wwPDB EM Validation Summary Report

May 23, 2022 – 04:40 pm BST

PDB ID	:	7OIM
EMDB ID	:	EMD-12932
Title	:	Mouse RNF213, with mixed nucleotides bound
Authors	:	Grabarczyk, D.; Ahel, J.; Clausen, T.
Deposited on	:	2021-05-11
Resolution	:	4.00 Å(reported)
Based on initial model	:	6TAX

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

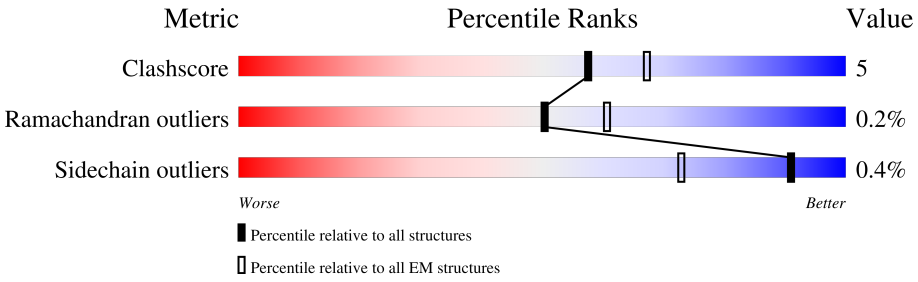
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	78% 14% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35597 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
			Total	C	N	O	S		
1	A	4426	35505	22641	6093	6561	210	0	0

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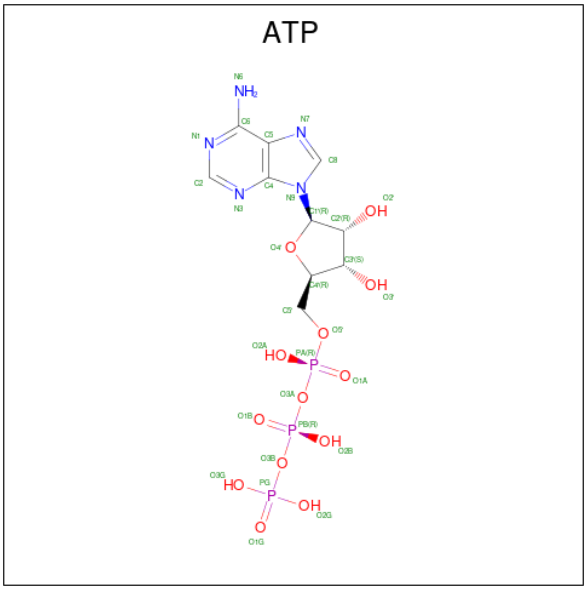
Chain	Residue	Modelled	Actual	Comment	Reference
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

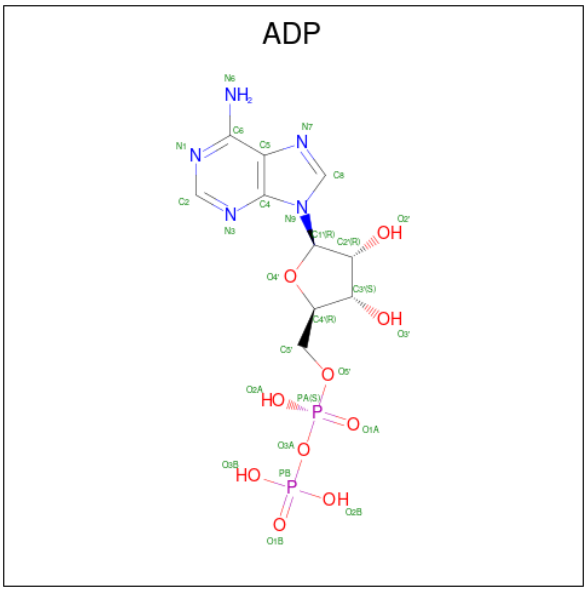
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

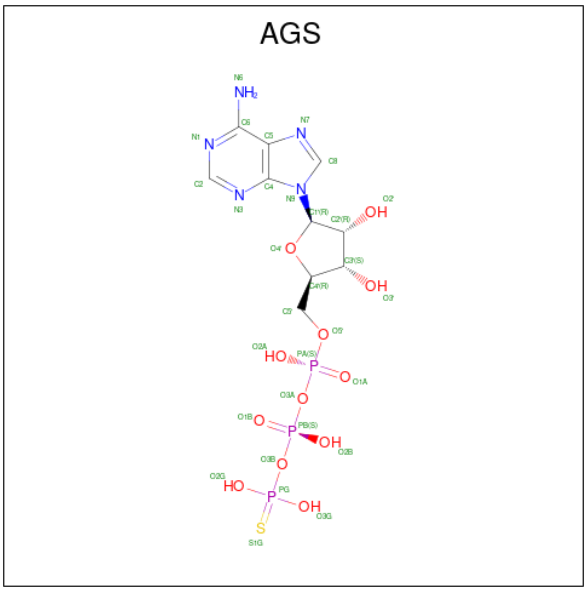
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



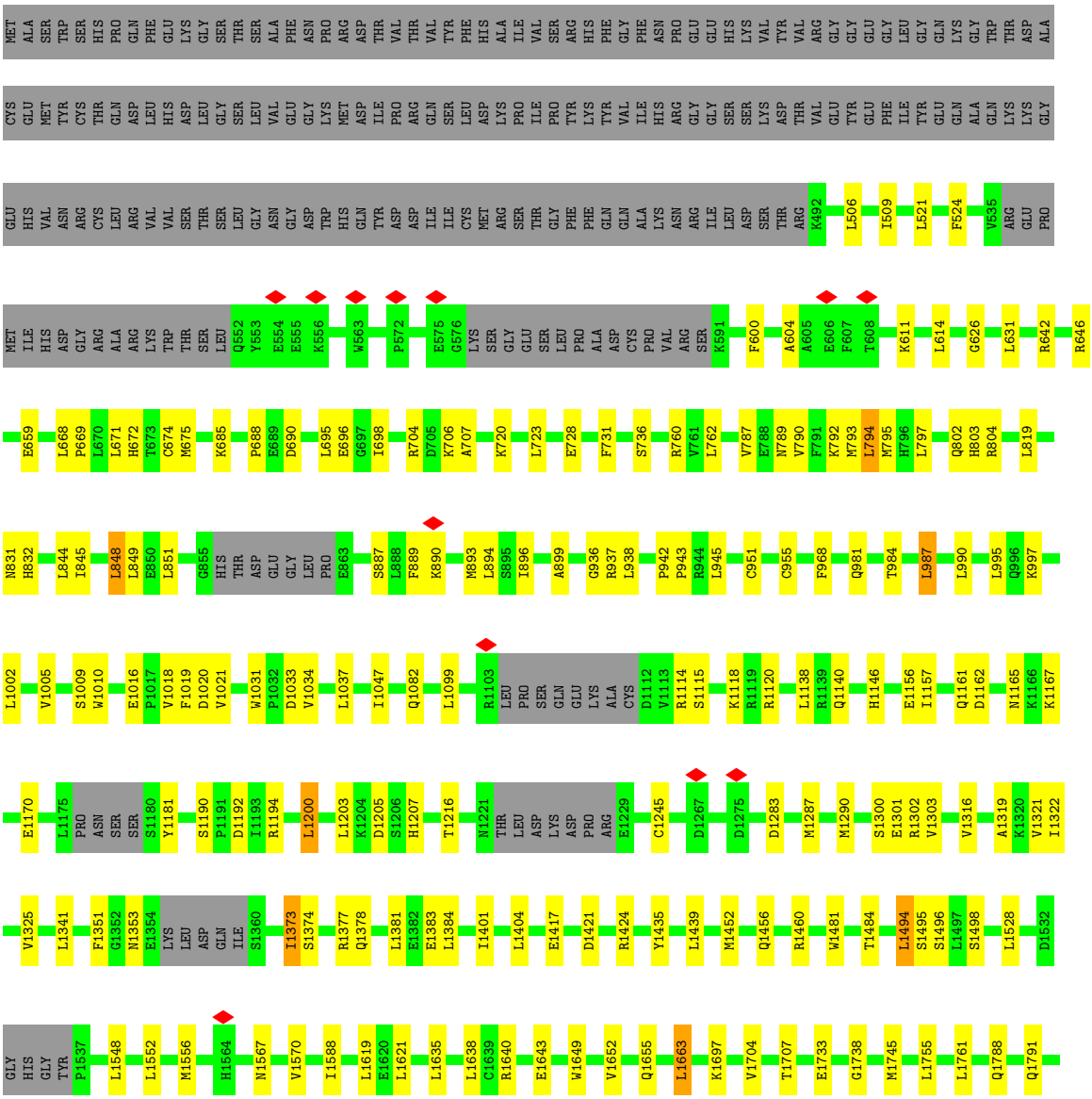
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

