



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 06:04 PM EST

PDB ID : 7JSG
EMDB ID : EMD-22453
Title : Adeno-Associated Virus 2 Rep68 HD-Heptamer-ssDNA with ATPgS
Authors : Escalante, C.R.
Deposited on : 2020-08-14
Resolution : 5.20 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

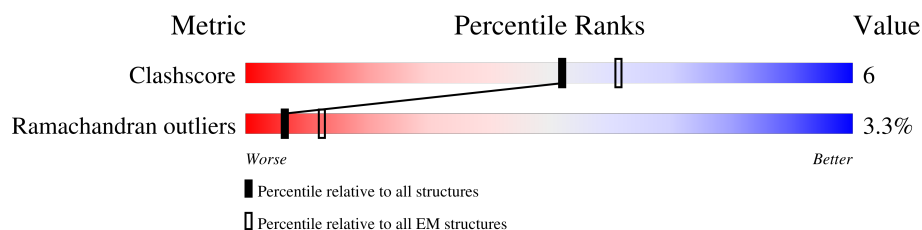
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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

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

Mol	Chain	Length	Quality of chain
1	A	537	<div> <div>6%</div> <div>47%</div> <div>49%</div> </div>
1	B	537	<div> <div>8%</div> <div>49%</div> <div>49%</div> </div>
1	C	537	<div> <div>11%</div> <div>47%</div> <div>49%</div> </div>
1	D	537	<div> <div>10%</div> <div>48%</div> <div>49%</div> </div>
1	E	537	<div> <div>10%</div> <div>48%</div> <div>49%</div> </div>
1	F	537	<div> <div>8%</div> <div>47%</div> <div>49%</div> </div>
1	G	537	<div> <div>9%</div> <div>47%</div> <div>49%</div> </div>
2	N	17	<div> <div>100%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7956 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 Protein Rep68.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	272	Total	C	N	O	0	0
			1088	544	272	272		
1	B	272	Total	C	N	O	0	0
			1088	544	272	272		
1	C	272	Total	C	N	O	0	0
			1088	544	272	272		
1	D	272	Total	C	N	O	0	0
			1088	544	272	272		
1	E	272	Total	C	N	O	0	0
			1088	544	272	272		
1	F	272	Total	C	N	O	0	0
			1088	544	272	272		
1	G	272	Total	C	N	O	0	0
			1088	544	272	272		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P03132
A	1	PRO	-	expression tag	UNP P03132
A	17	GLU	GLY	conflict	UNP P03132
A	151	SER	CYS	engineered mutation	UNP P03132
B	0	GLY	-	expression tag	UNP P03132
B	1	PRO	-	expression tag	UNP P03132
B	17	GLU	GLY	conflict	UNP P03132
B	151	SER	CYS	engineered mutation	UNP P03132
C	0	GLY	-	expression tag	UNP P03132
C	1	PRO	-	expression tag	UNP P03132
C	17	GLU	GLY	conflict	UNP P03132
C	151	SER	CYS	engineered mutation	UNP P03132
D	0	GLY	-	expression tag	UNP P03132
D	1	PRO	-	expression tag	UNP P03132
D	17	GLU	GLY	conflict	UNP P03132
D	151	SER	CYS	engineered mutation	UNP P03132

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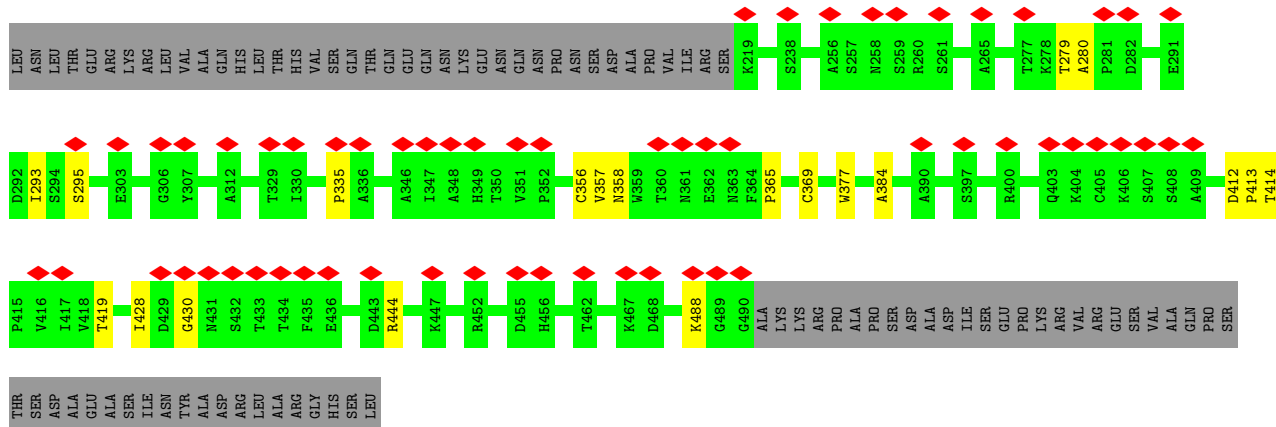
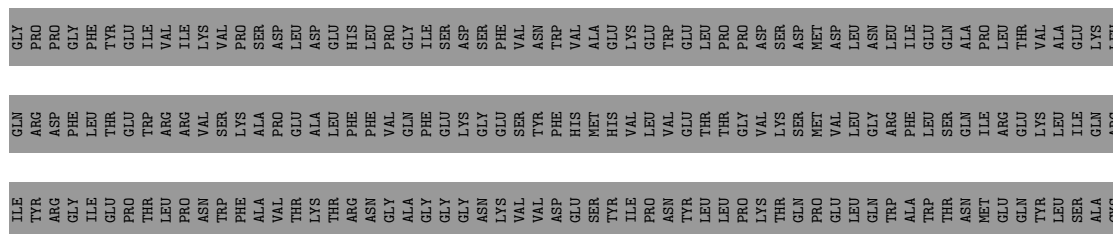
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P03132
E	1	PRO	-	expression tag	UNP P03132
E	17	GLU	GLY	conflict	UNP P03132
E	151	SER	CYS	engineered mutation	UNP P03132
F	0	GLY	-	expression tag	UNP P03132
F	1	PRO	-	expression tag	UNP P03132
F	17	GLU	GLY	conflict	UNP P03132
F	151	SER	CYS	engineered mutation	UNP P03132
G	0	GLY	-	expression tag	UNP P03132
G	1	PRO	-	expression tag	UNP P03132
G	17	GLU	GLY	conflict	UNP P03132
G	151	SER	CYS	engineered mutation	UNP P03132

