



## wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 08:43 PM EDT

PDB ID : 6BZO / pdb\_00006bzo  
EMDB ID : EMD-7319  
Title : Mtb RNAP Holo/RbpA/Fidaxomicin/upstream fork DNA  
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.  
Deposited on : 2017-12-25  
Resolution : 3.38 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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.43.1

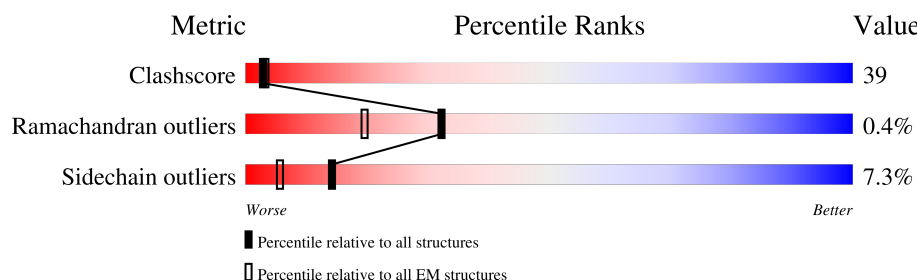
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.38 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.



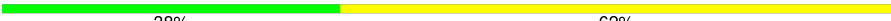
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1181	
3	D	1324	
4	E	110	
5	F	531	
6	J	111	
7	O	31	

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Mol	Chain	Length	Quality of chain
8	P	26	 38% 62%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27336 atoms, of which 74 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	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8556	5361	1504	1652	39		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879
C	1186	GLY	-	expression tag	UNP V9Z879
C	1187	ALA	-	expression tag	UNP V9Z879

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1263	Total	C	N	O	S	0	0
			9857	6175	1791	1850	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	326	Total	C	N	O	S	0	0
			2588	1617	467	495	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	107	Total	C	N	O	S	0	0
			872	539	162	168	3		

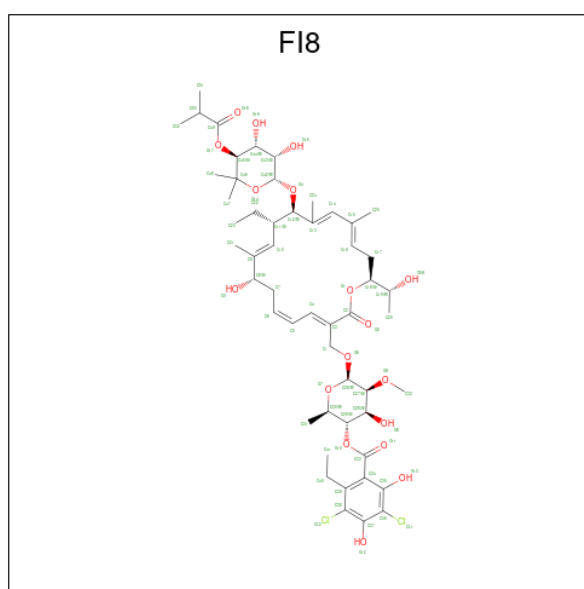
- Molecule 7 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	31	Total	C	N	O	P	0	0
			634	305	114	185	30		

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	26	Total	C	N	O	P	0	0
			526	254	94	153	25		

- Molecule 9 is Fidaxomicin (CCD ID: FI8) (formula:  $C_{52}H_{74}Cl_2O_{18}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	Cl	H	O	0
			146	52	2	74	18	

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	C	2	Total 2	O 2	0
12	D	4	Total 4	O 4	0