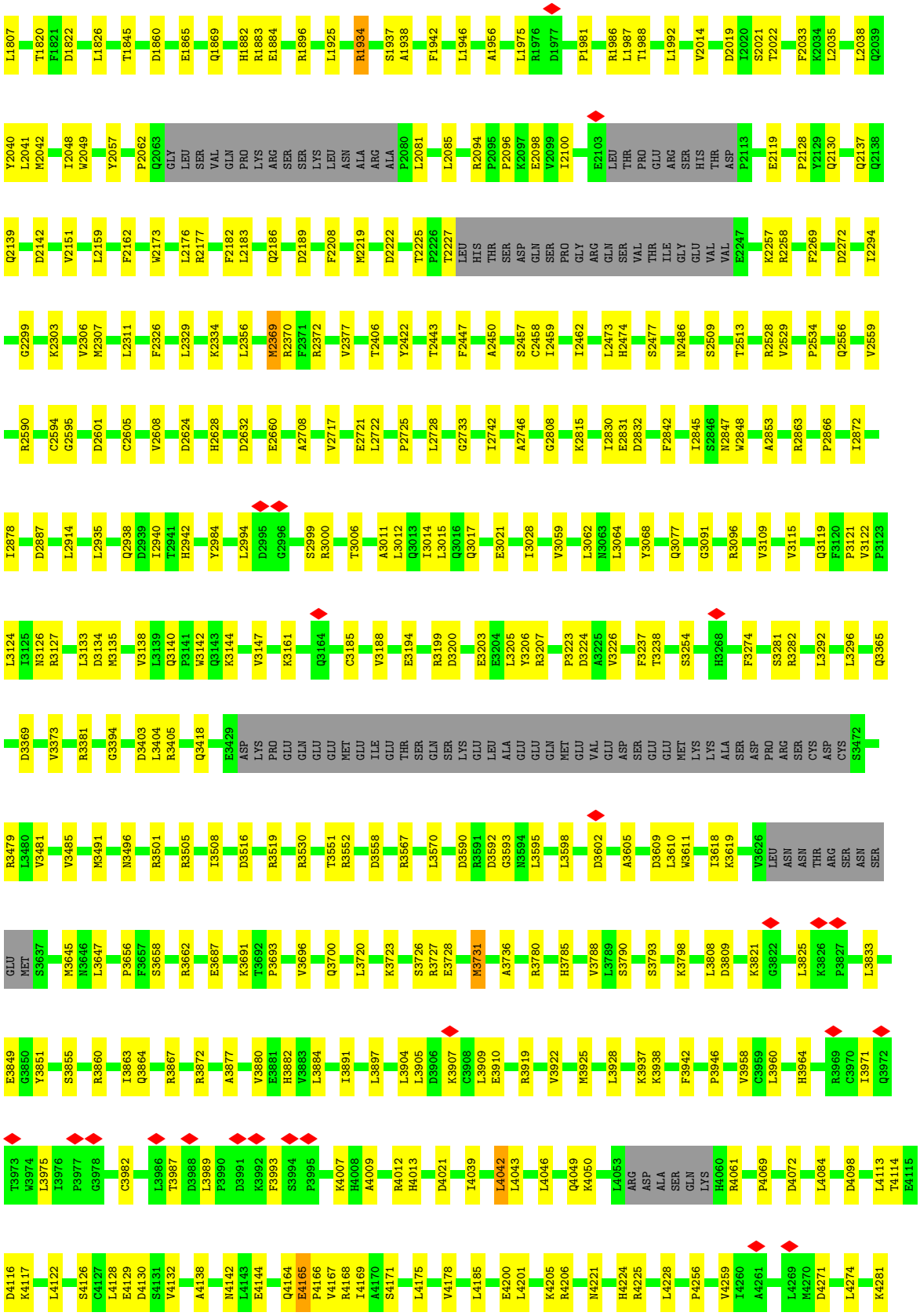
3 Residue-property plots (i)

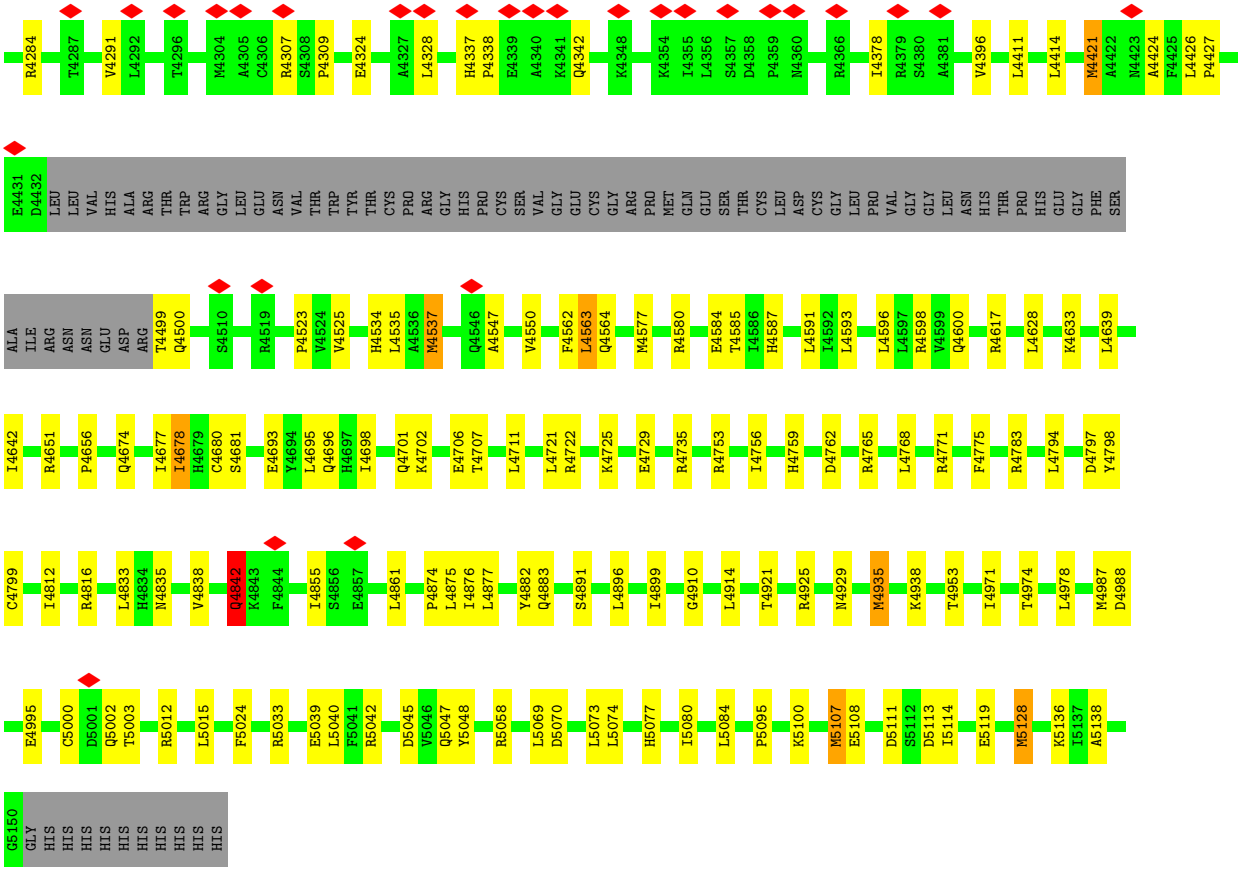
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase RNF213

Chain A:




