



## wwPDB EM Validation Summary Report ⓘ

Dec 2, 2025 – 12:37 pm GMT

PDB ID : 9I1J / pdb\_00009i1j  
EMDB ID : EMD-52571  
Title : Cryo-EM structure of mouse RNF213:UBE2L3 transthiolation intermediate, chemically stabilized, and ATPgS  
Authors : Grabarczyk, D.B.; Ahel, J.; Clausen, T.  
Deposited on : 2025-01-16  
Resolution : 3.80 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.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

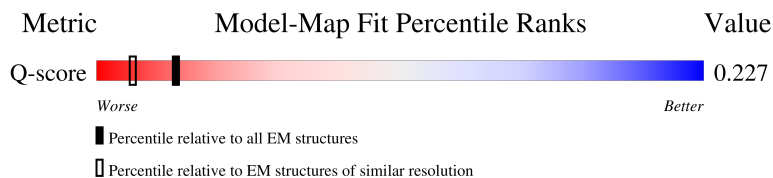
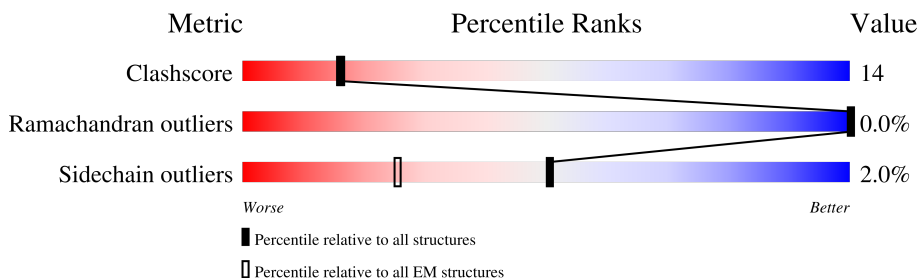
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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	4836	
2	B	166	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ADP	A	5205	-	-	X	-
6	ADP	A	5206	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36793 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4423	Total	C	N	O	S	0	0
			35465	22611	6087	6556	211		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	MET	-	initiating methionine	UNP E9Q555
A	327	ALA	-	expression tag	UNP E9Q555
A	328	SER	-	expression tag	UNP E9Q555
A	329	TRP	-	expression tag	UNP E9Q555
A	330	SER	-	expression tag	UNP E9Q555
A	331	HIS	-	expression tag	UNP E9Q555
A	332	PRO	-	expression tag	UNP E9Q555
A	333	GLN	-	expression tag	UNP E9Q555
A	334	PHE	-	expression tag	UNP E9Q555
A	335	GLU	-	expression tag	UNP E9Q555
A	336	LYS	-	expression tag	UNP E9Q555
A	337	GLY	-	expression tag	UNP E9Q555
A	338	SER	-	expression tag	UNP E9Q555
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

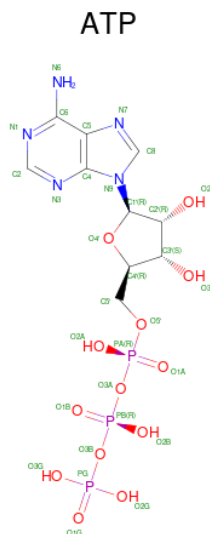
- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	153	Total	C	N	O	S	0	0
			1240	792	214	230	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLY	-	expression tag	UNP P68036
B	-10	TRP	-	expression tag	UNP P68036
B	-9	SER	-	expression tag	UNP P68036
B	-8	HIS	-	expression tag	UNP P68036
B	-7	PRO	-	expression tag	UNP P68036
B	-6	GLN	-	expression tag	UNP P68036
B	-5	PHE	-	expression tag	UNP P68036
B	-4	GLU	-	expression tag	UNP P68036
B	-3	LYS	-	expression tag	UNP P68036
B	-2	PRO	-	expression tag	UNP P68036
B	-1	GLY	-	expression tag	UNP P68036
B	0	SER	-	expression tag	UNP P68036
B	17	SER	CYS	conflict	UNP P68036
B	137	SER	CYS	conflict	UNP P68036

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Zn 2 2	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

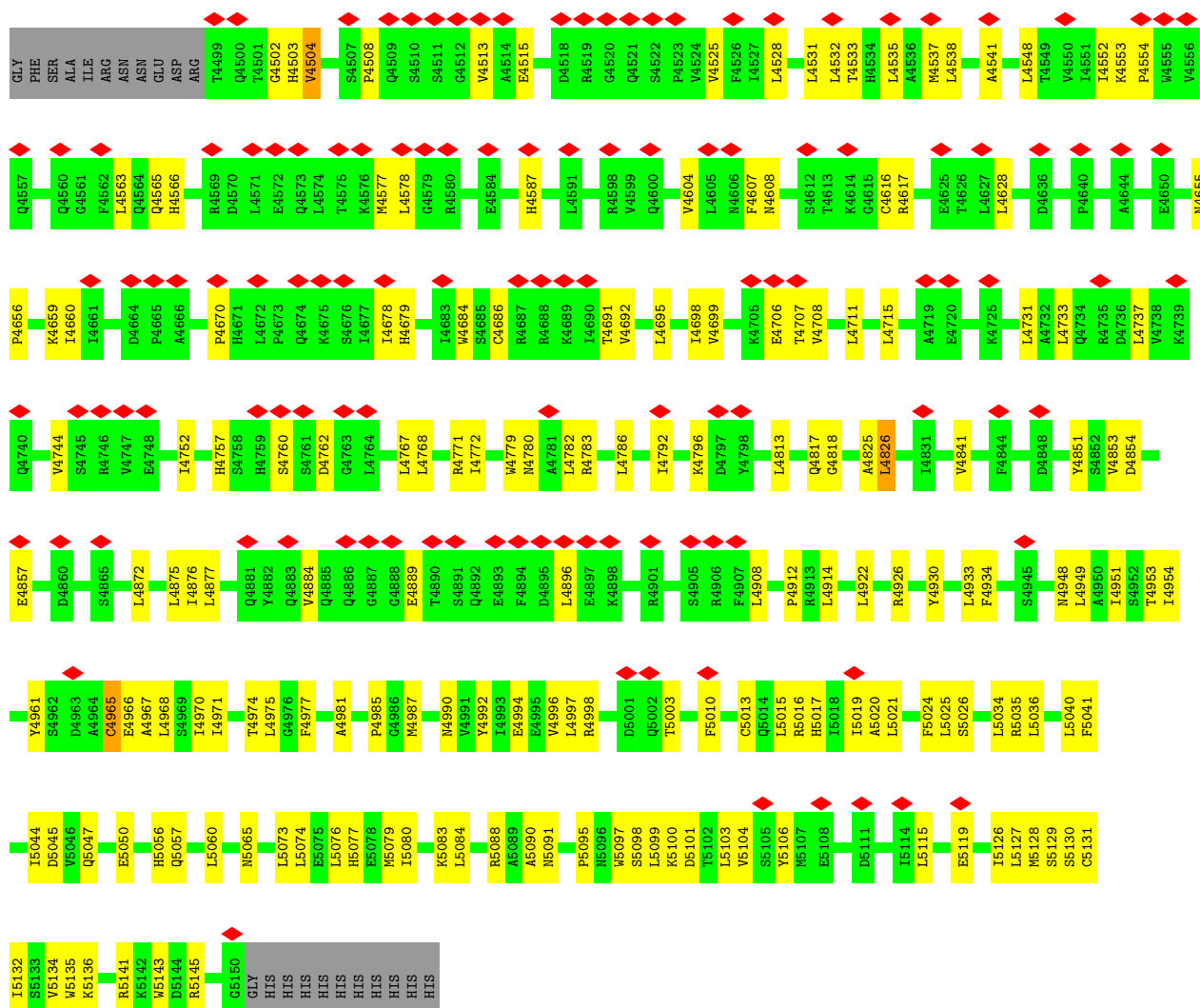




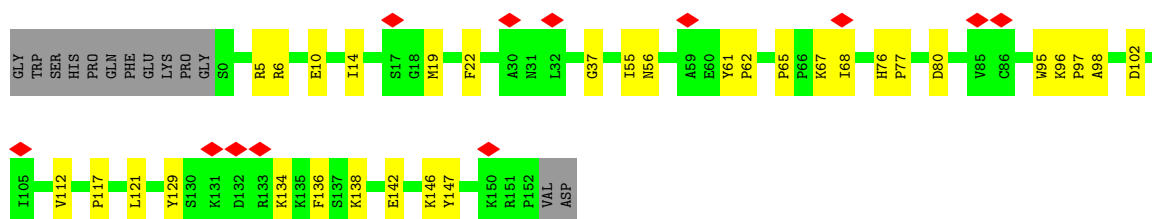
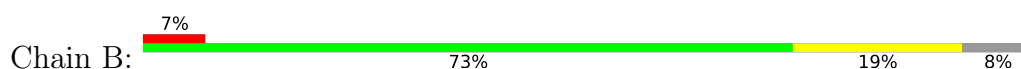