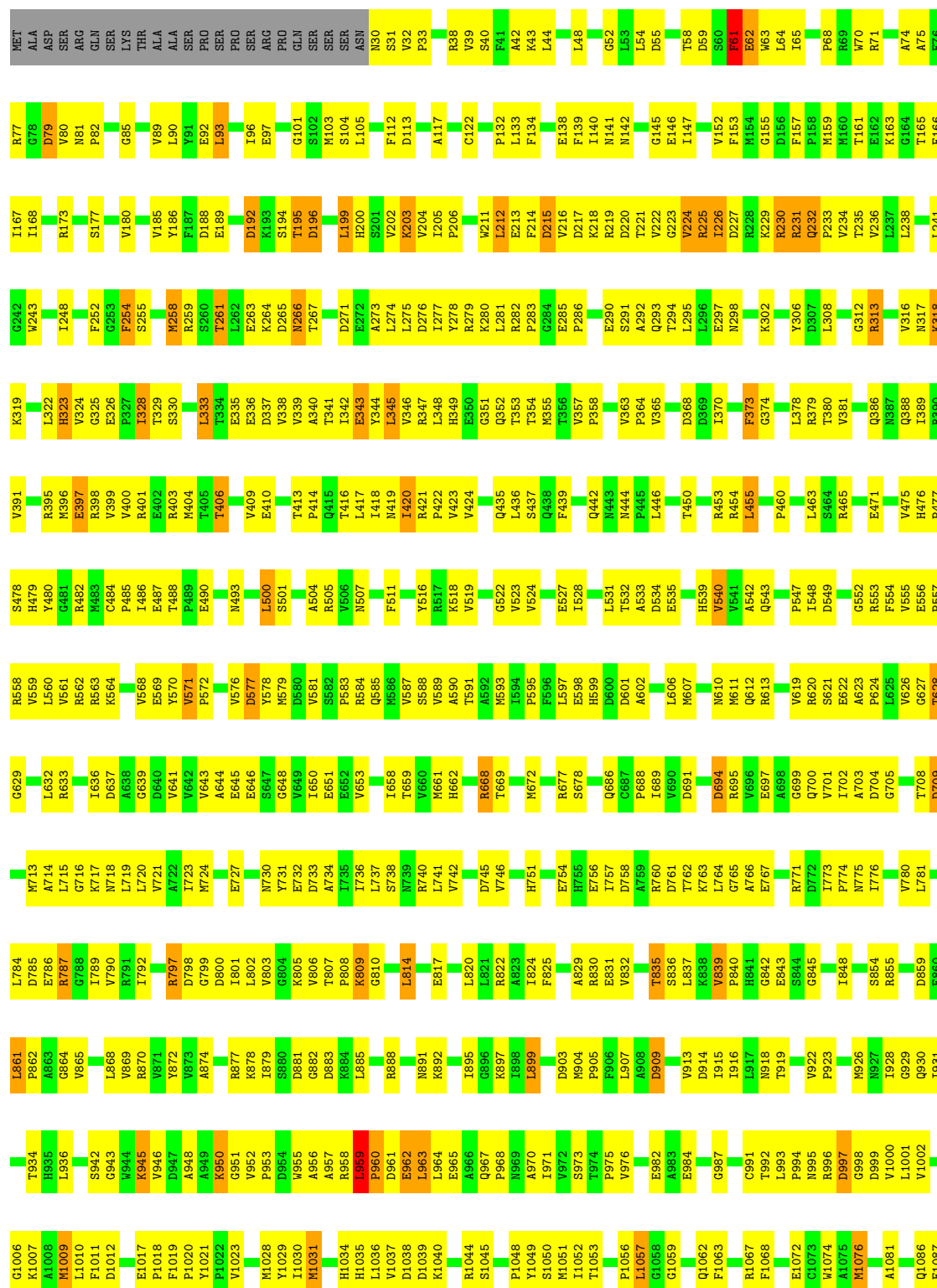




ALA  
TYR  
GLU  
GLN  
ASP  
TYR  
ALA  
GLU  
THR  
GLU  
GLN  
LEU

● Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 42% 46% 5% 6%



L1088	L1091	L1092	S1093	R1099	V1102	Y1103	E1104	Y1107	E1110	N1111	I1112	T1117	F1118	E1119	V1123	L1124	L1125	K1126	E1127	Q1129	V1135	S1140	ASP	GLY	ALA	ALA	TLE	GLU	LEU	ARG	GLU	ASP	ASP	LEU	GLU	ARG	ALA	ALA	ASN	ASN	GLY	TLE	ASN	LEU	SER
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ARG	ASN	GLU	SER	ALA	SER	VAL	GLU	ASP	LEU	ALA	ALA	ARG	HIS	GLY	GLY	SER	GLY	ALA
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• Molecule 3: DNA-directed RNA polymerase subunit beta'



RET	LEU	ASP	V4	N5	E9	L10	R11	I12	D19	I104	H103	I20	H105	R21	Q22	Y25	P31	N35	Y36	R37	T38	L39	E49	R50	I51	F52	G53	P54	T55	R56	D57	W58	E59	C60	Y61	G62	G63	K64	Y65	K66	R67	I73	E76	R77	C78	G79	V80	E81	H82	A83	T84	E85	A86	V87
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R88	R89	E90	R91	N92	E96	V101	T102	H103	I104	H105	I106	F107	P111	S112	R113	Y116	L117	L118	D119	D120	A121	P122	R123	D124	L125	F126	G127	I128	I129	Y130	Y134	Y135	I136	T137	S138	V139	D140	E141	E142	M143	R144	H145	N146	E147	L148	S149	T150	L151	E152	A153	T83	R84	E85	M155	A156	V157
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E158	R159	A160	A161	V162	E163	D164	Q165	R166	E169	L170	I171	A172	R173	A174	Q175	K176	L177	E178	A179	E185	A186	E187	G188	L189	K190	A191	D192	A193	K196	V197	R198	D199	G200	E201	E202	R203	E204	R205	R206	Q207	T208	R211	A212	Q213	R214	E215	L216	D217	R218	L219	E220	D221	I222
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K223	S224	T225	F226	T227	K228	L229	A230	P231	K232	L234	T235	V236	D237	E238	N239	L240	Y241	R242	E243	L244	V245	D246	R247	Y248	G249	E250	F251	F252	T253	M256	L261	Q262	K263	F268	D269	L270	E273	A274	E275	S276	L277	R278	D279	V280	Q287	L290	L293	K294	R295	L296	K297
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V298	V299	M310	V313	L314	D315	A316	V317	V318	V319	T320	P321	P322	E323	L324	K327	V328	L330	D331	G332	G333	R334	F335	A336	T337	S338	D339	L340	N341	Y344	R345	L348	N349	L354	L357	L360	G361	A362	P363	E364	L365	L366	V367	N368	N369	E370	K371	R372	K373	L374	Q375
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F382	N383	N384	G385	R386	R387	T392	R397	P398	L399	K400	S401	L402	L405	L406	K407	G408	K409	Q410	Q411	R412	F413	R414	K420	R421	Y429	T430	V431	V432	Q433	P434	Q435	L436	G442	L443	P444	M447	A448	L449	Q450	L451	F452	K453	P454	F455	V456	R459	L460	L463	K464
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H465	A466	Q467	N468	L469	K470	S471	A472	N475	V476	E477	R478	Q479	L485	V486	L487	E488	E489	V490	L491	H494	P495	N499	R500	T503	L504	H505	R506	P512	E513	P514	N515	L516	V517	K520	A521	L522	Q523	L524	H525	P526	L527	A534	D535	D539	Q540	L545
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P546	L547	E554	L557	L558	H559	S561	S567	R572	P573	L574	A575	N576	P577	R578	L579	N580	E581	V582	F587	L588	T589	T590	D595	T596	G597	E598	Y599	Q600	P601	H606	P607	E608	T609	G610	V611	S614	P615	A616	E617	M620	A621	A622	D623	R624	E625	V626	L627	S628	V629
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R630	A631	K632	L633	K634	V635	R636	L637	T638	Q639	L640	R641	P642	T646	E647	A648	E649	L650	D660	A661	M662	N663	A664	E665	T666	K673	L676	L677	P678	L679	V684	N685	K686	Q687	N688	L697	L698	L699	L700	R703	Y704	P705	M706	I707
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V708	V709	A710	Q711	T712	V713	L716	K717	D718	F721	P722	W723	A724	T725	R726	T730	V731	S732	M733	A734	D735	V736	L737	V738	P739	R740	R741	R742	K743	E744	L745	L746	Y749	E750	A753	L757	E757	F760	L765	N766	H767	Y769	R770	N771	L774	V775	D776	E777	L778	W779	L780	A781
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T782	D783	A784	V785	R790	E791	L792	H793	N797	L798	T799	T800	A807	T808	F811	L817	N820	K821	G822	L823	V824	G827	E828	R829	S830	F831	T832	P833	R834	P835	V836	K837	F840	R841	L844	T845	V846	L847	E848	Y849	F850	L851	N852	T853	H854	G855	L856	R857	L860	A861
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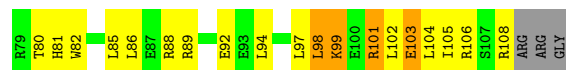
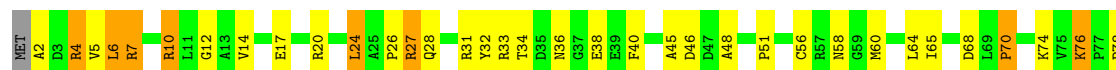
D862	T863	A864	L865	R866	T867	L873	T874	R875	R876	L877	S880	S881	Q882	D883	V884	L885	V886	R887	E888	H889	D890	C891	Q892	T893	E894	N895	R896	L897	V898	V899	T900	L901	A902	E903	R904	A905	G908	T909	L910	R911	R912	D913	P914	Y915	Y916	E917	Y921	A922	R923	T924	L925	G926	T927	T928	A929
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V930	D931	E932	A933	R934	G935	V936	I937	V938	E939	R940	G941	D942	D943	L944	D946	P947	E948	L952	A955	G956	I957	V960	R961	V962	R963	G964	V965	L966	T967	C968	A969	T970	G973	V974	C975	A976	T977	C978	Y979	G980	R981	S982	V989	D990	I991	G992	E993	E1005	T1008	Q1009	L1010
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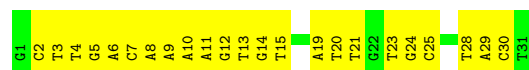