L1807 T1820 F1821 D1822 L1826 T1845 D1860 E1865 Q1869 H1882 R1883 E1884 R1896 L1925 R1934 S1937 A1938 F1942 L1946 A1956 L1975 R1976 D1977 P1981 R1986 L1987 T1988 L1992 V2014 D2019 I2020 S2021 T2022 F2033 K2034 L2035 L2038 Q2039
Y2040 L2041 M2042 I2048 W2049 Y2057 P2062 Q2063 GLY LEU SER VAL GLN PRO LYS ARG SER SER LYS LEU ASN ALA ARG ALA P2080 L2081 L2085 R2094 P2095 P2096 K2097 E2098 V2099 I2100 E2103 LEU THR PRO GLU ARG SER HIS THR ASP P2113 E2119 P2128 Y2129 Q2130 Q2137 Q2138
Q2139 D2142 V2151 L2159 F2162 W2173 L2176 R2177 F2182 L2183 Q2186 D2189 F2208 M2219 D2222 T2225 P2226 T2227 LEU HIS THR SER ASP GLN SER PRO GLY ARG GLN SER VAL THR ILE GLY GLU VAL VAL E2247 K2257 R2258 F2269 D2272 I2294
G2299 K2303 V2306 M2307 L2311 F2326 L2329 K2334 L2356 M2369 R2370 F2371 R2372 V2377 T2406 Y2422 T2443 F2447 A2450 S2457 C2458 I2459 I2462 L2473 H2474 S2477 N2486 S2509 T2513 R2528 V2529 P2534 Q2556 V2559
R2590 C2594 G2595 D2601 C2605 V2608 D2624 H2628 D2632 E2660 A2708 V2717 E2721 L2722 P2725 L2728 G2733 I2742 A2746 G2808 K2815 I2830 E2831 D2832 F2842 I2845 S2846 N2847 W2848 A2853 R2863 P2866 I2872
I2878 D2887 L2914 L2935 Q2938 D2939 I2940 T2941 H2942 Y2984 L2994 D2995 G2996 S2999 R3000 T3006 A3011 L3012 Q3013 I3014 L3015 Q3016 Q3017 E3021 I3028 V3059 L3062 N3063 L3064 Y3068 Q3077 G3091 R3096 V3109 V3115 Q3119 F3120 P3121 V3122 P3123
L3124 I3125 N3126 R3127 L3133 D3134 M3135 V3138 L3139 Q3140 P3141 W3142 Q3143 K3144 V3147 K3161 Q3164 C3185 V3188 E3194 R3199 D3200 E3203 E3204 L3205 Y3206 R3207 P3223 D3224 A3225 V3226 F3237 T3238 S3254 H3268 F3274 S3281 R3282 L3292 L3296 Q3365
D3369 V3373 R3381 G3394 D3403 L3404 R3405 Q3418 E3429 ASP LYS PRO GLU GLN GLU GLU GLU MET GLU ILE GLU THR SER GLN SER LYS GLU LEU ALA GLU GLU GLN MET GLU VAL GLU ASP SER GLU GLU MET LYS LYS ALA SER ASP PRO ARG SER CYS ASP CYS S3472
R3479 L3480 V3481 V3485 M3491 N3496 R3501 R3505 I3508 D3516 R3519 R3530 T3551 R3552 D3558 R3567 L3570 D3590 R3591 D3592 G3593 N3594 L3595 L3598 D3602 A3605 D3609 L3610 W3611 I3618 K3619 V3626 LEU ASN ASN THR ARG SER ASN SER
GLU MET S3637 M3645 N3646 L3647 P3656 F3657 S3658 R3662 E3687 K3691 T3692 P3693 V3696 Q3700 L3720 K3723 S3726 R3727 E3728 M3731 A3736 R3780 H3785 V3788 L3789 S3790 S3793 K3798 L3808 D3809 K3821 G3822 L3825 K3826 P3827 L3833
E3849 G3850 Y3851 S3855 R3860 I3863 Q3864 R3867 R3872 A3877 V3880 E3881 H3882 V3883 L3884 I3891 L3897 L3904 L3905 D3906 K3907 C3908 L3909 E3910 R3919 V3922 M3925 L3928 K3937 K3938 F3942 P3946 V3958 C3959 L3960 H3964 R3969 C3970 I3971 Q3972
T3973 W3974 L3975 I3976 P3977 G3978 C3982 L3986 T3987 D3988 L3989 P3990 D3991 K3992 P3993 S3994 P3995 K4007 H4008 A4009 R4012 H4013 D4021 I4039 L4042 L4043 L4046 Q4049 K4050 L4063 ARG ASP ALA SER GLN LYS H4060 R4061 P4069 D4072 L4084 D4098 L4113 T4114 E4115
D4116 K4117 L4122 S4126 C4127 L4128 E4129 D4130 S4131 V4132 A4138 N4142 L4143 E4144 Q4164 E4165 P4166 V4167 R4168 I4169 A4170 S4171 L4175 V4178 L4185 E4200 L4201 K4205 R4206 N4221 H4224 R4225 L4228 P4256 V4259 I4260 A4261 L4269 M4270 D4271 L4274 K4281


R4284 T4287 V4291 L4292 T4296 M4304 A4305 C4306 R4307 S4308 P4309 E4324 A4327 L4328 H4337 P4338 E4339 A4340 K4341 Q4342 K4348 K4354 I4355 L4356 S4357 D4358 P4359 N4360 R4366 I4378 R4379 S4380 A4381 V4396 L4411 L4414 M4421 A4422 N4423 A4424 F4425 L4426 P4427
E4431 D4432 LEU LEU VAL HIS ALA ARG THR TRP ARG GLY LEU GLU ASN VAL THR TRP TYR THR CYS PRO ARG GLY HIS PRO CYS SER VAL GLY GLU CYS GLY ARG PRO MET GLN GLU SER THR CYS LEU ASP CYS GLY LEU PRO VAL GLY GLY LEU ASN HIS THR PRO HIS GLU GLY PHE SER
ALA ILE ARG ASN ASN GLU ASP ARG T4499 Q4500 S4510 R4519 P4523 V4524 V4525 H4534 L4535 A4536 M4537 Q4546 A4547 V4550 F4562 L4563 Q4564 M4577 R4580 E4584 T4585 I4586 H4587 L4591 I4592 L4593 L4596 L4597 R4598 V4599 Q4600 R4617 L4628 K4633 L4639
I4642 R4651 P4656 Q4674 I4677 I4678 H4679 C4680 S4681 E4693 Y4694 L4695 Q4696 H4697 I4698 Q4701 K4702 E4706 T4707 L4711 L4721 R4722 K4725 E4729 R4735 R4753 I4756 H4759 D4762 R4765 L4768 R4771 F4775 R4783 L4794 D4797 Y4798
C4799 I4812 R4816 L4833 H4834 N4835 V4838 Q4842 K4843 F4844 I4855 S4856 E4857 L4861 P4874 L4875 I4876 L4877 Y4882 Q4883 S4891 L4896 I4899 G4910 L4914 T4921 R4925 N4929 M4935 K4938 T4953 I4971 T4974 L4978 M4987 D4988
E4995 C5000 D5001 Q5002 T5003 R5012 L5015 F5024 R5033 E5039 L5040 F5041 R5042 D5045 V5046 Q5047 Y5048 R5058 L5069 D5070 L5073 L5074 H5077 I5080 L5084 P5095 K5100 M5107 E5108 D5111 S5112 D5113 I5114 E5119 M5128 K5136 I5137 A5138
G5150 GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	336000	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 ($e^-/Å^2$)	45, 40.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	370.656, 370.656, 370.656	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AGS, ZN, ATP

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	0.32	0/36242	0.75	71/49026 (0.1%)

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	6

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	671	LEU	CA-CB-CG	9.41	136.93	115.30
1	A	4421	MET	CA-CB-CG	9.06	128.69	113.30
1	A	762	LEU	CA-CB-CG	9.05	136.12	115.30
1	A	1494	LEU	O-C-N	8.98	137.07	122.70
1	A	1975	LEU	CA-CB-CG	8.69	135.29	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1170	GLU	Peptide
1	A	1373	ILE	Peptide
1	A	659	GLU	Peptide
1	A	688	PRO	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	35505	0	35642	355	0
2	A	31	0	12	3	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	27	0	12	0	0
6	A	31	0	12	2	0
All	All	35597	0	35678	355	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 5.

The worst 5 of 355 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:731:PHE:HB3	1:A:760:ARG:HH21	1.47	0.78
1:A:4935:MET:SD	1:A:4938:LYS:NZ	2.60	0.74
1:A:942:PRO:HB3	1:A:3207:ARG:HE	1.54	0.72
1:A:3292:LEU:O	1:A:3296:LEU:HB2	1.91	0.70
1:A:942:PRO:HB3	1:A:3207:ARG:HH21	1.56	0.70

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4394/4836 (91%)	4028 (92%)	358 (8%)	8 (0%)	47 79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3122	VAL
1	A	4600	GLN
1	A	1374	SER
1	A	3496	ASN
1	A	4166	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3970/4342 (91%)	3955 (100%)	15 (0%)	91 94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3798	LYS
1	A	4842	GLN
1	A	3919	ARG
1	A	5058	ARG
1	A	4598	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4564	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	AGS	A	5206	-	26,33,33	0.71	1 (3%)	26,52,52	1.18	2 (7%)
5	ADP	A	5205	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
2	ATP	A	5201	3	26,33,33	0.60	0	31,52,52	0.79	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	AGS	A	5206	-	-	4/17/38/38	0/3/3/3
5	ADP	A	5205	-	-	5/12/32/32	0/3/3/3
2	ATP	A	5201	3	-	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)
5	A	5205	ADP	C5-C4	2.43	1.47	1.40
6	A	5206	AGS	PG-S1G	2.10	1.95	1.90

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5206	AGS	PA-O3A-PB	-4.64	116.90	132.83
5	A	5205	ADP	N3-C2-N1	-3.36	123.43	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5205	ADP	PA-O3A-PB	-2.98	122.60	132.83
5	A	5205	ADP	C4-C5-N7	-2.77	106.51	109.40
5	A	5205	ADP	C3'-C2'-C1'	2.53	104.78	100.98

