



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 03:55 PM EDT

PDB ID : 9BI5 / pdb_00009bi5
EMDB ID : EMD-44559
Title : Apo form Mre11-Rad50 complex
Authors : Yu, Y.; Patel, D.J.
Deposited on : 2024-04-22
Resolution : 3.60 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.dev126
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

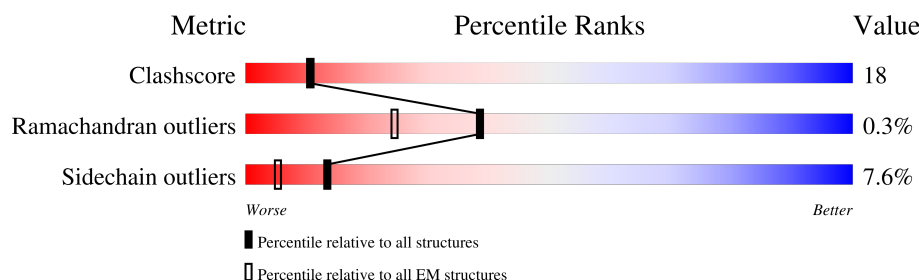
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	C	1312	
1	D	1312	
2	A	706	
2	B	706	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12413 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 repair protein RAD50.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	408	Total	C	N	O	S	0	0
			3217	2032	556	614	15		
1	C	334	Total	C	N	O	S	0	0
			2631	1661	459	499	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1235	GLN	GLU	engineered mutation	UNP P12753
C	1235	GLN	GLU	engineered mutation	UNP P12753

- Molecule 2 is a protein called Double-strand break repair protein MRE11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	411	Total	C	N	O	S	0	0
			3237	2048	553	618	18		
2	B	412	Total	C	N	O	S	0	0
			3262	2066	555	622	19		

There are 28 discrepancies between the modelled and reference sequences:

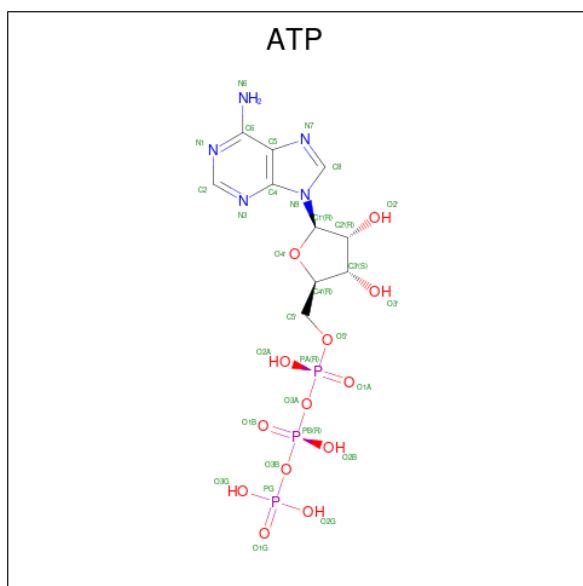
Chain	Residue	Modelled	Actual	Comment	Reference
A	693	TYR	-	expression tag	UNP P32829
A	694	ASP	-	expression tag	UNP P32829
A	695	TYR	-	expression tag	UNP P32829
A	696	LYS	-	expression tag	UNP P32829
A	697	ASP	-	expression tag	UNP P32829
A	698	ASP	-	expression tag	UNP P32829
A	699	ASP	-	expression tag	UNP P32829
A	700	ASP	-	expression tag	UNP P32829
A	701	LYS	-	expression tag	UNP P32829
A	702	HIS	-	expression tag	UNP P32829
A	703	HIS	-	expression tag	UNP P32829

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Chain	Residue	Modelled	Actual	Comment	Reference
A	704	HIS	-	expression tag	UNP P32829
A	705	HIS	-	expression tag	UNP P32829
A	706	HIS	-	expression tag	UNP P32829
B	693	TYR	-	expression tag	UNP P32829
B	694	ASP	-	expression tag	UNP P32829
B	695	TYR	-	expression tag	UNP P32829
B	696	LYS	-	expression tag	UNP P32829
B	697	ASP	-	expression tag	UNP P32829
B	698	ASP	-	expression tag	UNP P32829
B	699	ASP	-	expression tag	UNP P32829
B	700	ASP	-	expression tag	UNP P32829
B	701	LYS	-	expression tag	UNP P32829
B	702	HIS	-	expression tag	UNP P32829
B	703	HIS	-	expression tag	UNP P32829
B	704	HIS	-	expression tag	UNP P32829
B	705	HIS	-	expression tag	UNP P32829
B	706	HIS	-	expression tag	UNP P32829

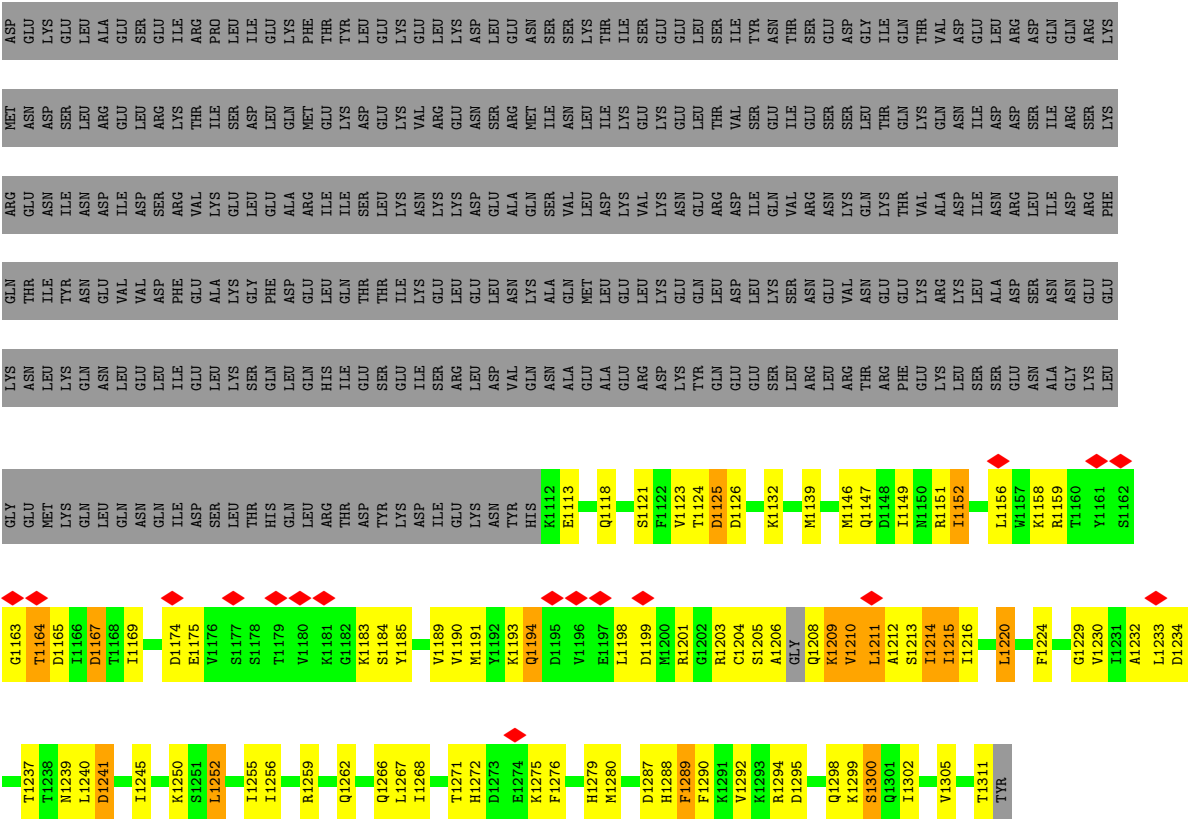
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