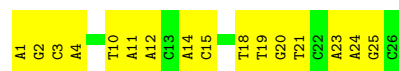
• Molecule 6: RNA polymerase-binding protein RbpA



• Molecule 7: DNA (32-MER)



• Molecule 8: DNA (26-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173509	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 ( $e^-/\text{\AA}^2$ )	6.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.278	Depositor
Minimum map value	-1.545	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.347	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FI8, 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	A	0.10	0/1750	0.30	0/2380
1	B	0.10	0/1802	0.31	0/2454
2	C	0.10	0/8714	0.33	2/11824 (0.0%)
3	D	0.15	0/10021	0.33	0/13549
4	E	0.10	0/662	0.29	0/901
5	F	0.10	0/2622	0.29	0/3538
6	J	0.41	2/888 (0.2%)	0.42	0/1199
7	O	0.18	0/710	0.37	0/1095
8	P	0.20	0/589	0.39	0/906
All	All	0.14	2/27758 (0.0%)	0.33	2/37846 (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	C	0	3
3	D	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	10	ARG	C-O	-6.83	1.16	1.23
6	J	10	ARG	CA-C	-6.33	1.44	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	254	PHE	CA-C-N	5.37	131.37	121.70
2	C	254	PHE	C-N-CA	5.37	131.37	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	61	PHE	Peptide
2	C	958	ARG	Peptide
2	C	960	PRO	Peptide
3	D	1194	VAL	Peptide
3	D	600	GLN	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	A	1724	0	1768	130	0
1	B	1775	0	1809	178	0
2	C	8556	0	8459	769	0
3	D	9857	0	9920	807	0
4	E	649	0	645	57	0
5	F	2588	0	2602	230	0
6	J	872	0	852	61	0
7	O	634	0	350	39	0
8	P	526	0	296	38	0
9	C	72	74	0	3	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
12	C	2	0	0	0	0
12	D	4	0	0	3	0
All	All	27262	74	26701	2122	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 39.

The worst 5 of 2122 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)
2:C:948:ALA:HB2	2:C:953:PRO:HD3	1.27	1.16
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.33	1.08
2:C:633:ARG:NH1	2:C:637:ASP:OD2	1.87	1.07
2:C:225:ARG:HB2	2:C:231:ARG:HA	1.34	1.06
2:C:960:PRO:HG2	2:C:963:LEU:HD12	1.35	1.04

There are no symmetry-related clashes.

## 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	224/347 (65%)	206 (92%)	18 (8%)	0	100	100
1	B	235/347 (68%)	200 (85%)	35 (15%)	0	100	100
2	C	1109/1181 (94%)	961 (87%)	141 (13%)	7 (1%)	22	50
3	D	1257/1324 (95%)	1148 (91%)	105 (8%)	4 (0%)	37	66
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
5	F	324/531 (61%)	306 (94%)	18 (6%)	0	100	100
6	J	105/111 (95%)	89 (85%)	15 (14%)	1 (1%)	13	39
All	All	3335/3951 (84%)	2985 (90%)	338 (10%)	12 (0%)	32	60

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	GLU
2	C	323	HIS
3	D	909	THR
3	D	910	LEU
3	D	904	ARG



### 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	195/297 (66%)	186 (95%)	9 (5%)	23	50
1	B	197/297 (66%)	179 (91%)	18 (9%)	7	26
2	C	924/997 (93%)	865 (94%)	59 (6%)	14	40
3	D	1041/1103 (94%)	967 (93%)	74 (7%)	12	37
4	E	69/89 (78%)	64 (93%)	5 (7%)	12	37
5	F	272/429 (63%)	246 (90%)	26 (10%)	7	24
6	J	93/97 (96%)	80 (86%)	13 (14%)	3	11
All	All	2791/3309 (84%)	2587 (93%)	204 (7%)	14	36

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	478	ARG
3	D	957	ILE
6	J	97	LEU
3	D	506	ARG
3	D	733	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	325	ASN
5	F	388	GLN
2	C	1066	GLN
2	C	986	GLN
5	F	414	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	FI8	C	1201	-	74,75,75	1.89	19 (25%)	96,109,109	1.58	18 (18%)

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
9	FI8	C	1201	-	-	20/75/118/118	0/3/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	FI8	C1-C3	5.34	1.57	1.50
9	C	1201	FI8	C14-C15	4.52	1.54	1.45
9	C	1201	FI8	O1-C18	-4.10	1.39	1.46
9	C	1201	FI8	O1-C2	3.96	1.43	1.34
9	C	1201	FI8	O17-C49	3.83	1.43	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	FI8	C18-C17-C16	-4.88	104.00	112.94
9	C	1201	FI8	O14-C46-C45	4.60	115.06	107.67
9	C	1201	FI8	C31-C30-C29	-4.34	106.94	113.39
9	C	1201	FI8	O1-C2-C3	3.81	117.40	112.11
9	C	1201	FI8	C7-C6-C5	-3.73	120.69	125.44