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

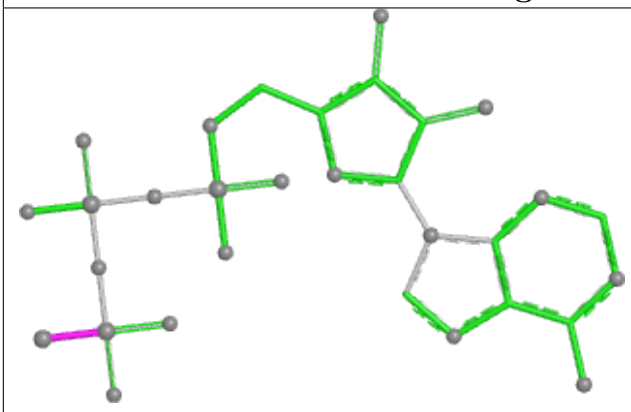
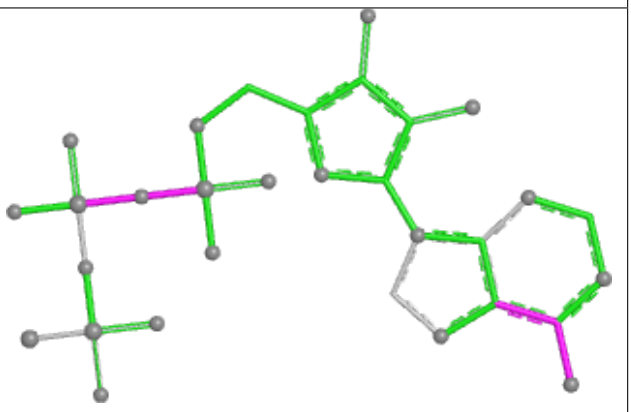
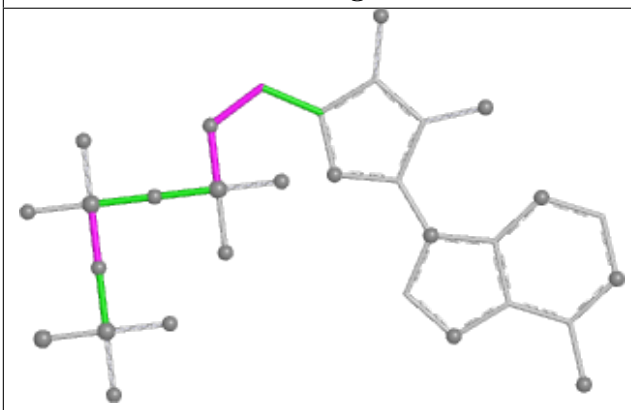
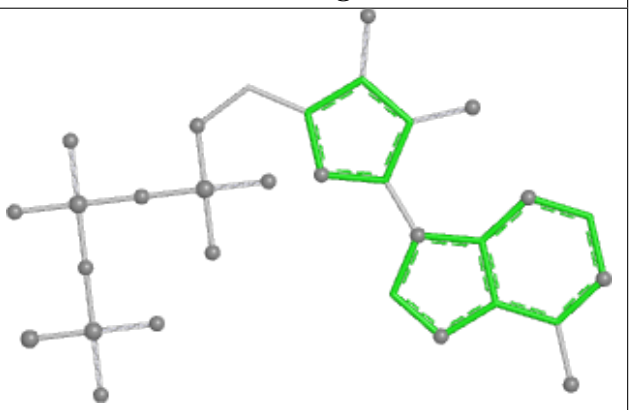
Mol	Chain	Res	Type	Atoms
2	A	5201	ATP	C5'-O5'-PA-O1A
2	A	5201	ATP	C5'-O5'-PA-O2A
2	A	5201	ATP	O4'-C4'-C5'-O5'
5	A	5205	ADP	C5'-O5'-PA-O3A
5	A	5205	ADP	O4'-C4'-C5'-O5'

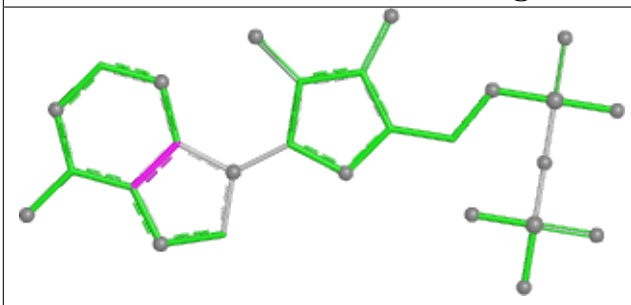
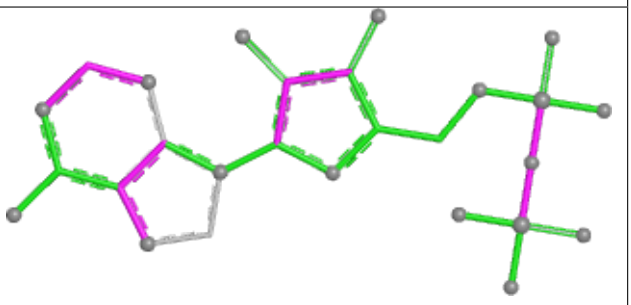
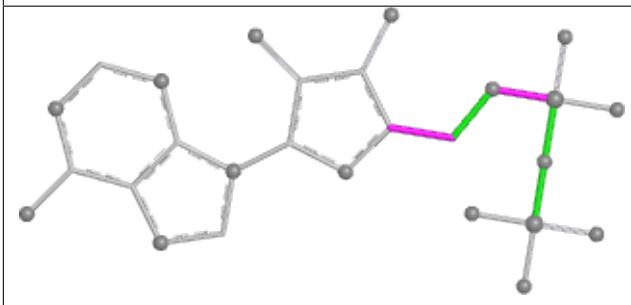
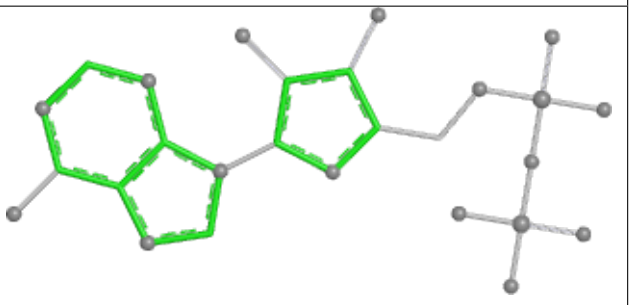
There are no ring outliers.

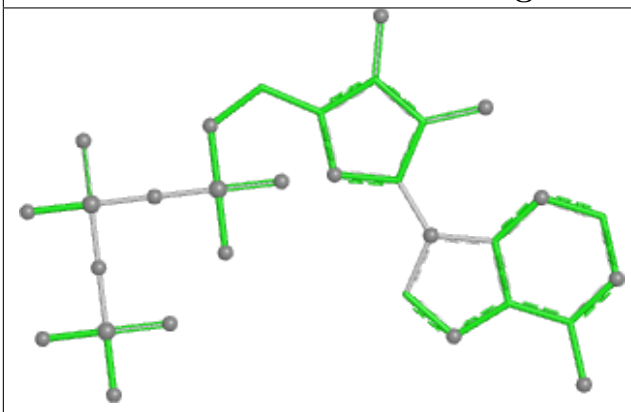
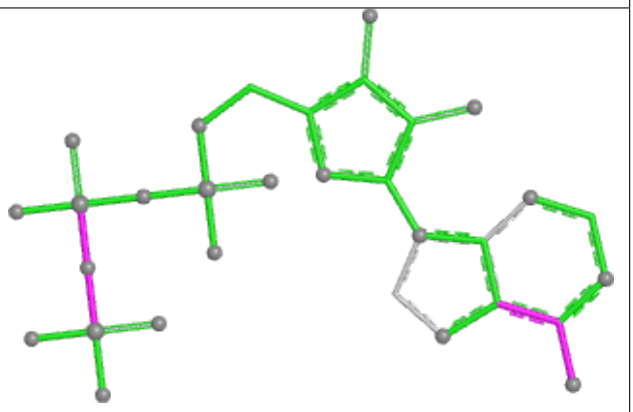
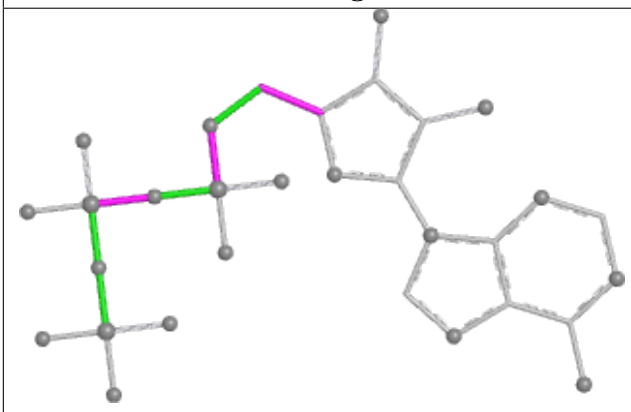
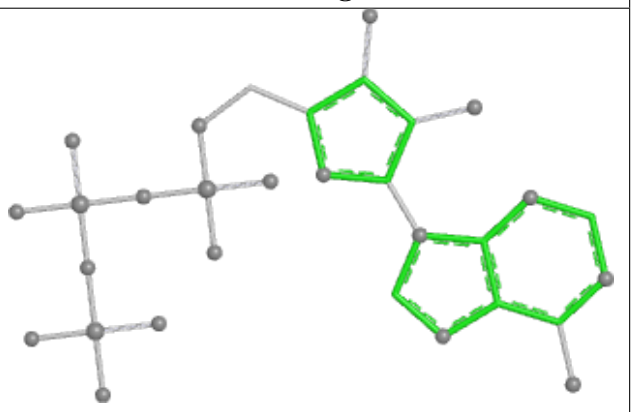
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5206	AGS	2	0
2	A	5201	ATP	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS A 5206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 5205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP A 5201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

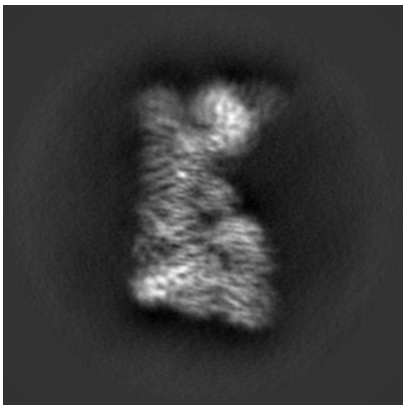
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12932. These allow visual inspection of the internal detail of the map and identification of artifacts.

