



# wwPDB EM Validation Summary Report ⓘ

Mar 11, 2024 – 01:12 AM EDT

PDB ID : 6PSU  
EMDB ID : EMD-20464  
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi2)  
with TraR and rpsT P2 promoter  
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2019-07-13  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev70  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

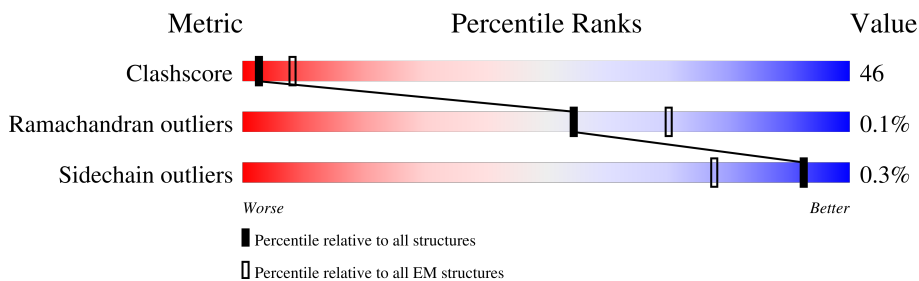
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 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	N	72	44% (Green), 56% (Yellow)
2	G	329	32% (Green), 38% (Yellow), 30% (Grey)
2	H	329	24% (Green), 42% (Yellow), 34% (Grey)
2	M	329	9% (Red), 13% (Orange), 78% (Grey)
3	I	1342	36% (Green), 63% (Yellow)
4	J	1430	6% (Red), 34% (Green), 59% (Yellow), 6% (Grey)
5	K	91	27% (Green), 52% (Yellow), 21% (Grey)
6	L	616	12% (Red), 25% (Green), 61% (Yellow), 14% (Grey)

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Mol	Chain	Length	Quality of chain
7	O	85	
8	P	85	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 32323 atoms, of which 156 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 Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	72	571	353	105	108	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	230	1775	1108	314	347	6	0	0
2	H	217	1668	1043	293	326	6	0	0
2	M	73	572	362	100	108	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	1340	10567	6631	1841	2052	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	1344	10433	6556	1856	1971	50	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	72	577	352	110	114	1	0	0

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	529	4277	2677	753	821	26	0	0

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 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	42	863	411	168	242	42	0	0

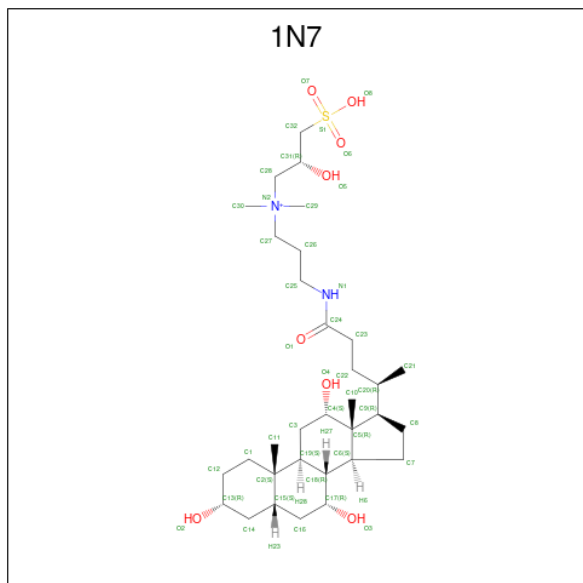
- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	37	752	363	117	235	37	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	N	1	1	1	0
9	J	2	2	2	0

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula: C<sub>32</sub>H<sub>59</sub>N<sub>2</sub>O<sub>8</sub>S).



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

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

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

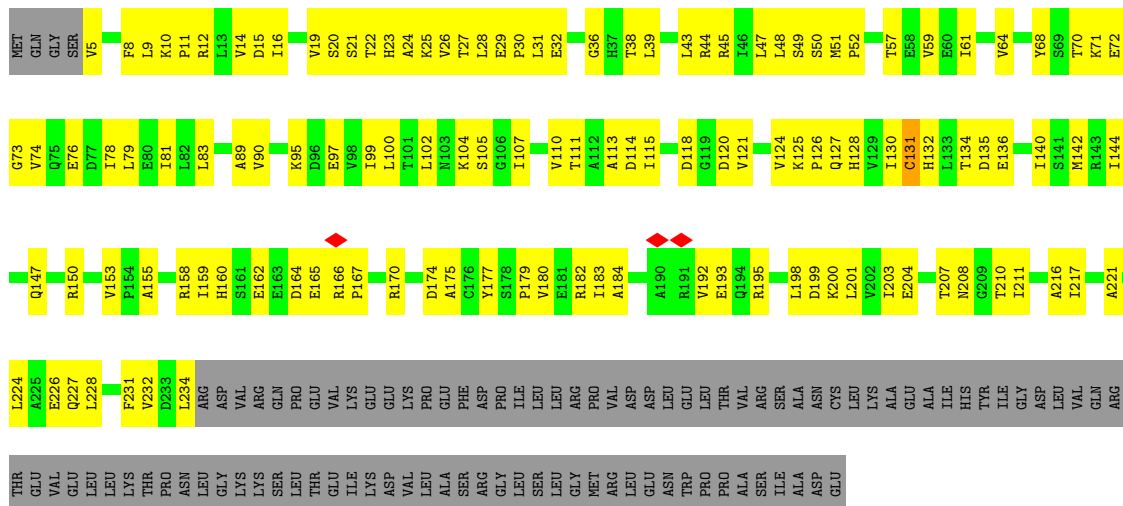
- Molecule 1: Protein TraR

Chain N: 




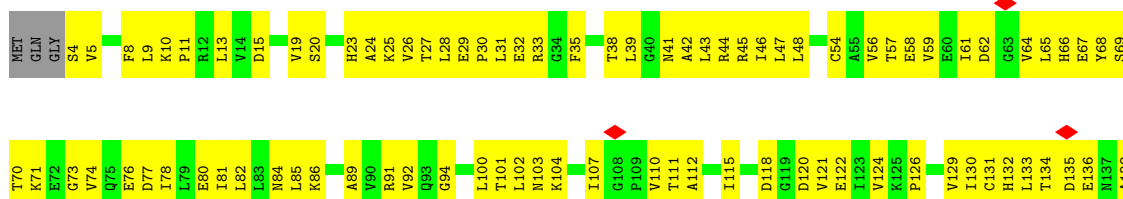
- Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain G: 

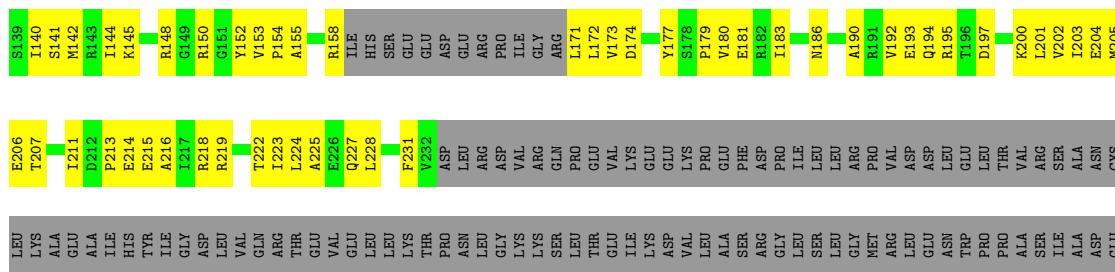


- Molecule 2: DNA-directed RNA polymerase subunit alpha

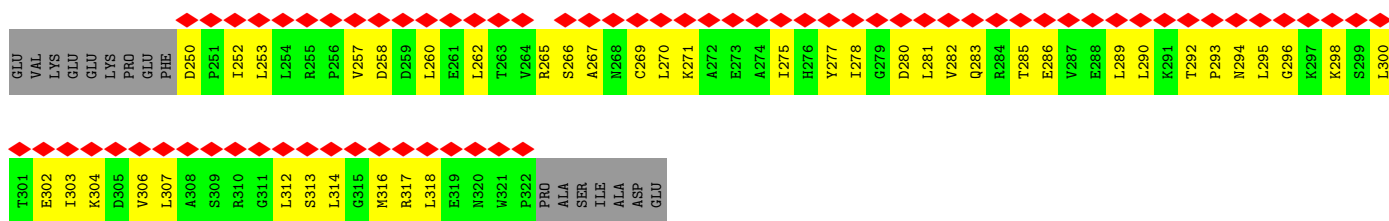
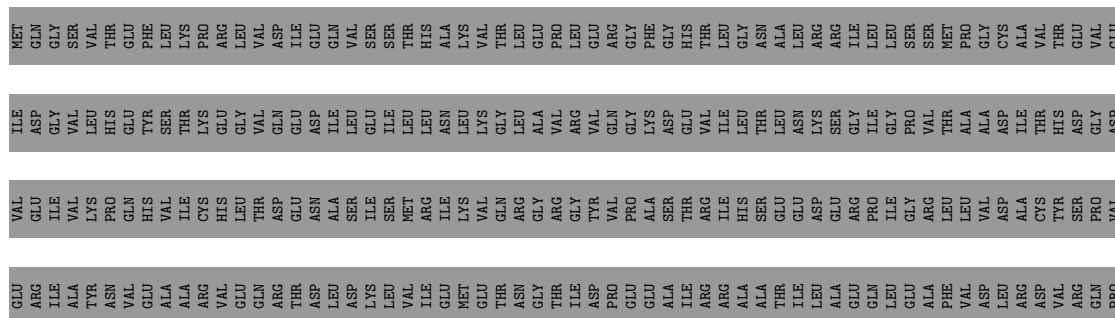
Chain H: 



