



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:54 AM UTC

PDB ID : 7Z88 / pdb_00007z88
EMDB ID : EMD-14546
Title : DNA-PK in the intermediate state
Authors : Liang, S.; Blundell, T.L.
Deposited on : 2022-03-16
Resolution : 3.33 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

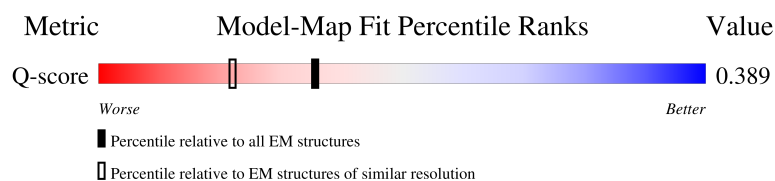
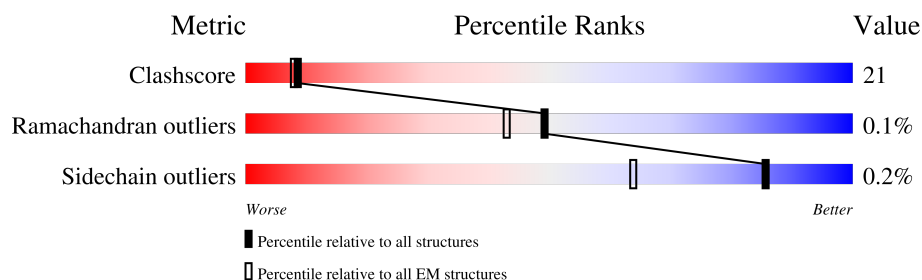
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14484 (2.83 - 3.83)

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

Mol	Chain	Length	Quality of chain
1	A	4128	15% 49% 37% 13%
2	B	609	10% 46% 34% 20%
3	C	732	43% 52% 39% 10%
4	D	26	12% 50% 50%

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Mol	Chain	Length	Quality of chain
5	E	26	15%46%54%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38754 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3599	Total	C	N	O	S	0	0
			28443	18257	4823	5179	184		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3937	2525	667	728	17		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			5274	3372	882	994	26		

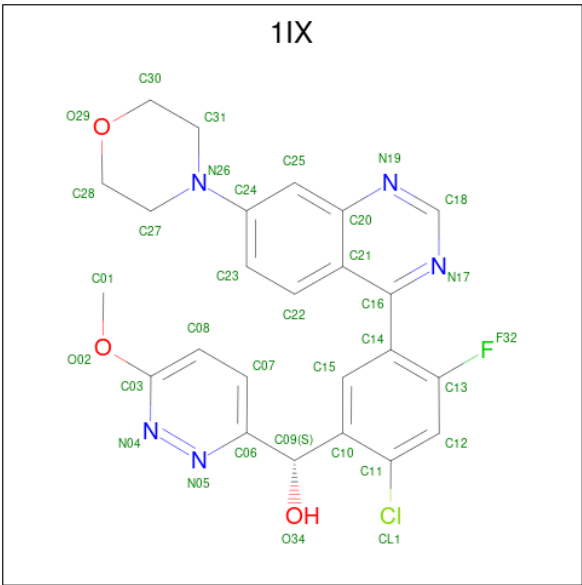
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	26	Total	C	N	O	P	0	0
			526	250	92	158	26		

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	26	Total	C	N	O	P	0	0
			540	254	106	154	26		

- Molecule 6 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (CCD ID: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).

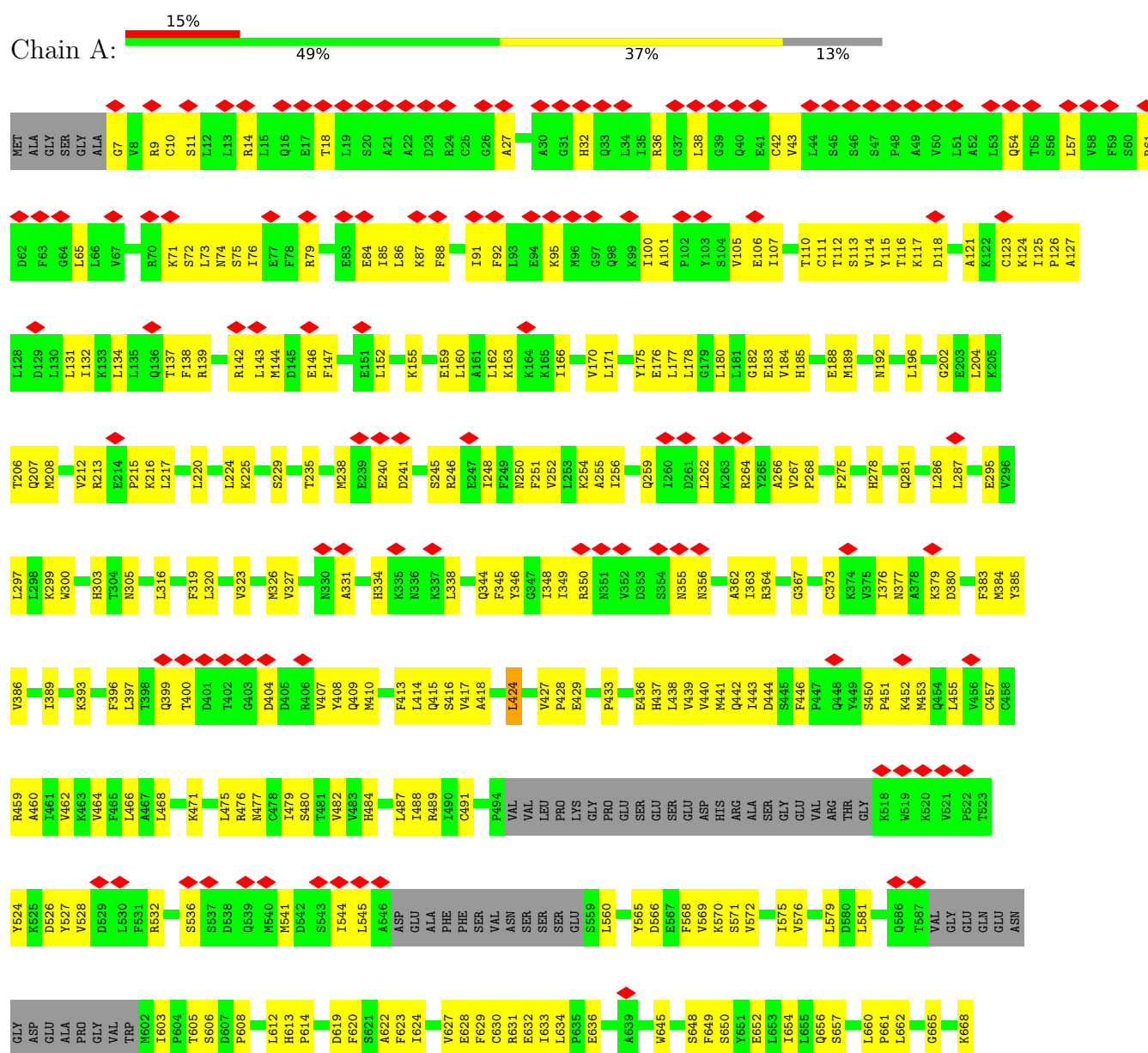


Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
6	A	1	34	24	1	1	5	3	0

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.