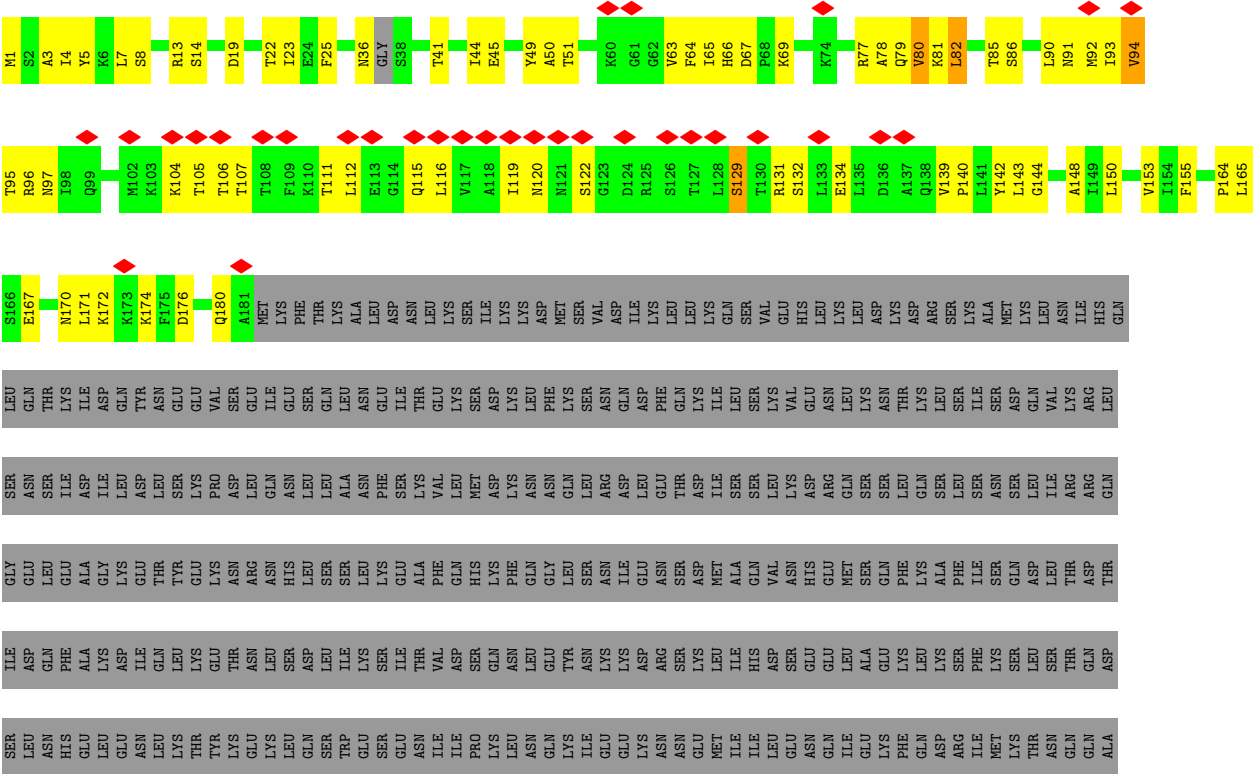
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mn 2	0
4	B	2	Total 2	Mn 2	0



● Molecule 1: DNA repair protein RAD50





L174	E88	L89	Y68	L175	L90	Y69	L176	L91	Y70	L177	L92	Y71	L178	L93	Y72	L179	L94	Y73	L180	L95	Y74	L181	L96	Y75	L182	L97	Y76	L183	L98	Y77	L184	L99	Y78	L185	L100	Y79	L186	L101	Y80	L187	L102	Y81	L188	L103	Y82	L189	L104	Y83	L190	L105	Y84	L191	L106	Y85	L192	L107	Y86	L193	L108	Y87	L194	L109	Y88	L195	L110	Y89	L196	L111	Y90	L197	L112	Y91	L198	L113	Y92	L199	L114	Y93	L200	L115	Y94	L201	L116	Y95	L202	L117	Y96	L203	L118	Y97	L204	L119	Y98	L205	L120	Y99	L206	L121	Y00	L207	L122	Y01	L208	L123	Y02	L209	L124	Y03	L210	L125	Y04	L211	L126	Y05	L212	L127	Y06	L213	L128	Y07	L214	L129	Y08	L215	L130	Y09	L216	L131	Y10	L217	L132	Y11	L218	L133	Y12	L219	L134	Y13	L220	L135	Y14	L221	L136	Y15	L222	L137	Y16	L223	L138	Y17	L224	L139	Y18	L225	L140	Y19	L226	L141	Y20	L227	L142	Y21	L228	L143	Y22	L229	L144	Y23	L230	L145	Y24	L231	L146	Y25	L232	L147	Y26	L233	L148	Y27	L234	L149	Y28	L235	L150	Y29	L236	L151	Y30	L237	L152	Y31	L238	L153	Y32	L239	L154	Y33	L240	L155	Y34	L241	L156	Y35	L242	L157	Y36	L243	L158	Y37	L244	L159	Y38	L245	L160	Y39	L246	L161	Y40	L247	L162	Y41	L248	L163	Y42	L249	L164	Y43	L250	L165	Y44	L251	L166	Y45	L252	L167	Y46	L253	L168	Y47	L254	L169	Y48	L255	L170	Y49	L256	L171	Y50	L257	L172	Y51	L258	L173	Y52	L259	L174	Y53	L260	L175	Y54	L261	L176	Y55	L262	L177	Y56	L263	L178	Y57	L264	L179	Y58	L265	L180	Y59	L266	L181	Y60	L267	L182	Y61	L268	L183	Y62	L269	L184	Y63	L270	L185	Y64	L271	L186	Y65	L272	L187	Y66	L273	L188	Y67	L274	L189	Y68	L275	L190	Y69	L276	L191	Y70	L277	L192	Y71	L278	L193	Y72	L279	L194	Y73	L280	L195	Y74	L281	L196	Y75	L282	L197	Y76	L283	L198	Y77	L284	L199	Y78	L285	L200	Y79	L286	L201	Y80	L287	L202	Y81	L288	L203	Y82	L289	L204	Y83	L290	L205	Y84	L291	L206	Y85	L292	L207	Y86	L293	L208	Y87	L294	L209	Y88	L295	L210	Y89	L296	L211	Y90	L297	L212	Y91	L298	L213	Y92	L299	L214	Y93	L300	L215	Y94	L301	L216	Y95	L302	L217	Y96	L303	L218	Y97	L304	L219	Y98	L305	L220	Y99	L306	L221	Y00	L307	L222	Y01	L308	L223	Y02	L309	L224	Y03	L310	L225	Y04	L311	L226	Y05	L312	L227	Y06	L313	L228	Y07	L314	L229	Y08	L315	L230	Y09	L316	L231	Y10	L317	L232	Y11	L318	L233	Y12	L319	L234	Y13	L320	L235	Y14	L321	L236	Y15	L322	L237	Y16	L323	L238	Y17	L324	L239	Y18	L325	L240	Y19	L326	L241	Y20	L327	L242	Y21	L328	L243	Y22	L329	L244	Y23	L330	L245	Y24	L331	L246	Y25	L332	L247	Y26	L333	L248	Y27	L334	L249	Y28	L335	L250	Y29	L336	L251	Y30	L337	L252	Y31	L338	L253	Y32	L339	L254	Y33	L340	L255	Y34	L341	L256	Y35	L342	L257	Y36	L343	L258	Y37	L344	L259
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232521	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 ($e^-/\text{\AA}^2$)	51.22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.547	Depositor
Minimum map value	-1.463	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	303.24, 303.24, 303.24	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	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: MN, 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	C	0.22	0/2669	0.48	0/3596
1	D	0.22	0/3263	0.52	2/4393 (0.0%)
2	A	0.25	0/3316	0.43	0/4508
2	B	0.22	0/3342	0.41	0/4541
All	All	0.23	0/12590	0.46	2/17038 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1204	CYS	N-CA-C	7.39	119.28	108.86
1	D	64	PHE	N-CA-C	-6.75	105.67	114.04

There are no chirality outliers.