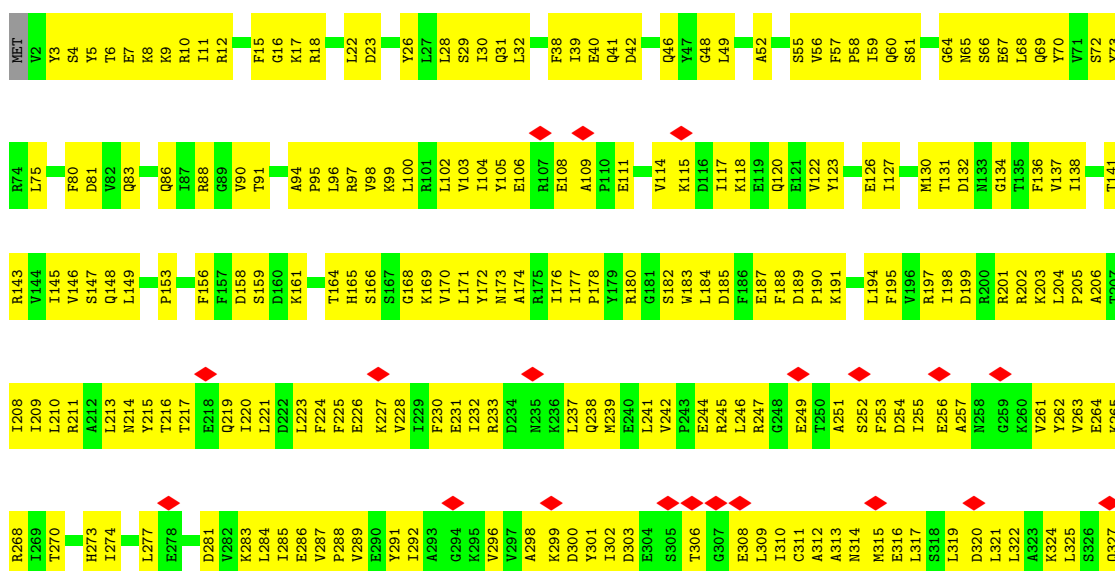




• Molecule 2: DNA-directed RNA polymerase subunit alpha



• Molecule 3: DNA-directed RNA polymerase subunit beta

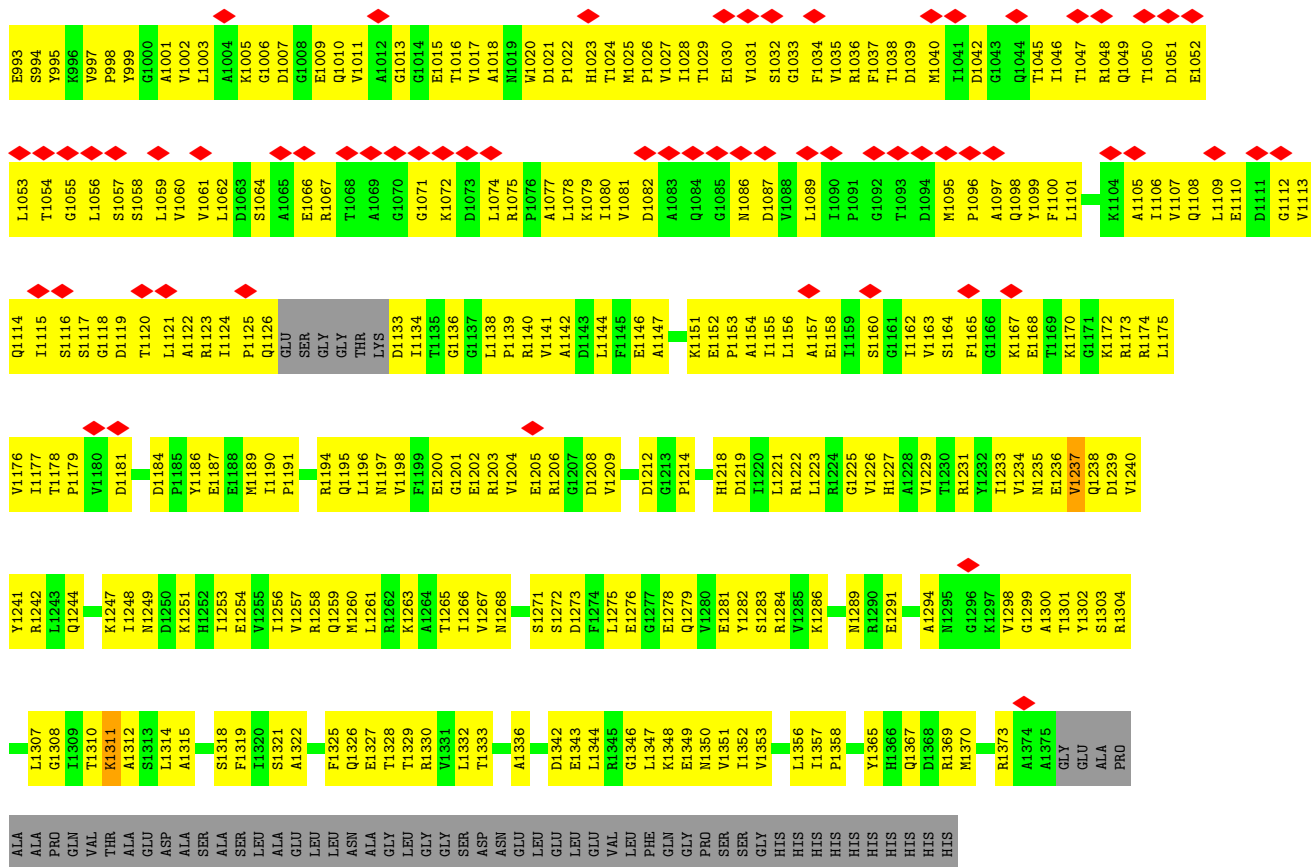


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K1158	V1159	L1160	L1161	F1164	S1165	D1166	E1167	E1168	V1169	M1170	R1171	L1172	A1173	R1176	L1177	K1178	M1180	P1181	I1182	A1183	T1184	P1185	F1186	V1187	F1187	G1188	G1189	G1190	K1191	K1192	L1192	L1193	I1194	I1195	K1196	E1197	L1198	L1204	P1205	Q1209	I1210	R1211	L1212	Y1213	D1214	G1215	R1216	T1217	G1218	E1219	Q1220	Q1289	E1222	R1223	V1225			
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K331	R332	I333	E334	T335	L336	F337	T338	N339	D340	L341	H342	D343	G344	P345	Y346	G417	I418	P489	S421	K422	I425	I426	D354	P355	D358	R359	L360	S361	I362	L363	V364	I365	I366	Y367	R368	M369	M370	R371	P372	G373	E374	T377	R378	E379	A380	A381	E382	S383	N387	L388	F389	Q463	F464	R465	S390	F391	R394	Y395
D396	L397	G401	R402	M403	K404	F405	M406	L409	E413	S417	G418	I419	L420	S421	K422	I425	I426	D427	K430	K431	L432	I433	D434	I435	R436	M437	G438	K439	G440	E441	D444	I445	D446	H447	L448	G449	M450	R451	I453	V456	M459	A460	E461	F462	Q463	F464	R465	S390	F391	R394	Y395							
L468	V469	R470	V471	E472	V475	K476	G482	D483	L484	T486	L487	M488	P489	Q490	M492	I493	M494	I498	S499	V502	F505	F506	L511	F514	M515	G516	Q517	N518	N519	P520	L521	H447	E522	S523	I524	K527	R528	R529	I530	L533	L538	Q541	R542	F545	E546	V547												
R548	D549	V550	H551	T552	G556	R557	V558	C559	P560	I561	E562	T563	P564	E565	G566	P567	N568	G570	I571	I572	N573	S576	V577	Y578	A579	Q580	T581	N582	E583	Y584	G585	G586	L587	E588	T589	P590	Y591	R592	K593	V594	T595	D596	G597	I603	H604	Y605	L606	S607	E610	E611	Y614							
V615	I616	A617	Q618	A619	M622	L623	D624	G627	H628	F629	V630	L633	V634	T635	C636	R637	E641	S642	V643	V644	F645	S646	V650	V650	D651	Y652	M653	D654	V655	S656	T657	Q658	Q659	V660	V661	S662	A665	S666	L667	F670	L671	E672	H673	A676	N677	R678	M681	G682	N684									
M685	Q686	R687	Q688	A689	V690	L693	L699	V700	E705	R706	V707	V708	D711	S712	G713	V714	T715	A716	V717	A718	K719	G722	V723	V724	Y725	T726	V727	R728	E729	V730	R731	I732	V733	I734	K735	E738	M741	Y742	P743	G744	E745	A746	G747	I748	D749	I750	Y751	N752	L753	V754	K755	Y756						
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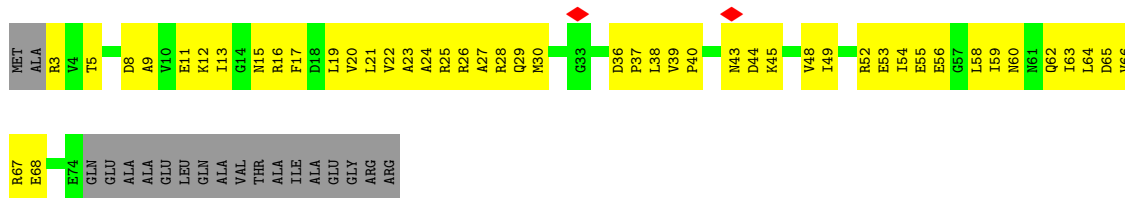
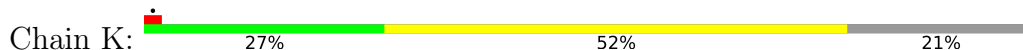
• Molecule 4: DNA-directed RNA polymerase subunit beta'