Q3260	A3261	H3262	L3263	R3264	K3265	T3266	H3267	H3268	E3269	C3185	C3270	S3187	A3186	V3188	V3189	L3190	L3191	Q3192	V3097	K3098	H3102	L3107	E3112	V3115	V3116	F3120	P3121	V3122	P3123	L3124	I3125	K3130	H3131	V3132	L3133	D3134	M3135	V3138	W3142	Q3143	K3144	S3145	I3146	V3147	L3150	F3157	A3158	D3159	V3160	K3161	A3162	L3259						
D3163	Q3164	F3165	V3176	F3177	L3178	Q3179	Q3085	K3086	V3087	V3088	D3089	L3090	G3091	L3092	H3095	R3096	V3097	K3098	H3102	L3107	E3112	V3115	V3116	F3120	P3121	V3122	P3123	L3124	I3125	K3130	H3131	V3132	L3133	D3134	M3135	V3138	W3142	Q3143	K3144	S3145	I3146	V3147	L3150	F3157	A3158	D3159	V3160	K3161	A3162	L3259								
Q2981	N2982	I2983	Y2984	F2985	G2986	P2987	Q2988	A2989	S2990	S2991	R2992	G2993	L2994	D2995	G2996	A2997	Y3001	L3002	L3003	V3004	L3005	T3006	V3010	A3011	L3012	Q3013	L3014	L3015	Q3016	Q3017	T3018	F3019	F3020	Q3023	Q3024	P3025	I3028	F3029	G3030	S3031	P3034	Q3035	I3046	V3049	M3053	M3058	L3061	L3062										
C2786	Q2791	S2800	V2801	V2802	V2803	L2804	V2807	G2808	L2809	A2810	S2813	F2814	K2815	L2816	P2817	L2818	K2819	T2820	L2821	H2822	P2823	L2824	L2825	T2830	E2831	Y2837	K2838	L2839	V2840	G2841	F2842	S2846	R2847	N2848	S2849	L2850	A2853	K2854	N2855	R2856	L2857	G2858	L2859	V2860	V2861	P2866	E2868	K2869										
I2872	E2876	G2877	L2878	C2879	L2884	V2885	Q2886	D2887	K2888	L2889	R2890	Y2900	L2914	R2915	Y2917	Y2918	S2919	L2920	I2921	K2922	M2923	V2924	F2925	K2932	L2935	I2940	T2941	L2945	R2946	N2947	F2948	S2949	L2957	F2960	T2961	A2967	R2968	Y2969	K2970	E2971	E2972	V2973	V2976	E2977	L2978													
Q2981	N2982	I2983	Y2984	F2985	G2986	P2987	Q2988	A2989	S2990	S2991	R2992	G2993	L2994	D2995	G2996	A2997	Y3001	L3002	L3003	V3004	L3005	T3006	V3010	A3011	L3012	Q3013	L3014	L3015	Q3016	Q3017	T3018	F3019	F3020	Q3023	Q3024	P3025	I3028	F3029	G3030	S3031	P3034	Q3035	I3046	V3049	M3053	M3058	L3061	L3062										
N3066	L3075	Y3079	Q3085	K3086	V3087	V3088	D3089	L3090	G3091	L3092	H3095	R3096	V3097	K3098	H3102	L3107	E3112	V3115	V3116	F3120	P3121	V3122	P3123	L3124	I3125	K3130	H3131	V3132	L3133	D3134	M3135	V3138	W3142	Q3143	K3144	S3145	I3146	V3147	L3150	F3157	A3158	D3159	V3160	K3161	A3162	L3259												
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Q3260	A3261	H3262	L3263	R3264	K3265	T3266	H3267	H3268	E3269	C3185	C3270	S3187	A3186	V3188	V3189	L3190	L3191	Q3192	V3097	K3098	H3102	L3107	E3112	V3115	V3116	F3120	P3121	V3122	P3123	L3124	I3125	K3130	H3131	V3132	L3133	D3134	M3135	V3138	W3142	Q3143	K3144	S3145	I3146	V3147	L3150	F3157	A3158	D3159	V3160	K3161	A3162	L3259						
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D3200	L3201	T3202	K3203	S3204	R3205	H3206	L3207	T3208	F3209	G3210	S3211	R3212	A3213	V3214	T3215	L3216	T3217	V3218	H3219	K3220	L3221	E3222	V3223	F3224	G3225	H3226	T3227	P3228	L3229	M3230	N3231	O3232	A3233	B3234	C3235	D3236	E3237	F3238	G3239	H3240	I3241	J3242	K3243	L3244	M3245	N3246	O3247	P3248	Q3249	R3250	S3251	T3252	U3253	V3254	W3255	X3256	Y3257	Z3258
D3200	L3201	T3202	K3203	S3204	R3205	H3206	L3207	T3208	F3209	G3210	S3211	R3212	A3213	V3214	T3215	L3216	T3217	V3218	H3219	K3220	L3221	E3222	V3223	F3224	G3225	H3226	T3227	P3228	L3229	M3230	N3231	O3232	A3233	B3234	C3235	D3236	E3237	F3238	G3239	H3240	I3241	J3242	K3243	L3244	M3245	N3246	O3247	P3248	Q3249	R3250	S3251	T3252	U3253	V3254	W3255	X3256	Y3257	Z3258
D3200	L3201	T3202	K3203	S3204	R3205	H3206	L3207	T3208	F3209	G3210	S3211	R3212	A3213	V3214	T3215	L3216	T3217	V3218	H3219	K3220	L3221	E3222	V3223	F3224	G3225	H3226	T3227	P3228	L3229	M3230	N3231	O3232	A3233	B3234	C3235	D3236	E3237	F3238	G3239	H3240	I3241	J3242	K3243	L3244	M3245	N3246	O3247	P3248	Q3249	R3250	S3251	T3252	U3253	V3254	W3255	X3256	Y3257	Z3258
D3200	L3201	T3202	K3203	S3204	R3205	H3206	L3207	T3208	F3209	G3210	S3211	R3212	A3213	V3214	T3215	L3216	T3217	V3218	H3219	K3220	L3221	E3222	V3223	F3224	G3225	H3226	T3227	P3228	L3229	M3230	N3231	O3232	A3233	B3234	C3235	D3236	E3237	F3238	G3239	H3240	I3241	J3242	K3243	L3244	M3245	N3246	O3247	P3248	Q3249	R3250	S3251	T3252	U3253	V3254	W3255	X3256	Y3257	Z3258
D3200	L3201	T3202	K3203	S3204	R3205	H3206	L3207	T3208	F3209	G3210	S3211	R3212	A3213	V3214	T3215	L3216	T3217	V3218	H3219</																																							





• Molecule 2: Ubiquitin-conjugating enzyme E2 L3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0047	Depositor
Map size (Å)	379.96, 379.96, 379.96	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	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, ADP, ATP, 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	0.15	0/36204	0.41	4/48982 (0.0%)
2	B	0.16	0/1271	0.40	0/1719
All	All	0.15	0/37475	0.41	4/50701 (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	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	4604	VAL	N-CA-C	-5.66	106.97	112.29
1	A	748	GLU	CA-C-N	-5.57	113.41	122.65
1	A	748	GLU	C-N-CA	-5.57	113.41	122.65
1	A	3711	GLN	CA-CB-CG	5.27	124.64	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4165	GLU	Peptide
1	A	641	ILE	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	35465	0	35592	1019	0
2	B	1240	0	1240	25	0
3	A	31	0	12	6	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	54	0	24	28	0
All	All	36793	0	36868	1037	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 14.

The worst 5 of 1037 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)
1:A:2704:ALA:HB3	6:A:5206:ADP:N6	1.45	1.31
1:A:2704:ALA:CB	6:A:5206:ADP:HN61	1.65	1.09
1:A:2922:LYS:NZ	6:A:5206:ADP:H1'	1.85	0.92
1:A:717:MET:HE1	1:A:749:ASN:HD21	1.40	0.86
1:A:2757:PHE:HA	1:A:2760:LEU:HD12	1.57	0.84

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	4393/4836 (91%)	4059 (92%)	332 (8%)	2 (0%)	100 100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	151/166 (91%)	150 (99%)	1 (1%)	0	100	100
All	All	4544/5002 (91%)	4209 (93%)	333 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3122	VAL
1	A	4166	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	3968/4342 (91%)	3887 (98%)	81 (2%)	50	68
2	B	135/148 (91%)	135 (100%)	0	100	100
All	All	4103/4490 (91%)	4022 (98%)	81 (2%)	50	68

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3579	THR
1	A	4752	ILE
1	A	3678	THR
1	A	4262	GLN
1	A	4965	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2981	GLN
1	A	3673	GLN
1	A	3016	GLN
1	A	3541	ASN
1	A	3777	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	ADP	A	5206	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
6	ADP	A	5205	-	24,29,29	0.97	1 (4%)	29,45,45	1.45	5 (17%)
3	ATP	A	5201	-	26,33,33	0.59	0	31,52,52	0.82	2 (6%)

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	ADP	A	5206	-	-	7/12/32/32	0/3/3/3
6	ADP	A	5205	-	-	7/12/32/32	0/3/3/3
3	ATP	A	5201	-	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5205	ADP	C5-C4	2.60	1.47	1.40
6	A	5206	ADP	C5-C4	2.51	1.47	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5206	ADP	PA-O3A-PB	-4.05	118.92	132.83
6	A	5205	ADP	PA-O3A-PB	-3.56	120.62	132.83
6	A	5206	ADP	N3-C2-N1	-3.05	123.91	128.68
6	A	5205	ADP	N3-C2-N1	-3.02	123.96	128.68
6	A	5206	ADP	C3'-C2'-C1'	3.00	105.50	100.98