There are no planarity outliers.

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	C	2631	0	2639	110	0
1	D	3217	0	3260	162	0
2	A	3237	0	3108	126	0
2	B	3262	0	3149	86	0
3	D	62	0	24	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	12413	0	12180	452	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 18.

The worst 5 of 452 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:A:412:ARG:HB3	2:A:412:ARG:HH11	1.13	1.12
1:D:115:GLN:HE21	1:D:127:THR:CG2	1.64	1.09
2:B:119:PHE:HB3	2:B:149:PHE:HE2	1.17	1.05
1:D:44:ILE:HD11	1:D:1268:ILE:HD13	1.38	1.03
2:B:119:PHE:HB3	2:B:149:PHE:CE2	1.96	1.00

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	C	324/1312 (25%)	280 (86%)	44 (14%)	0	100	100
1	D	402/1312 (31%)	355 (88%)	43 (11%)	4 (1%)	13	46
2	A	409/706 (58%)	382 (93%)	27 (7%)	0	100	100
2	B	410/706 (58%)	384 (94%)	25 (6%)	1 (0%)	44	73
All	All	1545/4036 (38%)	1401 (91%)	139 (9%)	5 (0%)	38	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	168	PRO
1	D	1167	ASP
1	D	1210	VAL
1	D	180	GLN
2	B	118	VAL

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	C	289/1234 (23%)	263 (91%)	26 (9%)	8	32
1	D	358/1234 (29%)	324 (90%)	34 (10%)	7	30
2	A	359/635 (56%)	337 (94%)	22 (6%)	15	44
2	B	364/635 (57%)	342 (94%)	22 (6%)	16	45
All	All	1370/3738 (37%)	1266 (92%)	104 (8%)	13	37

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	THR
1	C	1165	ASP
2	B	266	VAL
1	C	82	LEU
1	C	116	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
2	B	401	ASN
1	C	1266	GLN
2	B	261	GLN
1	C	1244	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, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	ATP	D	1402	-	28,33,33	0.73	0	34,52,52	0.83	2 (5%)
3	ATP	D	1401	-	28,33,33	0.72	0	34,52,52	0.66	1 (2%)

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
3	ATP	D	1402	-	-	5/18/38/38	0/3/3/3
3	ATP	D	1401	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	ATP	C5-C6-N6	2.41	123.98	120.31
3	D	1402	ATP	O4'-C1'-N9	2.26	111.74	108.75
3	D	1401	ATP	C5-C6-N6	2.08	123.48	120.31

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

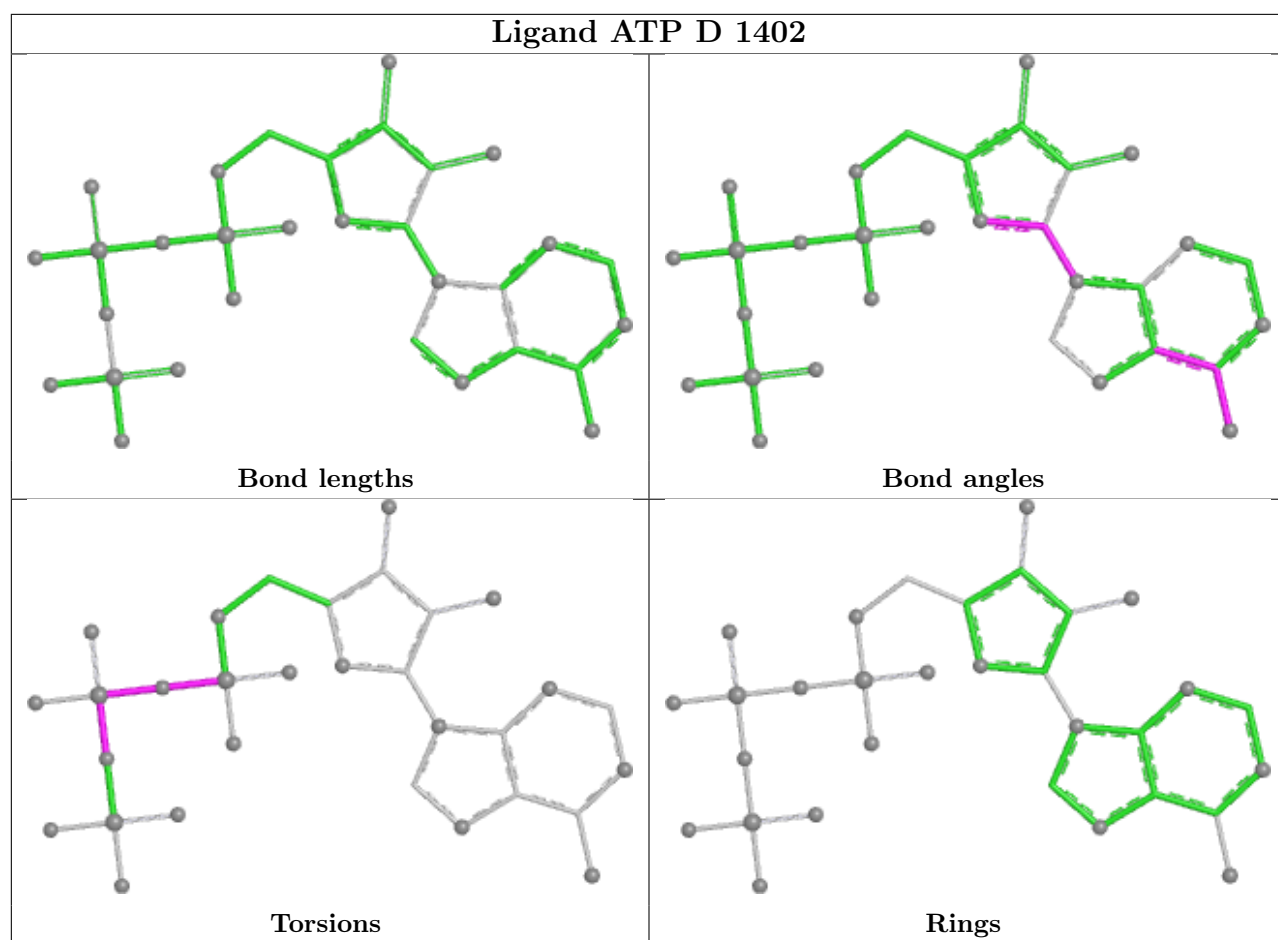
Mol	Chain	Res	Type	Atoms
3	D	1401	ATP	C3'-C4'-C5'-O5'
3	D	1401	ATP	O4'-C4'-C5'-O5'
3	D	1402	ATP	PG-O3B-PB-O1B
3	D	1402	ATP	PG-O3B-PB-O2B
3	D	1401	ATP	PA-O3A-PB-O1B