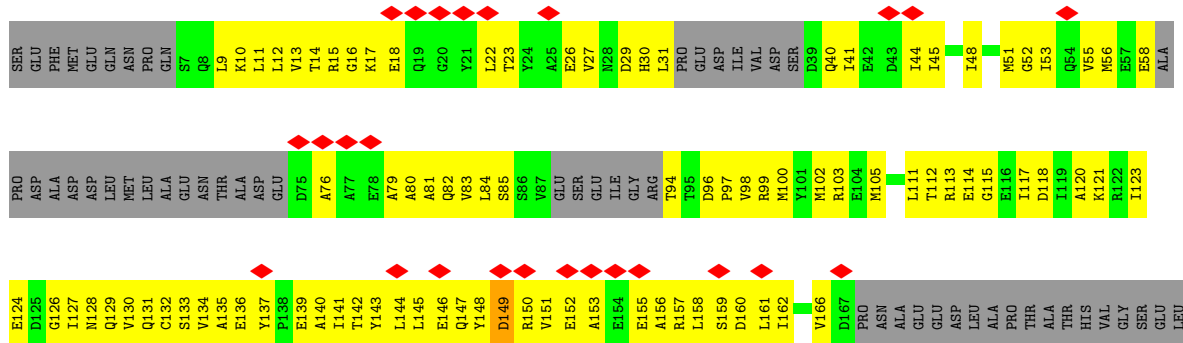
VAL	LYS	ASP	LEU	LEU	PHE	LEU	LEU	ALA	GLN	THR	LYS	THR	GLU	E16	F17	D18	A19	I20	S26	M29	I30	W33	S34	F35	G36	E37	V38	K39	K40	E42	T43	I44	M45	Y46	R47	T48	P51	E52	R53	D54	G55	L56	F57	C58	A59	R60	I61	G62	K66	D67	Y68	E69				
C70	L71	C72	G73	K74	Y75	L78	K79	H80	V83	C85	E86	L84	M151	T152	M153	C88	D89	V90	E91	V92	T93	Q94	T95	R88	R99	E100	R101	M102	G103	H104	I105	E106	L107	P110	T111	H113	I114	W115	F116	L117	K118	S119	L120	P121	S122	R123	I124	G125	L126	L127	I128	D129	M130	E131	L132	R133
D134	I135	R137	V138	L139	Y140	F141	V146	H80	I147	E148	M151	T152	M153	L154	E155	Q158	L159	L160	T161	E162	E163	Q164	L166	D167	E170	F171	E172	G173	D174	E175	F176	D177	A178	K179	M180	G181	A182	I185	L188	L189	D183	L194	E195	Q196	E197	C198	E199	Q200	R201	L202	L203	F203				
E204	E211	K216	L217	T218	K219	R220	L221	K222	E225	A226	F227	V228	Q229	Q158	P234	L160	T161	E162	V241	P243	V244	P246	L249	R250	F251	L252	V253	P254	R259	F260	A261	T262	L265	N266	R267	L268	Y269	L286	R270	R271	L285	L194	E195	Q196	E197	C198	E199	Q200	R201	L202	L203	D284				
L285	A286	A287	P288	D289	L290	L291	V292	R293	N294	E295	K296	R297	M298	Q300	D304	A305	L306	L307	D308	R311	T317	G318	R322	K325	S326	L327	R329	K330	I331	K332	G333	K334	Q335	G336	R337	R338	R339	Q340	R341	L342	L343	G344	R345	R346	V347	D348	Y349	S350	G351	R352	S353	V354				
I355	F356	V357	G358	P359	L361	R362	L363	H364	N365	C366	G367	L368	P369	K370	K371	M372	A373	L374	E375	L376	F377	K378	P379	Y382	G383	K384	L385	L390	T393	L394	K398	K399	M400	V401	E405	A406	V407	V408	W409	D410	L411	E414	V415	D348	Y349	S350	G351	R352	S353	V421						
L422	L423	M424	R425	A426	P427	T428	L429	H430	R431	L432	F437	E438	V439	W440	L441	L442	E443	G444	K445	Q448	L449	H450	P451	L452	V453	C454	N458	A459	P460	F461	D462	G463	D464	Q465	M466	A467	V468	H469	V470	P471	L472	L473	L474	E475	A476	Q477	L478	E479	A482	M483	M485	S486	T487	N488		
M489	L490	S492	M495	I499	S500	V501	P502	S503	V506	V507	L508	K509	L510	Y511	Y512	M513	T514	R515	P516	C517	V518	M519	M525	L527	P530	K531	E532	A533	L536	F537	R538	T607	G608	L541	A542	H545	A546	R547	V548	K549	V550	R551	T552	D553	Q554	E555	B556	K557	D558	A559						
E562	L563	V564	A565	K566	T567	S568	L569	K570	D571	T572	F573	Y574	G575	R576	L579	Y580	M581	L582	V583	P584	K585	C517	L587	P588	Y589	M590	L591	V592	A595	T601	S602	K603	M604	L605	T611	L612	K615	P616	I619	F620	D621	Q623	E554	L624	M625	K557	T627									
A632	A633	R634	V639	G640	L641	H642	M643	M644	V645	L646	P647	I653	E658	V661	L579	Y580	M581	L582	V583	P584	K585	C517	L587	P588	Y589	M590	L591	V592	A595	T601	S602	K603	M604	L605	T611	L612	K615	P616	I619	F620	D621	Q623	E554	L624	M625	K557	T627									
A632	A633	R634	V639	G640	L641	H642	M643	M644	V645	L646	P647	I653	E658	V661	L579	Y580	M581	L582	V583	P584	K585	C517	L587	P588	Y589	M590	L591	V592	A595	T601	S602	K603	M604	L605	T611	L612	K615	P616	I619	F620	D621	Q623	E554	L624	M625	K557	T627									
W717	S718	F719	N720	S721	L722	Y723	W724	M725	S728	H731	G732	S733	W734	A735	Q736	L737	R738	Q739	L740	E741	G742	G745	L746	W747	A748	K749	G750	D751	G752	S753	L754	L755	E756	W757	F758	L759	N762	L763	R764	E765	G766	L767	N768	Q771	L774	S775	R776	L779	A779	R780	K781	E782	L783			
T786	A787	L788	E867	M868	C869	D870	L871	R872	L873	L800	V801	D902	W803	A804	Q805	V806	W809	T810	E811	D812	D813	M821	H822	W823	A824	V825	L826	D830	H831	K832	L835	R836	R837	R838	V839	R842	T844	A845	E846	D847	V848	L849	K850	P851	D855	L856	L857	V858	R859	R860	R861					
T862	L863	H864	E865	E866	H868	C869	D870	L871	R872	L800	V801	D902	W803	A804	Q805	V806	W809	T810	E811	D812	D813	M821	H822	W823	A824	V825	L826	D830	H831	K832	L835	R836	R837	R838	V839	R842	T844	A845	E846	D847	V848	L849	K850	P851	D855	L856	L857	V858	R859	R860	R861					
H932	R933	T934	G937	GLY	GLY	ALA	ALA	ALA	ARG	ALA	ALA	ALA	GLU	S948	S949	I950	O951	V952	R953	N954	V885	G956	S957	I958	R959	L960	S961	R962	V963	K964	G965	V966	V967	N968	A969	R905	G906	H907	I908	N909	I910	K911	G912	E913	S914	A915	I918	I923	G924	E925	P926	G927	S928	V929	L930	T931