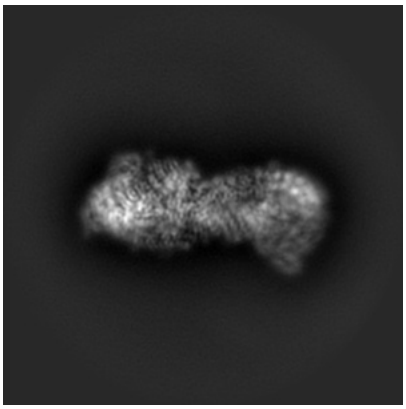
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

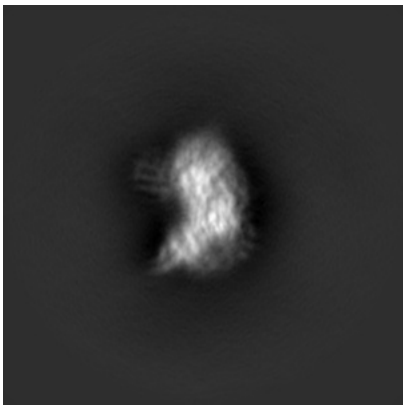
6.1.1 Primary map



X

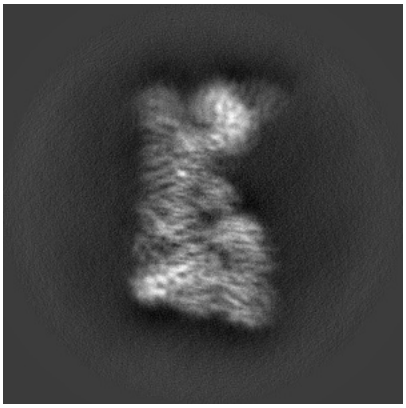


Y

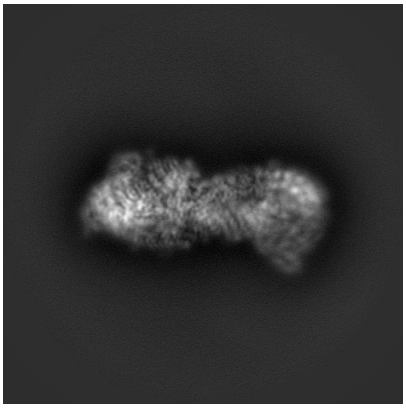


Z

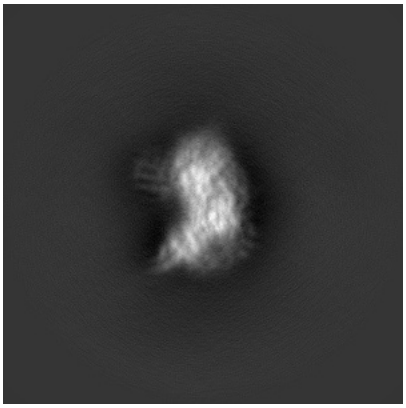
6.1.2 Raw map



X



Y

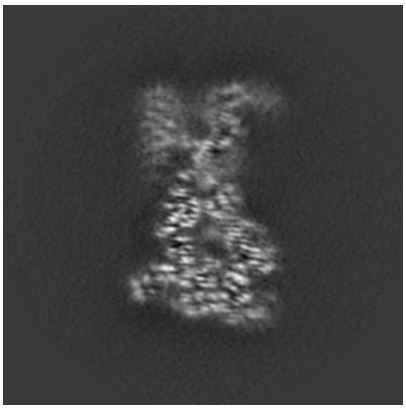


Z

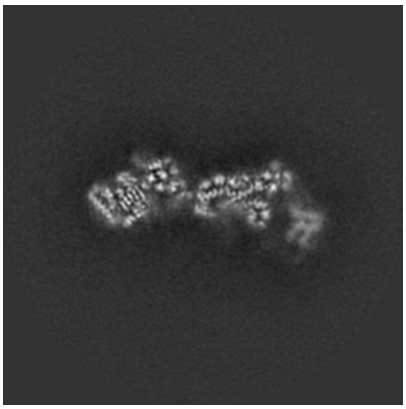
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

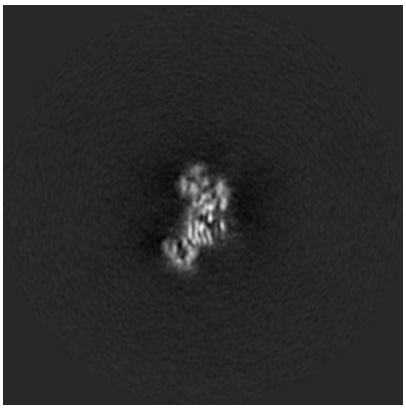
6.2.1 Primary map



X Index: 176

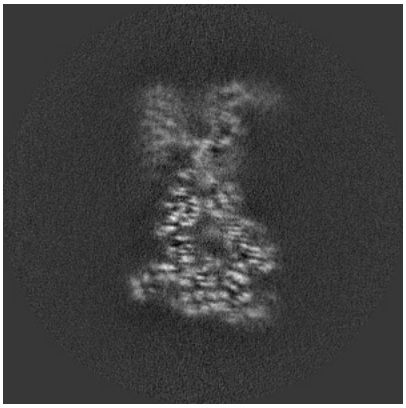


Y Index: 176

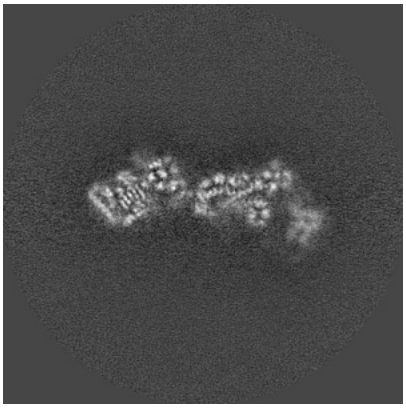


Z Index: 176

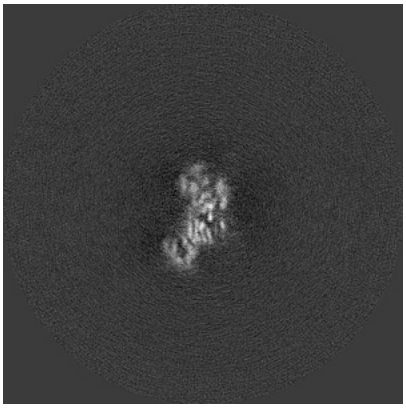
6.2.2 Raw map



X Index: 176



Y Index: 176

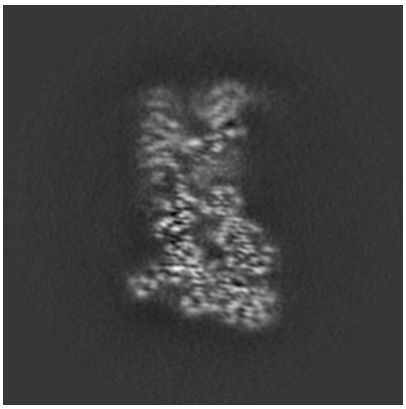


Z Index: 176

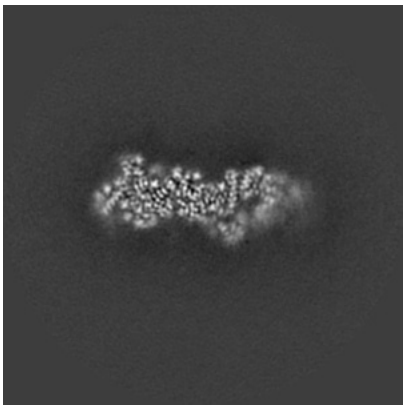
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