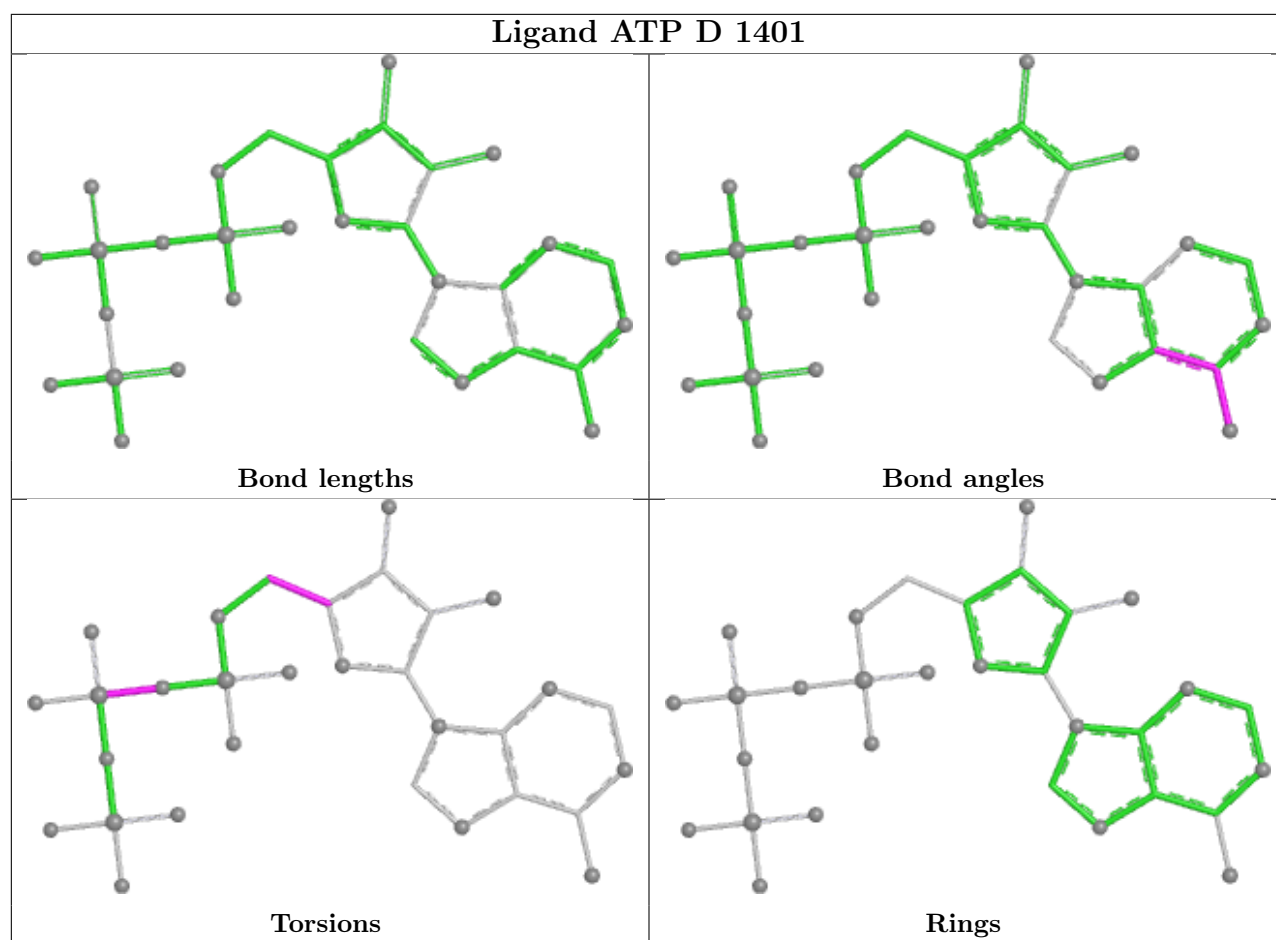
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1402	ATP	5	0
3	D	1401	ATP	8	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.

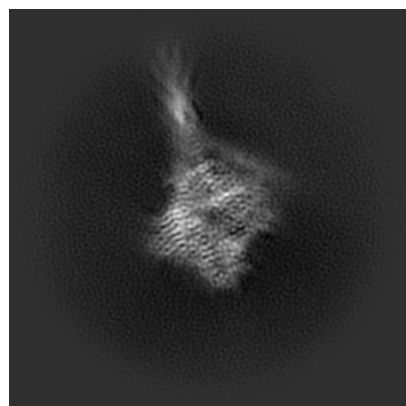
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44559. These allow visual inspection of the internal detail of the map and identification of artifacts.

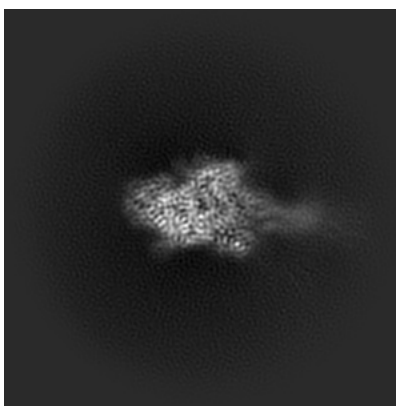
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

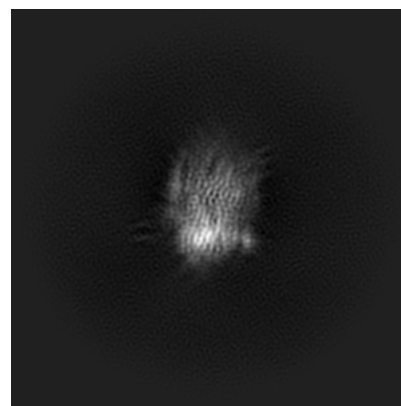
6.1.1 Primary map



X

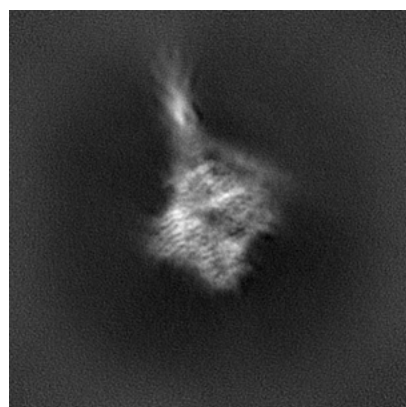


Y

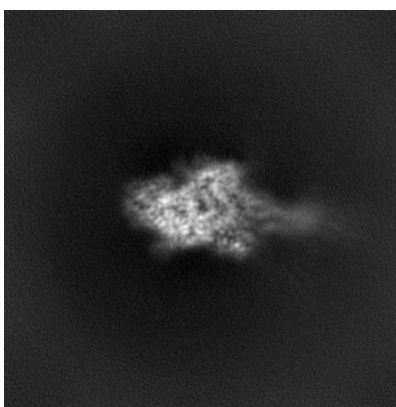


Z

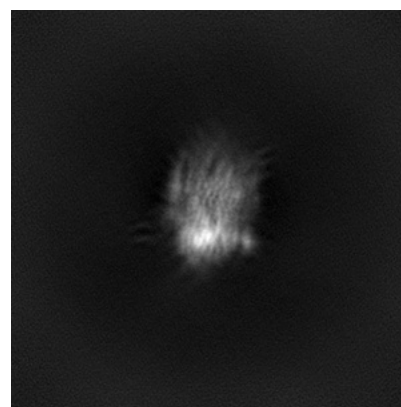
6.1.2 Raw map



X



Y

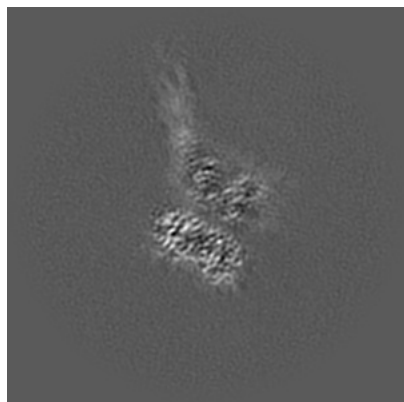


Z

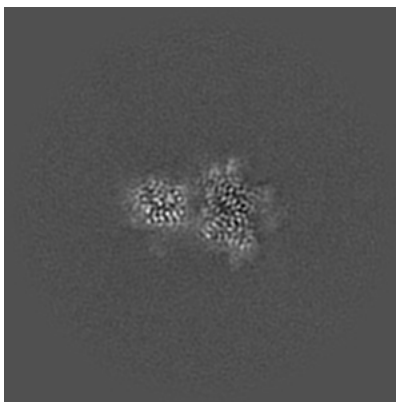
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