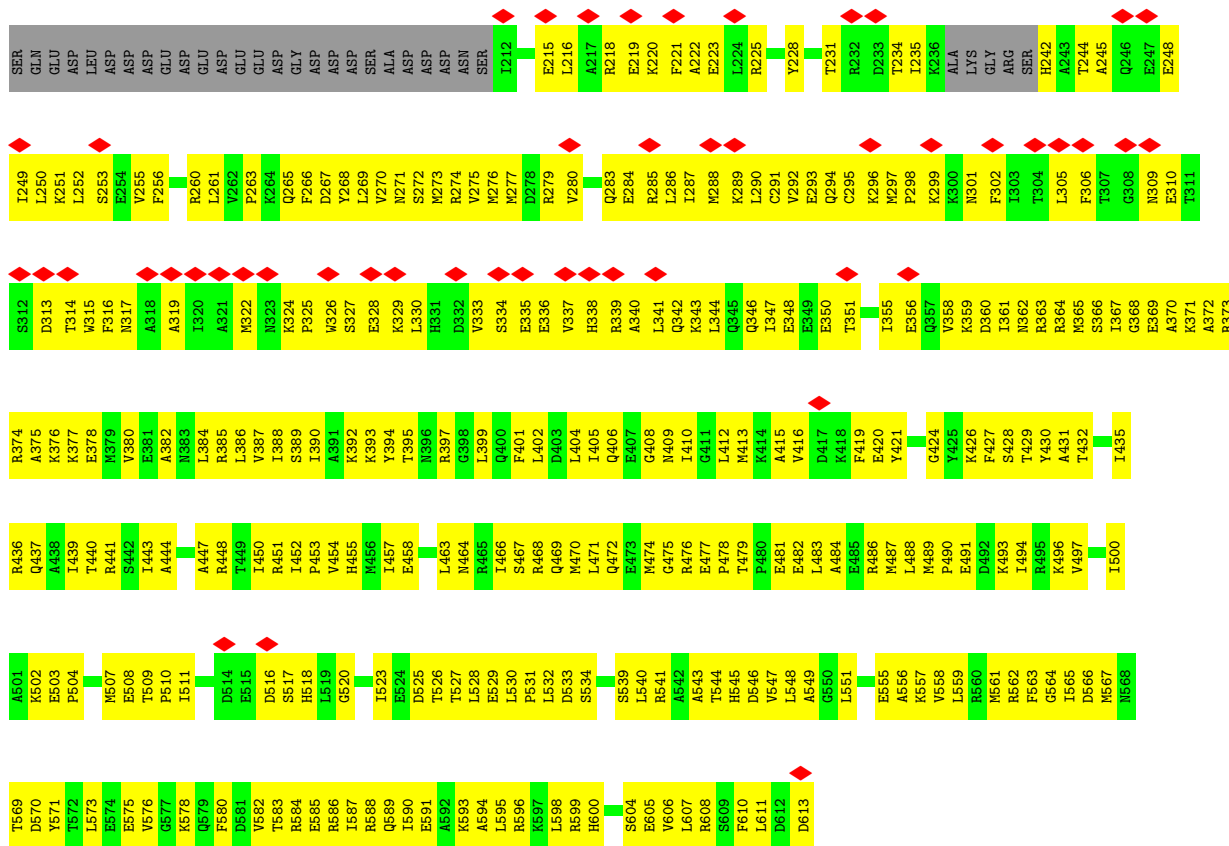


• Molecule 5: DNA-directed RNA polymerase subunit omega

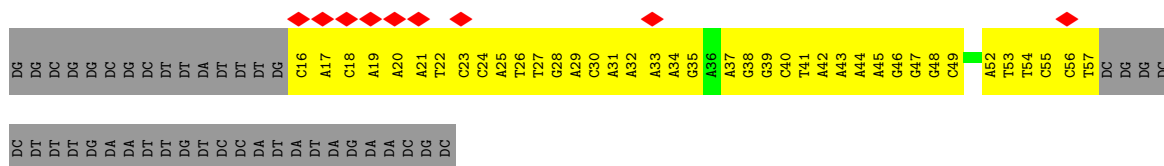


• Molecule 6: RNA polymerase sigma factor RpoD

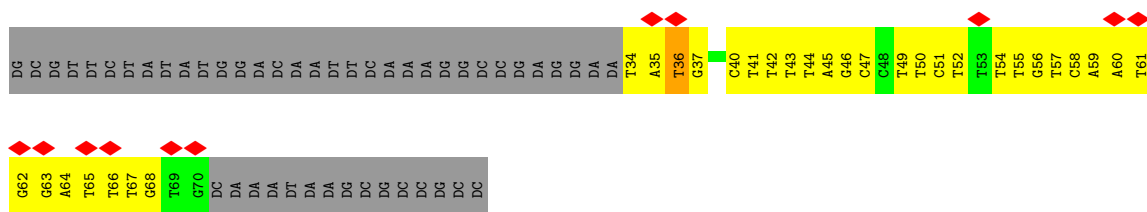




• Molecule 7: DNA (85-MER)



• Molecule 8: DNA (85-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46553	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 ( $e^-/\text{\AA}^2$ )	80	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	0.150	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, MG, 1N7

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	N	0.37	0/581	0.50	0/785
2	G	0.40	0/1797	0.53	0/2437
2	H	0.37	0/1687	0.54	0/2287
2	M	0.26	0/579	0.54	0/784
3	I	0.44	0/10736	0.55	1/14487 (0.0%)
4	J	0.41	0/10592	0.54	0/14308
5	K	0.32	0/579	0.49	0/779
6	L	0.29	0/4329	0.47	1/5820 (0.0%)
7	O	0.63	0/971	0.92	0/1495
8	P	0.59	0/837	1.06	1/1290 (0.1%)
All	All	0.41	0/32688	0.57	3/44472 (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
3	I	0	4
4	J	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1167	GLU	N-CA-C	5.85	126.79	111.00
6	L	149	ASP	CB-CG-OD2	5.24	123.01	118.30
8	P	36	DT	O4'-C4'-C3'	-5.22	102.41	104.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	1165	SER	Peptide
3	I	1166	ASP	Peptide
3	I	1240	ASP	Peptide
3	I	247	ARG	Peptide
4	J	47	ARG	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	N	571	0	556	50	0
2	G	1775	0	1803	131	0
2	H	1668	0	1702	175	0
2	M	572	0	602	61	0
3	I	10567	0	10585	1020	0
4	J	10433	0	10625	1022	0
5	K	577	0	588	53	0
6	L	4277	0	4325	530	0
7	O	863	0	471	74	0
8	P	752	0	426	74	0
9	J	2	0	0	0	0
9	N	1	0	0	0	0
10	I	27	39	39	7	0
10	J	27	39	38	4	0
10	L	27	39	37	3	0
10	N	27	39	38	4	0
11	J	1	0	0	0	0
All	All	32167	156	31835	2955	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 46.

The worst 5 of 2955 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)
10:L:701:1N7:C19	10:L:701:1N7:C3	1.83	1.57
10:N:102:1N7:C19	10:N:102:1N7:C3	1.83	1.51
10:I:1401:1N7:C3	10:I:1401:1N7:C19	1.82	1.51
10:J:1504:1N7:C19	10:J:1504:1N7:C3	1.83	1.50
6:L:284:GLU:HA	6:L:287:ILE:HB	1.36	1.07

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	N	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
2	G	228/329 (69%)	193 (85%)	35 (15%)	0	100	100
2	H	213/329 (65%)	169 (79%)	43 (20%)	1 (0%)	29	67
2	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
3	I	1338/1342 (100%)	1156 (86%)	182 (14%)	0	100	100
4	J	1338/1430 (94%)	1187 (89%)	150 (11%)	1 (0%)	51	84
5	K	70/91 (77%)	59 (84%)	11 (16%)	0	100	100
6	L	517/616 (84%)	464 (90%)	53 (10%)	0	100	100
All	All	3845/4538 (85%)	3363 (88%)	480 (12%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	859	PRO
2	H	94	GLY

### 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	N	61/61 (100%)	61 (100%)	0	100	100
2	G	196/286 (68%)	195 (100%)	1 (0%)	88	93
2	H	185/286 (65%)	185 (100%)	0	100	100
2	M	65/286 (23%)	65 (100%)	0	100	100
3	I	1155/1157 (100%)	1151 (100%)	4 (0%)	92	95
4	J	1122/1189 (94%)	1117 (100%)	5 (0%)	91	94
5	K	63/75 (84%)	63 (100%)	0	100	100
6	L	467/543 (86%)	467 (100%)	0	100	100
All	All	3314/3883 (85%)	3304 (100%)	10 (0%)	92	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	338	PHE
4	J	1237	VAL
4	J	1311	LYS
3	I	699	LEU
3	I	1216	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
6	L	147	GLN
6	L	472	GLN
6	L	246	GLN
6	L	409	ASN
3	I	1209	GLN

### 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
10	1N7	L	701	-	30,30,46	5.04	16 (53%)	47,48,72	2.17	14 (29%)
10	1N7	I	1401	-	30,30,46	4.84	15 (50%)	47,48,72	2.26	16 (34%)
10	1N7	J	1504	-	30,30,46	4.97	14 (46%)	47,48,72	2.11	14 (29%)
10	1N7	N	102	-	30,30,46	4.98	15 (50%)	47,48,72	2.26	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
10	1N7	L	701	-	-	5/7/72/92	0/4/4/4
10	1N7	I	1401	-	-	0/7/72/92	0/4/4/4
10	1N7	J	1504	-	-	1/7/72/92	0/4/4/4
10	1N7	N	102	-	-	7/7/72/92	0/4/4/4

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	701	1N7	C3-C19	18.02	1.83	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1504	1N7	C3-C19	17.74	1.83	1.53
10	N	102	1N7	C3-C19	17.63	1.83	1.53
10	I	1401	1N7	C3-C19	17.20	1.82	1.53
10	N	102	1N7	C3-C4	11.90	1.73	1.53

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	102	1N7	C7-C6-C18	-7.22	108.23	118.33
10	I	1401	1N7	C7-C6-C18	-6.08	109.83	118.33
10	J	1504	1N7	C7-C6-C18	-5.84	110.17	118.33
10	L	701	1N7	C9-C5-C4	-5.50	112.65	117.67
10	L	701	1N7	C7-C6-C18	-5.34	110.86	118.33

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	N	102	1N7	C9-C20-C22-C23
10	N	102	1N7	C21-C20-C22-C23
10	L	701	1N7	C22-C20-C9-C5
10	L	701	1N7	C20-C22-C23-C24
10	L	701	1N7	C21-C20-C9-C8

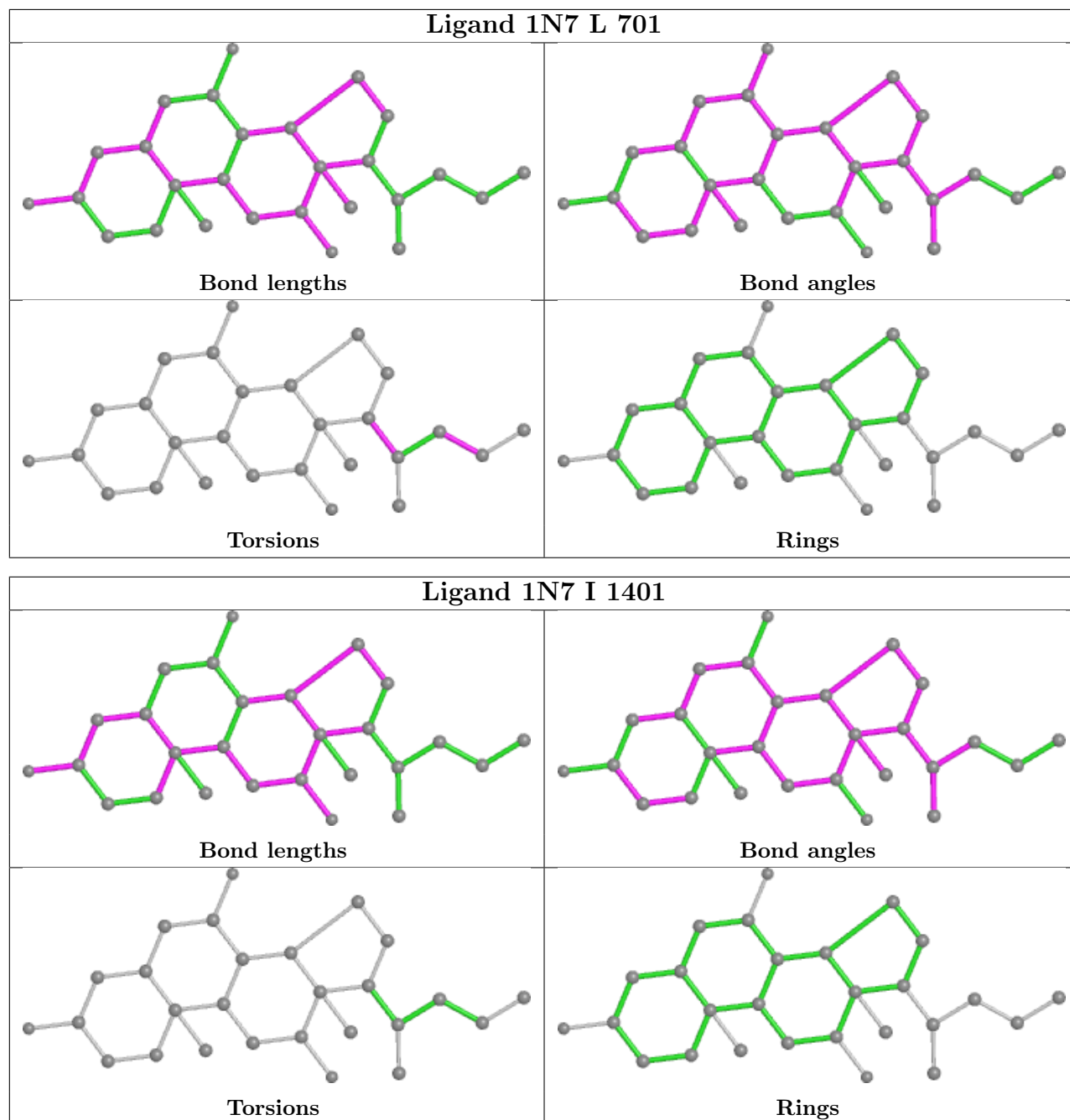
There are no ring outliers.