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

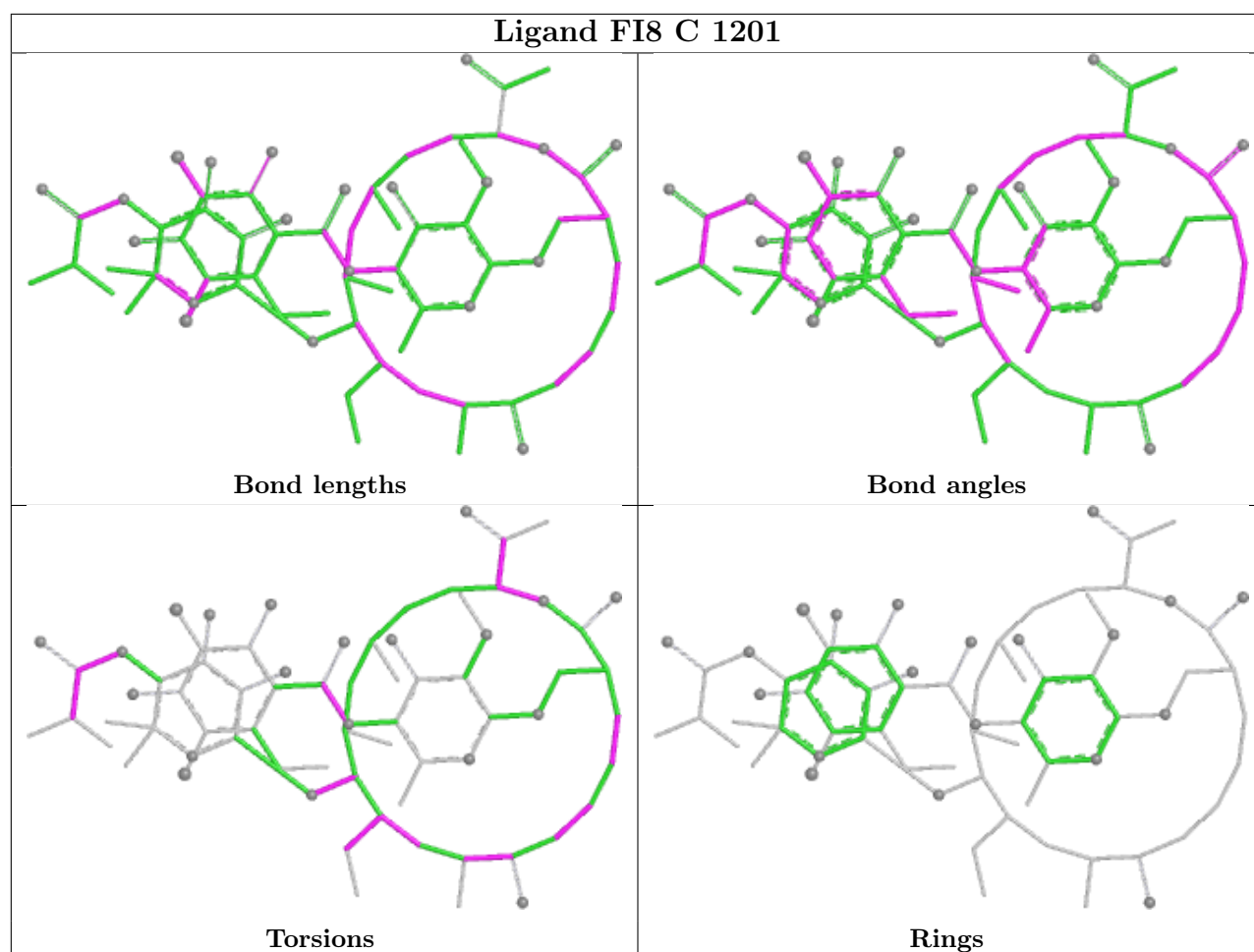
Mol	Chain	Res	Type	Atoms
9	C	1201	FI8	C9-C10-C11-C12
9	C	1201	FI8	C9-C10-C11-C22
9	C	1201	FI8	C10-C11-C22-C23
9	C	1201	FI8	C12-C11-C22-C23
9	C	1201	FI8	O1-C18-C19-O5A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	FI8	3	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.

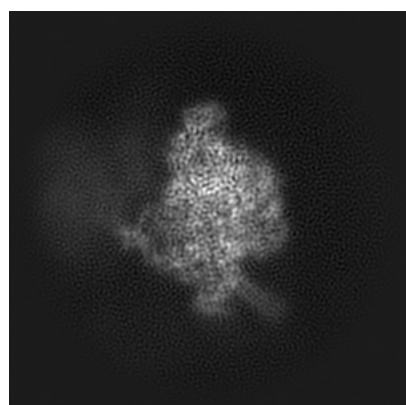
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7319. These allow visual inspection of the internal detail of the map and identification of artifacts.

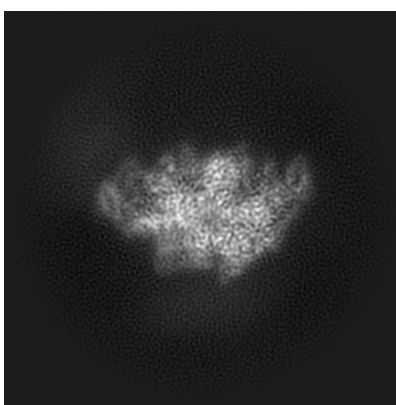
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

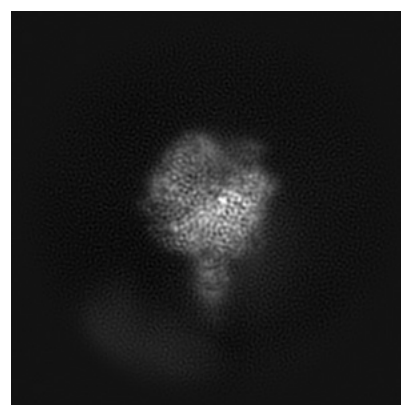
#### 6.1.1 Primary map



X



Y

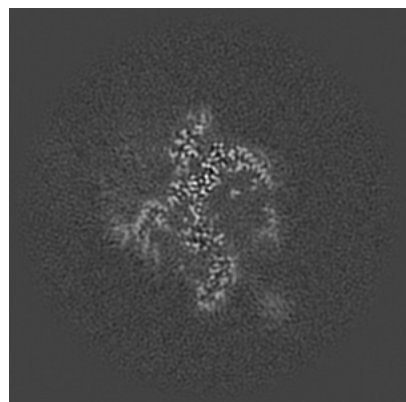


Z

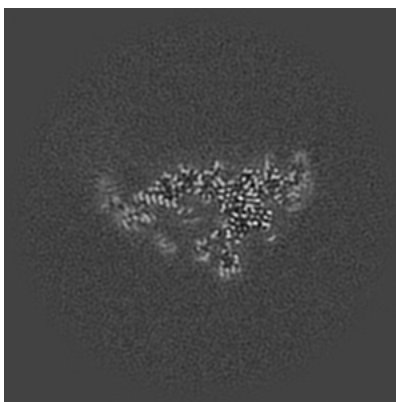
The images above show the map projected in three orthogonal directions.

