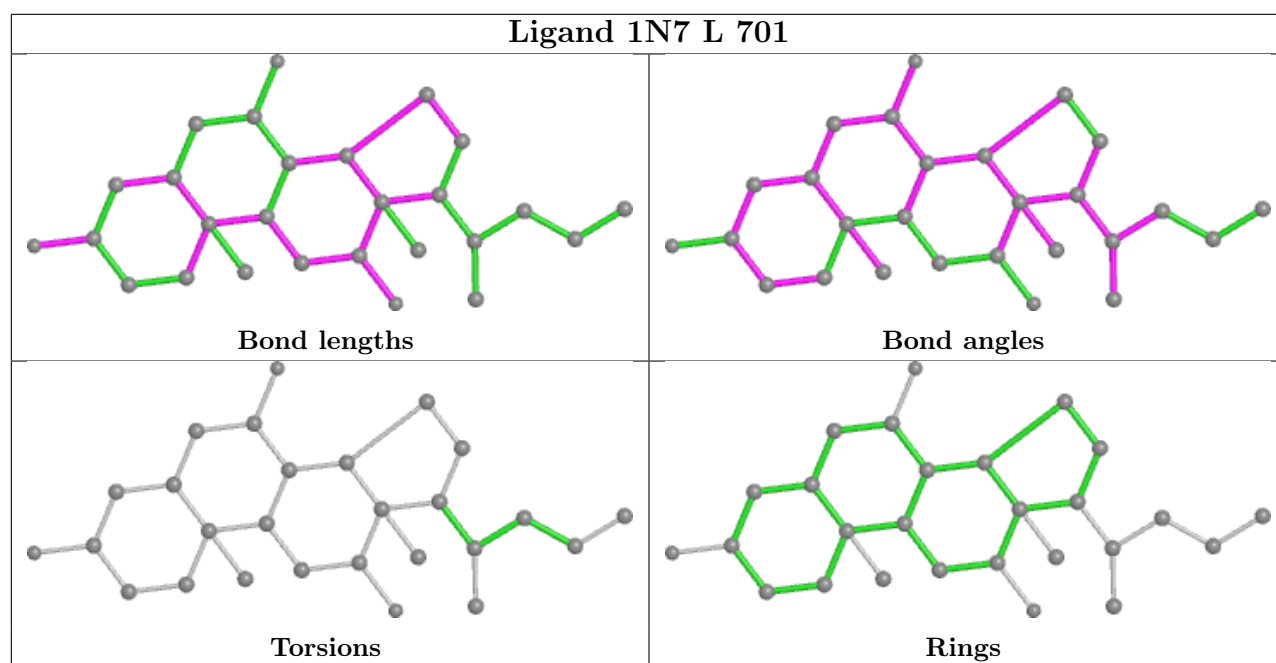
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

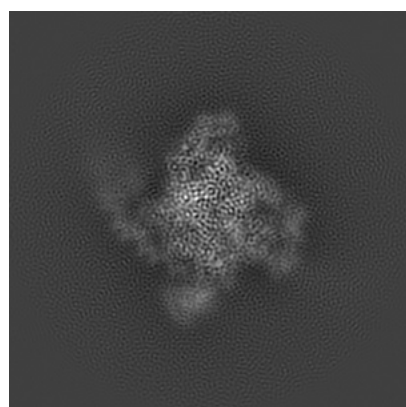
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20203. These allow visual inspection of the internal detail of the map and identification of artifacts.

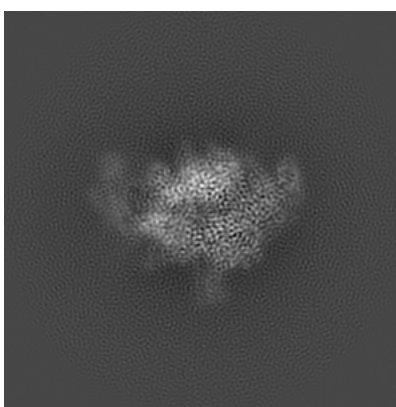
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