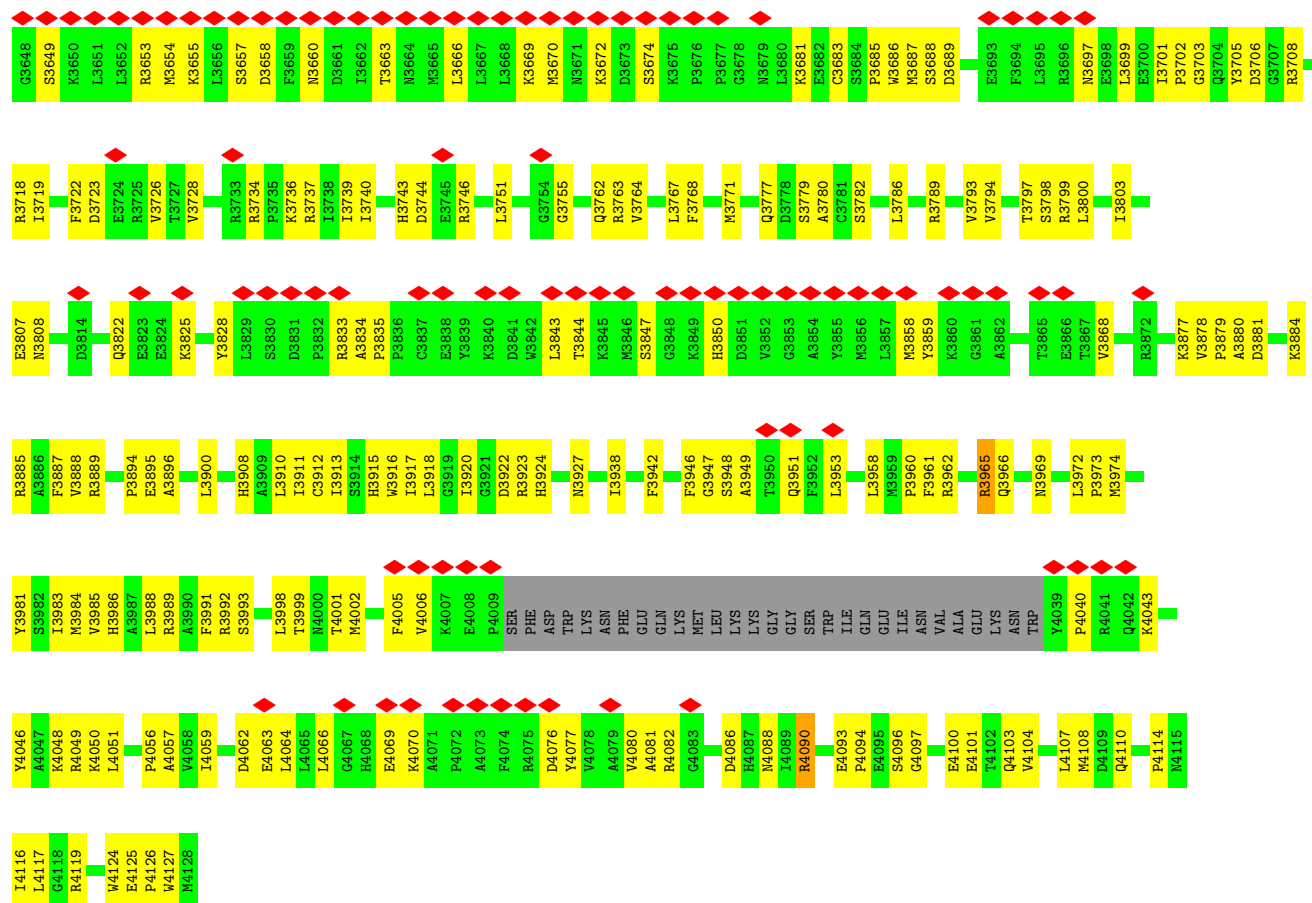
- Molecule 1: DNA-dependent protein kinase catalytic subunit