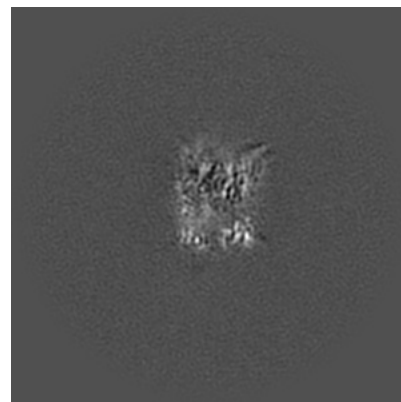
6.2.1 Primary map



X Index: 140

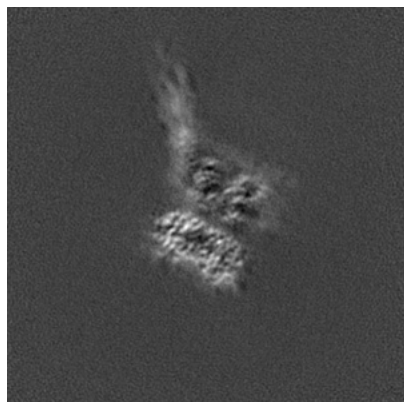


Y Index: 140

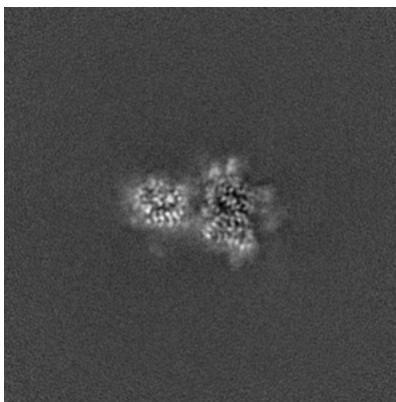


Z Index: 140

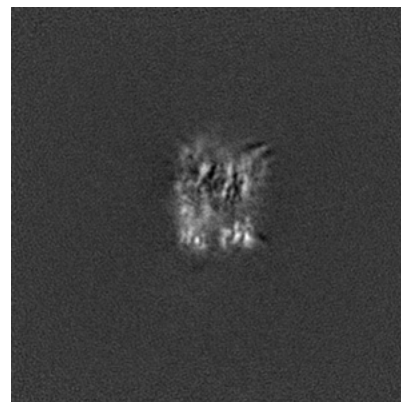
6.2.2 Raw map



X Index: 140



Y Index: 140

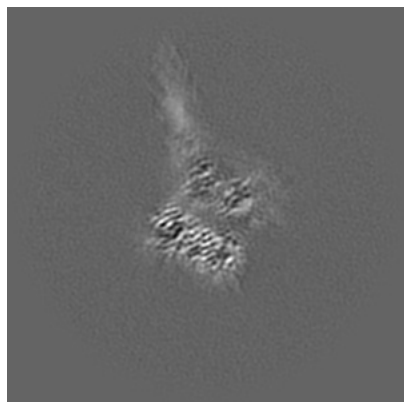


Z Index: 140

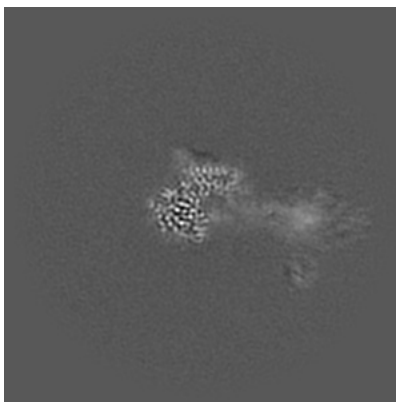
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

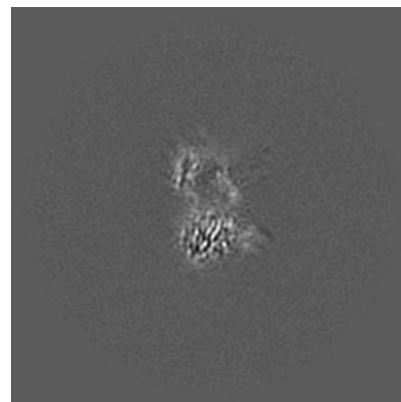
6.3.1 Primary map



X Index: 135

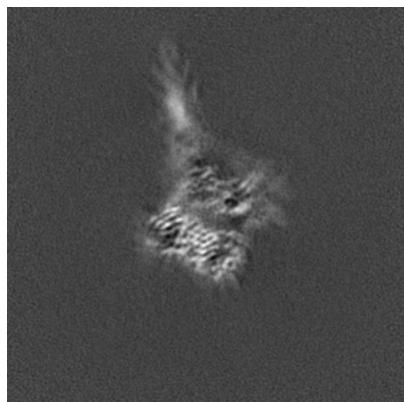


Y Index: 118

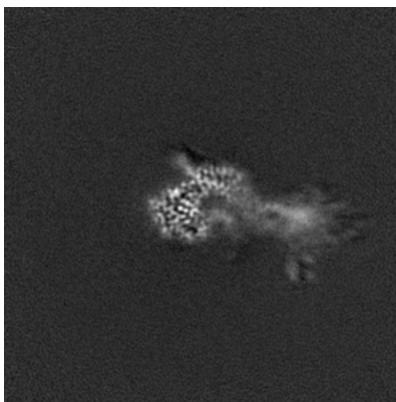


Z Index: 128

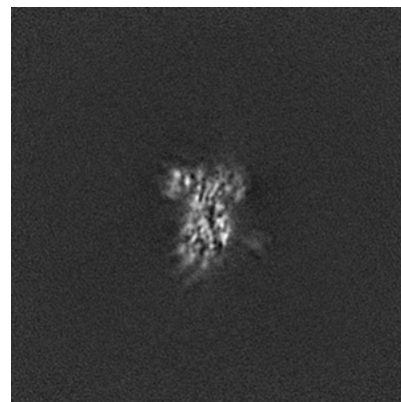
6.3.2 Raw map



X Index: 134



Y Index: 121

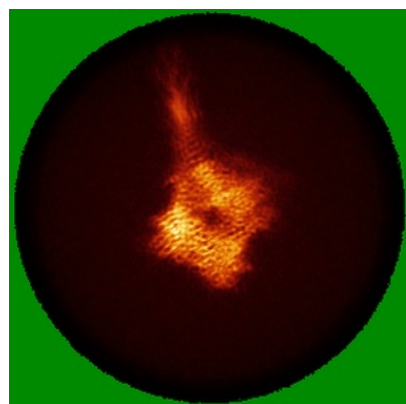


Z Index: 116

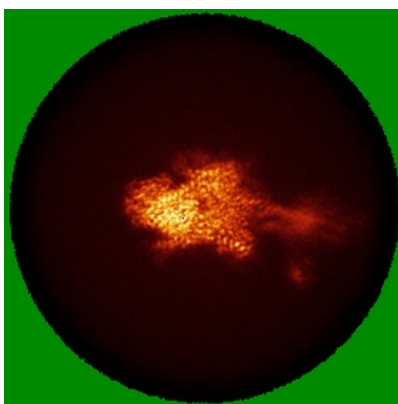
The images above show the largest variance slices of the map in three orthogonal directions.

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

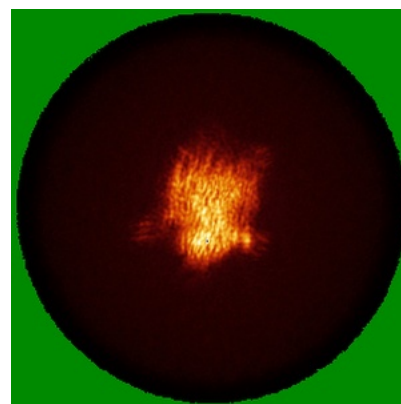
6.4.1 Primary map



X

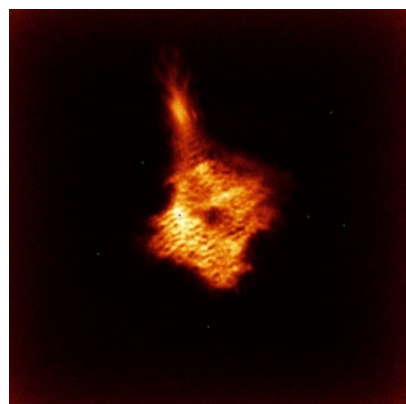


Y



Z

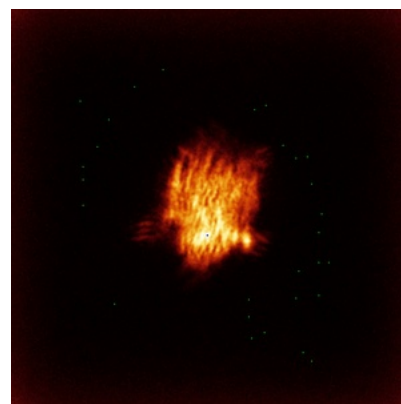
6.4.2 Raw map



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 0.25. 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.