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

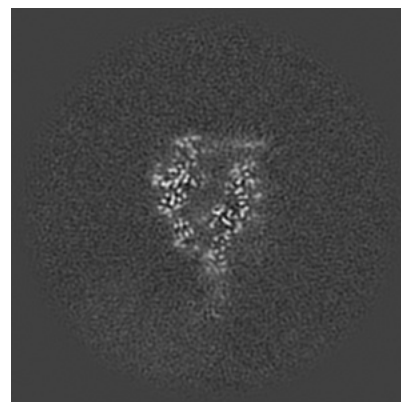
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

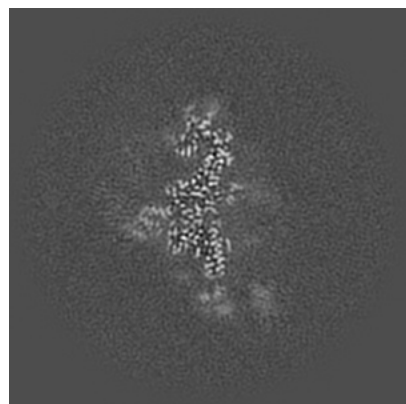


Z Index: 150

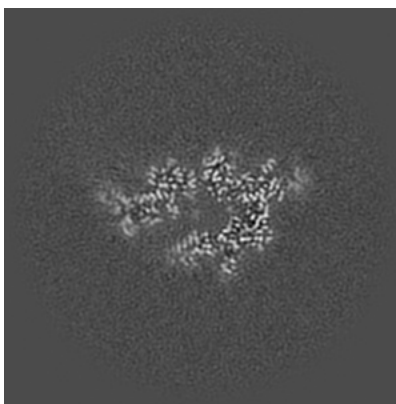
The images above show central slices of the map in three orthogonal directions.

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

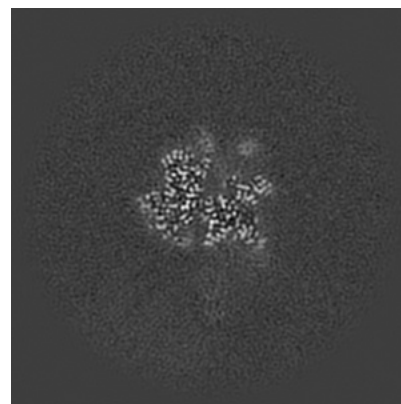
### 6.3.1 Primary map



X Index: 159



Y Index: 158

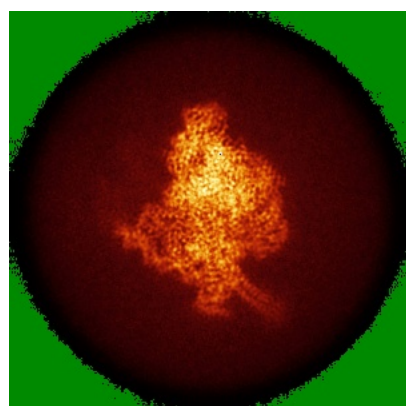


Z Index: 168

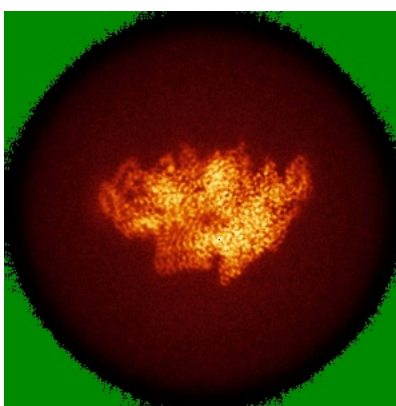
The images above show the largest variance slices of the map in three orthogonal directions.