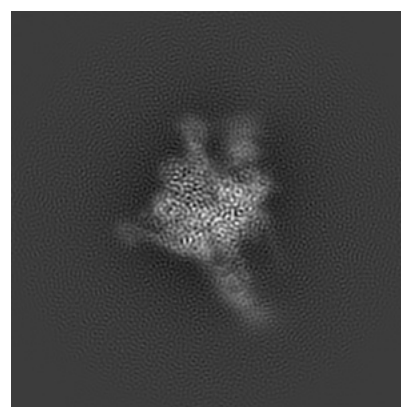
6.1.1 Primary map



X



Y

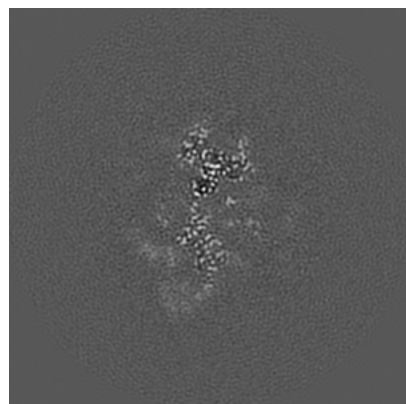


Z

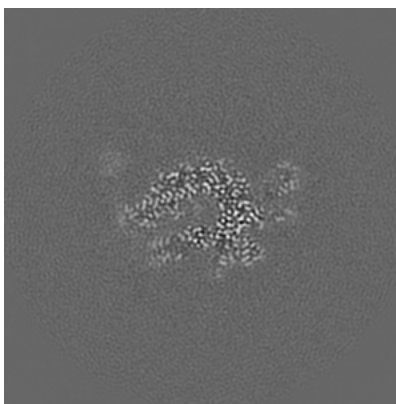
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

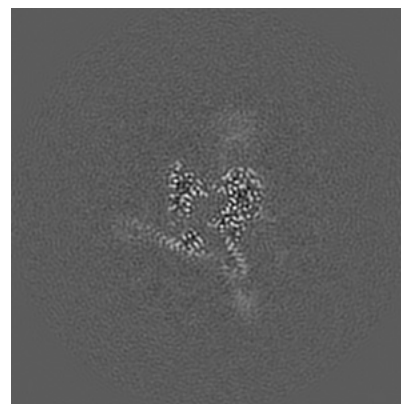
6.2.1 Primary map



X Index: 128



Y Index: 128

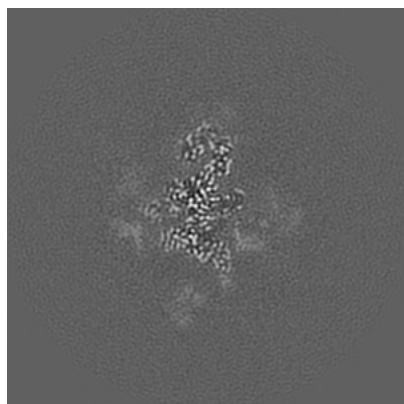


Z Index: 128

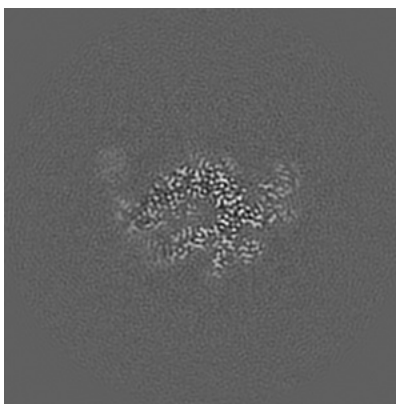
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