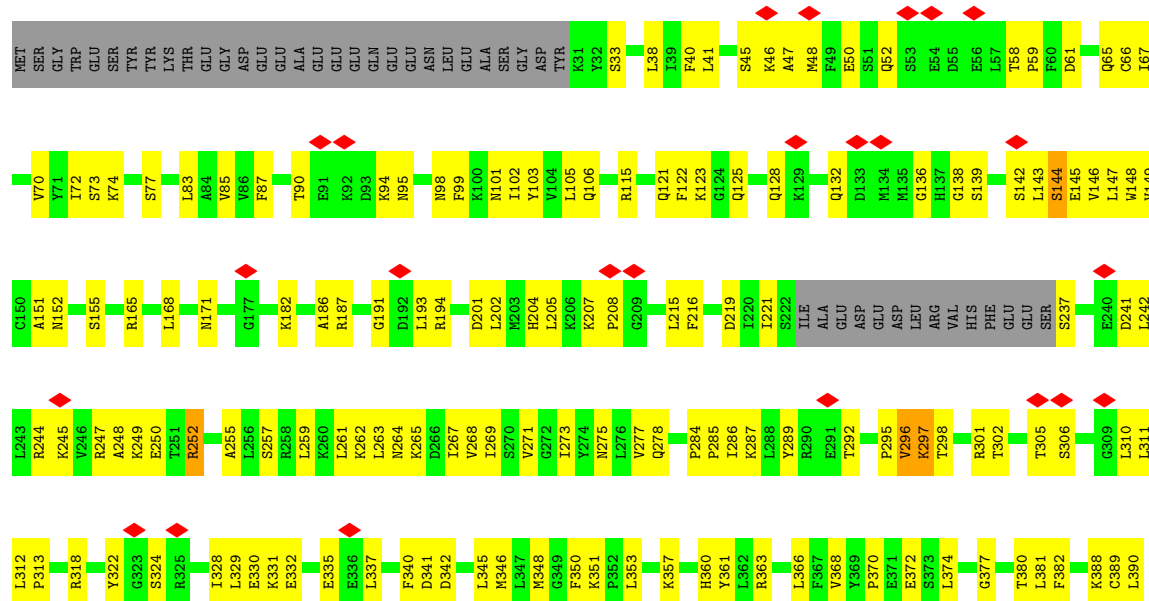


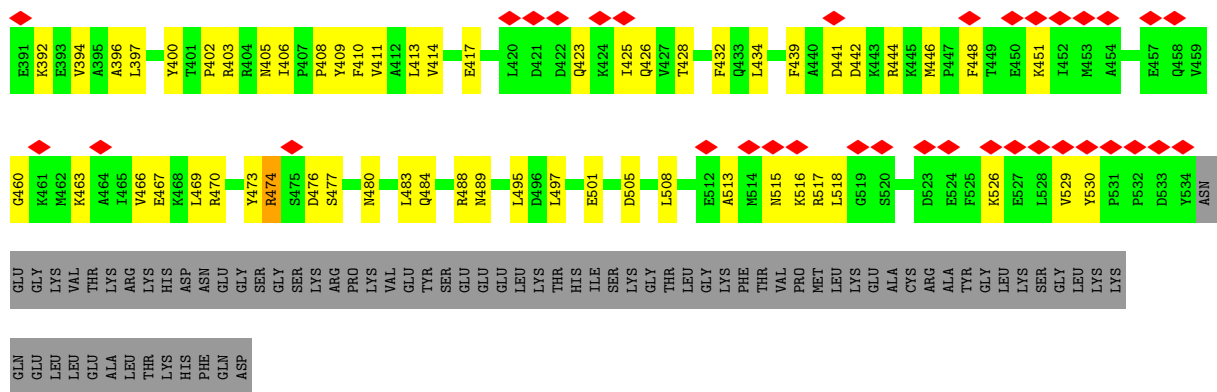


V3588	K3452	A3391	Q3326	L3259	F3189	V3119	I3045	L2976	P2887	PHE
S3589	A3453	ALA	N3327	L3262	L3190	L3120	R3046	N2977	V2888	HE
N3590	K3454	GLU	I3328	H3263	I3193	H3121	S3047	Q2978	K2978	ARG
D3591	K3455	GLU	L3329	K3264	E3194	H3122	K3048	Q2979	Q2807	ASP
V3592	A3461	ALA	G3331	E3265	E3195	Q3123	L3049	D2980	L2808	GLN
K3593	R3462	GLN	G3332	S3266	K3196	L3126	L3053	V2982	F2809	LEU
A3594	F3465	PRO	T3333	K3267	L3197	T3127	G3054	W2982	S2810	LEU
E3595	P3466	PRO	T3334	T3268	K3198	K3128	G3055	E2985	F2813	SER
L3596	R3467	TRP	R3335	R3269	L3199	L3129	G3056	E2986	E2819	LEU
A3597	K3468	SER	I3337	K3270	PRO	Q3130	Q3057	T2987	M2820	TVR
K3598	L3469	CYS	A3338	D3271	LEU	S3131	A3057	E2988	F2823	ARG
T3599	Q3470	GLY	N3339	K3272	PRO	Q3133	D3058	A2989	K2824	LYS
P3600	I3471	PRO	A3340	L3273	GLU	A3134	Q3059	E2990	F2829	GLY
V3601	I3472	A3407	L3341	V3274	ASN	L3135	S3060	K2991	K2836	VAL
K3602	E3473	G3408	S3275	S3275	SER	T3136	L3062	F2993	L2837	GLY
K3603	R3474	V3409	E3344	K3276	MET	Q3138	K3067	W2994	K2835	GLN
K3604	Y3475	I3410	P3345	V3277	ASN	Q3139	A3068	D3000	L2840	LYS
K3605	P3476	D3411	A3346	Q3278	VAL	F3141	M3069	N3003	F2841	TLE
K3606	E3477	A3412	C3347	S3279	GLN	I3142	E3072	H3004	N2841	LYS
E3607	E3478	T3415	L3348	C3281	ASP	F3144	L3073	L3005	L2844	GLU
T3608	L3479	L3416	A3349	R3282	ASP	I3145	Q3074	A3006	T2846	LYS
K3609	L3480	A3417	E3350	L3283	PRO	S3146	I3078	E3007	F2851	LYS
Y3610	S3481	D3418	I3351	S3284	SER	Q3147	E3079	W3008	P2852	GLN
K3611	T3484	F3419	E3352	C3286	ASP	Q3148	F3082	K3009	F2854	ALA
E3612	I3487	C3420	E3353	R3287	ARG	G3149	L3086	S3010	C2857	VAL
K3613	S3488	Y3421	D3354	S3290	GLU	N3150	L3089	E3012	L2856	VAL
F3614	S3489	Q3422	K3355	L3298	VAL	L3151	Y3090	R2951	Q2859	LEU
A3615	V3490	Q3423	A3356	T3299	GLN	L3152	L3091	S2932	D2860	TYR
K3616	F3495	L3424	R3357	V3300	GLU	Q3154	L3092	I2933	I2861	ARG
L3617	S3497	R3425	R3358	L3301	GLN	V3155	Q3093	A2927	Q2864	SER
K3618	W3498	K3426	L3359	K3302	GLU	L3157	D3094	L2939	L2868	HIS
D3619	I3499	E3429	E3362	S3305	GLU	K3158	D3095	I2942	L2871	GLY
P3620	S3500	ASN	SER	S3306	D3226	R3167	R3098	T2953	D2872	ASP
K3621	H3501	ALA	GLY	L3306	I3227	D3170	A3099	E2956	A2876	PRO
A3622	K3502	SER	SER	L3307	S3228	A3171	K3100	L2967	V2876	ASP
P3623	V3503	ILE	SER	L3308	S3229	K3172	Y3102	E2968	Q2784	ILE
K3624	A3504	ASP	GLU	D3309	S3230	M3173	I3103	A2969	G2879	LEU
L3625	L3505	SER	D3369	N3310	I3231	Q3176	Q3104	K2970	C2880	ARG
G3626	D3507	ALA	E3370	N3311	R3232	K3179	Q3108	Q2971	S2883	TYR
A3627	K3508	LEU	K3372	V3312	S3233	S3182	F3109	T2972	L2884	SER
F3628	D3509	Q3440	V3373	S3313	C3234	I3183	F3110	E2974	Q2885	GLY
K3629	Q3510	A3441	I3374	S3314	F3236	R3186	Q3112	E2975	Q2886	ASP
A3630	V3512	P3443	I3374	Y3315	R3241	C3187	Q3117			
K3631	A3513	A3444	I3374	V3316	K3242	F3188	N3113			
F3632	V3514	L3445	Y3378	L3316	M3243		S3116			
L3633	Q3515	V3446	A3381	S3317	I3243		I3117			
Q3634	E3519	F3447	H3384	K3318	D3244		Q3037			
T3635	E3520	K3449	L3385	N3319	R3247		Y3040			
F3636	I3521		S3386	L3320	Q3248		L3041			
K3637	T3522		E3387	L3321	Q3249		P3042			
K3638	L3583		A3388	A3322			Y3043			
E3639	L3584		V3389	R3323			M3044			
F3640	K3586		Q3390	D3325						
D3641										
K3642										
L3643										
F3644										
Q3645										
K3646										
G3647										

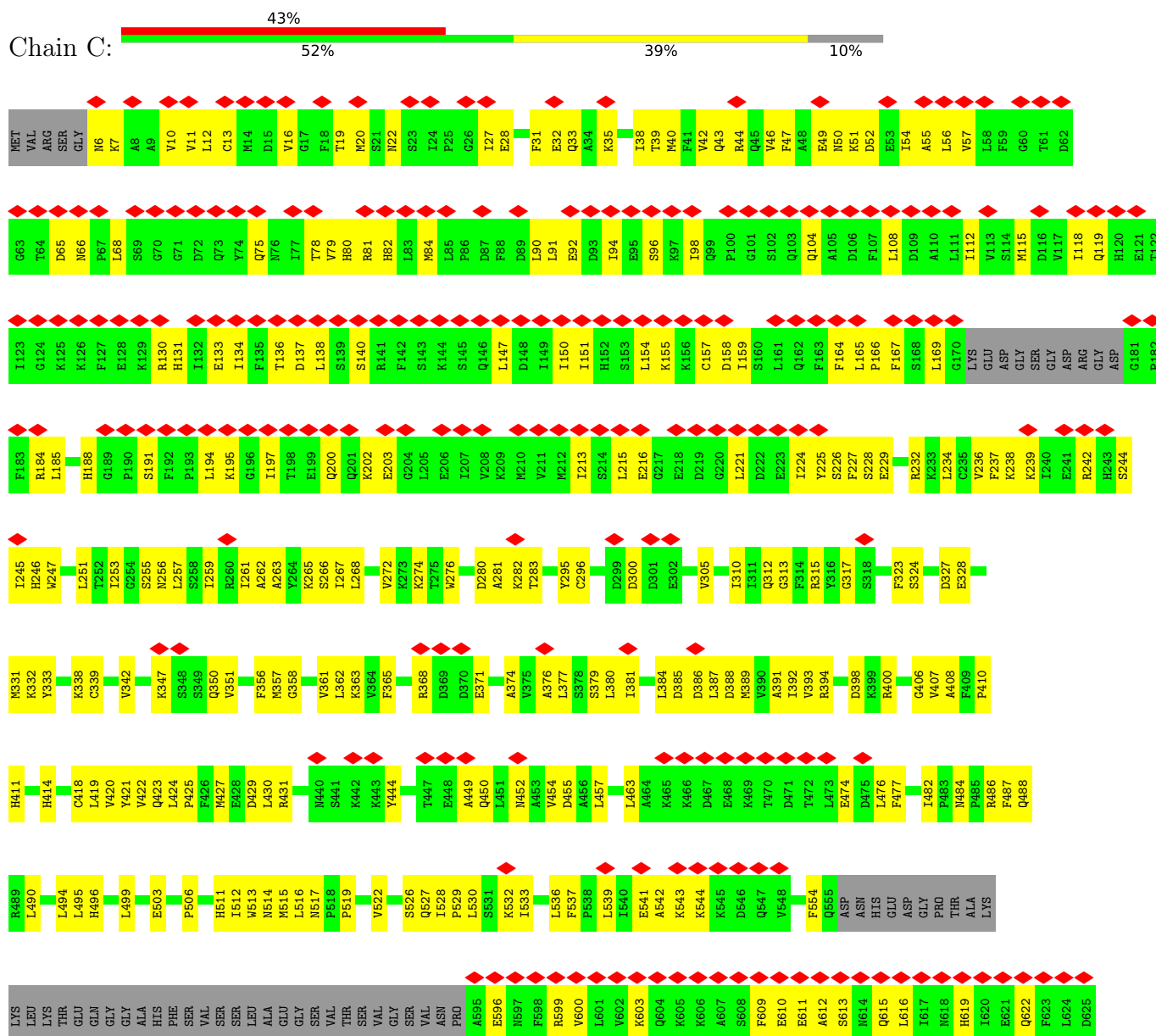


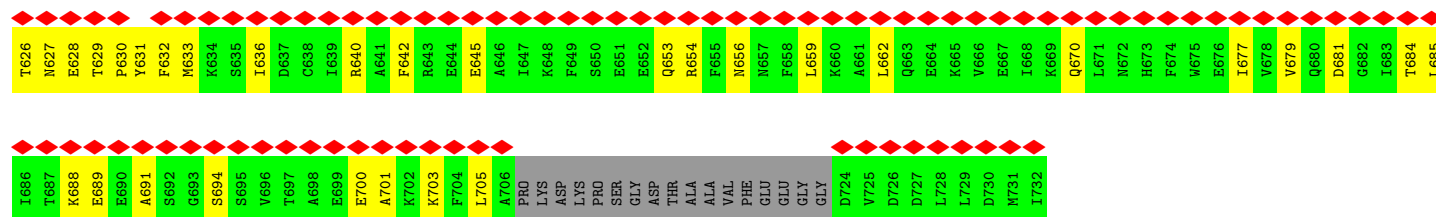
• Molecule 2: X-ray repair cross-complementing protein 6



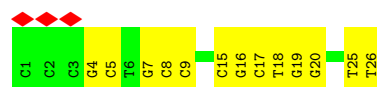


• Molecule 3: X-ray repair cross-complementing protein 5

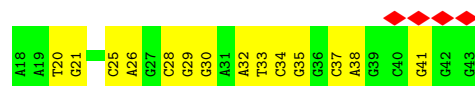




• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190498	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 ($e^-/\text{\AA}^2$)	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.648	Depositor
Minimum map value	-2.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IIX

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	0.23	0/29016	0.54	5/39251 (0.0%)
2	B	0.24	0/4014	0.56	0/5408
3	C	0.19	0/5374	0.46	0/7246
4	D	0.23	0/587	0.38	0/902
5	E	0.23	0/607	0.35	0/936
All	All	0.23	0/39598	0.53	5/53743 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	2
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2547	SER	CA-C-N	11.82	134.62	119.84
1	A	2547	SER	C-N-CA	11.82	134.62	119.84
1	A	407	VAL	N-CA-C	-6.28	107.38	113.53
1	A	3965	ARG	N-CA-C	6.04	118.64	111.33
1	A	976	VAL	N-CA-C	5.06	115.78	110.62

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1175	HIS	Peptide
1	A	3025	PRO	Peptide
1	A	3462	ARG	Peptide
2	B	252	ARG	Peptide

5.2 Too-close contacts

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	28443	0	28622	1225	0
2	B	3937	0	4013	198	0
3	C	5274	0	5275	261	0
4	D	526	0	293	12	0
5	E	540	0	291	14	0
6	A	34	0	0	0	0
All	All	38754	0	38494	1638	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 21.