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

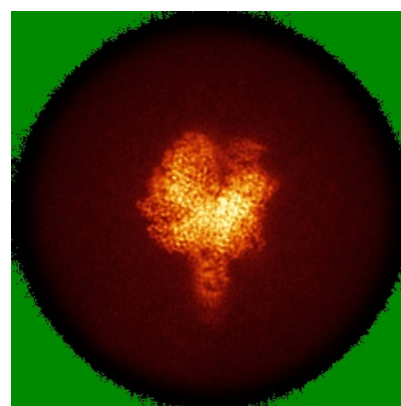
### 6.4.1 Primary map



X



Y

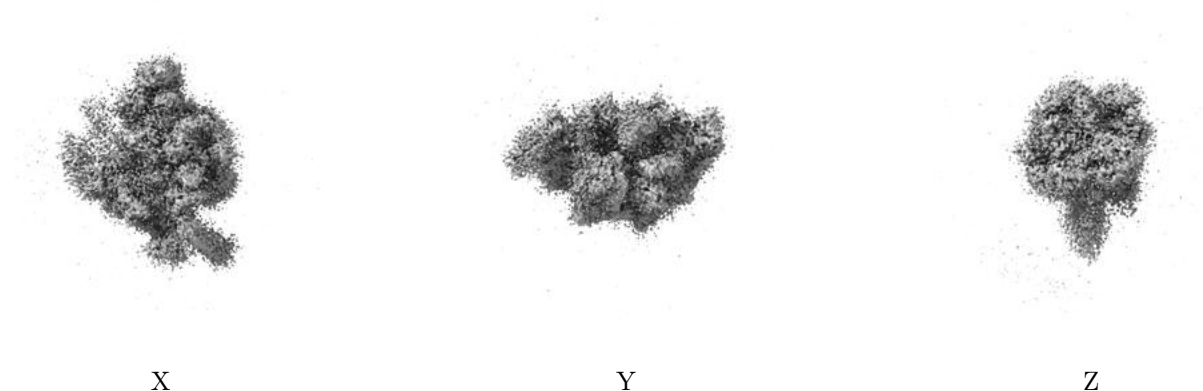


Z

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

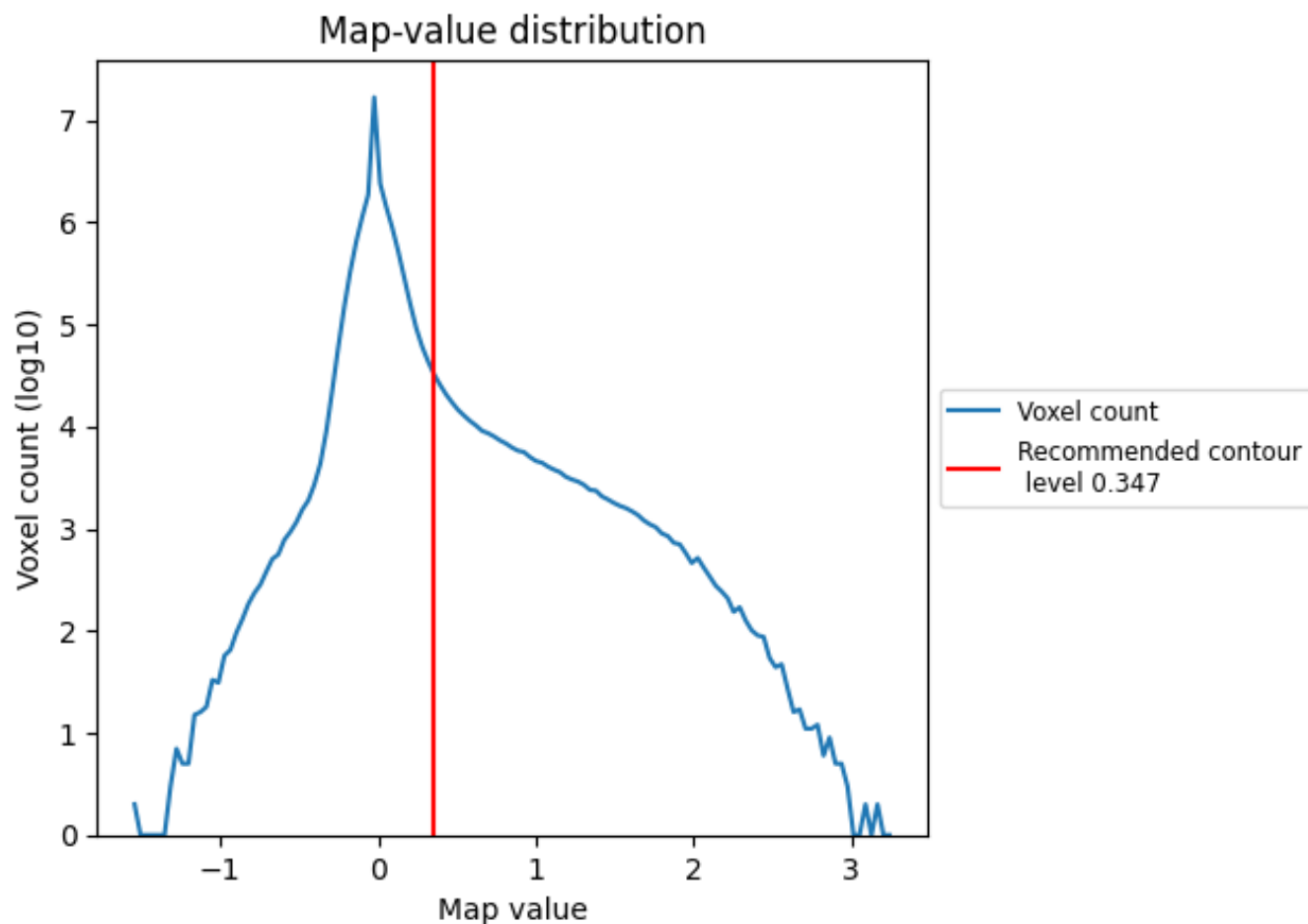
## 6.6 Mask visualisation [i](#)

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.

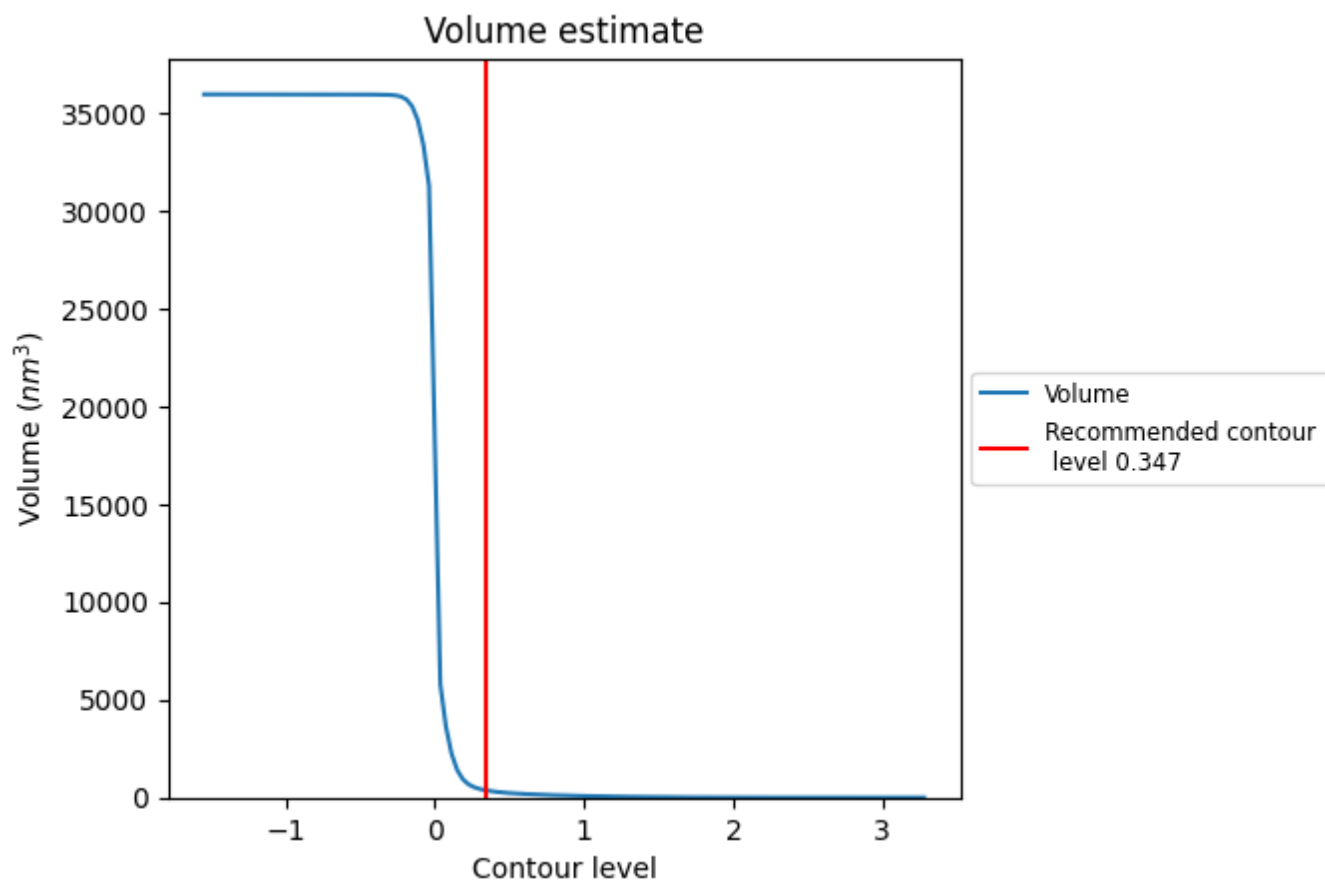
### 7.1 Map-value distribution [i](#)



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.