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

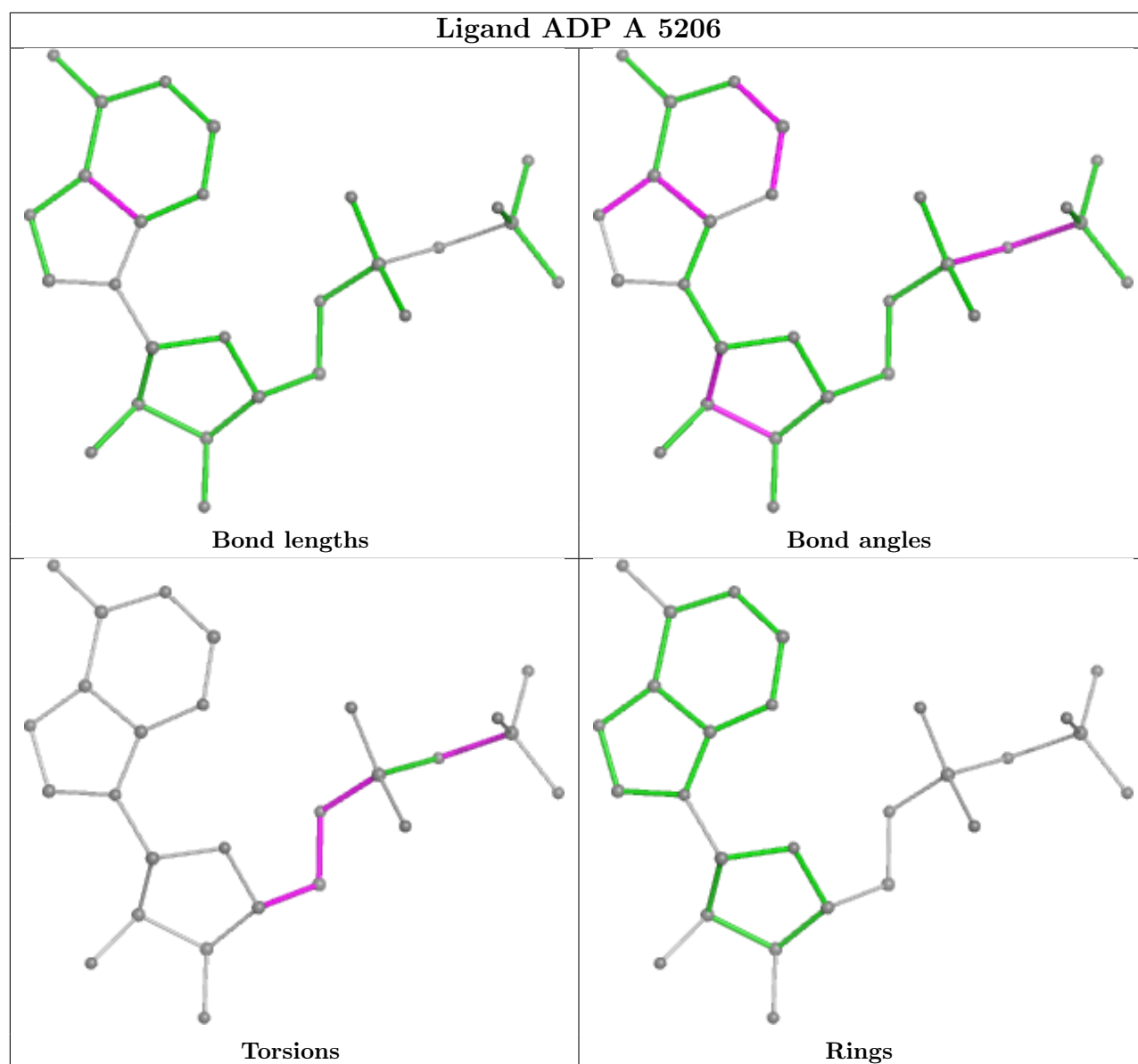
Mol	Chain	Res	Type	Atoms
3	A	5201	ATP	C5'-O5'-PA-O1A
3	A	5201	ATP	O4'-C4'-C5'-O5'
6	A	5205	ADP	C5'-O5'-PA-O1A
6	A	5205	ADP	C5'-O5'-PA-O2A
6	A	5205	ADP	C5'-O5'-PA-O3A

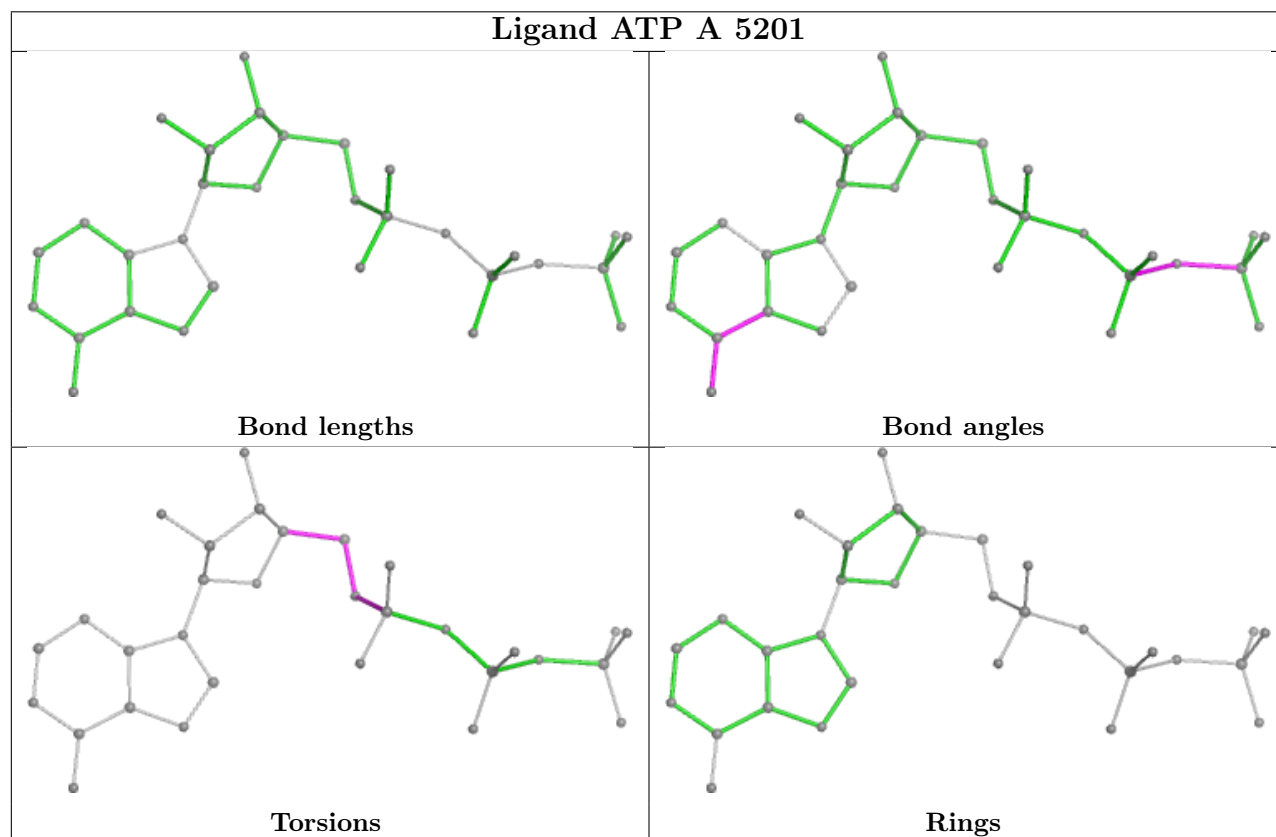
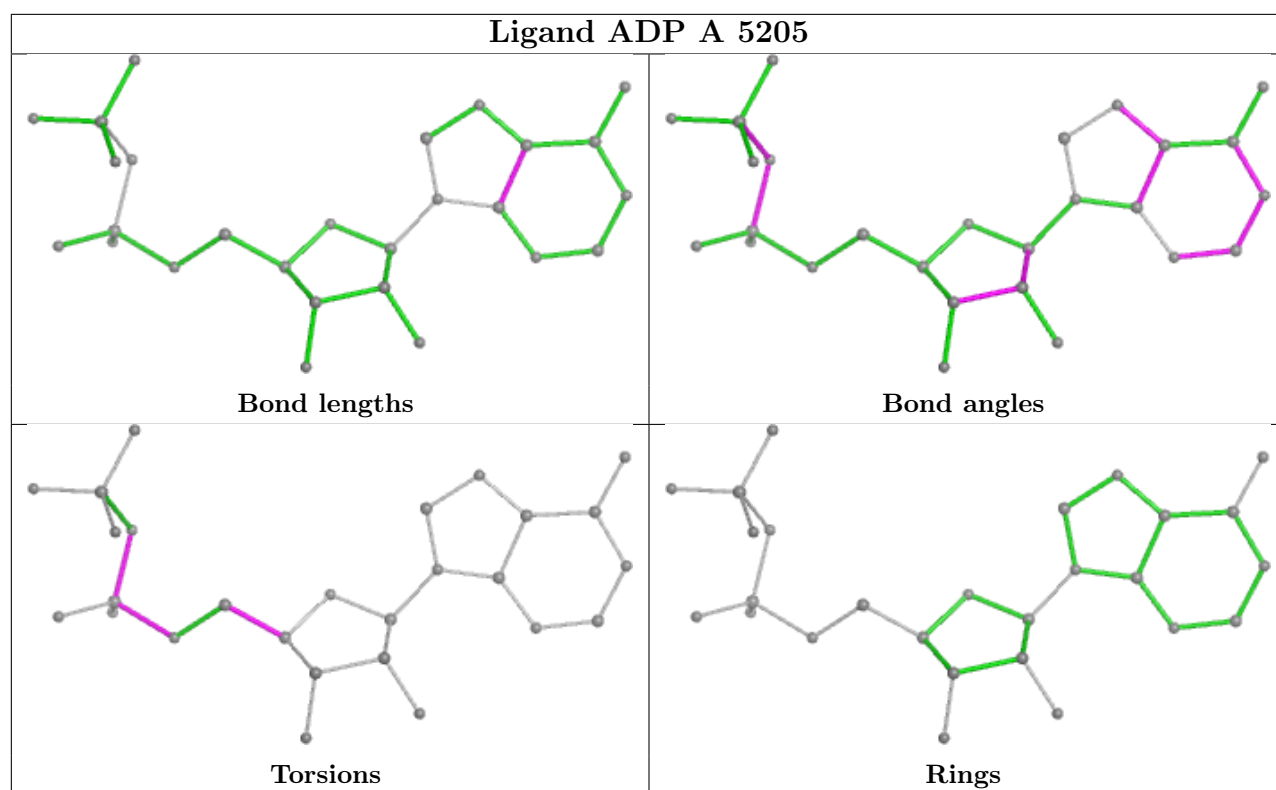
There are no ring outliers.