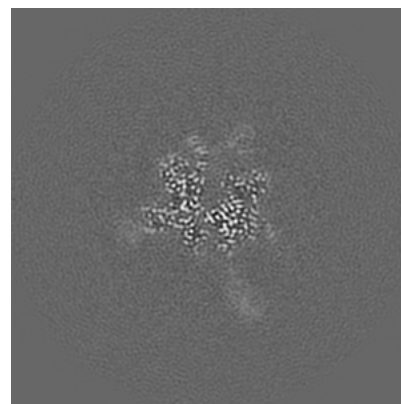
6.3.1 Primary map



X Index: 138



Y Index: 126

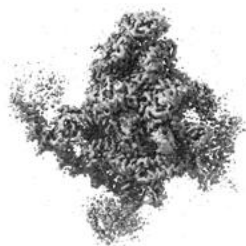


Z Index: 136

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

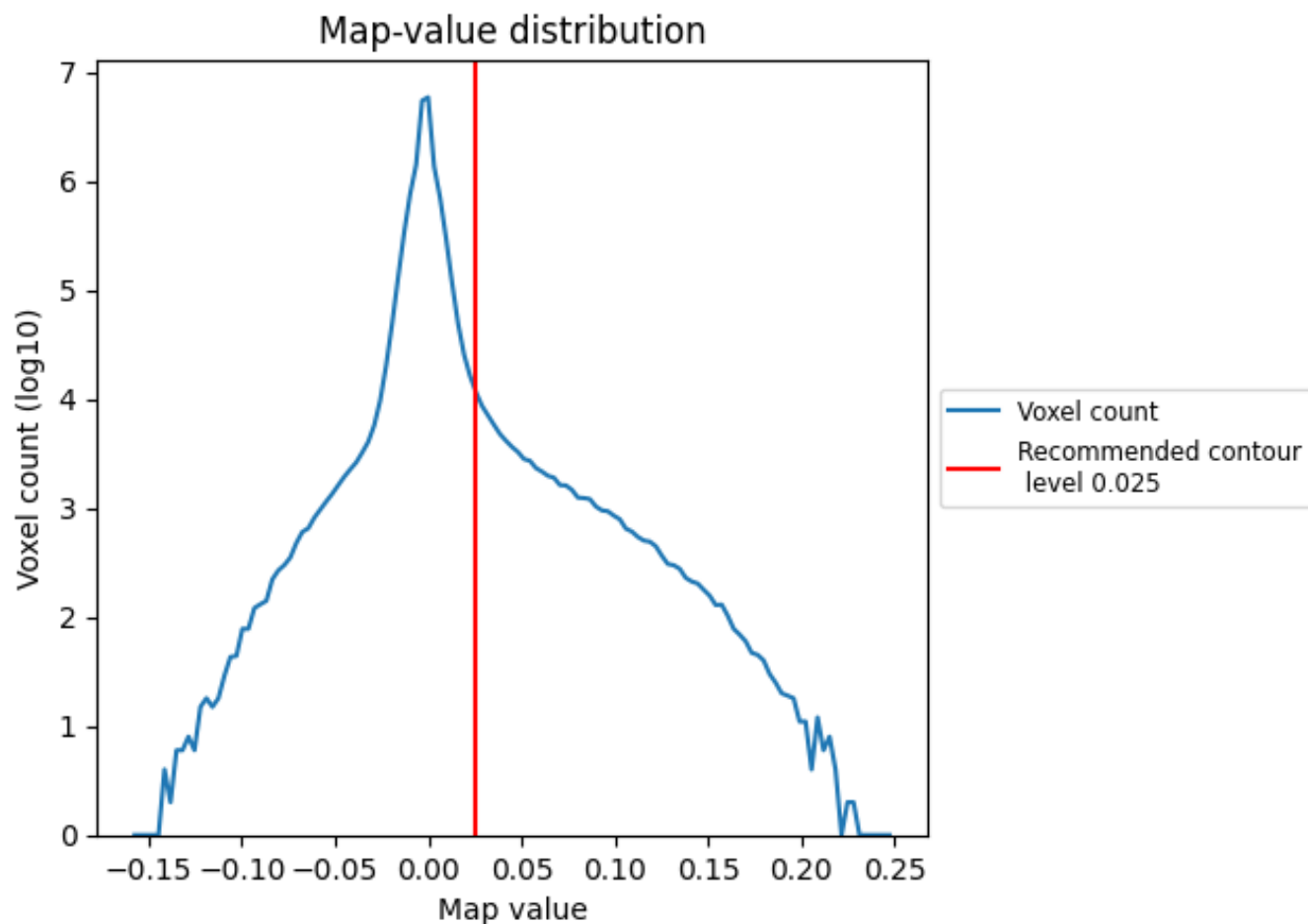
6.5 Mask visualisation