The worst 5 of 1638 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:B:322:TYR:CE2	3:C:274:LYS:HG3	1.64	1.32
3:C:323:PHE:CE1	3:C:328:GLU:HB3	1.82	1.13
2:B:322:TYR:HE2	3:C:274:LYS:CG	1.68	1.05
1:A:2225:HIS:ND1	1:A:2226:PRO:HD2	1.72	1.04
1:A:3190:LEU:HB3	1:A:3235:LYS:HZ2	1.27	0.98

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	3555/4128 (86%)	3157 (89%)	395 (11%)	3 (0%)	48	76
2	B	486/609 (80%)	418 (86%)	67 (14%)	1 (0%)	43	71
3	C	653/732 (89%)	585 (90%)	68 (10%)	0	100	100
All	All	4694/5469 (86%)	4160 (89%)	530 (11%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2548	PRO
1	A	1021	VAL
2	B	144	SER
1	A	1020	PRO

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	3121/3671 (85%)	3116 (100%)	5 (0%)	87	87
2	B	439/548 (80%)	437 (100%)	2 (0%)	81	82
3	C	585/649 (90%)	584 (100%)	1 (0%)	87	87
All	All	4145/4868 (85%)	4137 (100%)	8 (0%)	85	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	670	GLN
2	B	297	LYS
1	A	4090	ARG
1	A	2285	LEU
2	B	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3660	ASN
2	B	106	GLN
1	A	3743	HIS
1	A	3969	ASN
2	B	174	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
6	1IX	A	4201	-	38,38,38	2.25	10 (26%)	53,54,54	2.12	20 (37%)

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
6	1IX	A	4201	-	-	0/18/26/26	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.32	1.56	1.49
6	A	4201	1IX	C12-C13	5.72	1.47	1.37
6	A	4201	1IX	C11-CL1	4.27	1.83	1.73
6	A	4201	1IX	C21-C20	-3.67	1.36	1.42
6	A	4201	1IX	C24-N26	3.33	1.48	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C18-N19-C20	5.43	121.60	115.43
6	A	4201	1IX	C21-C16-N17	-5.33	119.52	123.04
6	A	4201	1IX	N19-C18-N17	-4.84	122.10	128.67
6	A	4201	1IX	C21-C20-N19	-4.22	118.34	122.82
6	A	4201	1IX	C10-C09-C06	-3.85	107.55	111.20

There are no chirality outliers.

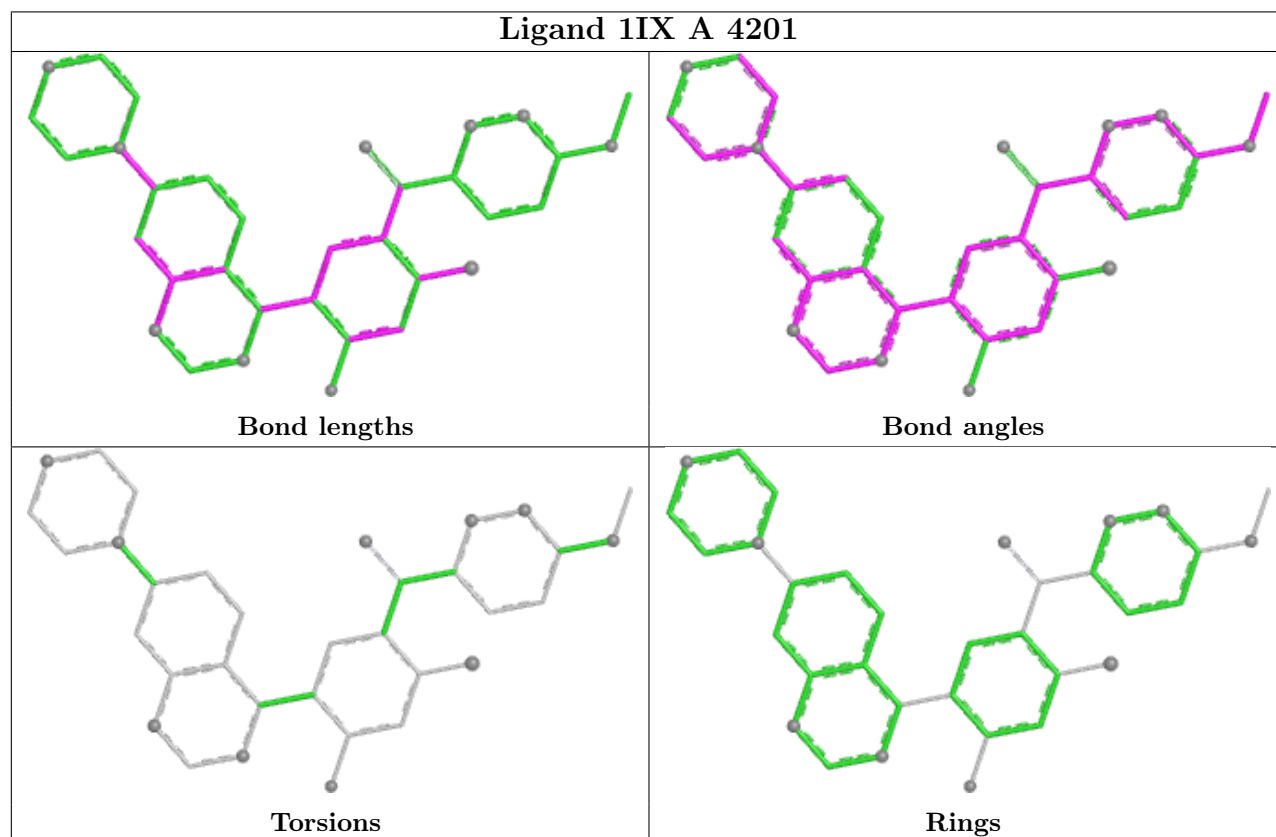
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

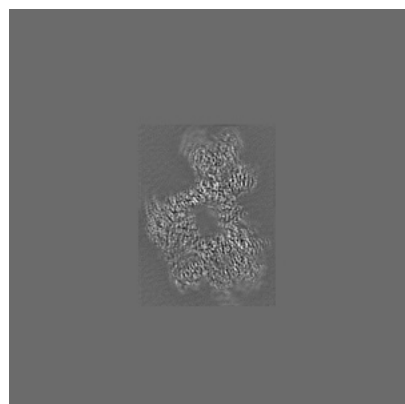
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14546. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