3 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5206	ADP	9	0
6	A	5205	ADP	19	0
3	A	5201	ATP	6	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.

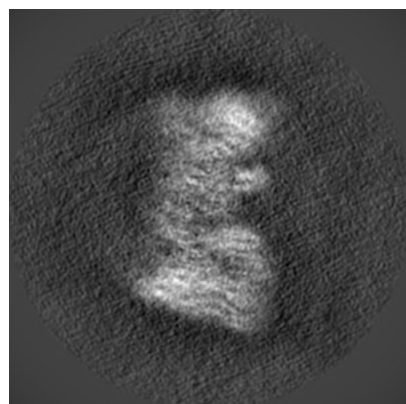
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52571. These allow visual inspection of the internal detail of the map and identification of artifacts.

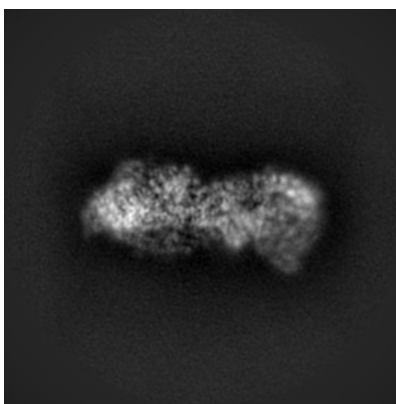
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

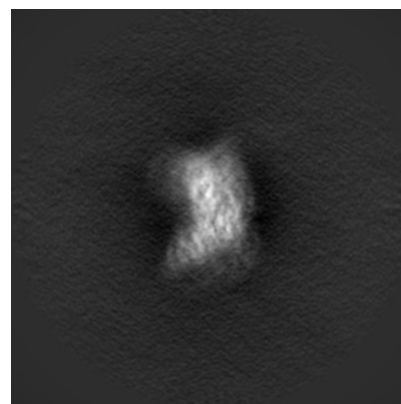
#### 6.1.1 Primary map



X

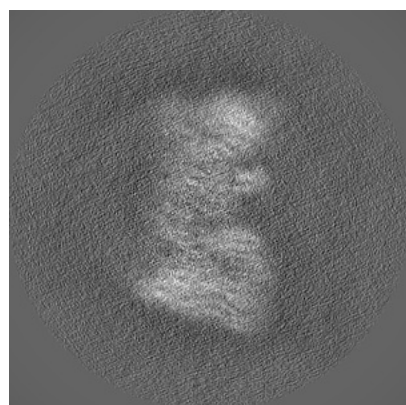


Y

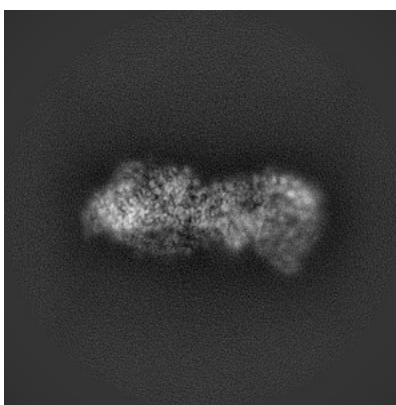


Z

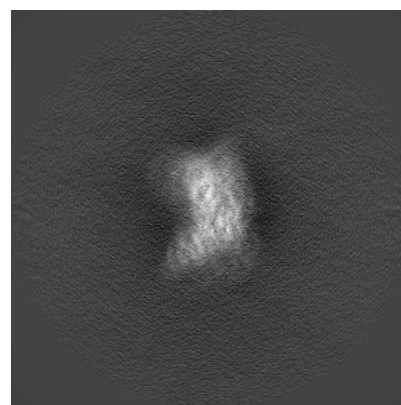
#### 6.1.2 Raw map



X



Y

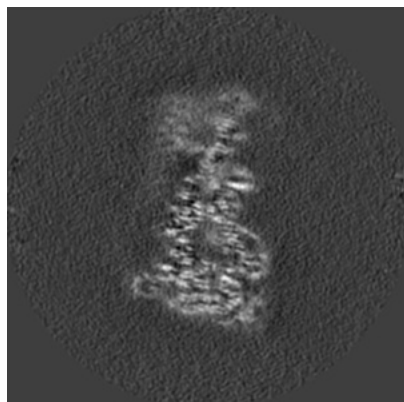


Z

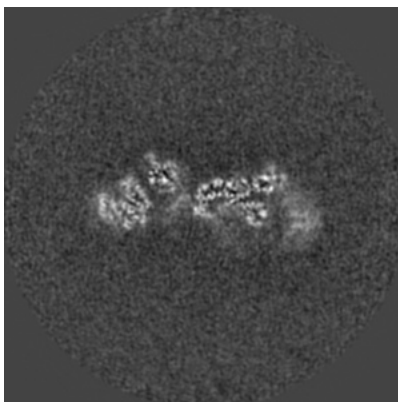
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