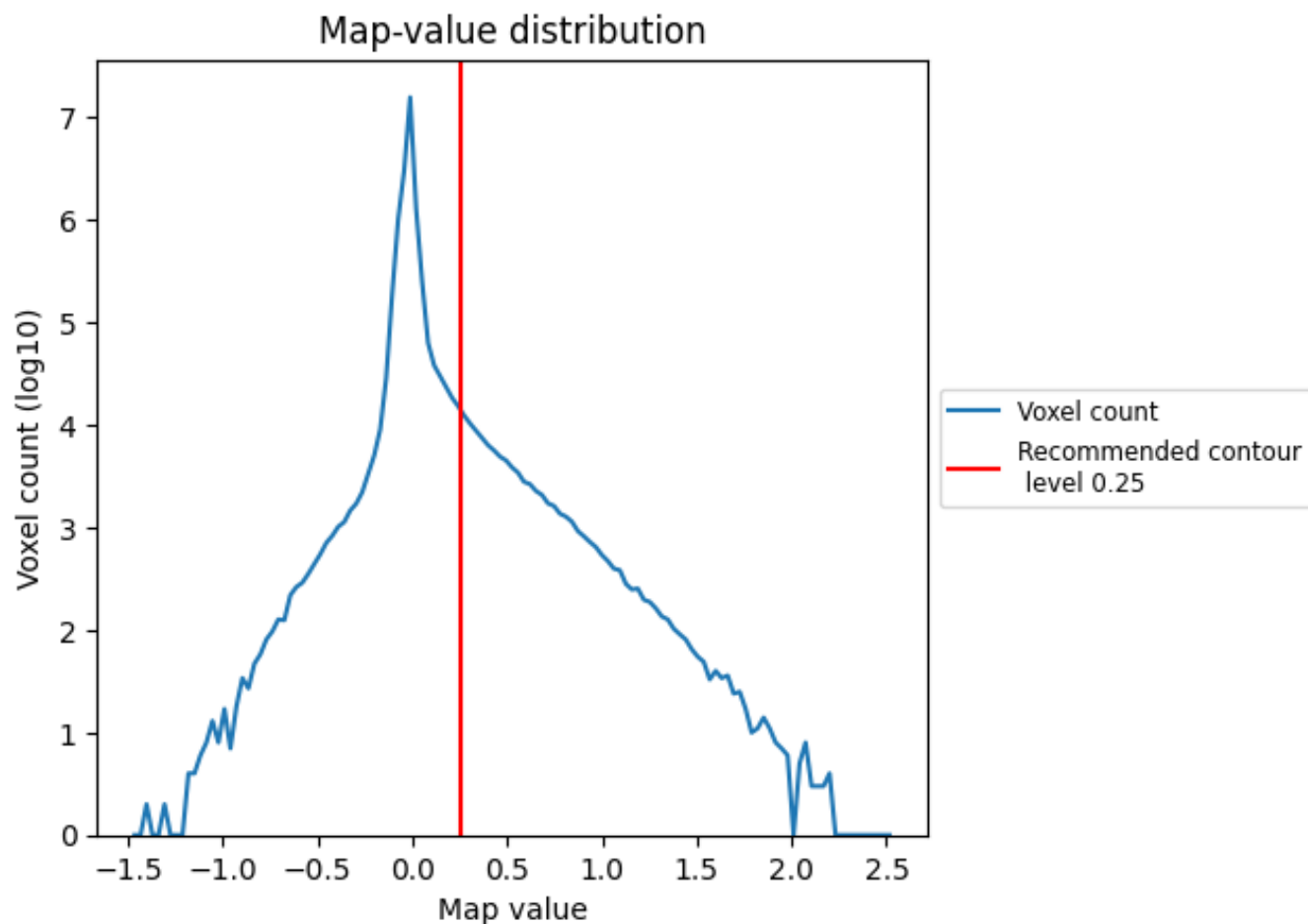
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

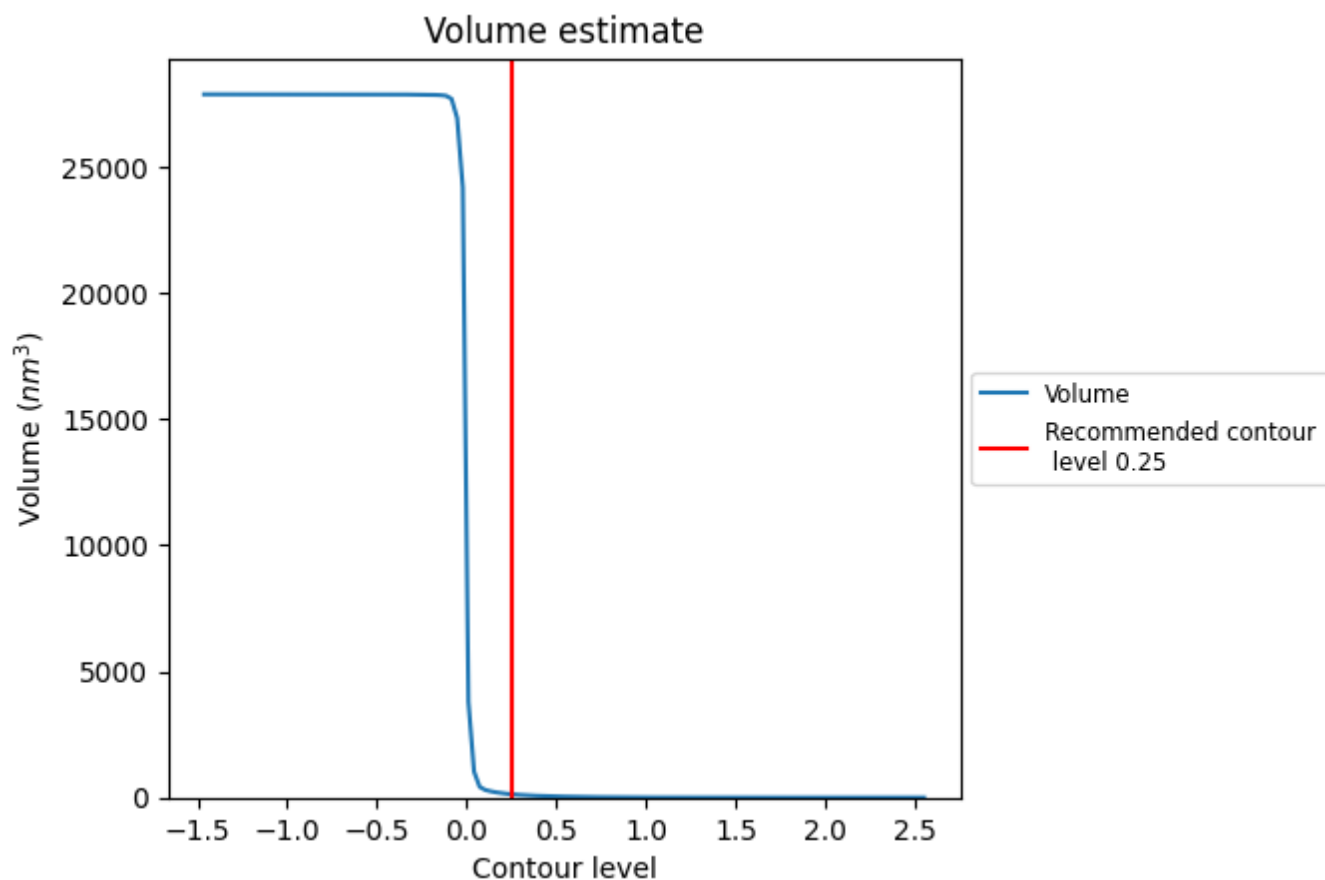
This section contains the results of statistical analysis of the map.