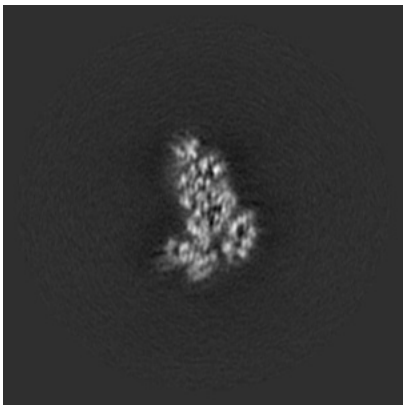
6.3.1 Primary map



X Index: 172

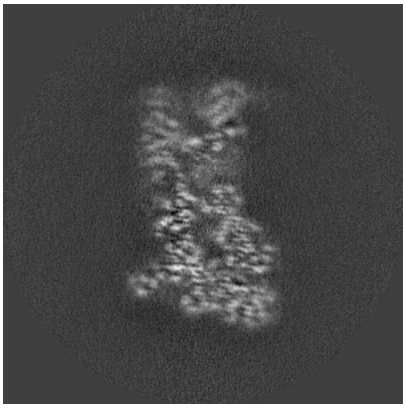


Y Index: 159

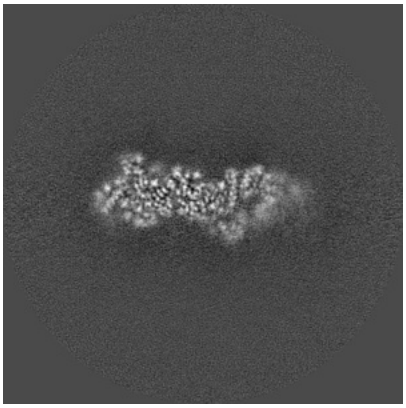


Z Index: 109

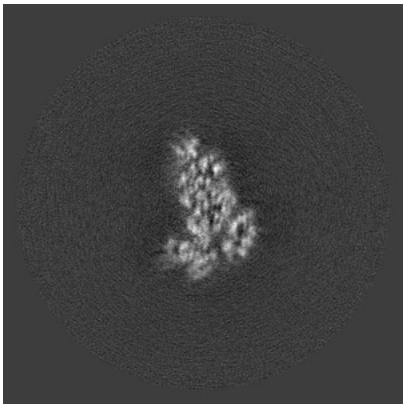
6.3.2 Raw map



X Index: 172



Y Index: 159



Z Index: 109

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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.

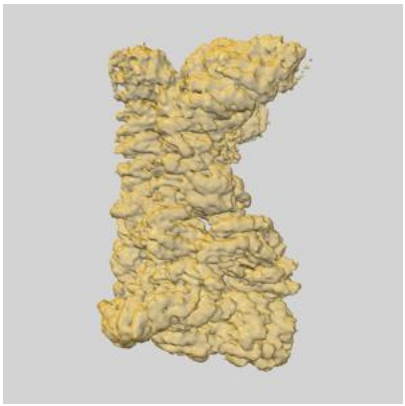
6.5 Mask visualisation

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

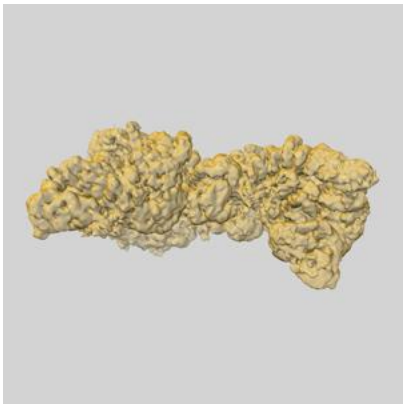
A mask typically either:

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

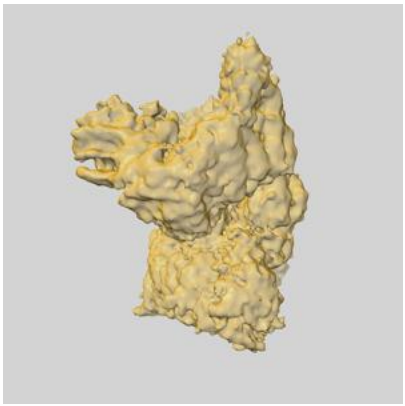
6.5.1 emd_12932_msk_2.map



X

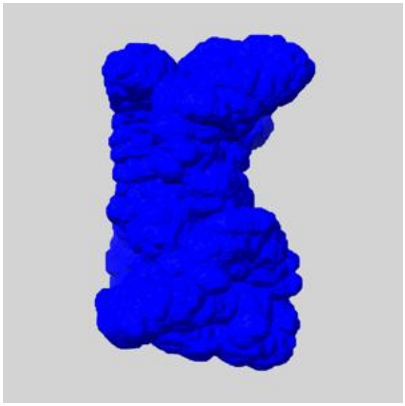


Y

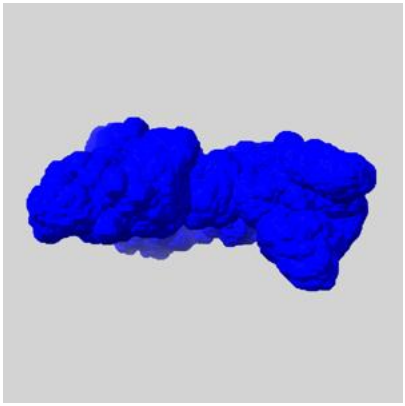


Z

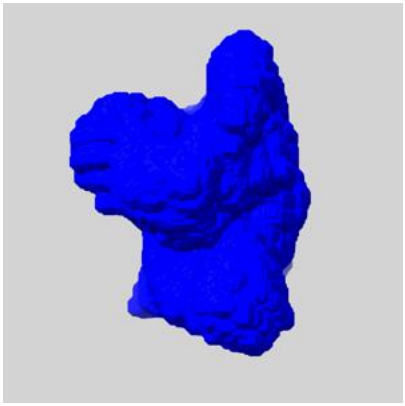
6.5.2 emd_12932_msk_1.map



X



Y

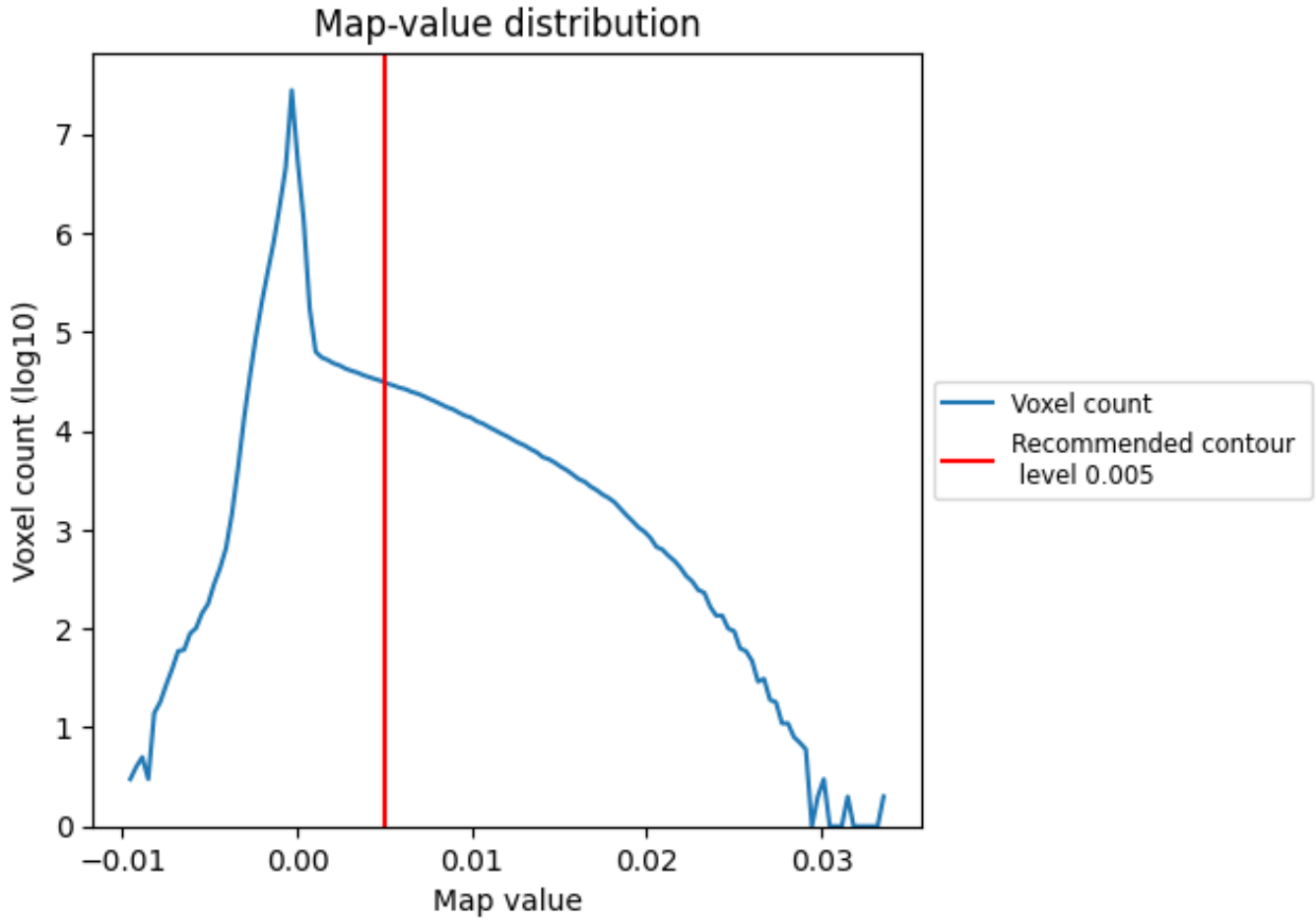


Z

7 Map analysis

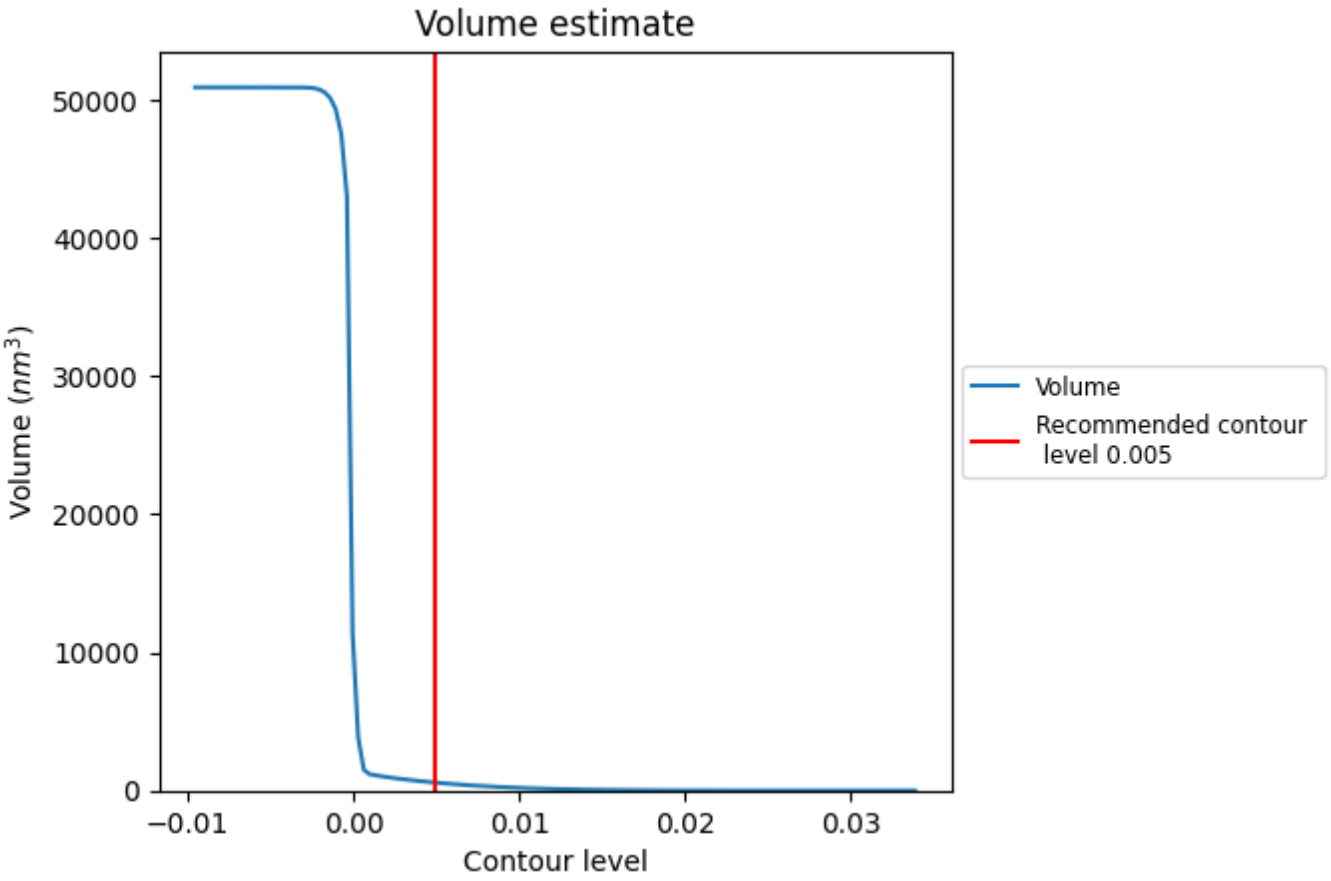
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

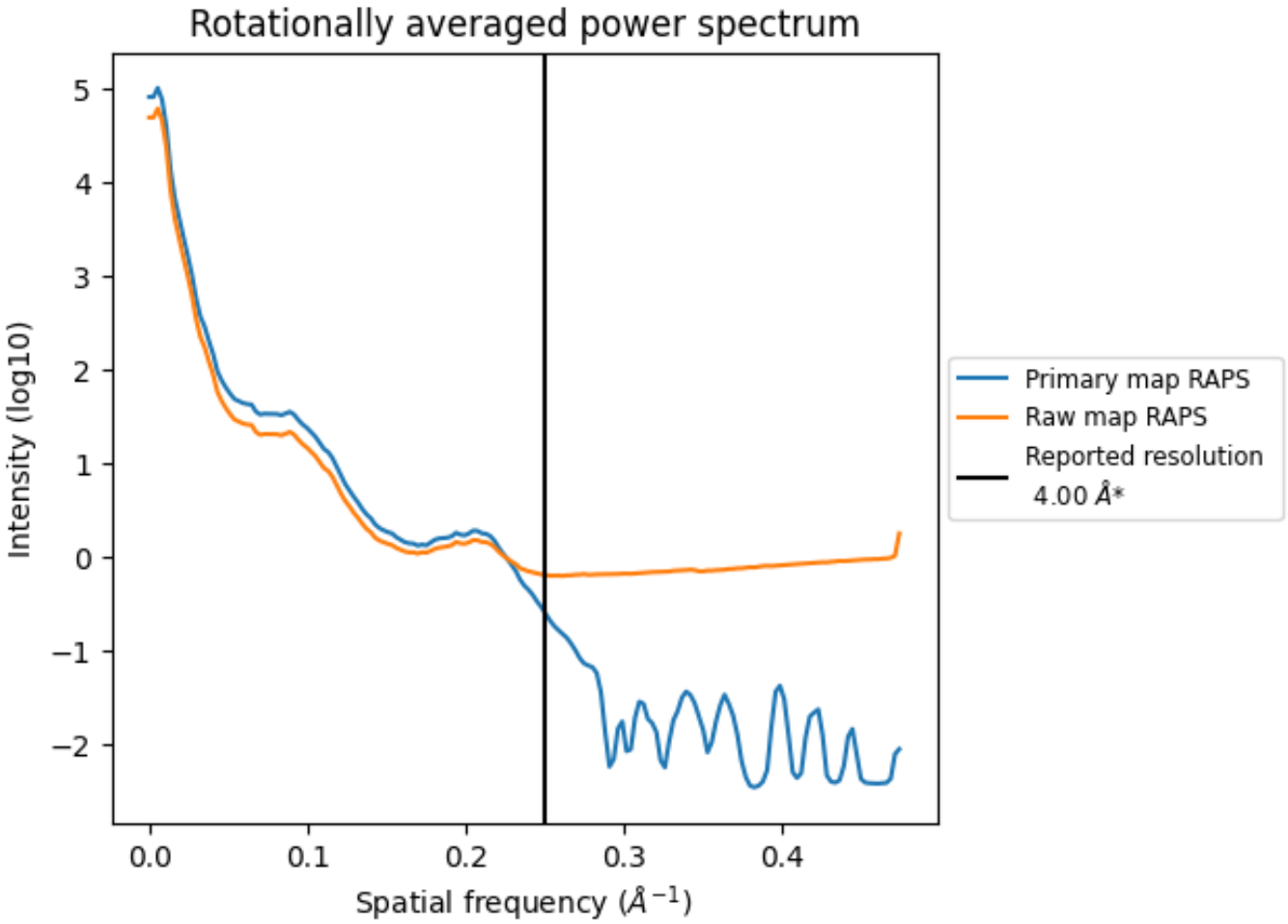
7.2 Volume estimate (i)



The volume at the recommended contour level is 572 nm^3; this corresponds to an approximate mass of 517 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