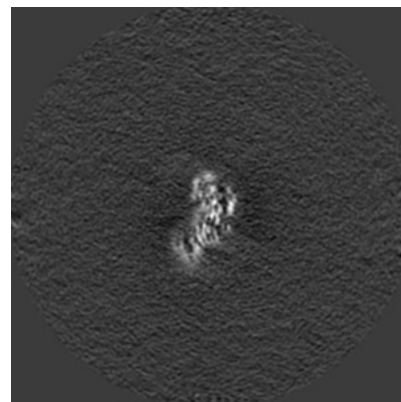
### 6.2.1 Primary map



X Index: 161

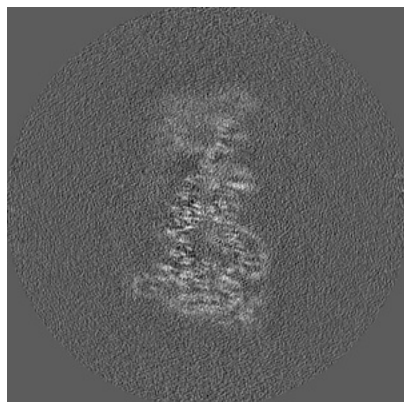


Y Index: 161

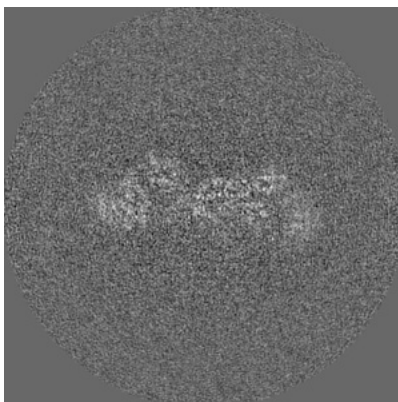


Z Index: 161

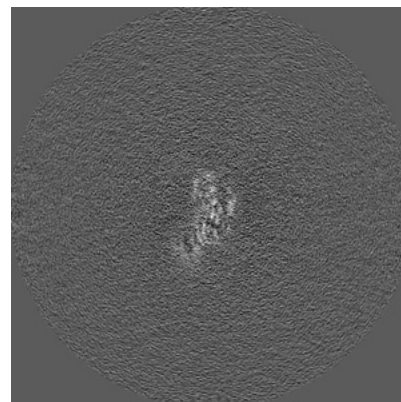
### 6.2.2 Raw map



X Index: 161



Y Index: 161



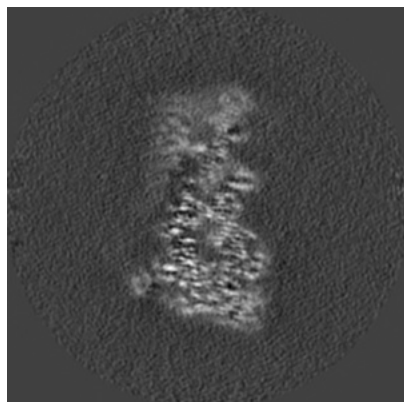
Z Index: 161

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

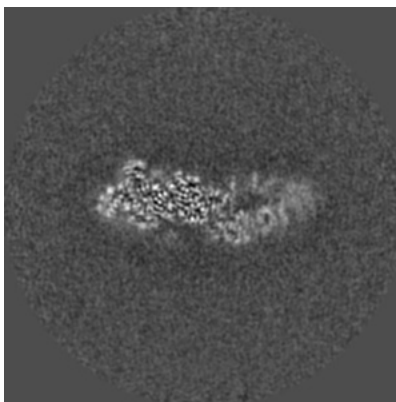


## 6.3 Largest variance slices [i](#)

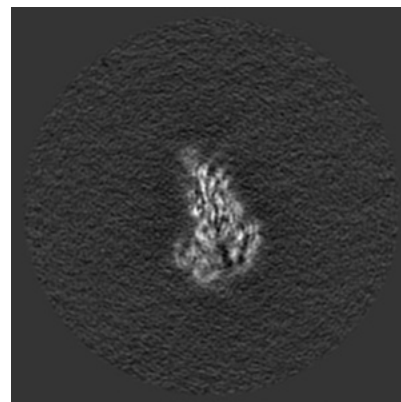
### 6.3.1 Primary map



X Index: 159

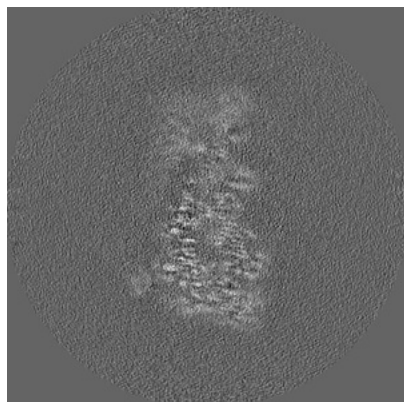


Y Index: 142

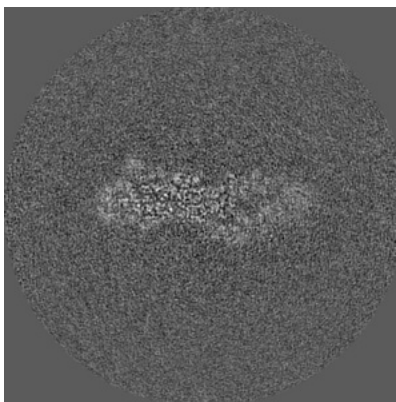


Z Index: 101

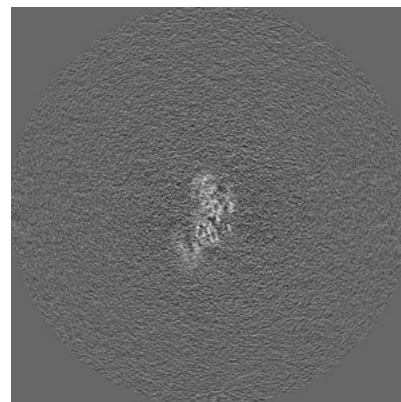
### 6.3.2 Raw map



X Index: 159



Y Index: 145



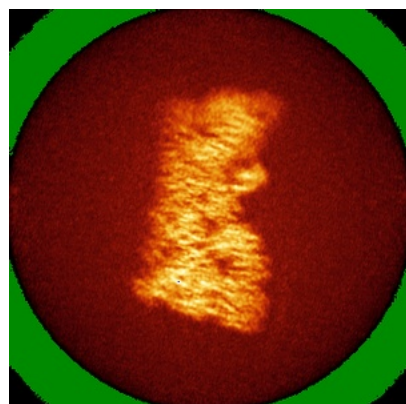
Z Index: 160

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

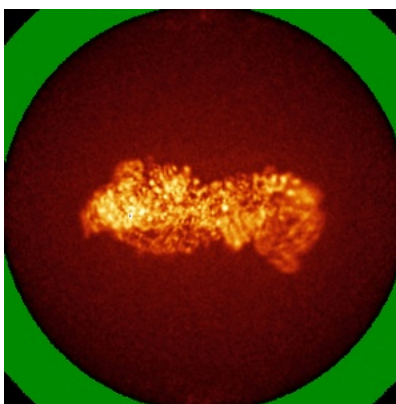


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

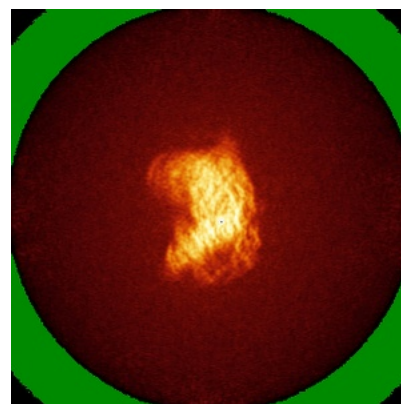
### 6.4.1 Primary map



X

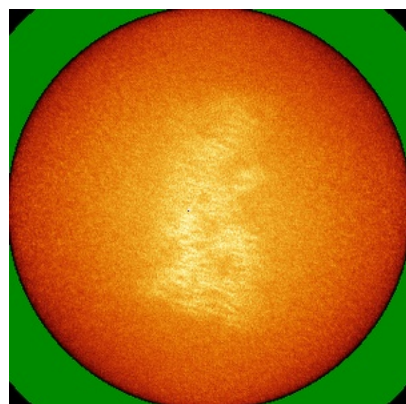


Y

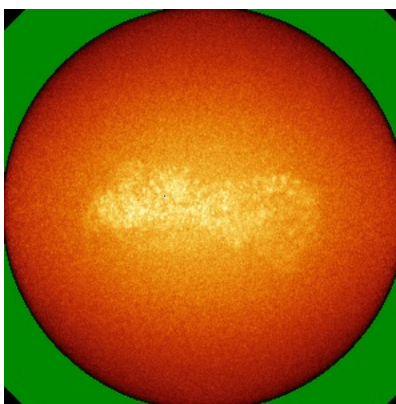


Z

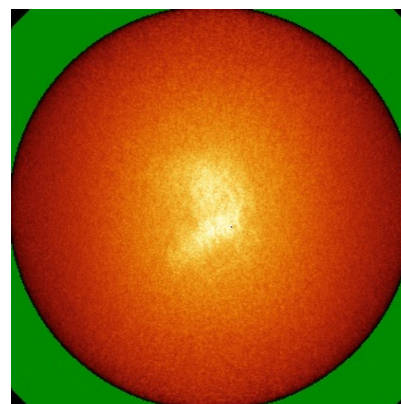
### 6.4.2 Raw map



X



Y

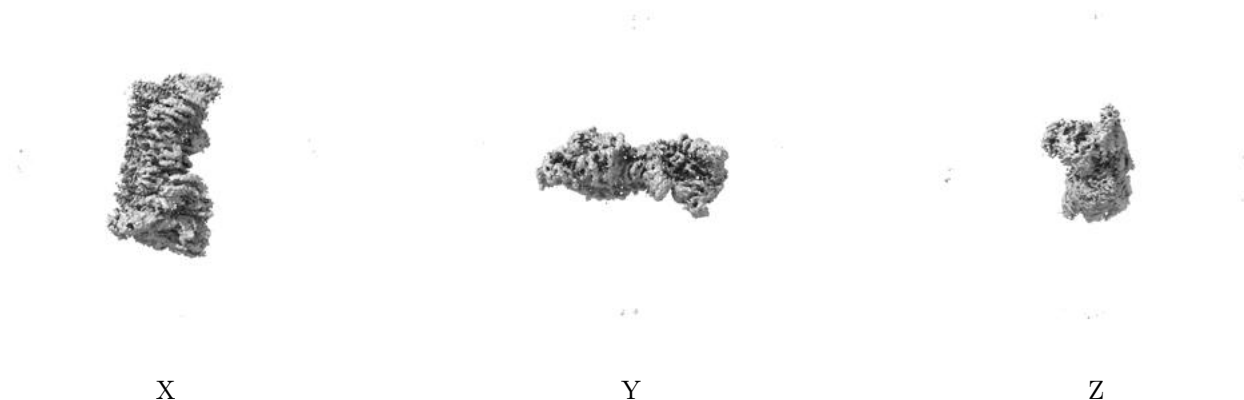


Z

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.