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

7 Map analysis [i](#)

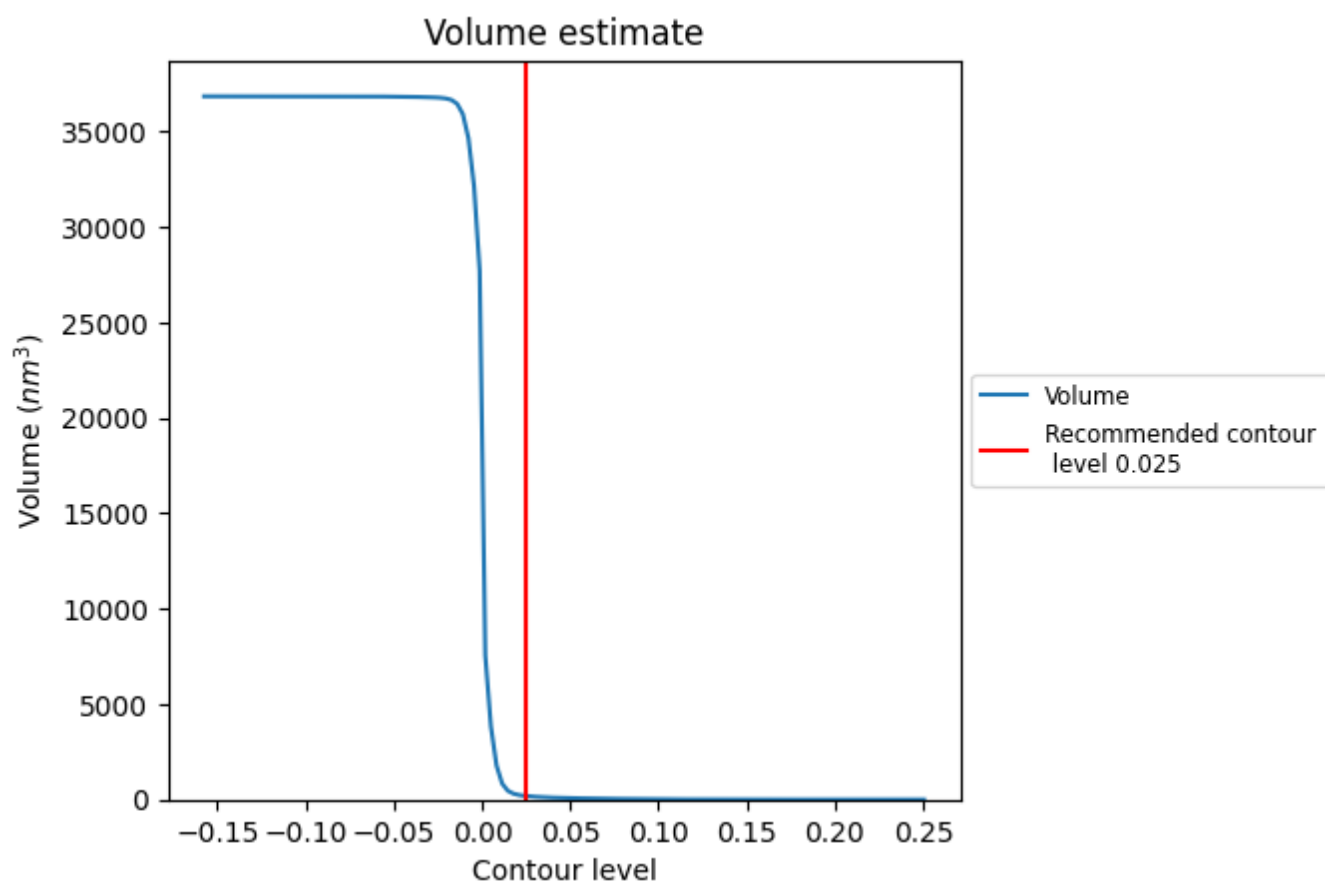
This section contains the results of statistical analysis of the map.

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.