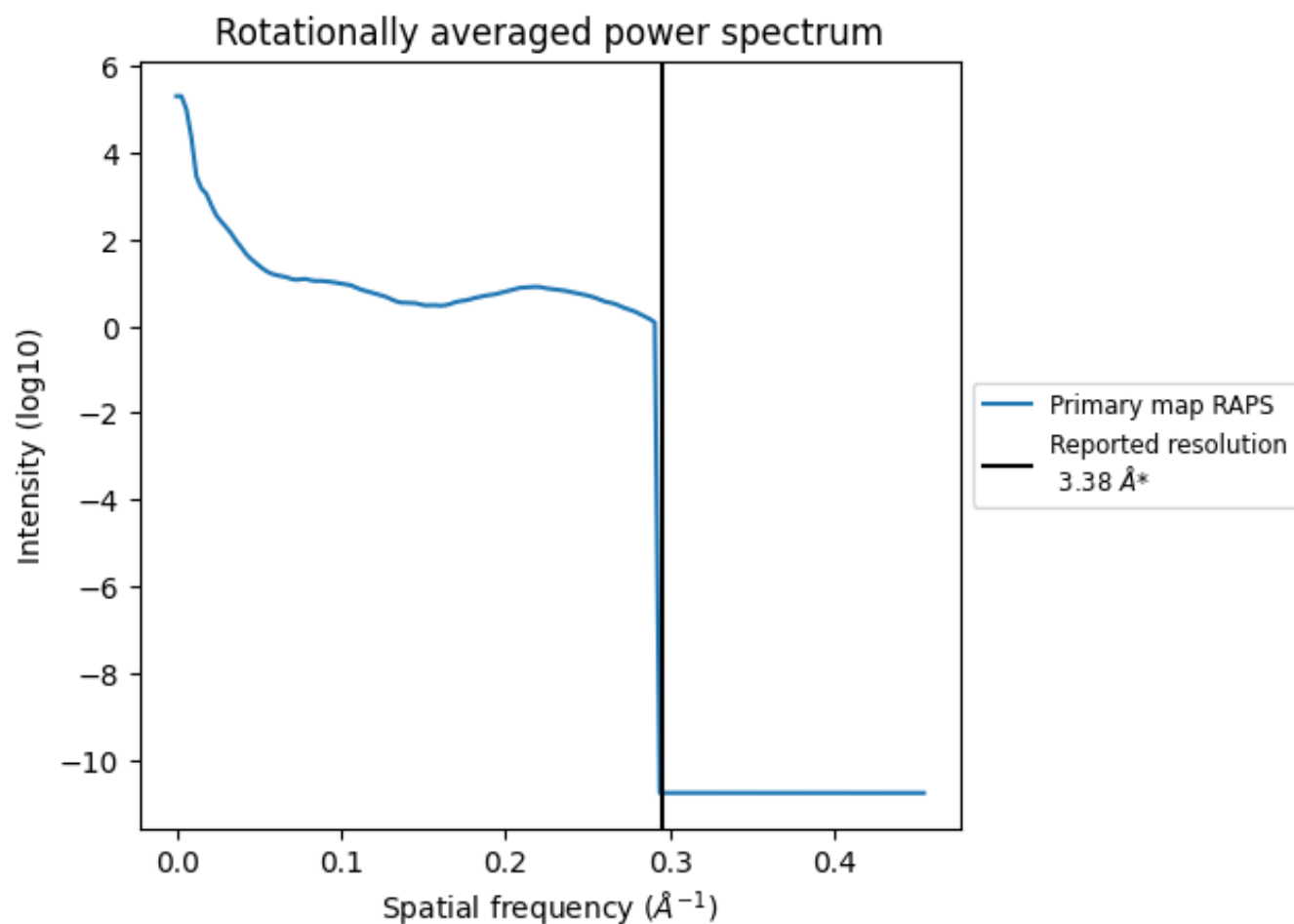
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365  $\text{nm}^3$ ; this corresponds to an approximate mass of 329 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 0.296 Å<sup>-1</sup>

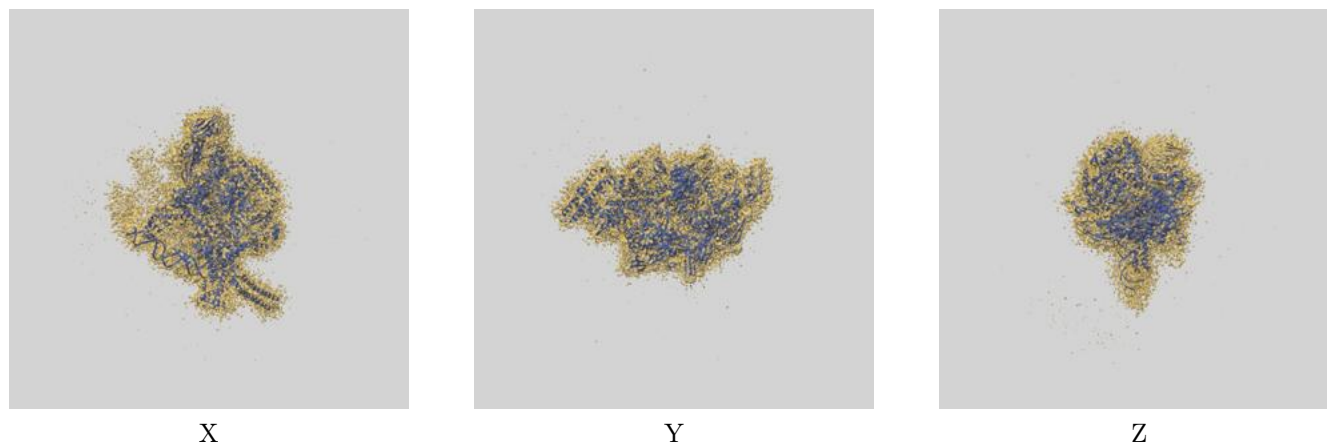
## 8 Fourier-Shell correlation

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

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

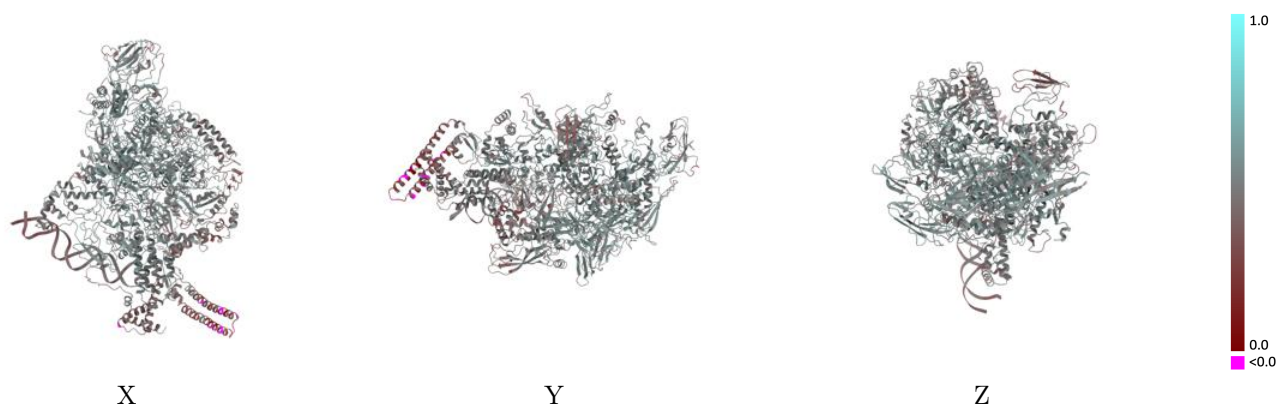
This section contains information regarding the fit between EMDB map EMD-7319 and PDB model 6BZO. Per-residue inclusion information can be found in section 3 on page 8.