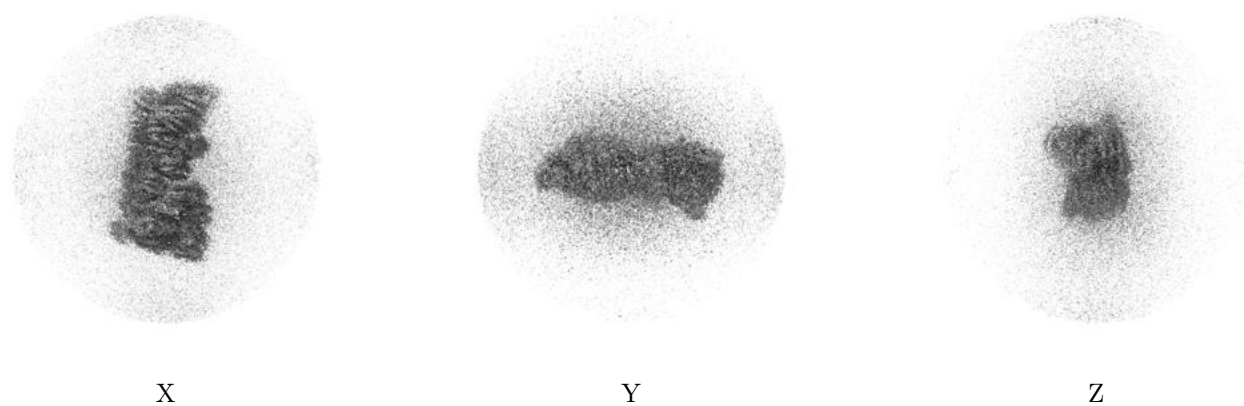
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0047. 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.

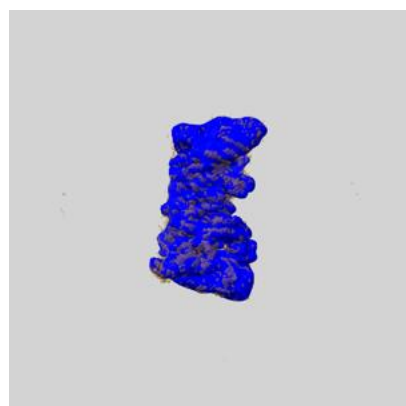
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

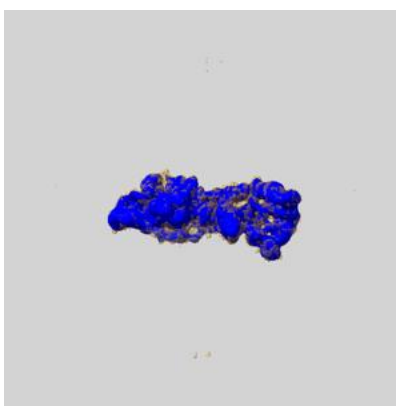
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

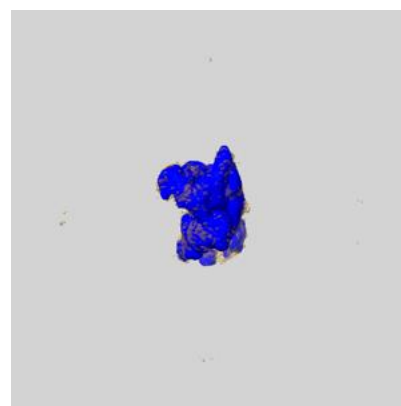
### 6.6.1 emd\_52571\_msk\_1.map [i](#)



X



Y

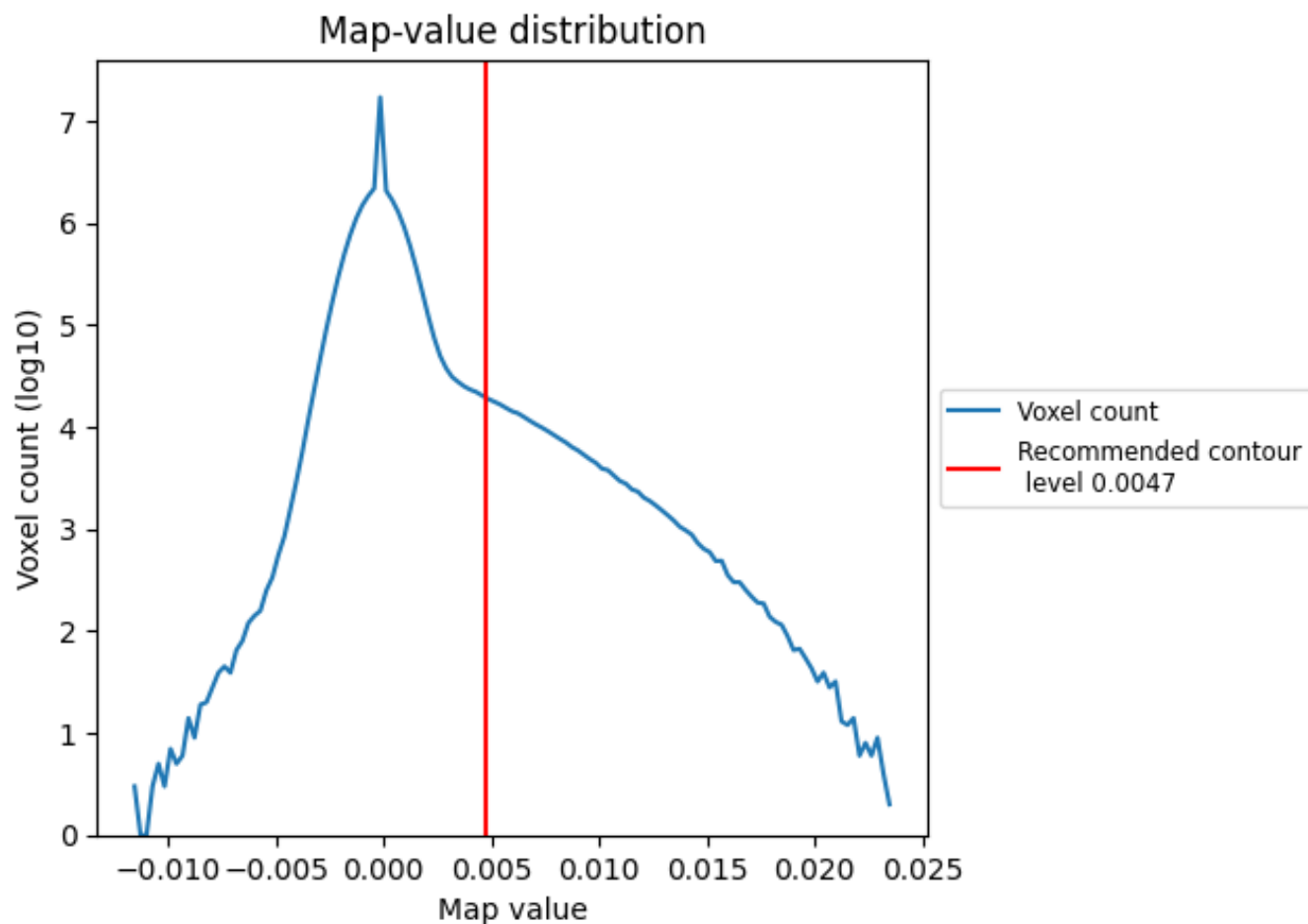


Z

## 7 Map analysis [i](#)

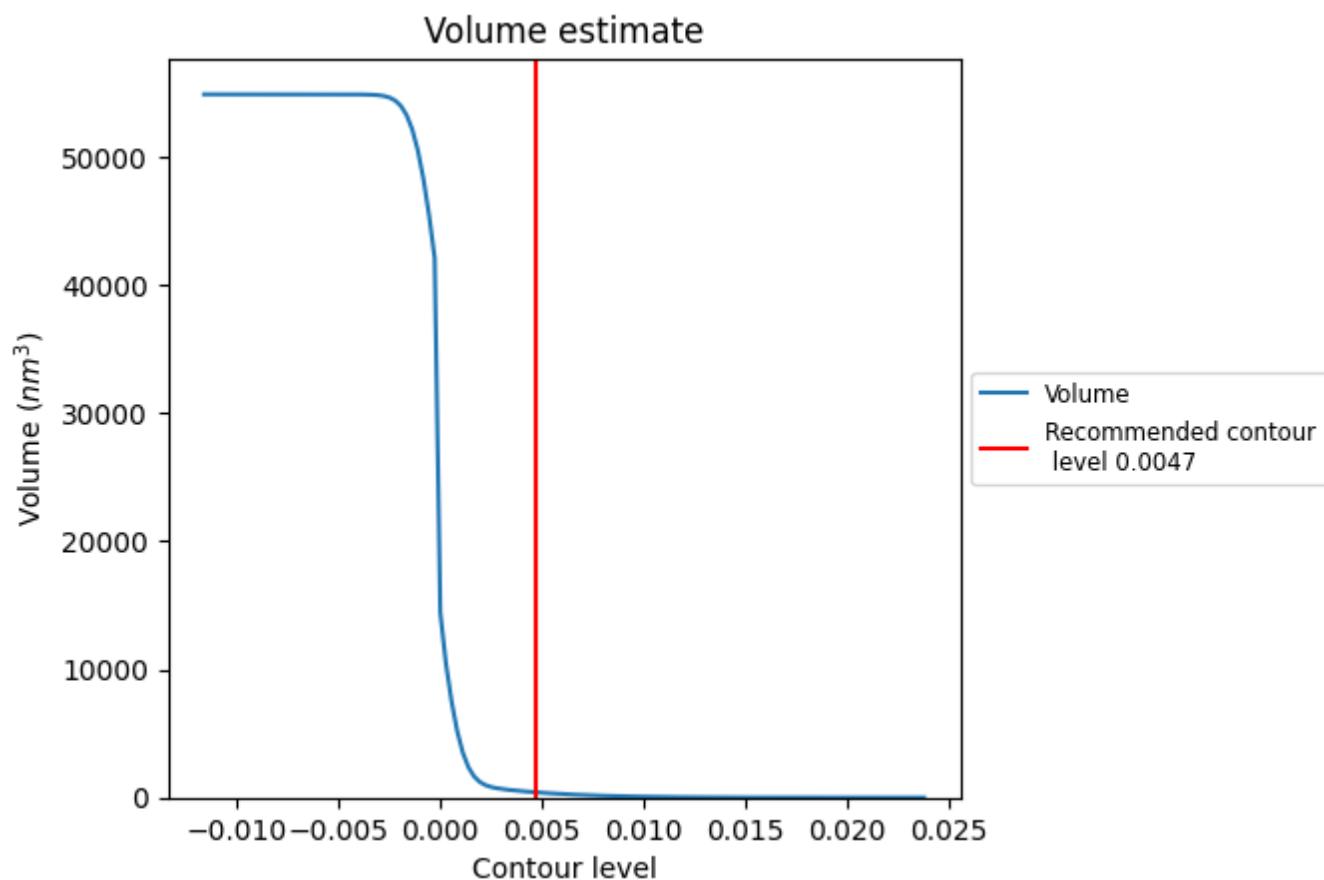
This section contains the results of statistical analysis of the map.