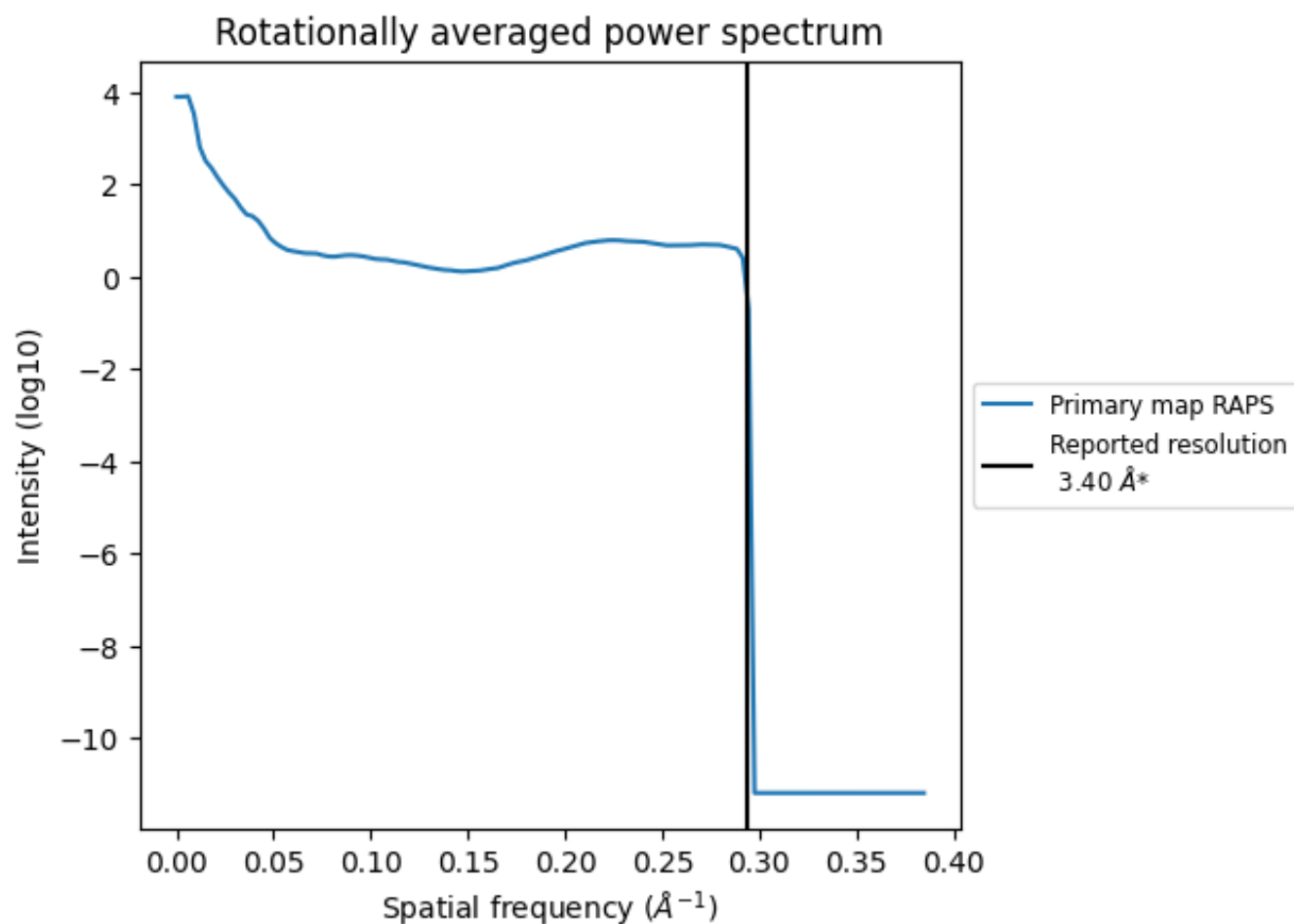
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 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 ⓘ