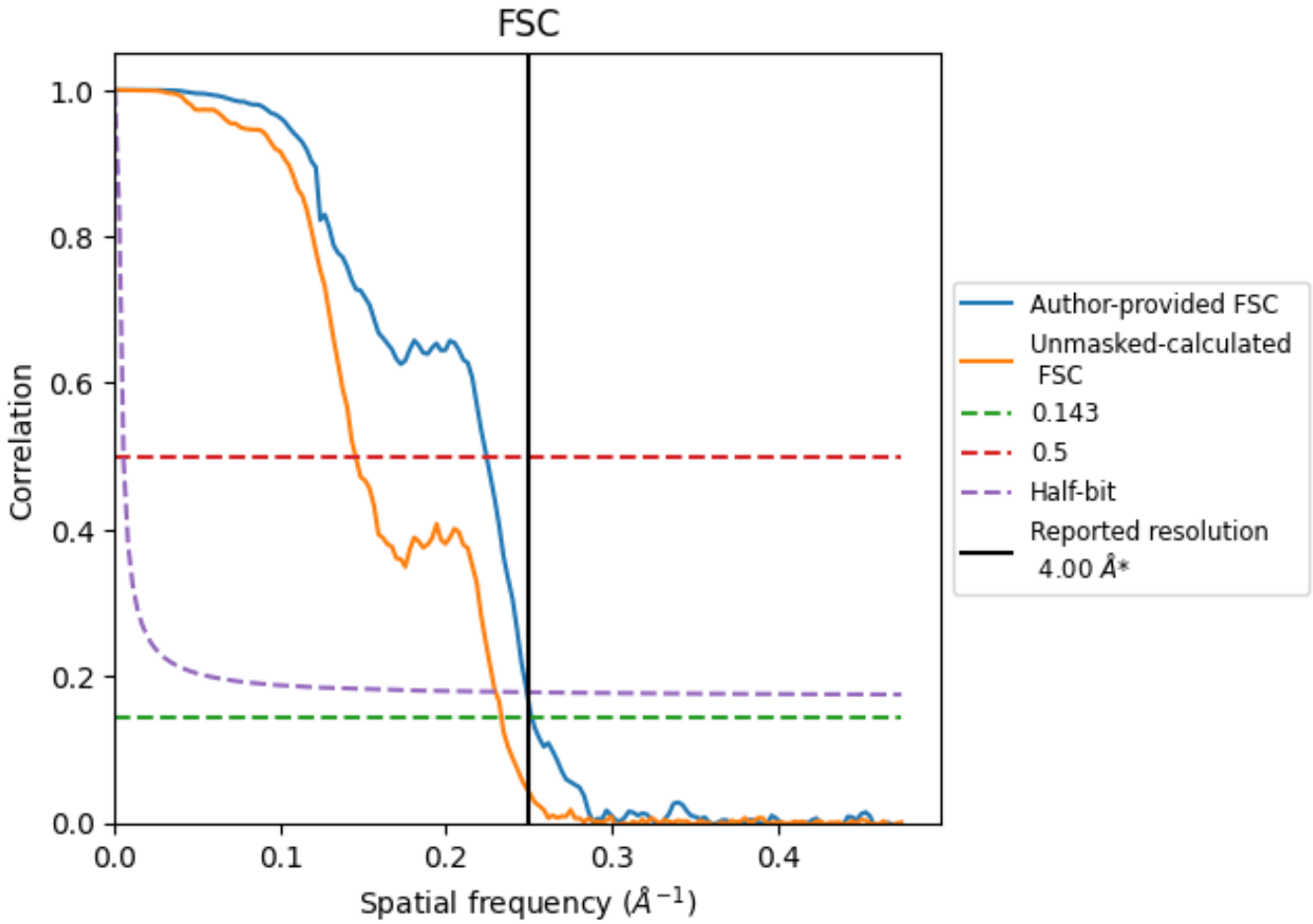


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

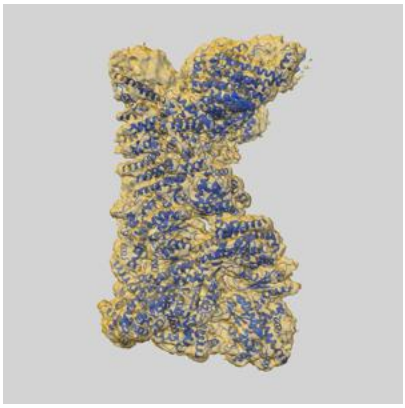
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.46	4.02
Unmasked-calculated*	4.28	6.88	4.35

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

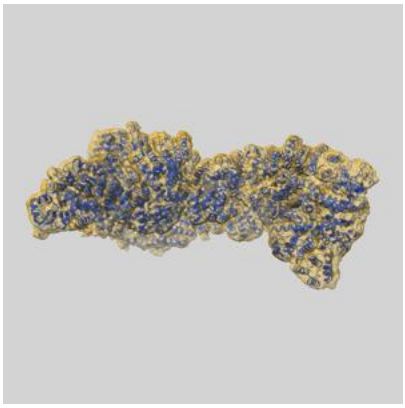
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12932 and PDB model 7OIM. Per-residue inclusion information can be found in section 3 on page 6.

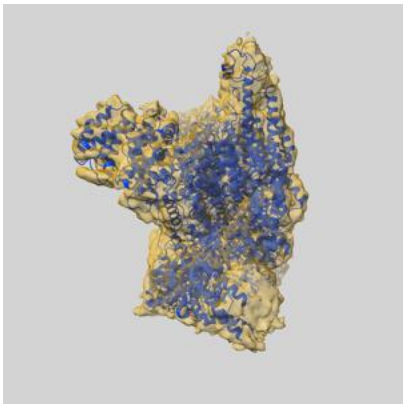
9.1 Map-model overlay



X



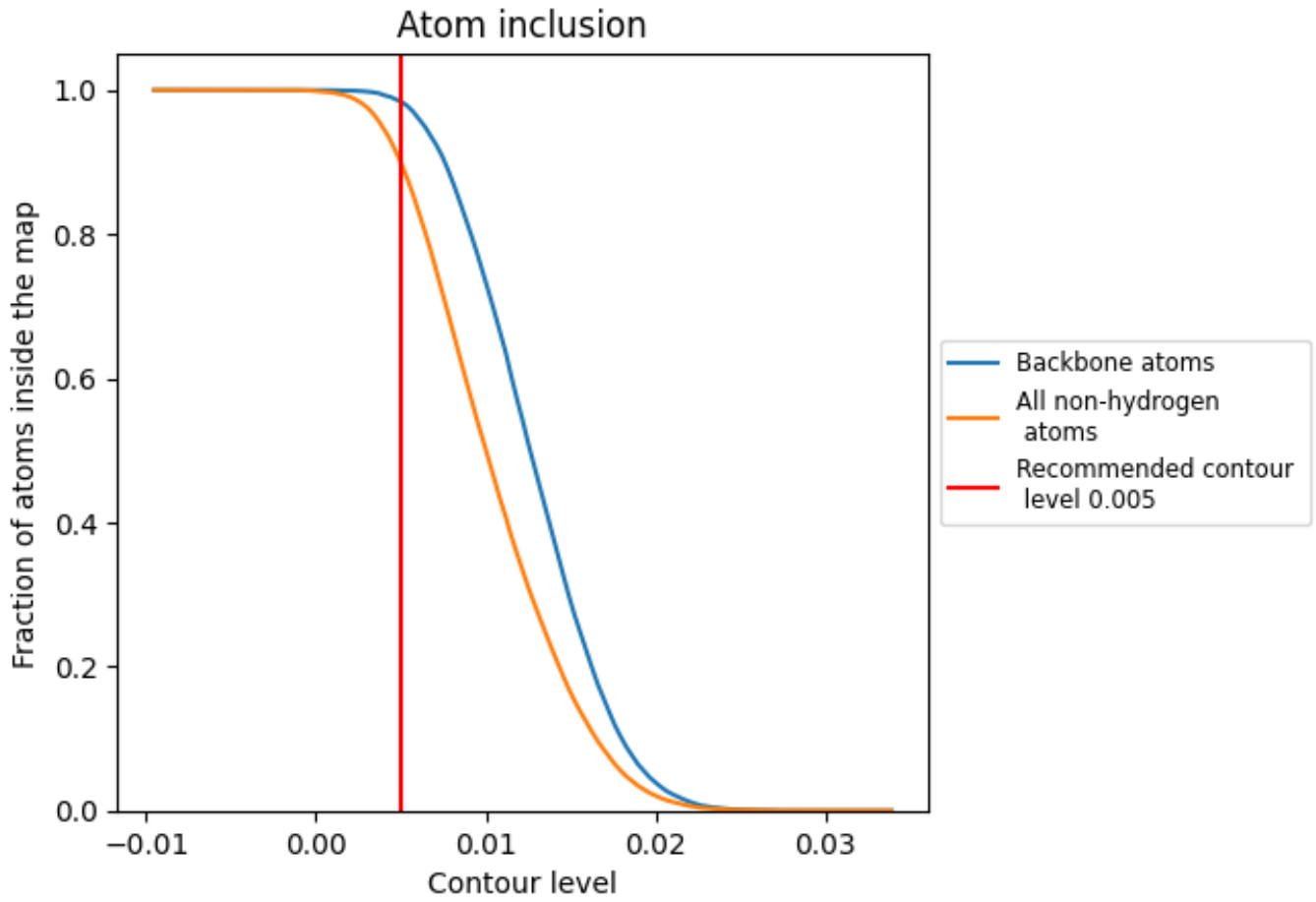
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.