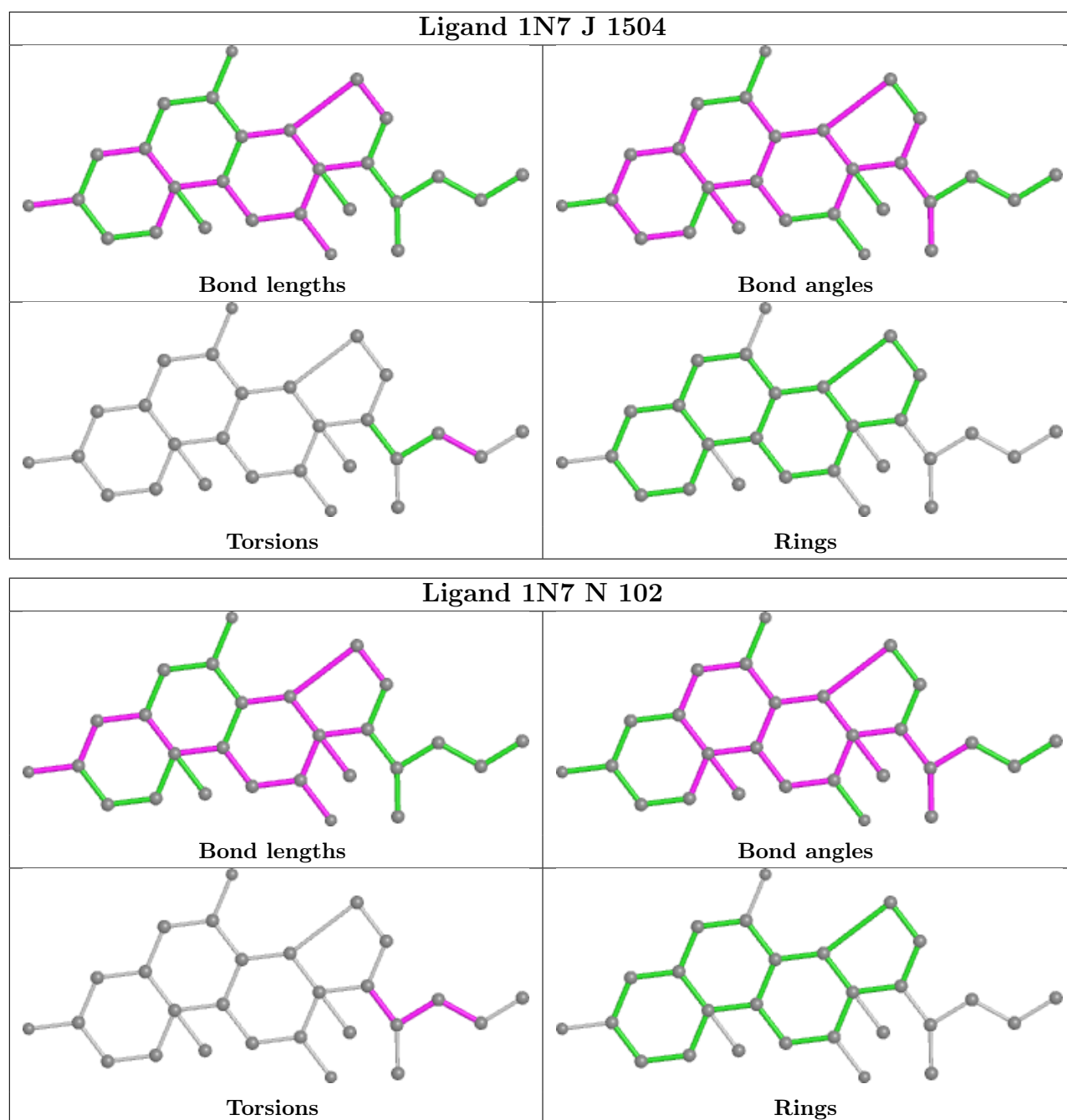
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	701	1N7	3	0
10	I	1401	1N7	7	0
10	J	1504	1N7	4	0
10	N	102	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.





## 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.

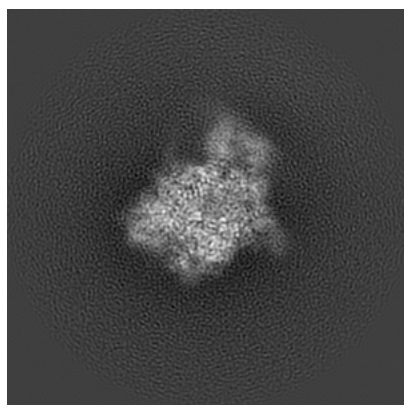
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20464. These allow visual inspection of the internal detail of the map and identification of artifacts.

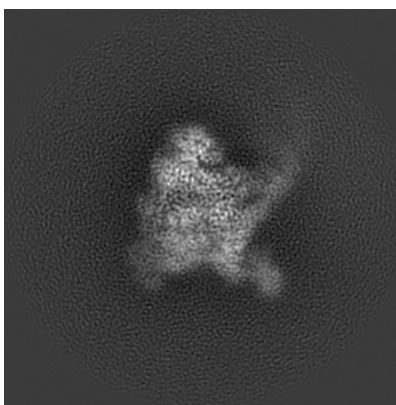
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

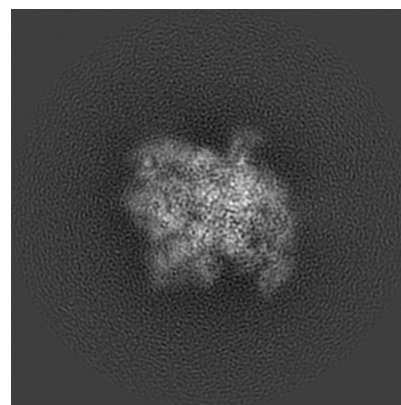
#### 6.1.1 Primary map



X



Y

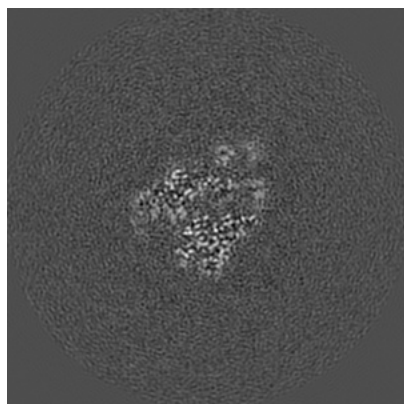


Z

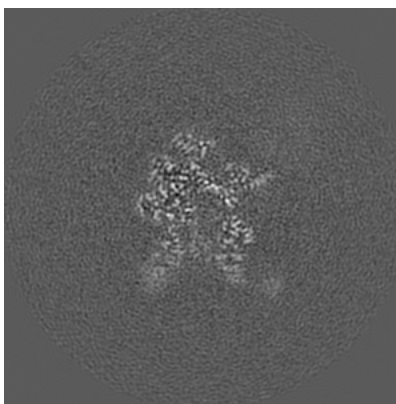
The images above show the map projected in three orthogonal directions.

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

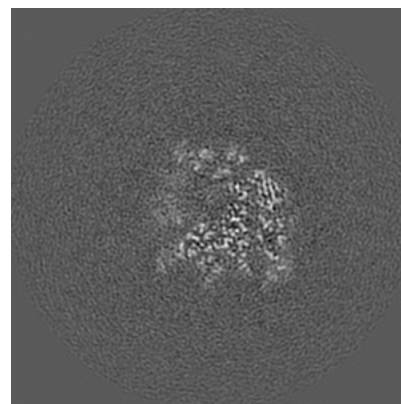
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



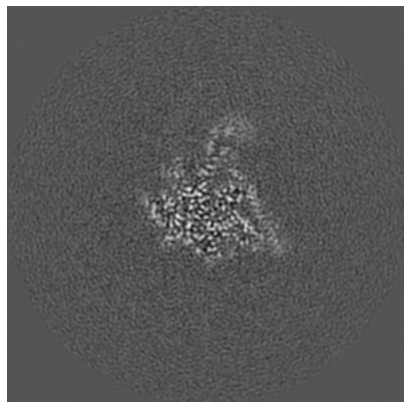
Z Index: 128



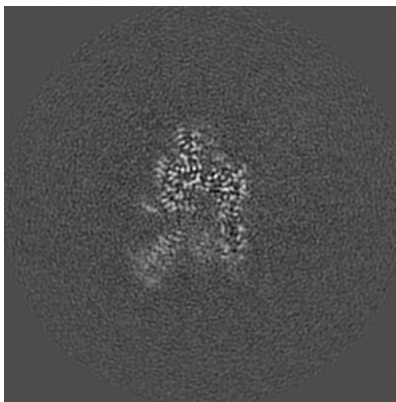
The images above show central slices of the map in three orthogonal directions.