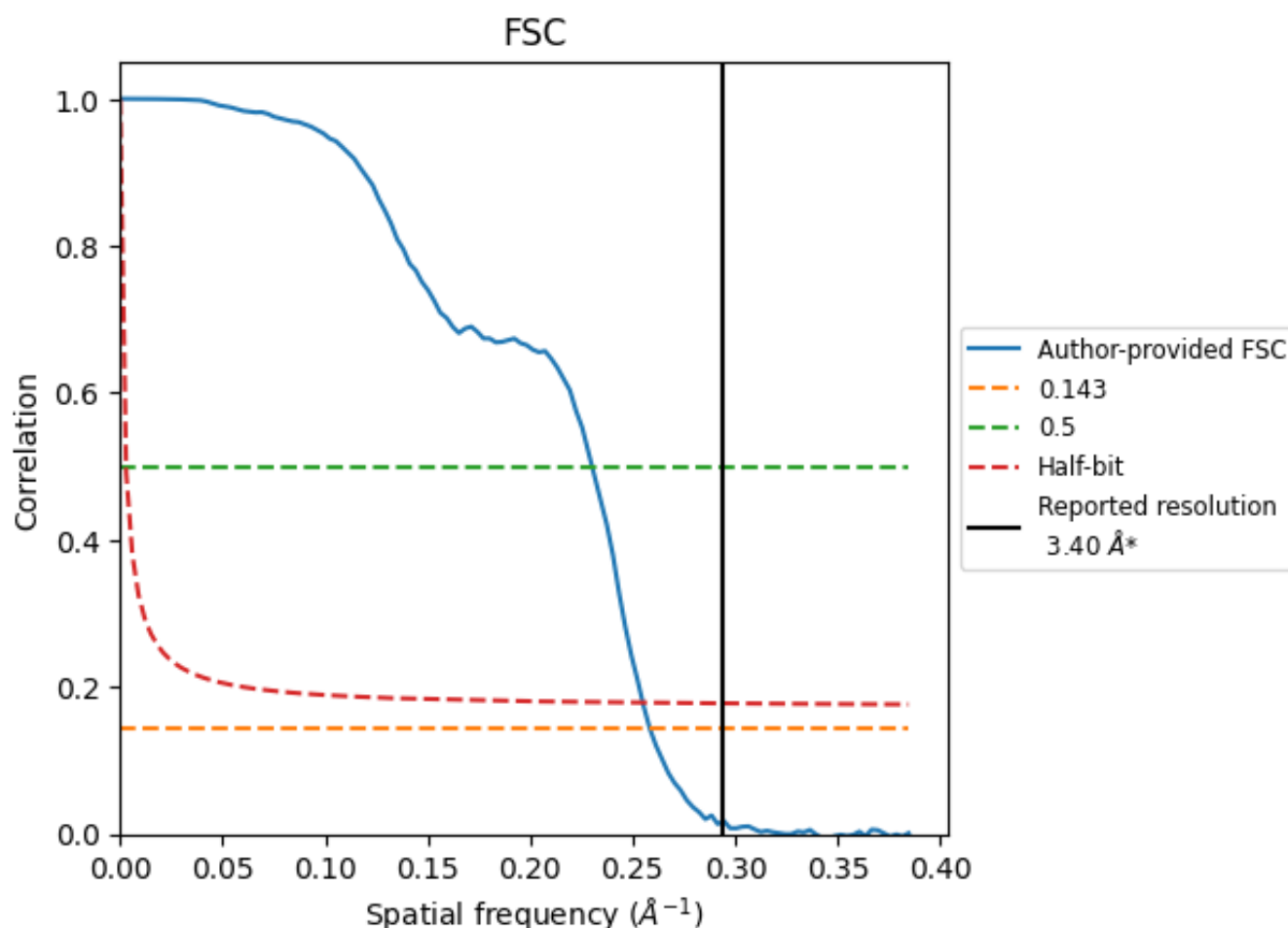


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

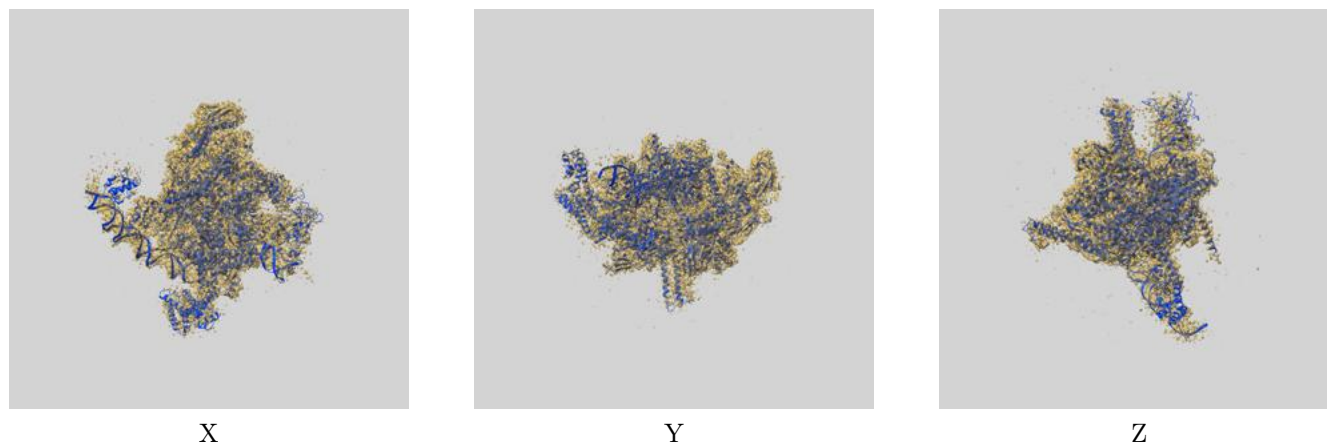
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.87	4.34	3.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