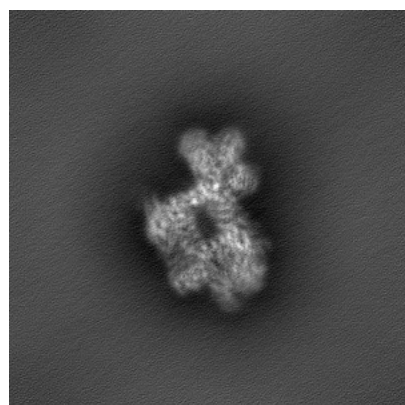


Y

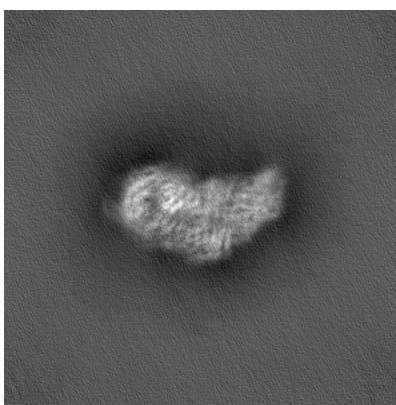


Z

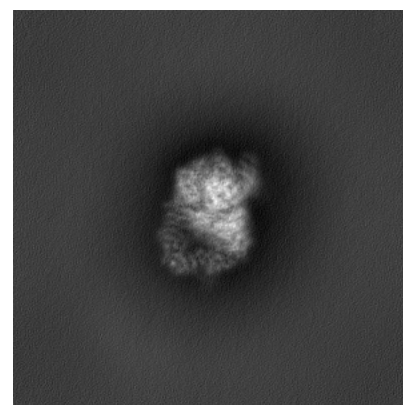
6.1.2 Raw map



X



Y

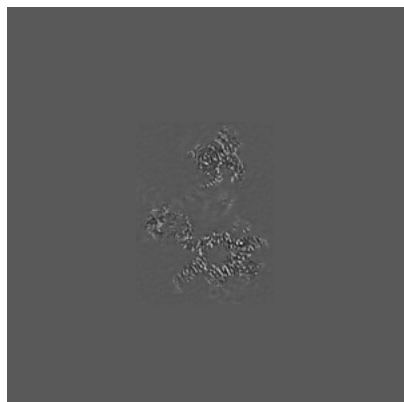


Z

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

6.2 Central slices [i](#)

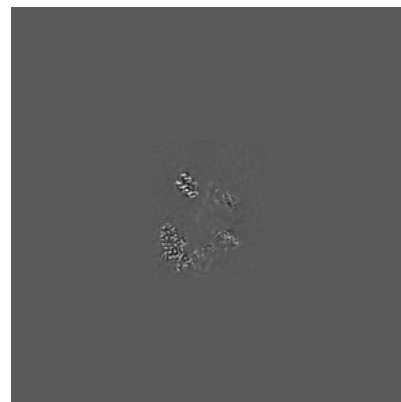
6.2.1 Primary map



X Index: 175

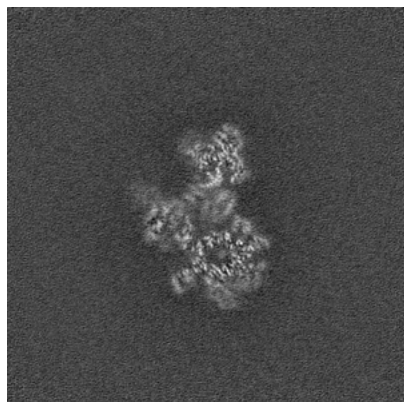


Y Index: 175

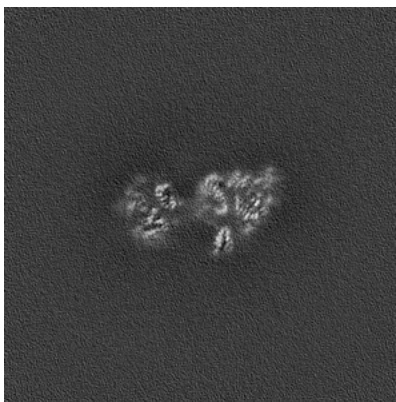


Z Index: 175

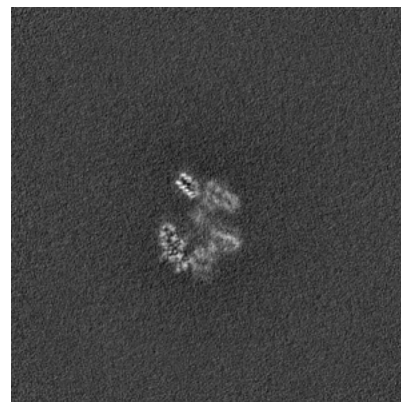
6.2.2 Raw map



X Index: 175



Y Index: 175

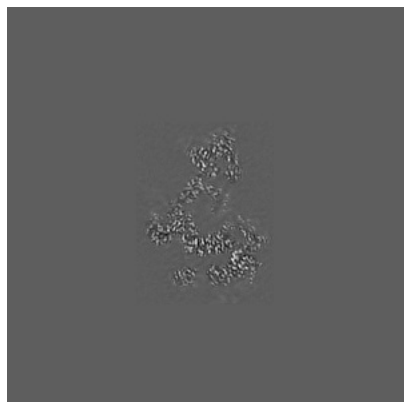


Z Index: 175

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

6.3 Largest variance slices [i](#)

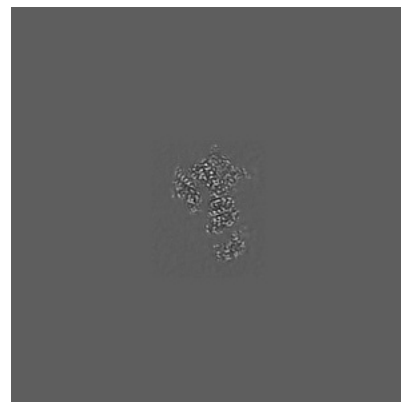
6.3.1 Primary map



X Index: 182

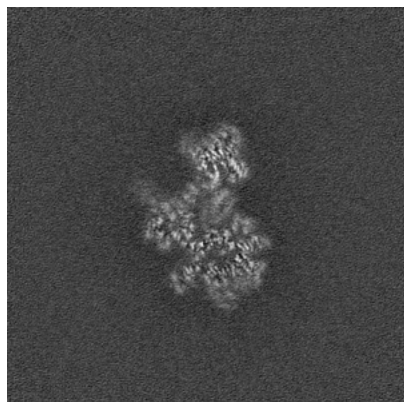


Y Index: 194

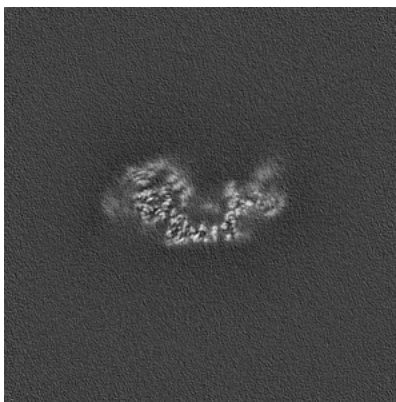


Z Index: 143

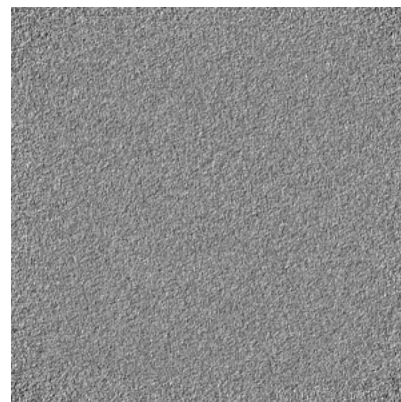
6.3.2 Raw map



X Index: 177



Y Index: 197

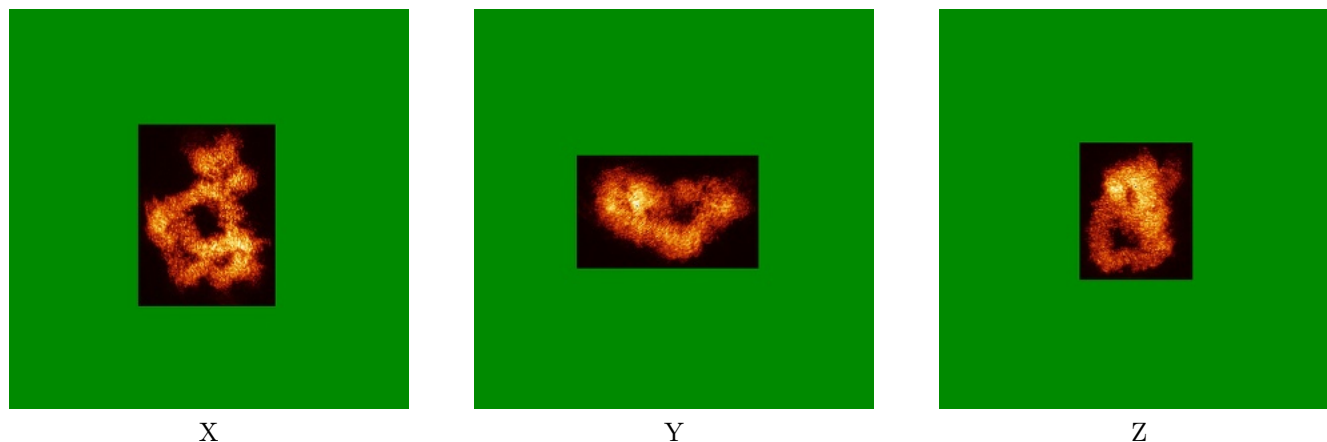


Z Index: 0

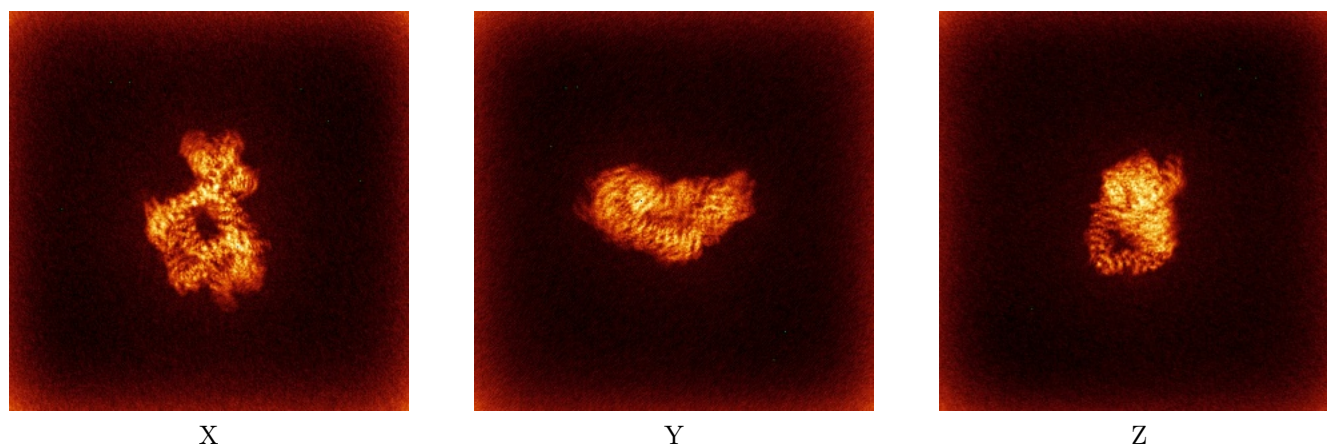
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