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

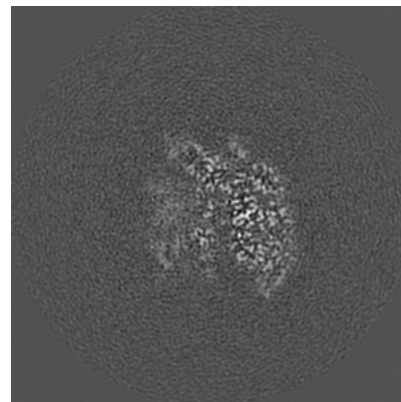
### 6.3.1 Primary map



X Index: 146



Y Index: 123

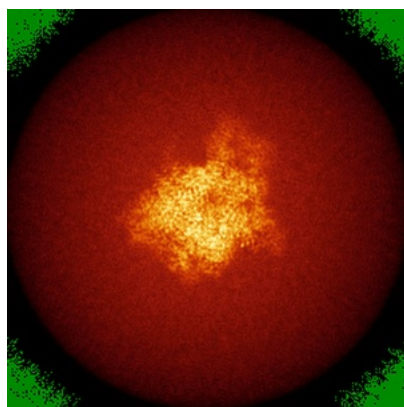


Z Index: 121

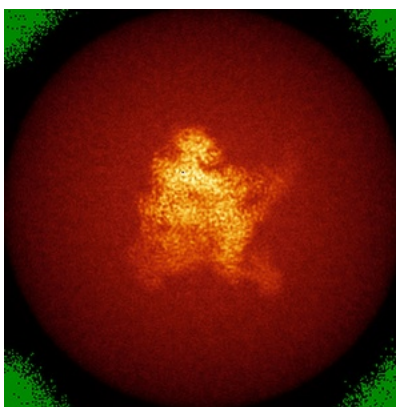
The images above show the largest variance slices of the map in three orthogonal directions.

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

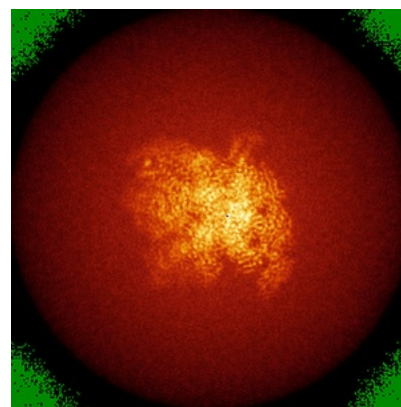
### 6.4.1 Primary map



X



Y



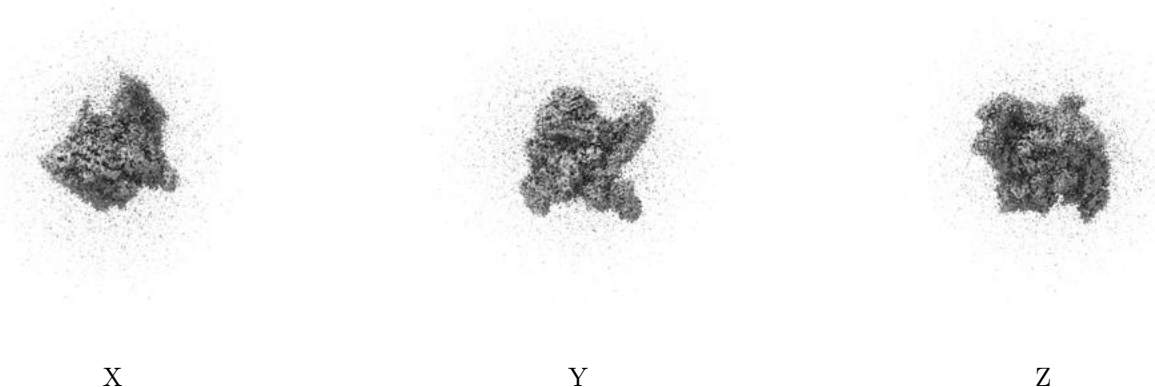
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

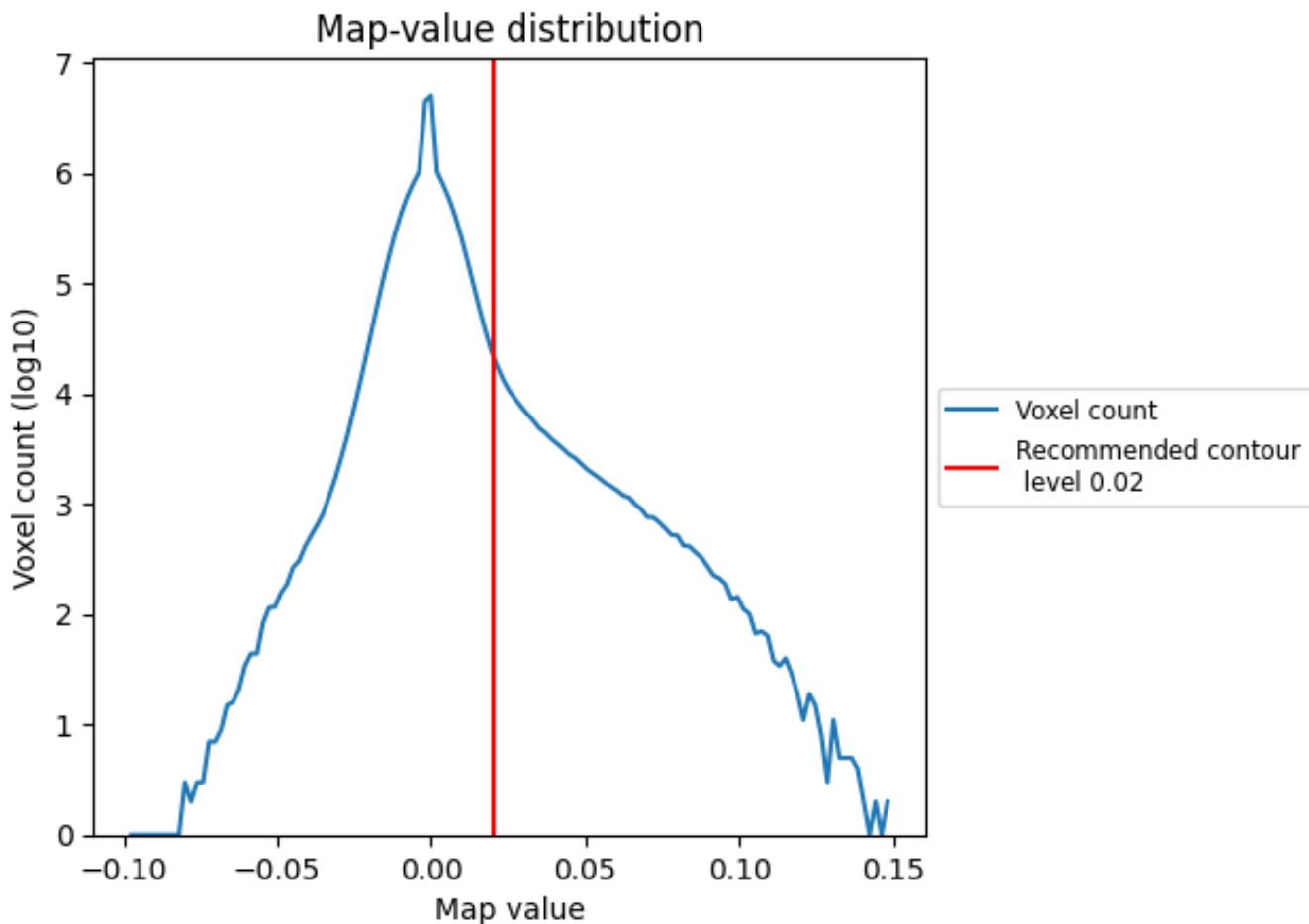
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