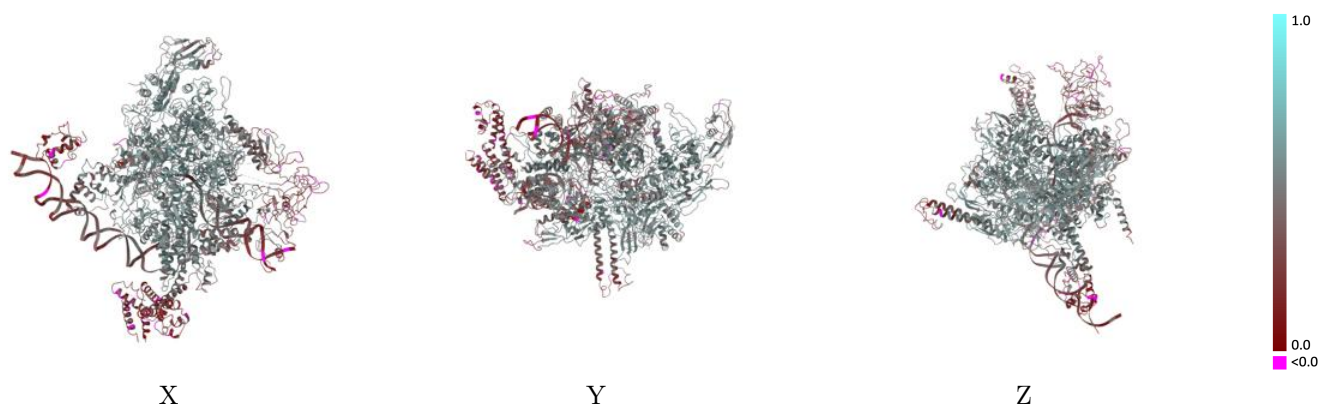
This section contains information regarding the fit between EMDB map EMD-20203 and PDB model 6OUL. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



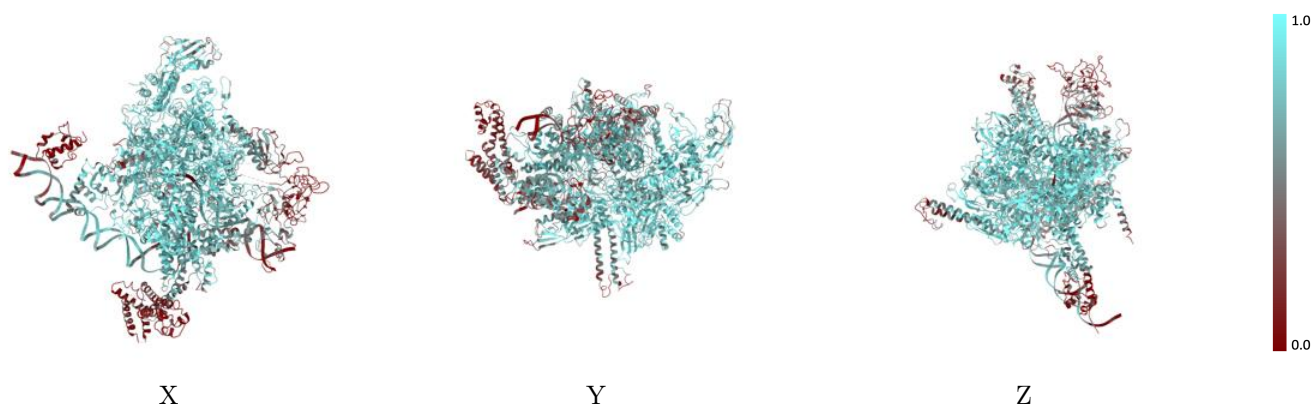
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