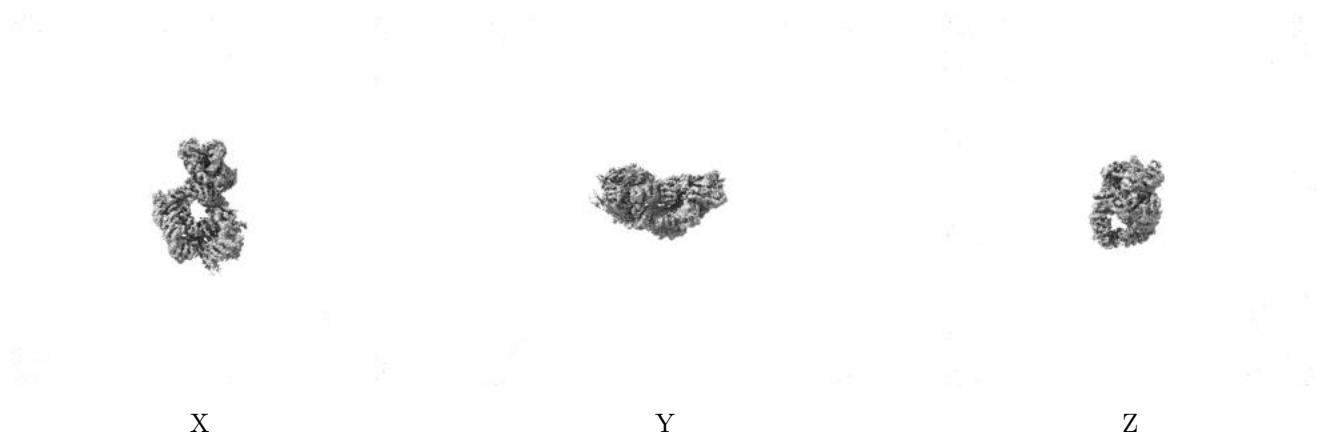
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

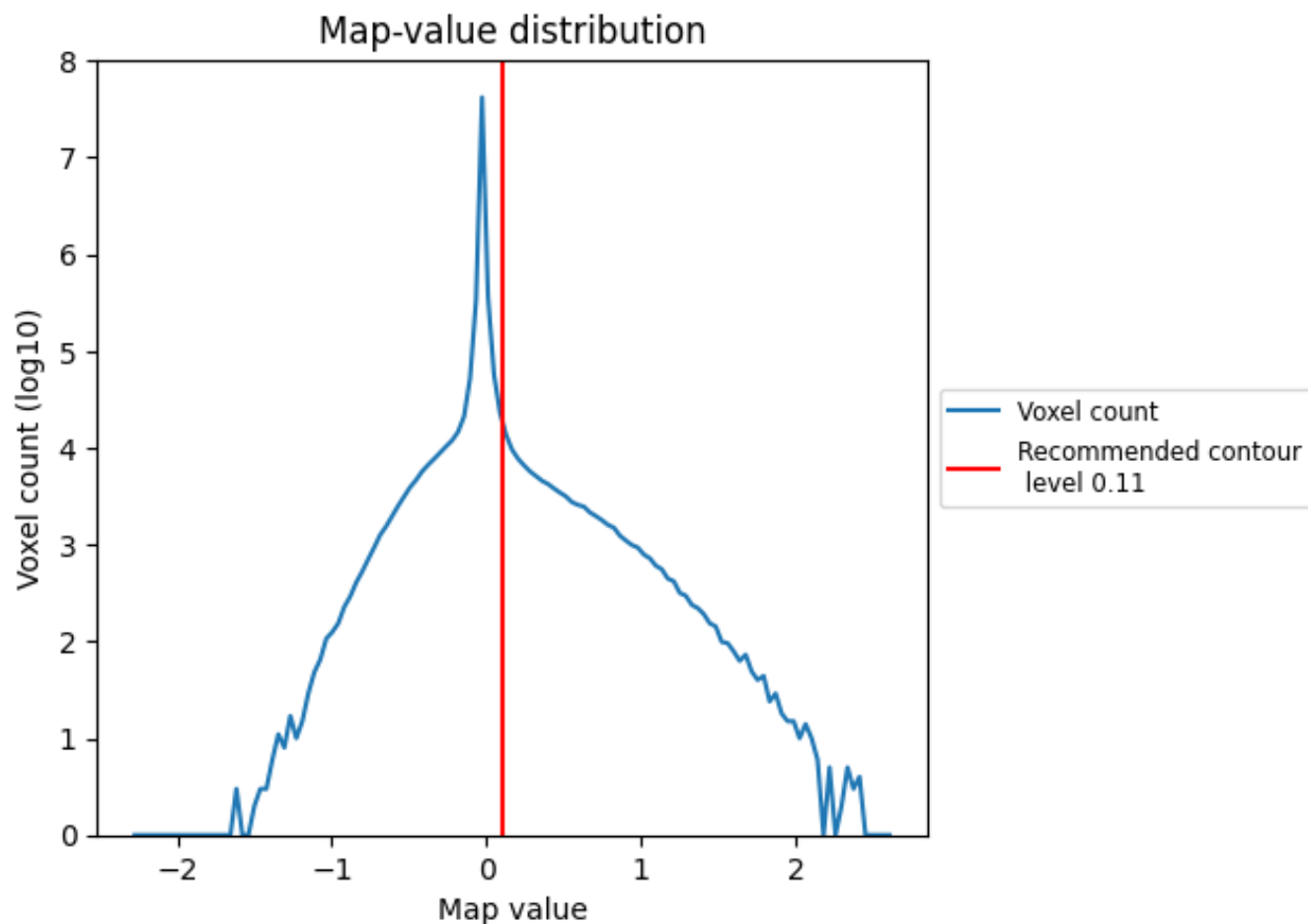
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