### 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.

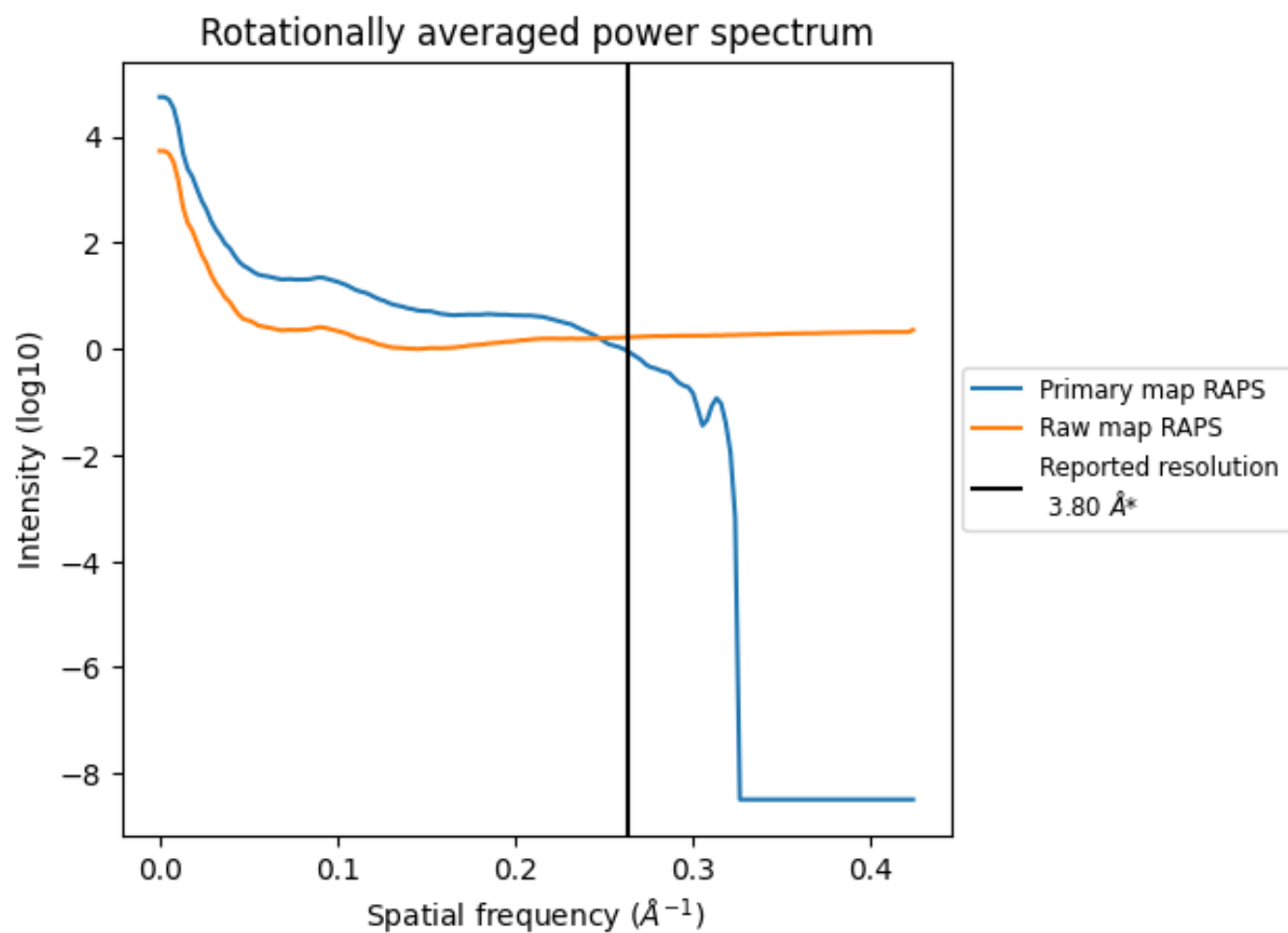
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm<sup>3</sup>; this corresponds to an approximate mass of 371 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 ⓘ

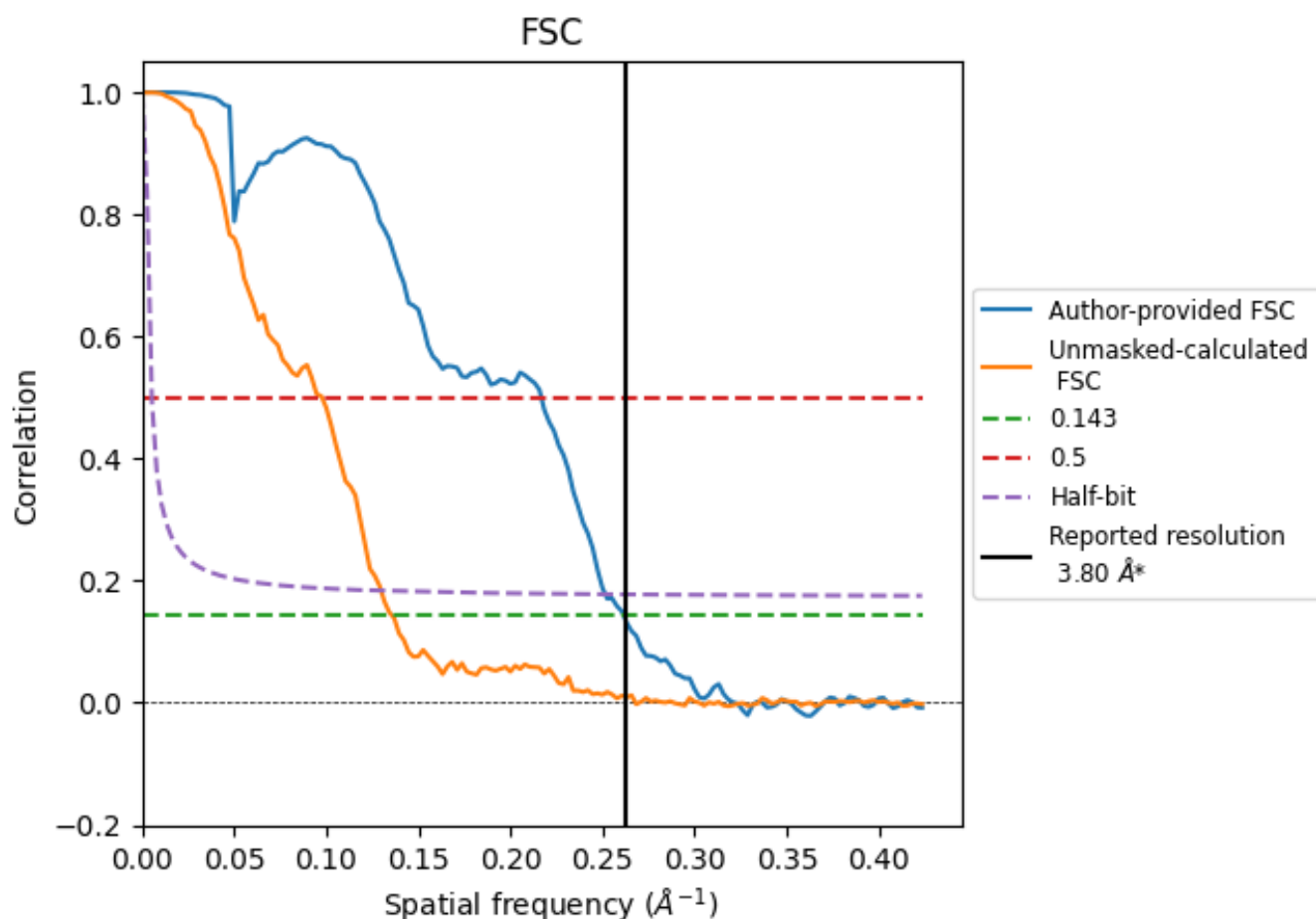


\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.61	3.97
Unmasked-calculated*	7.37	10.25	7.71