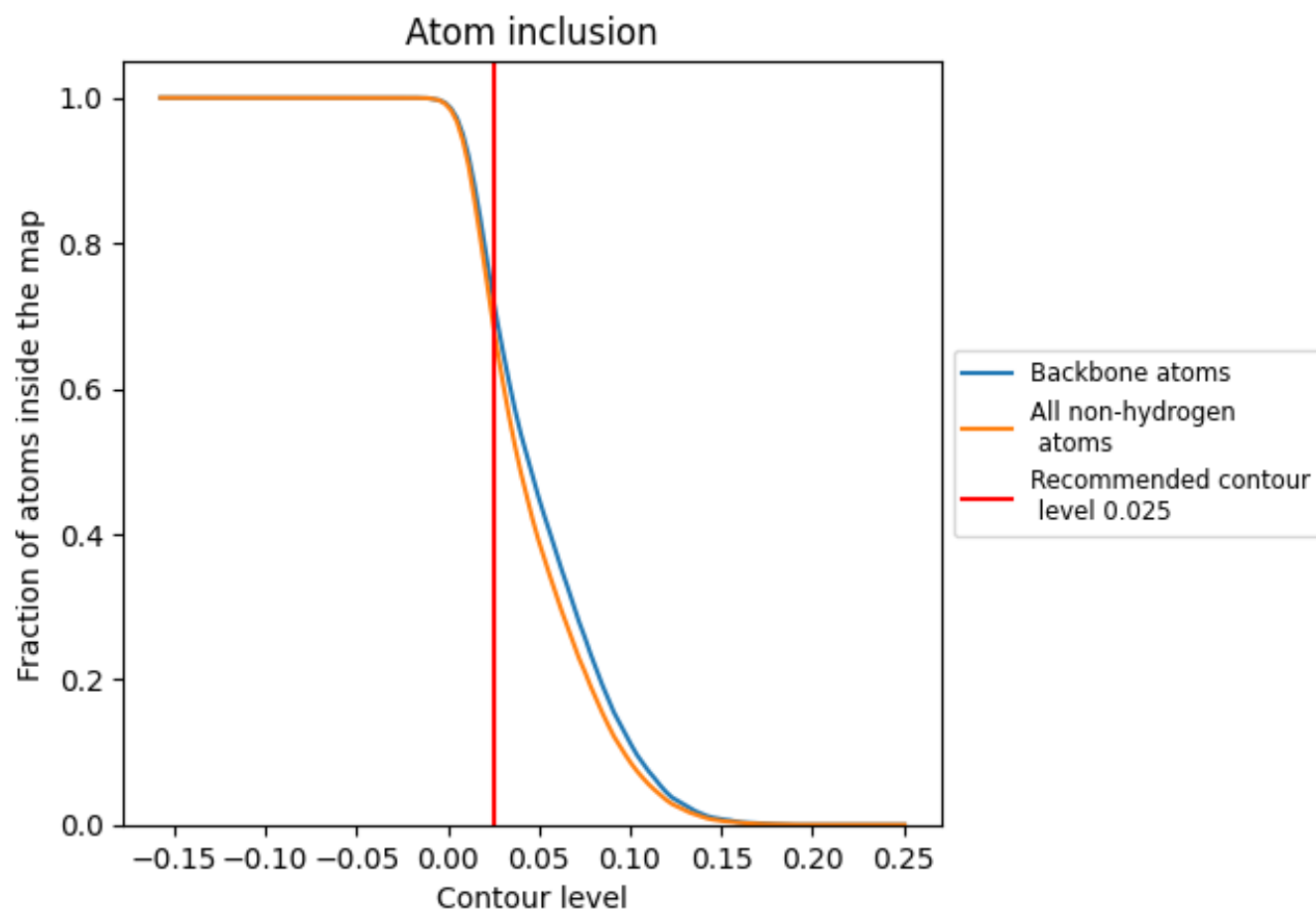
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 69% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6864	<div></div> 0.4600
G	<div></div> 0.7842	<div></div> 0.5150
H	<div></div> 0.7483	<div></div> 0.4900
I	<div></div> 0.7638	<div></div> 0.4990
J	<div></div> 0.7242	<div></div> 0.4850
K	<div></div> 0.6792	<div></div> 0.4830
L	<div></div> 0.5052	<div></div> 0.3730
P	<div></div> 0.5539	<div></div> 0.3180
Q	<div></div> 0.5381	<div></div> 0.2950
R	<div></div> 0.0768	<div></div> 0.2020

1.0

0.0

<0.0