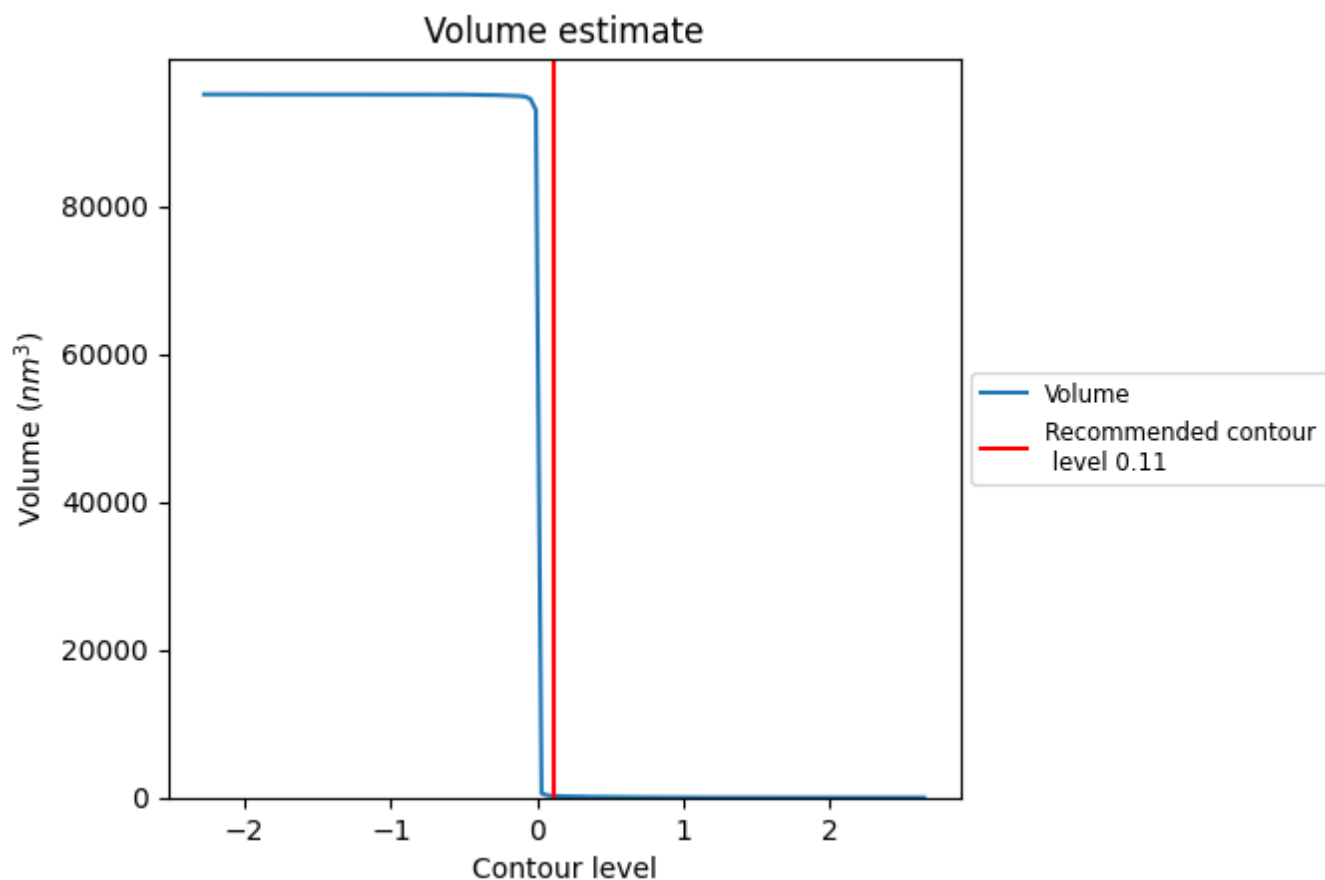
This section contains the results of statistical analysis of the map.

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.

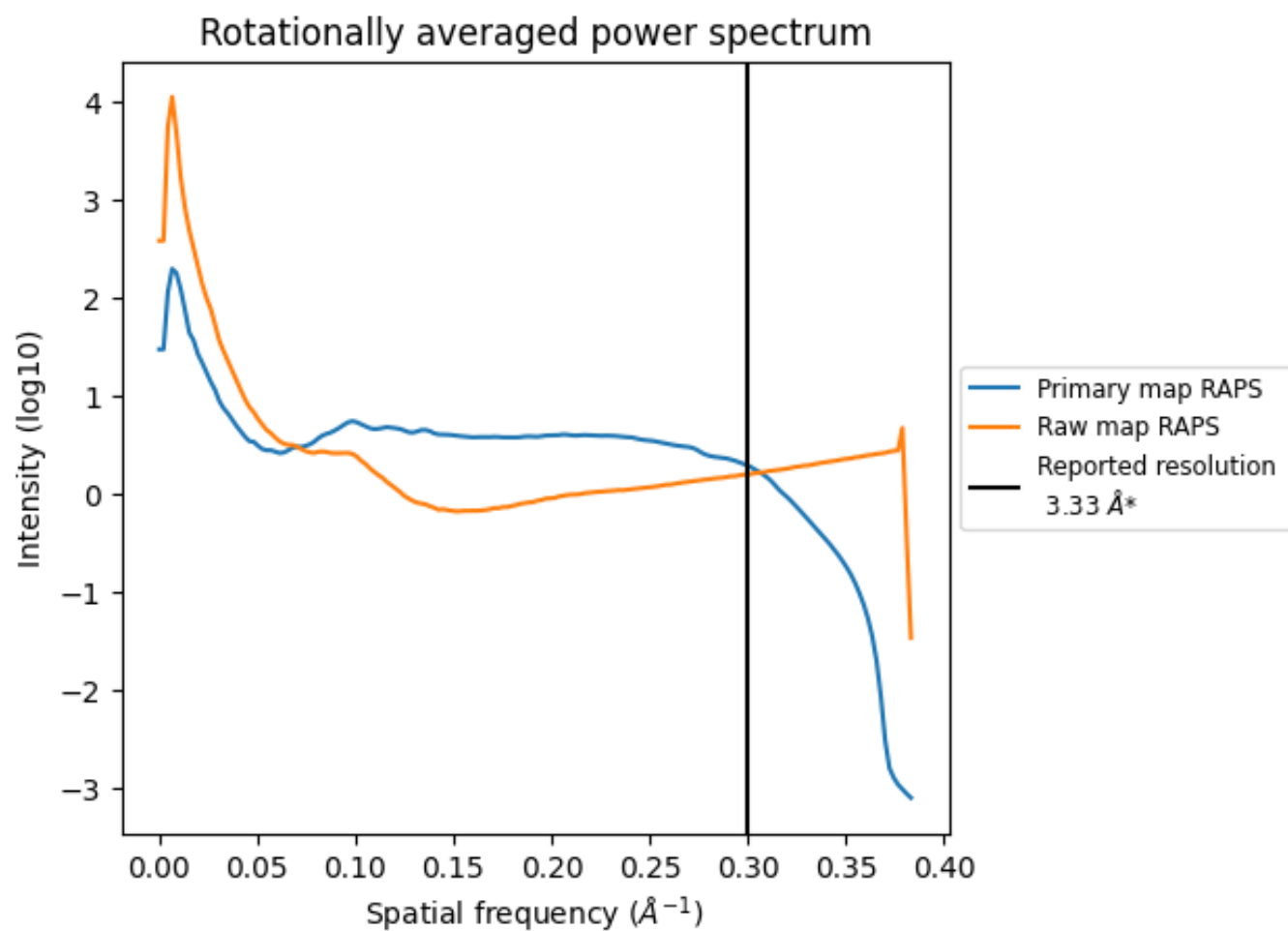
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm³; this corresponds to an approximate mass of 207 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 ⓘ

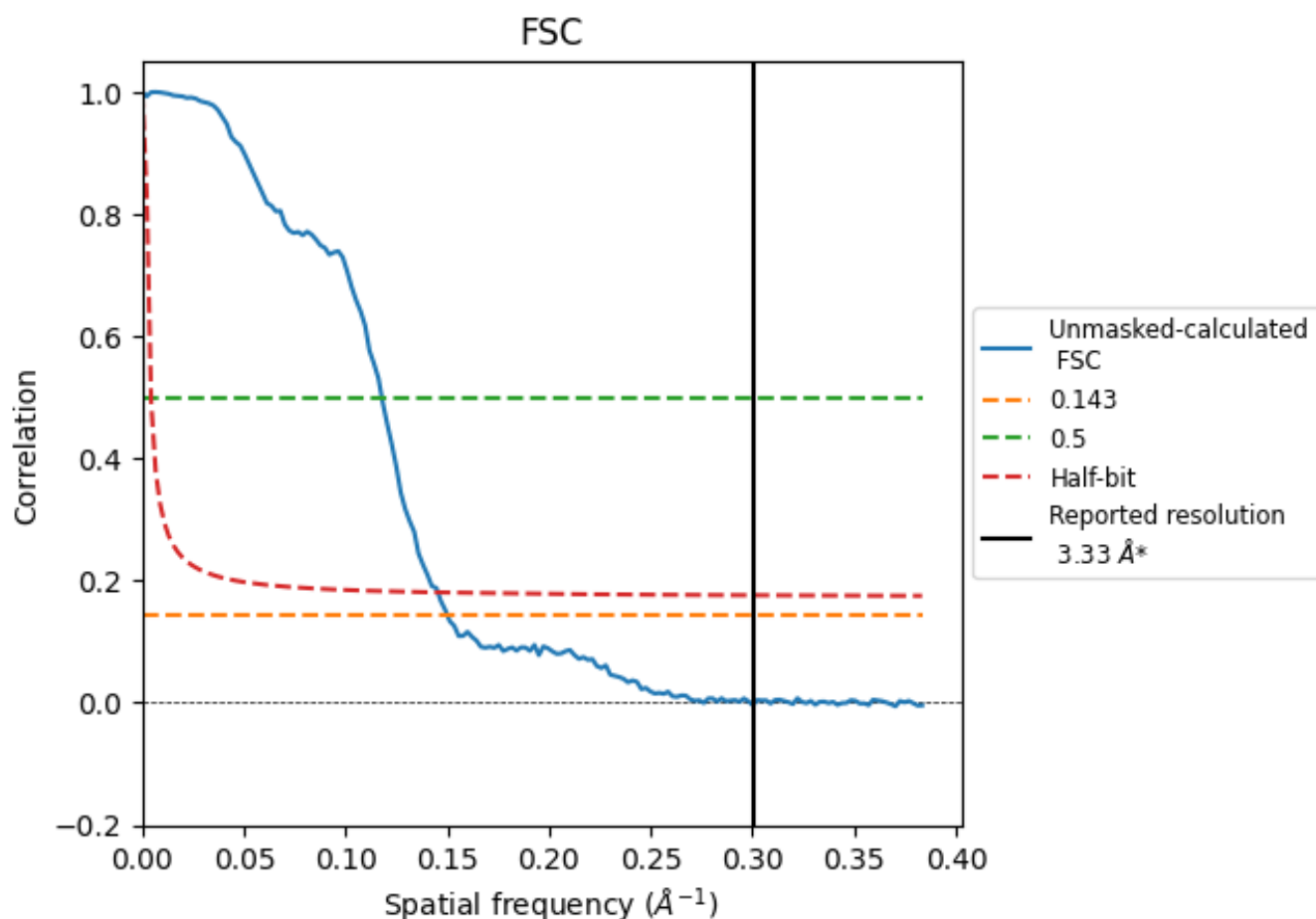


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

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 0.300 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