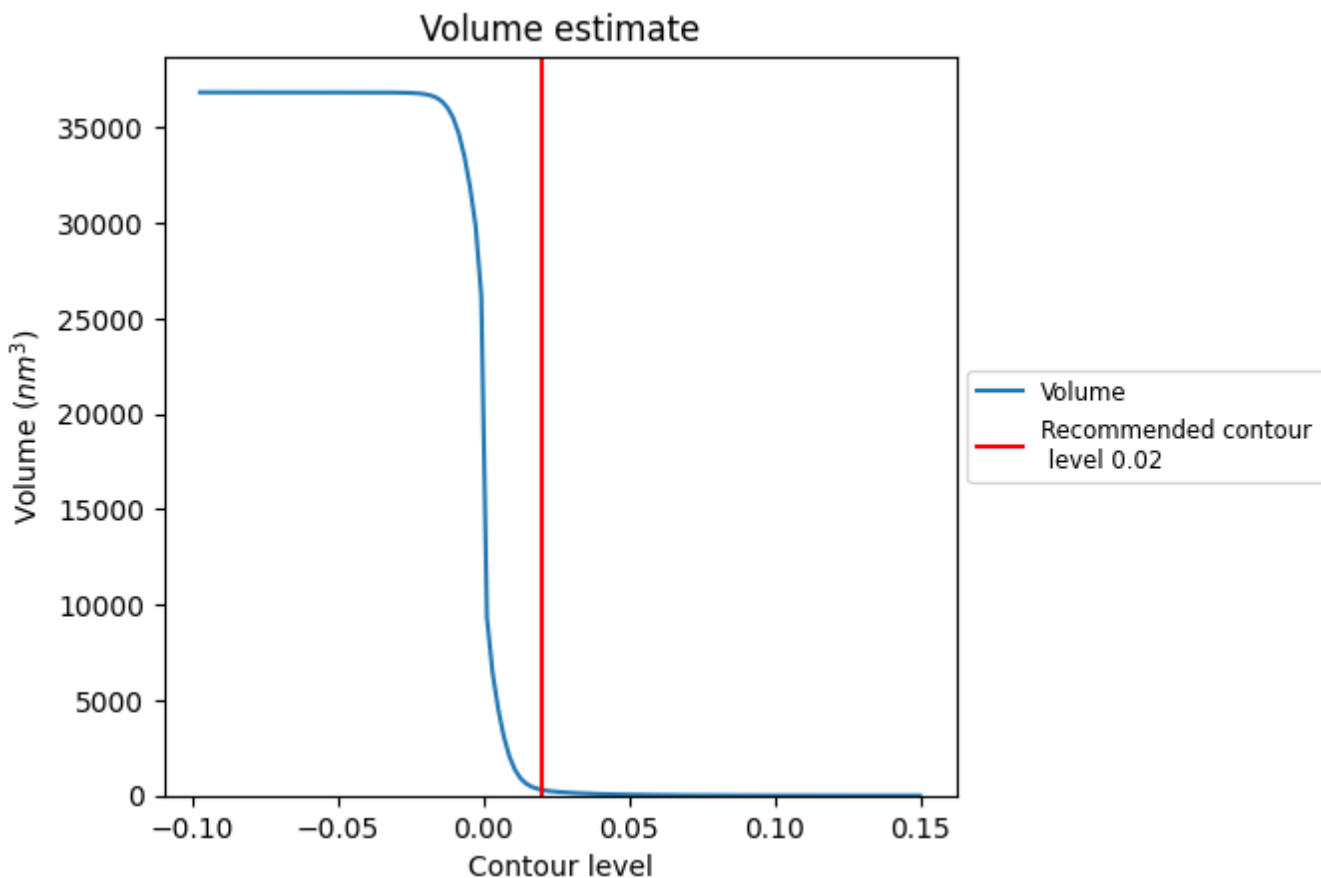
This section contains the results of statistical analysis of the map.

### 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.

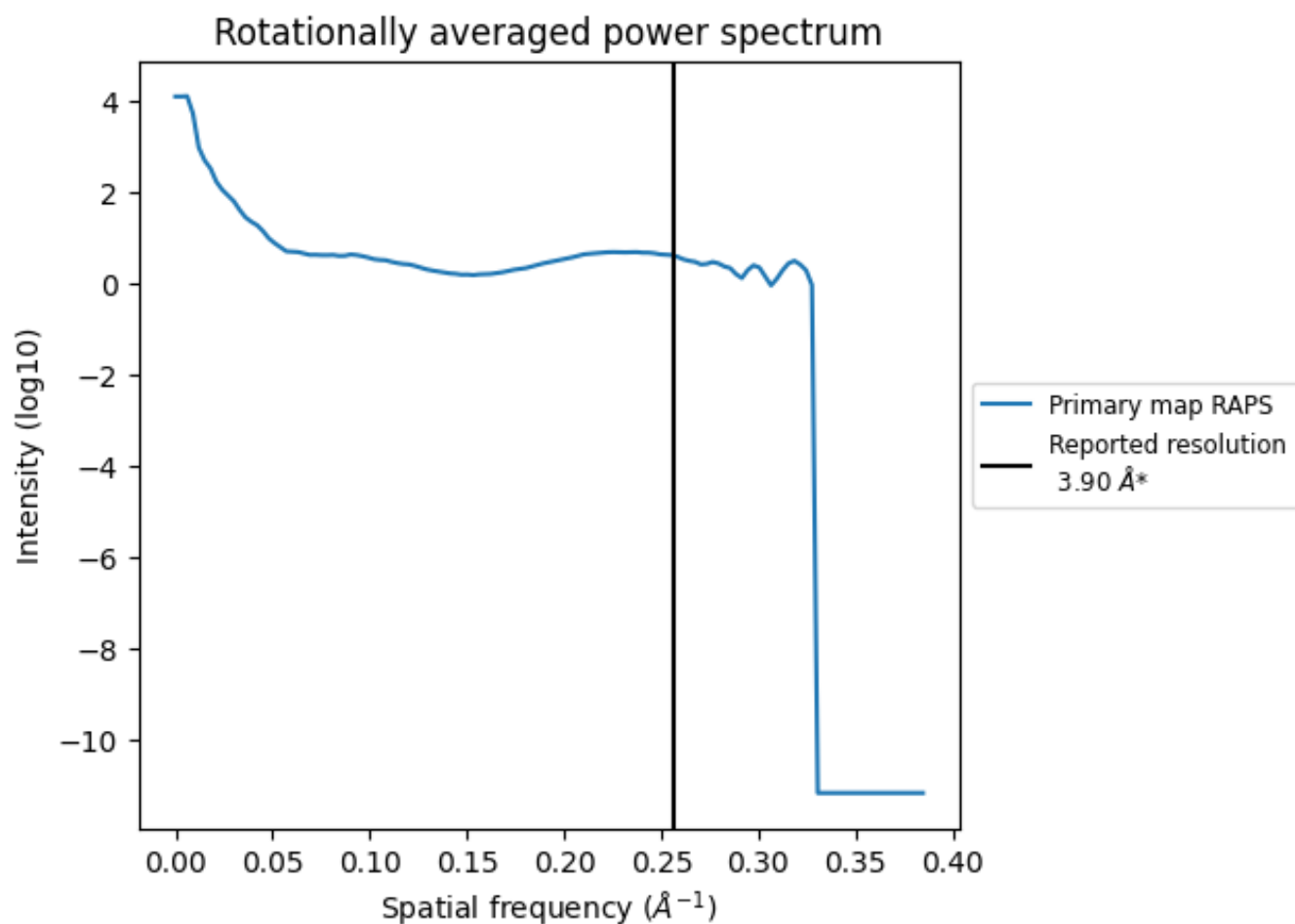
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 302 nm<sup>3</sup>; this corresponds to an approximate mass of 273 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 [\(i\)](#)