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



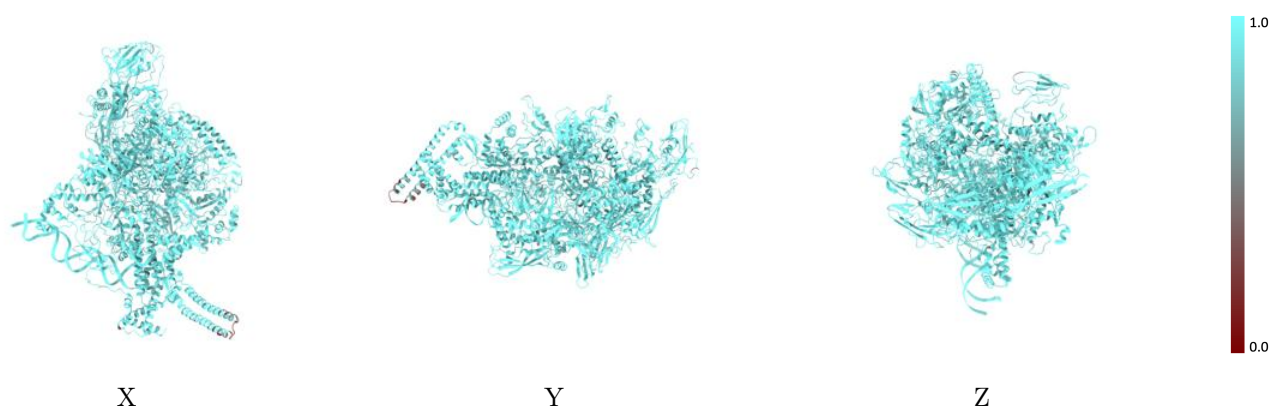
The images above show the 3D surface view of the map at the recommended contour level 0.347 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



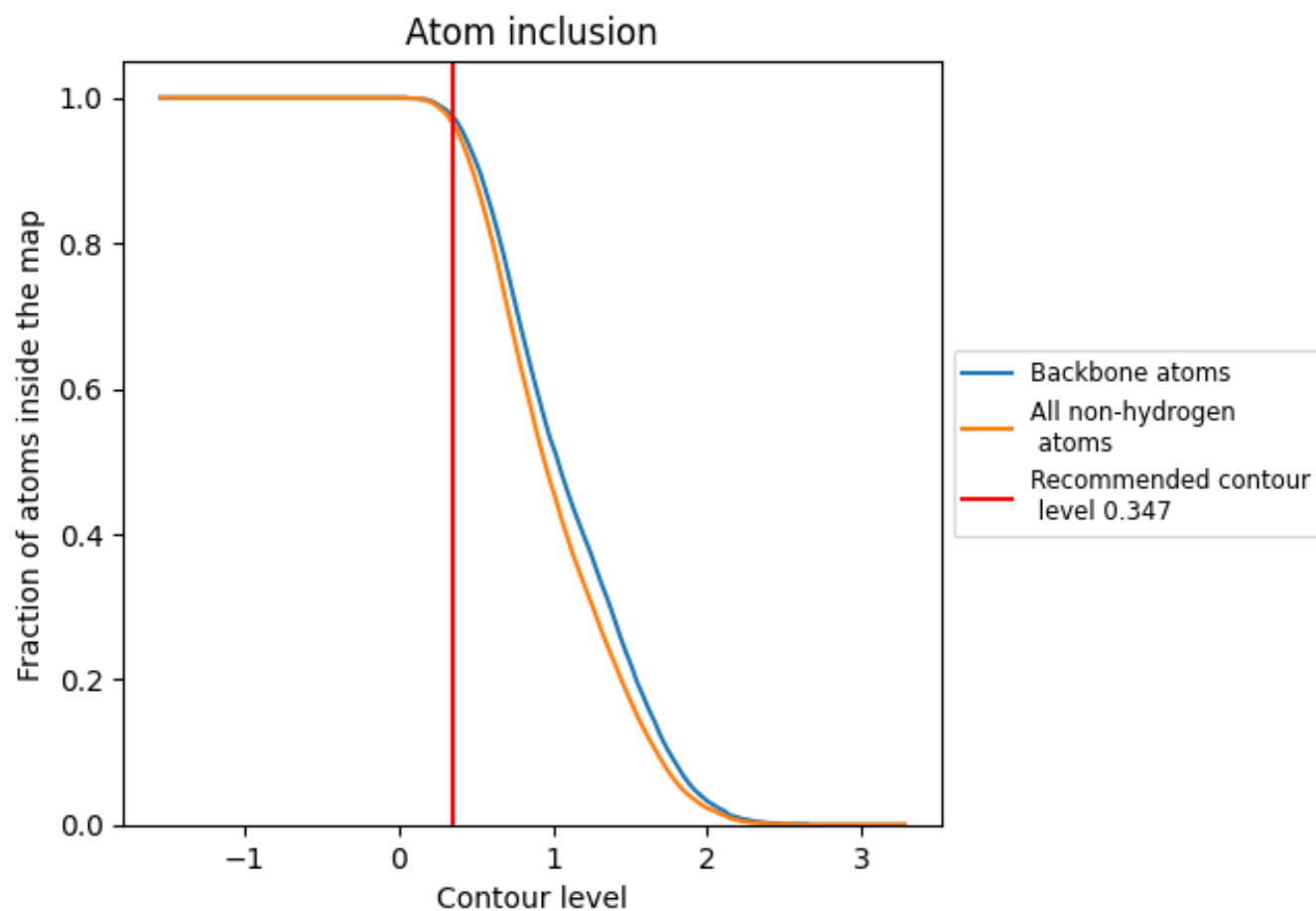
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.347).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.347) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9660	<div><div></div></div> 0.4890
A	<div><div></div></div> 0.9750	<div><div></div></div> 0.5130
B	<div><div></div></div> 0.9680	<div><div></div></div> 0.4960
C	<div><div></div></div> 0.9710	<div><div></div></div> 0.5050
D	<div><div></div></div> 0.9640	<div><div></div></div> 0.4910
E	<div><div></div></div> 0.9610	<div><div></div></div> 0.5010
F	<div><div></div></div> 0.9600	<div><div></div></div> 0.4520
J	<div><div></div></div> 0.9510	<div><div></div></div> 0.4750
O	<div><div></div></div> 0.9970	<div><div></div></div> 0.4080
P	<div><div></div></div> 0.9910	<div><div></div></div> 0.3890

1.0

0.0

<0.0