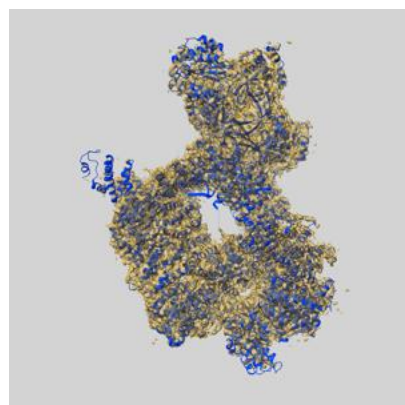
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	8.49	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 3.33 by more than 10 %

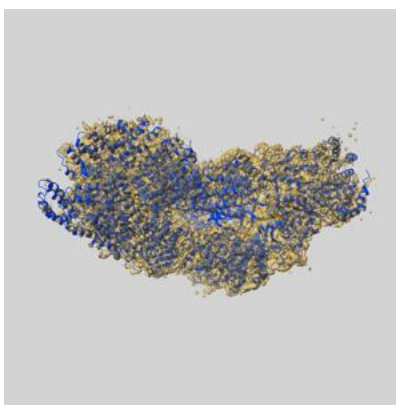
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14546 and PDB model 7Z88. Per-residue inclusion information can be found in section 3 on page 6.

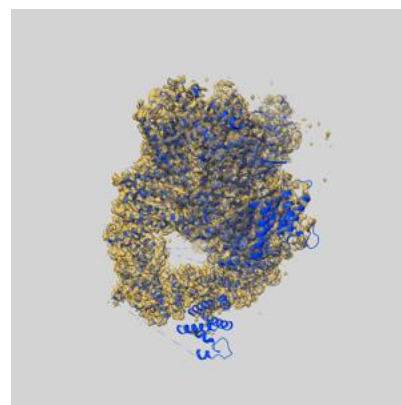
9.1 Map-model overlay [i](#)



X



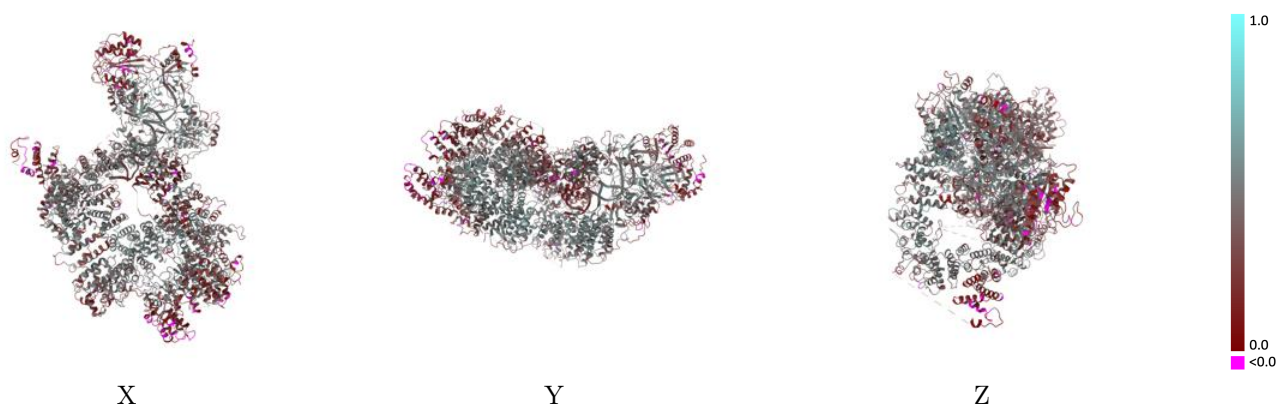
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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](#)

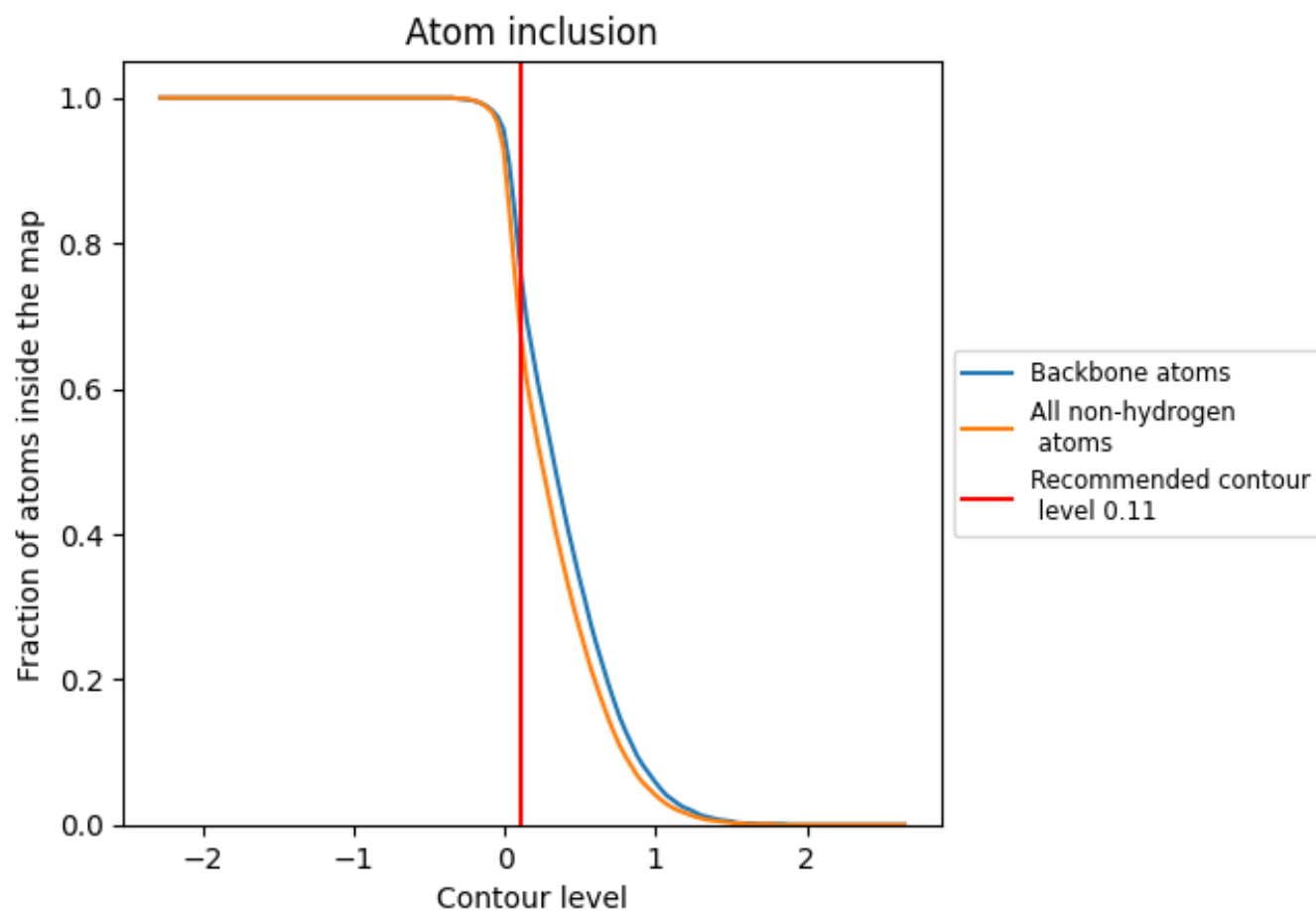


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.3890
A	0.7000	0.4010
B	0.7340	0.4110
C	0.4540	0.3040
D	0.7450	0.4420
E	0.6940	0.3990