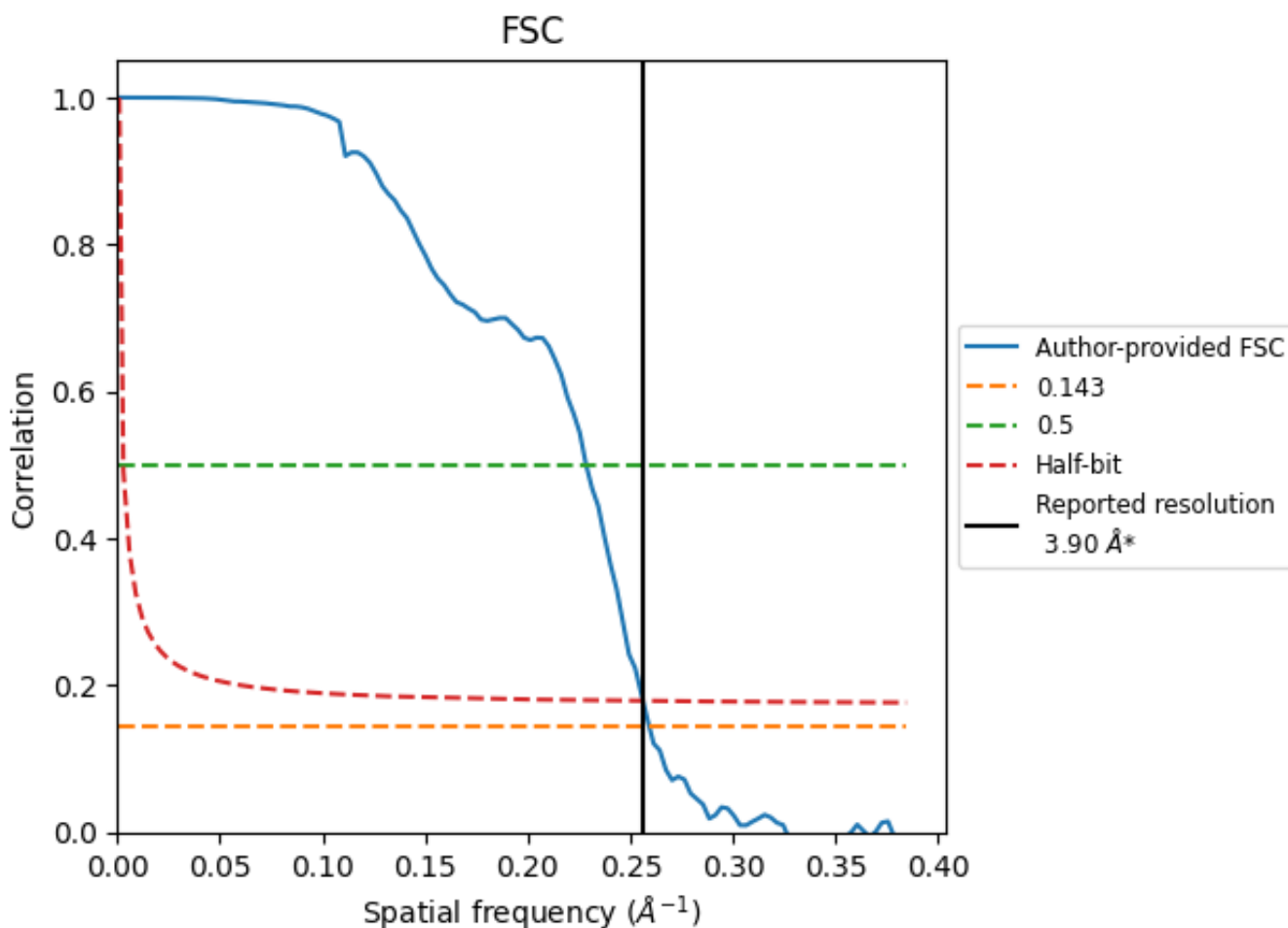


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

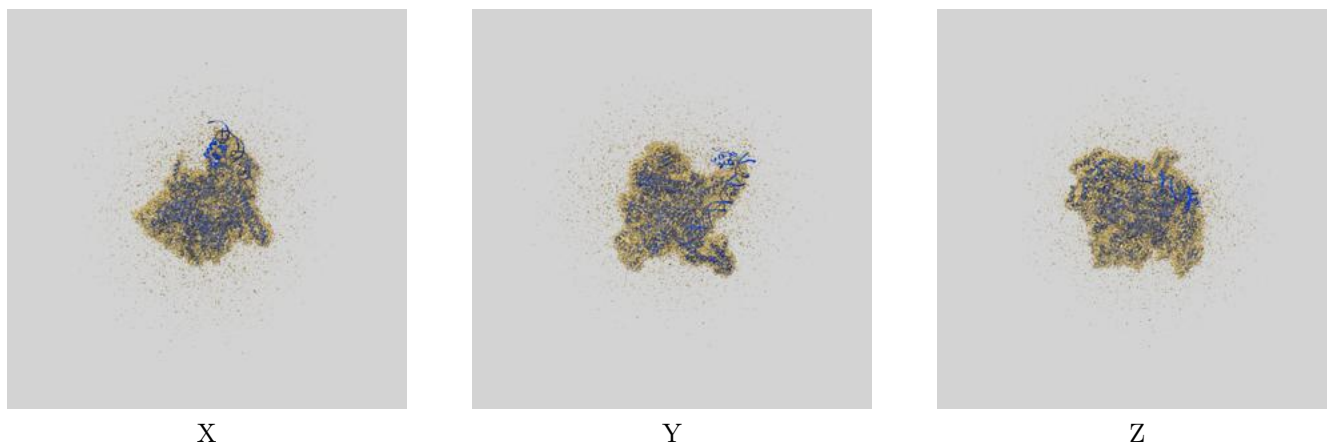
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	4.38	3.90
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

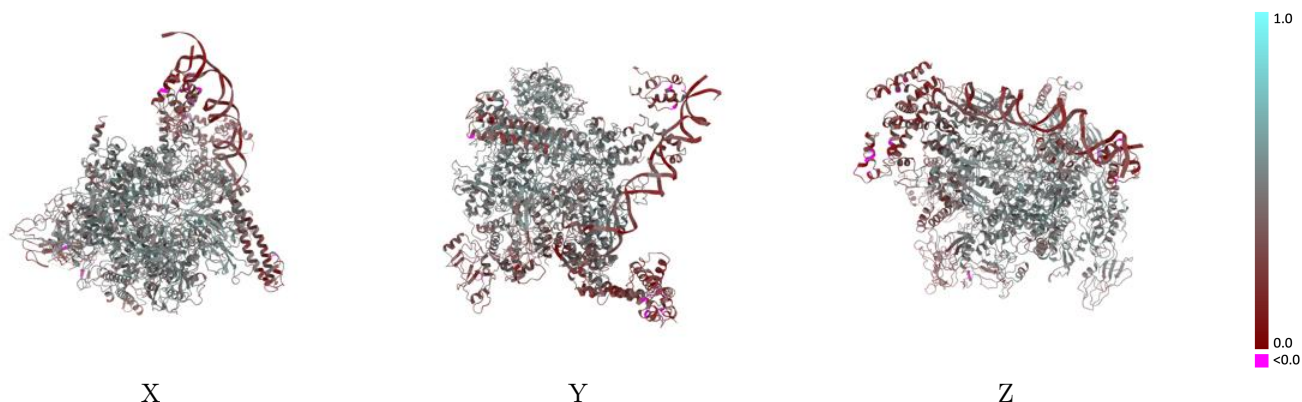
This section contains information regarding the fit between EMDB map EMD-20464 and PDB model 6PSU. Per-residue inclusion information can be found in section 3 on page 8.

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



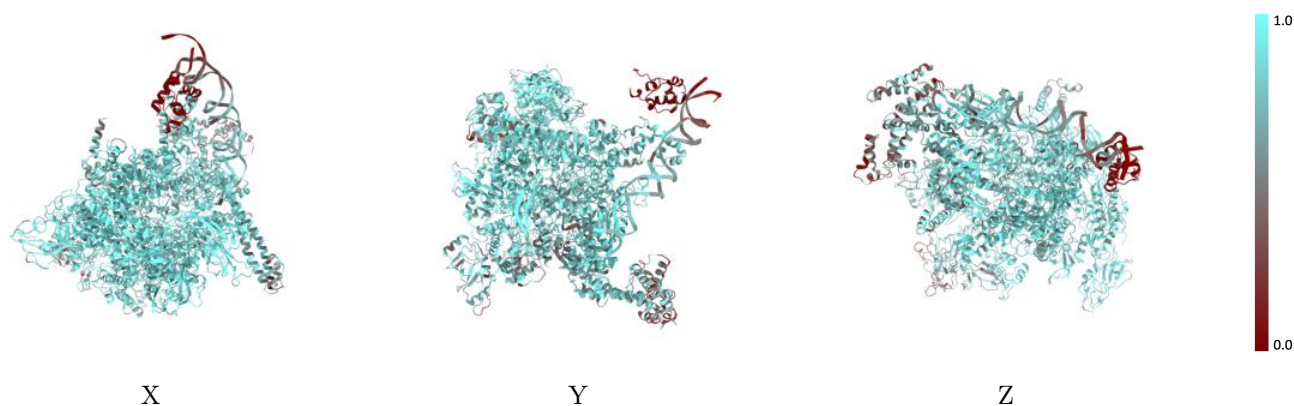
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

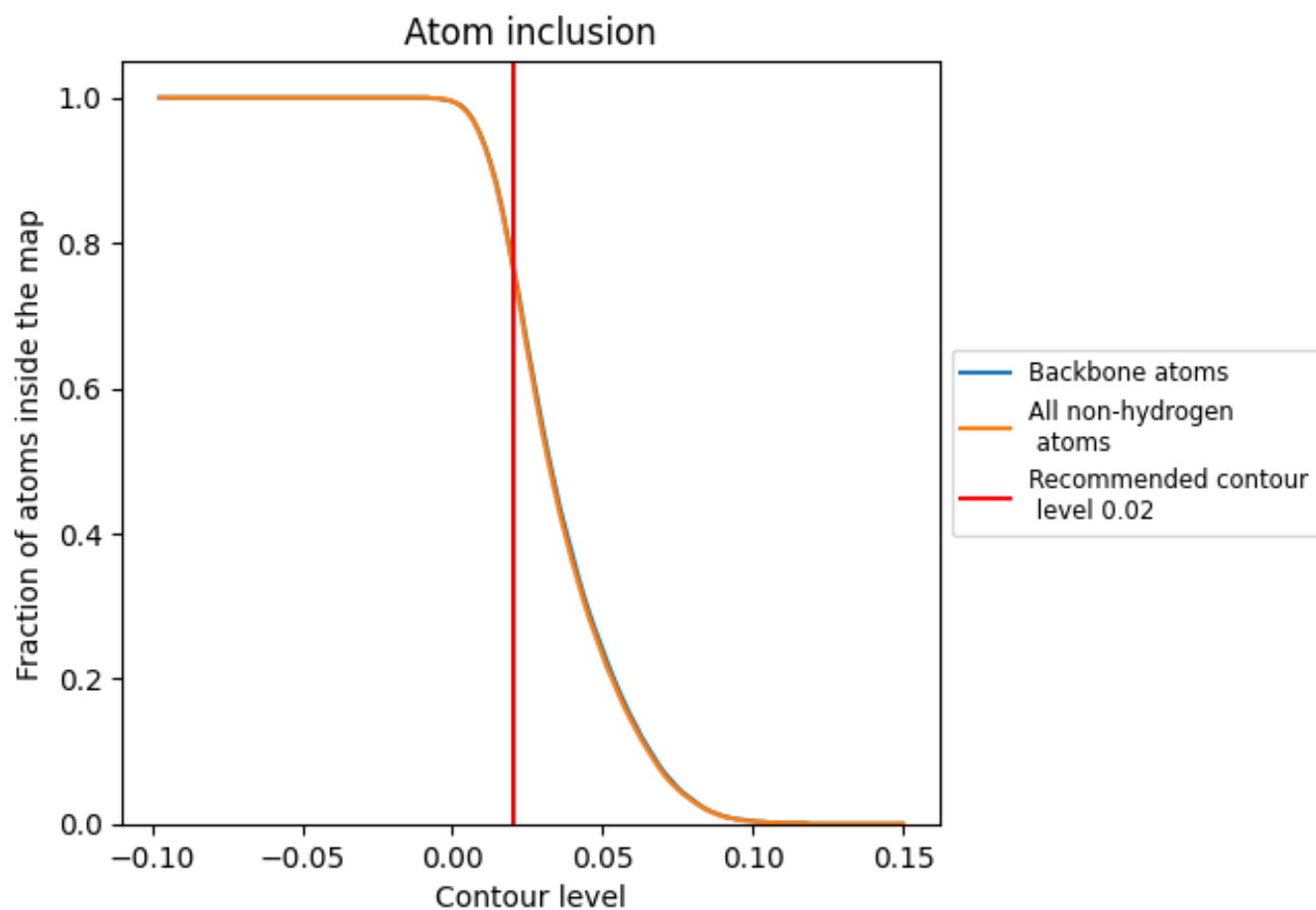
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4260
G	 0.8540	 0.4910
H	 0.8310	 0.4540
I	 0.8310	 0.4600
J	 0.8070	 0.4510
K	 0.6990	 0.4460
L	 0.6740	 0.3370
M	 0.0520	 0.2280
N	 0.8300	 0.4370
O	 0.5680	 0.2450
P	 0.5250	 0.2260