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.

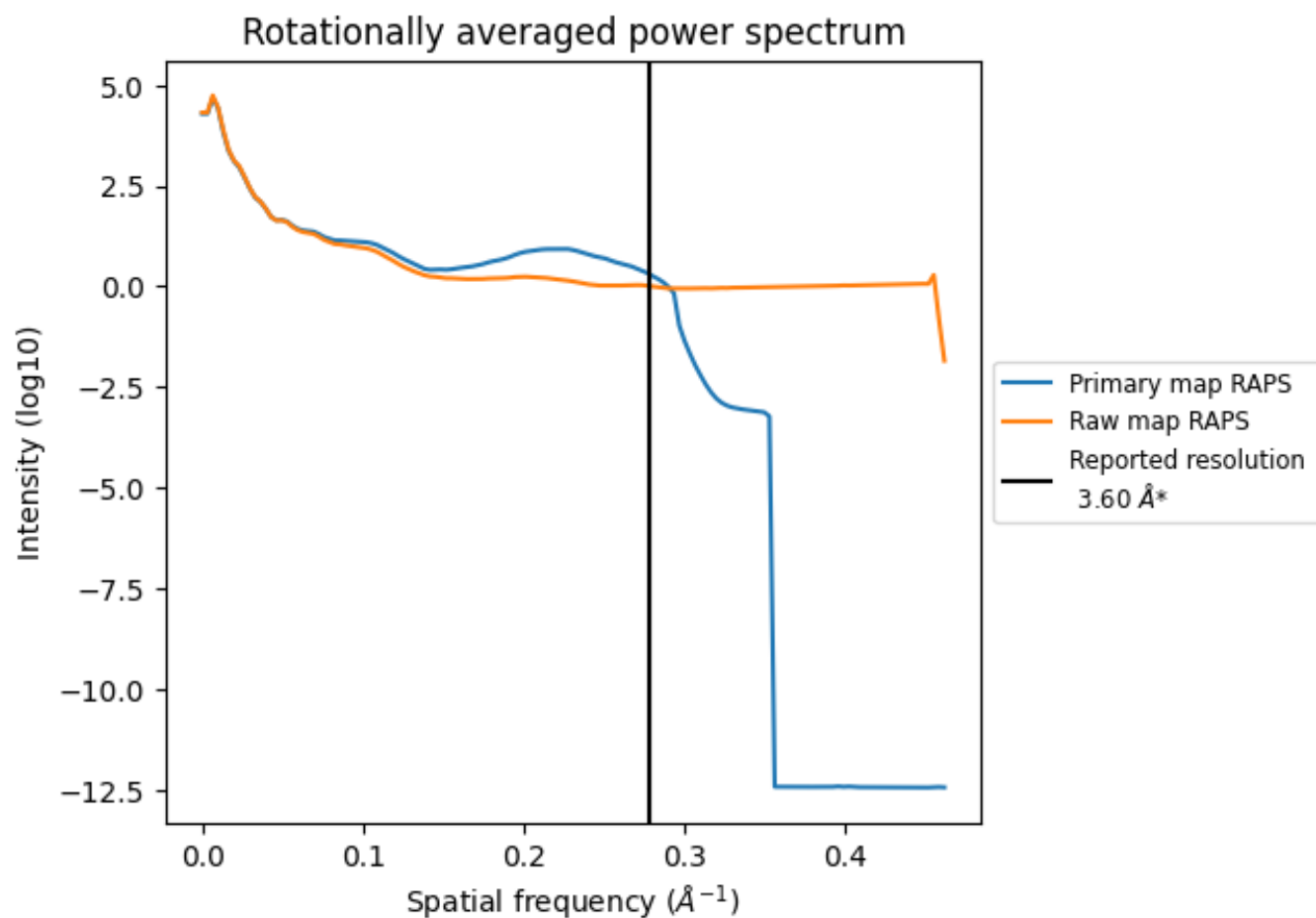
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm^3 ; this corresponds to an approximate mass of 119 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 ⓘ