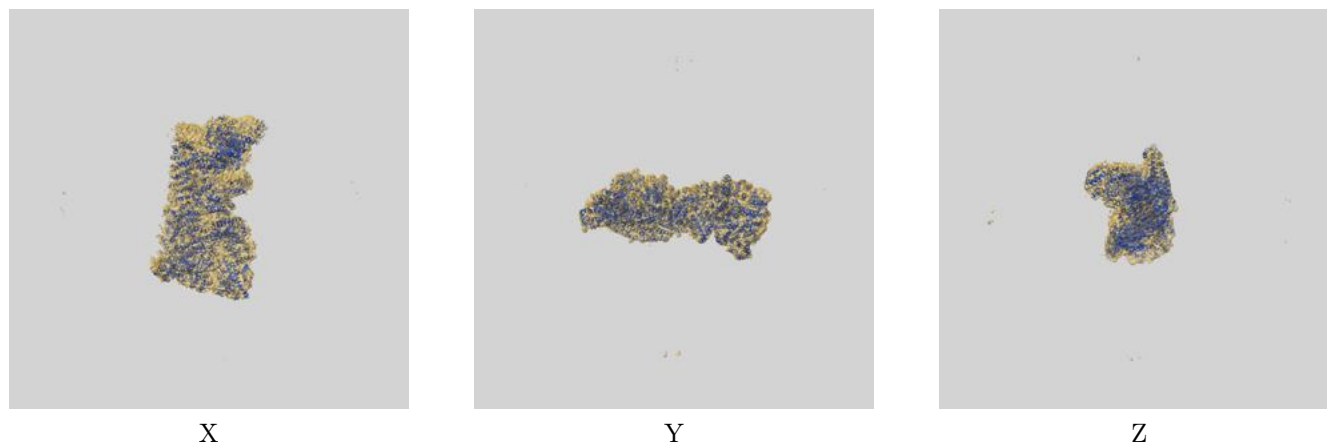
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.37 differs from the reported value 3.8 by more than 10 %



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

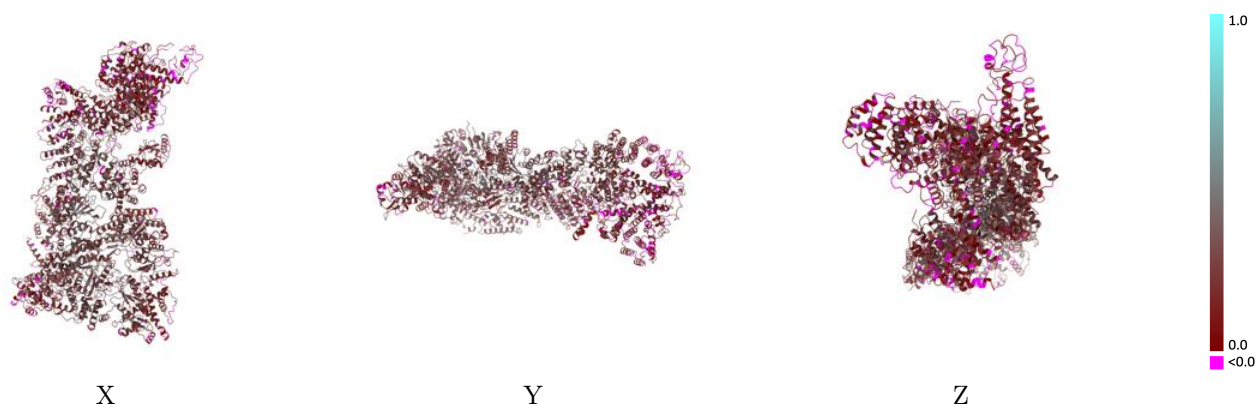
This section contains information regarding the fit between EMDB map EMD-52571 and PDB model 9I1J. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



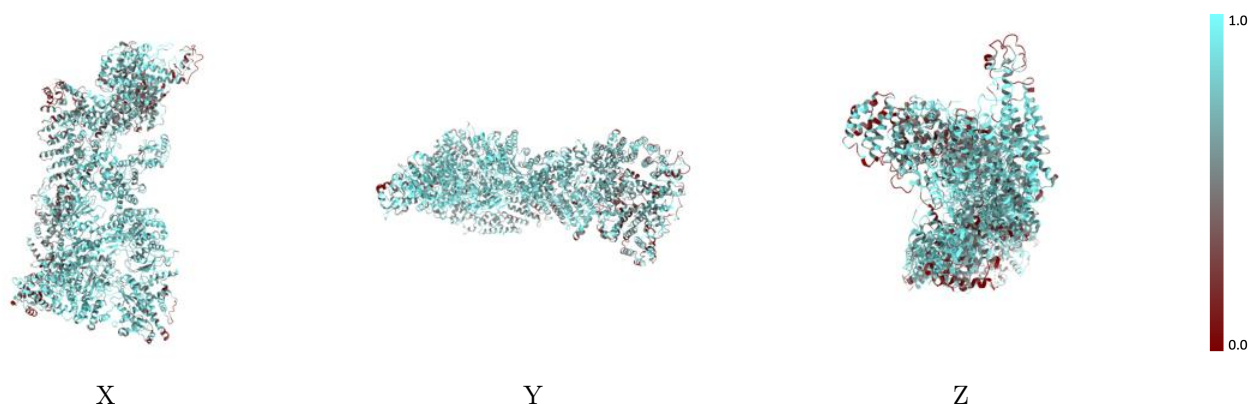
The images above show the 3D surface view of the map at the recommended contour level 0.0047 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



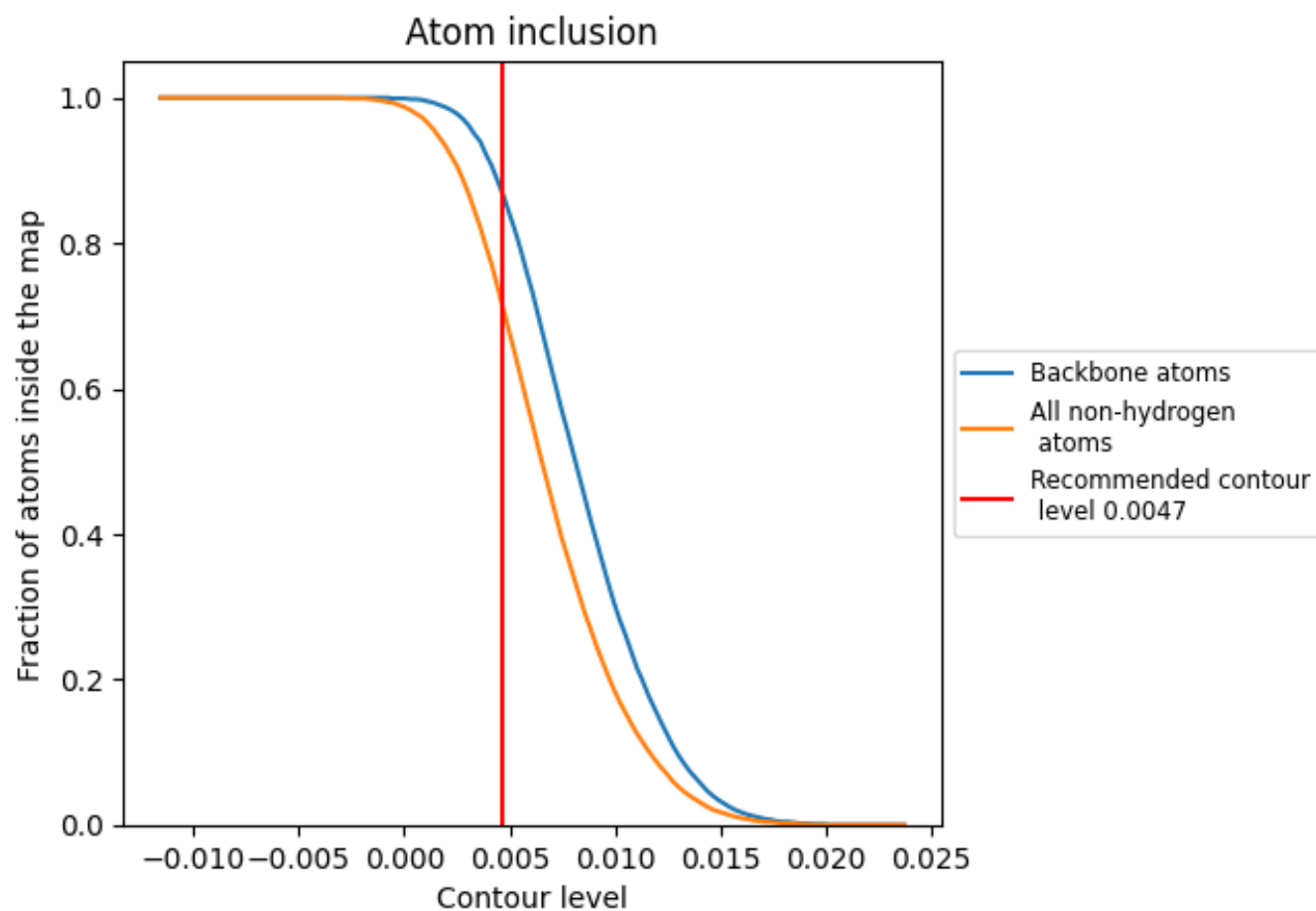
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0047).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7100	<div></div> 0.2270
A	<div></div> 0.7080	<div></div> 0.2290
B	<div></div> 0.7800	<div></div> 0.1800