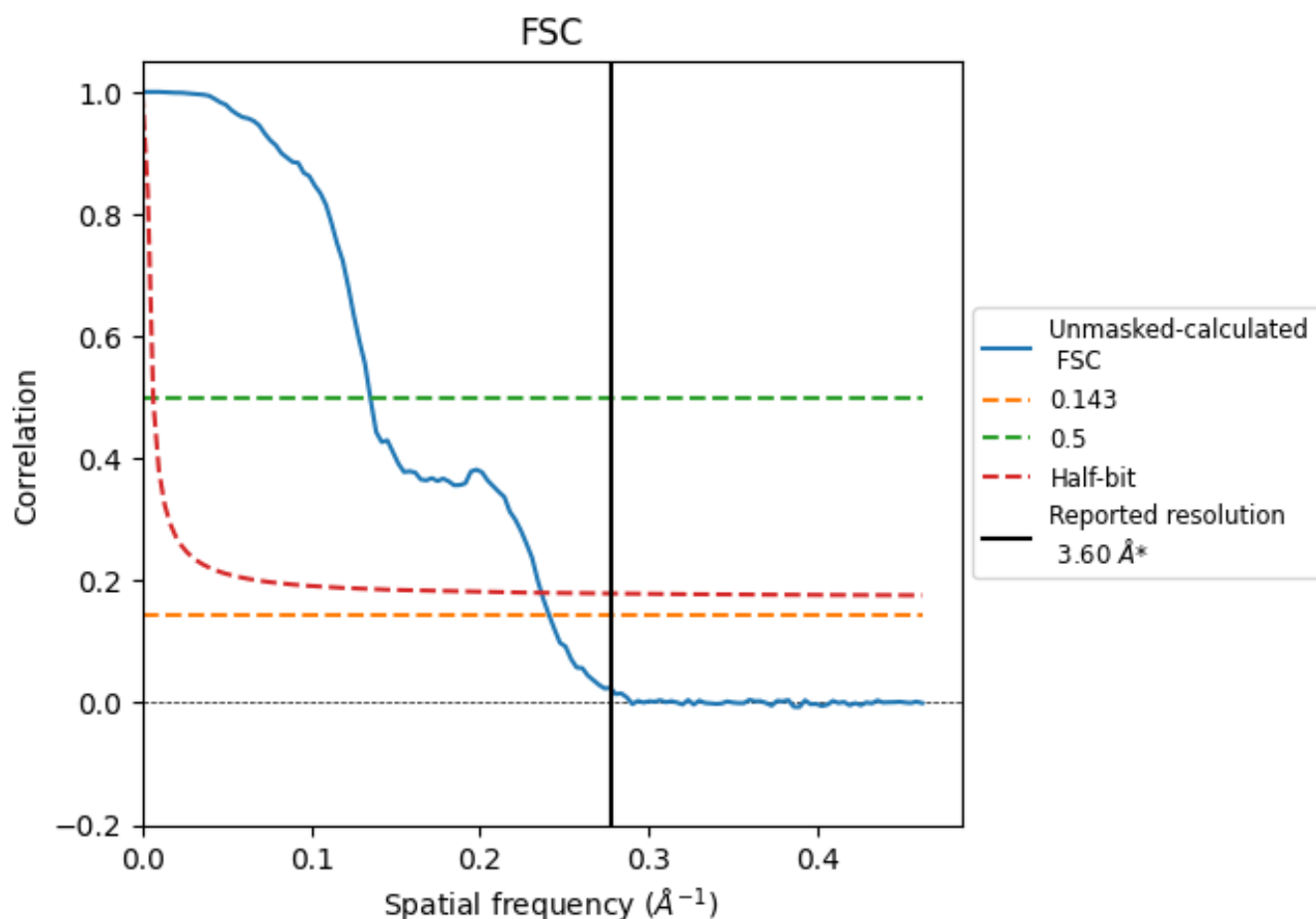


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

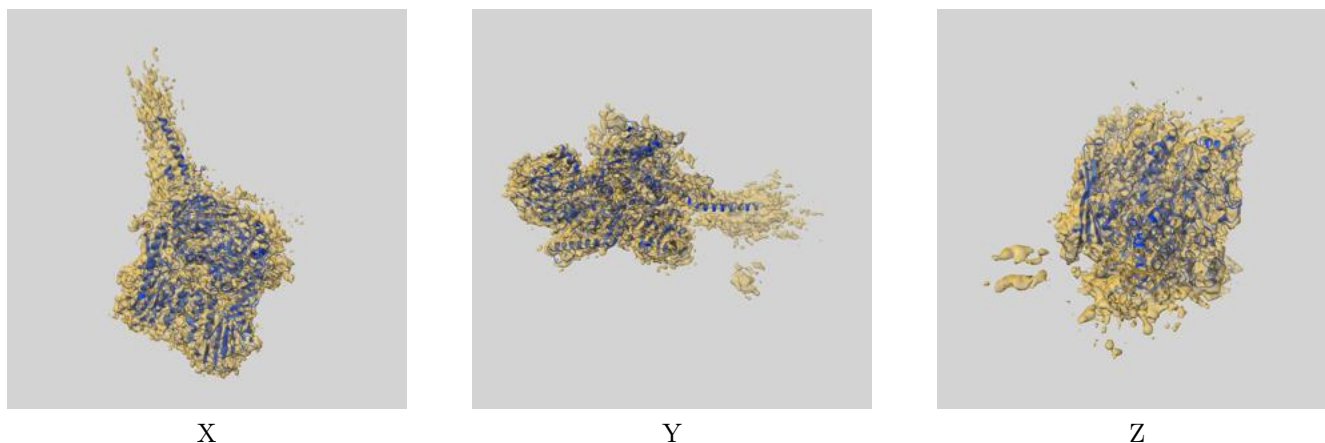
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.41	4.23

*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 4.15 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44559 and PDB model 9BI5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



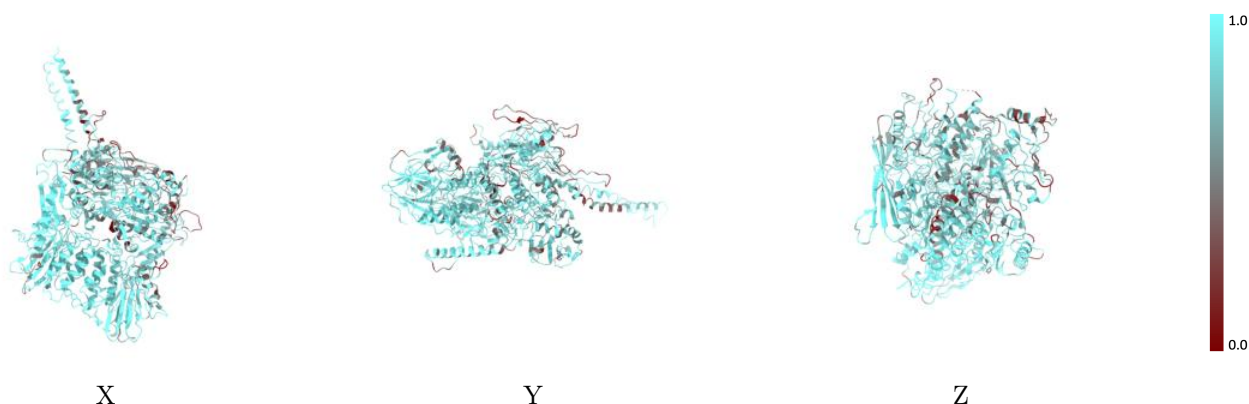
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



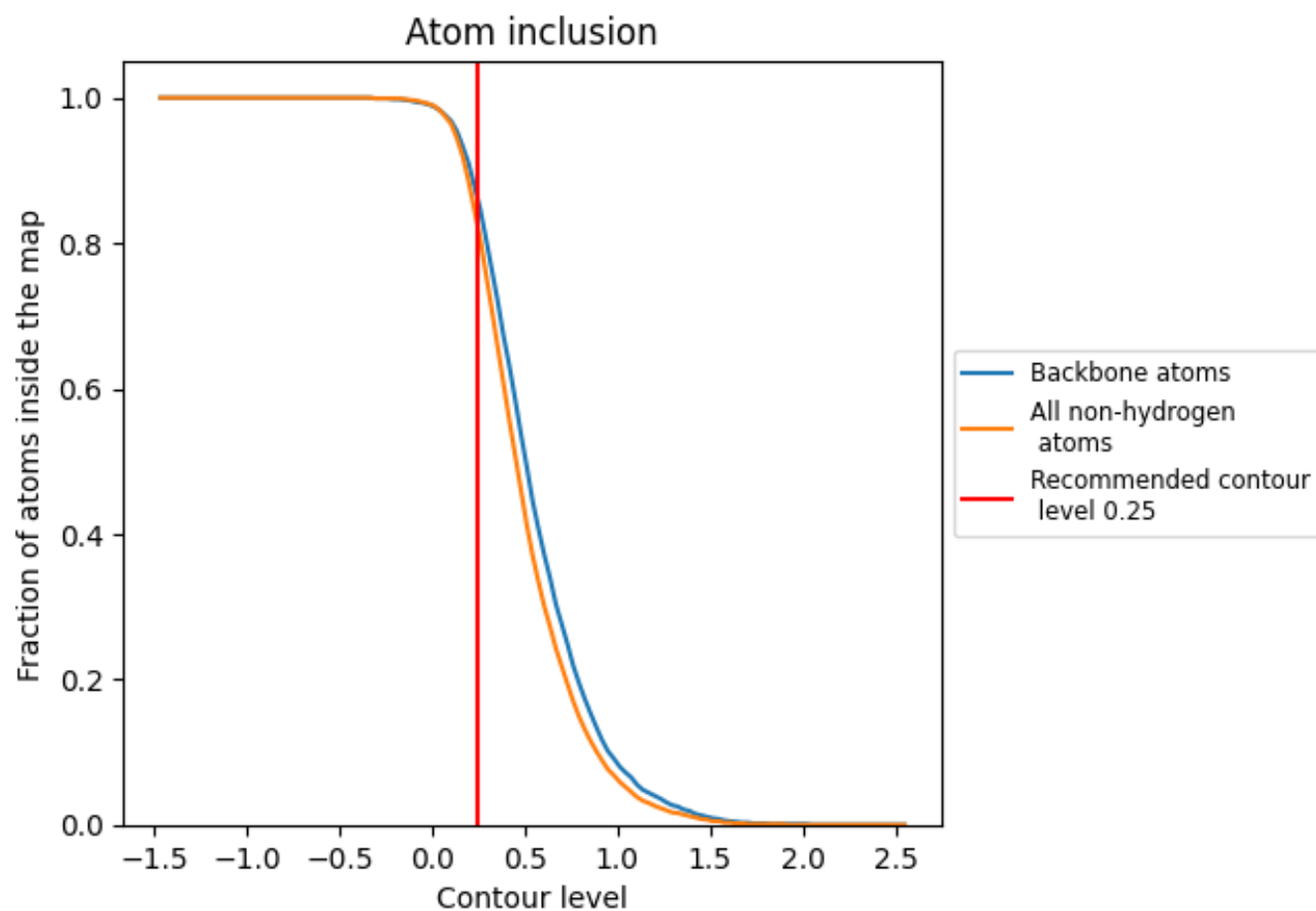
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8190	<div></div> 0.3970
A	<div></div> 0.8950	<div></div> 0.4270
B	<div></div> 0.8480	<div></div> 0.4150
C	<div></div> 0.7370	<div></div> 0.3610
D	<div></div> 0.7810	<div></div> 0.3790