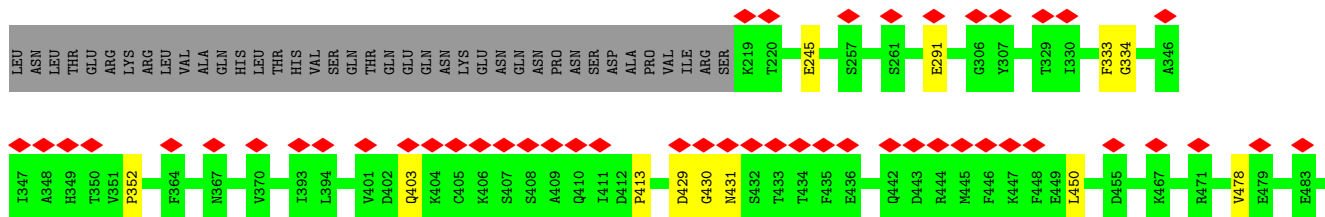
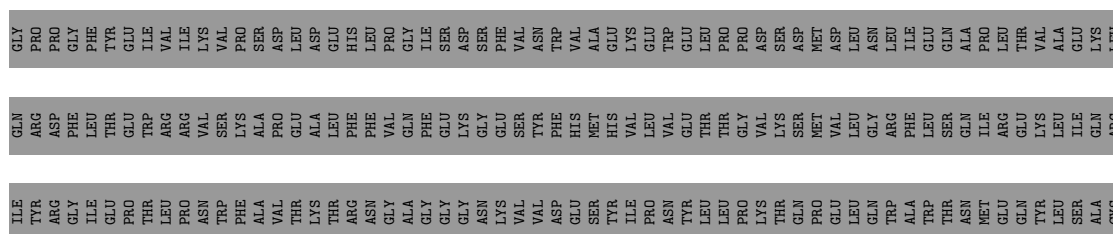
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

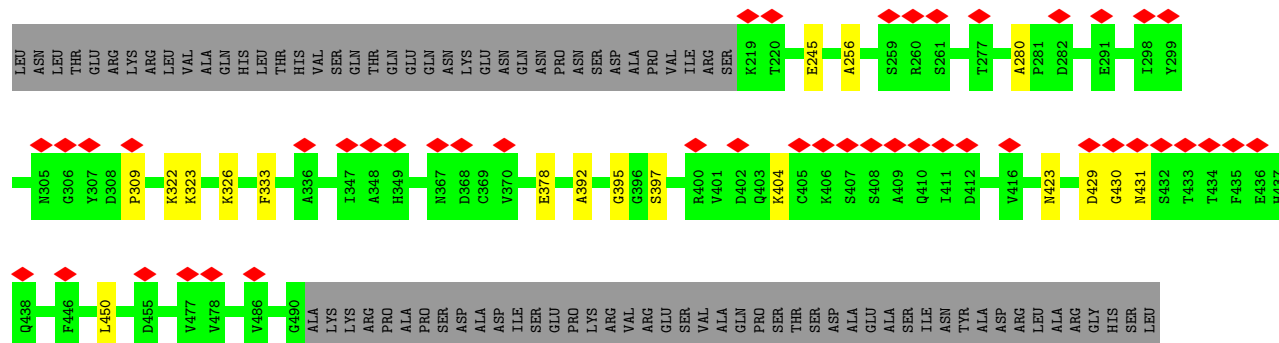
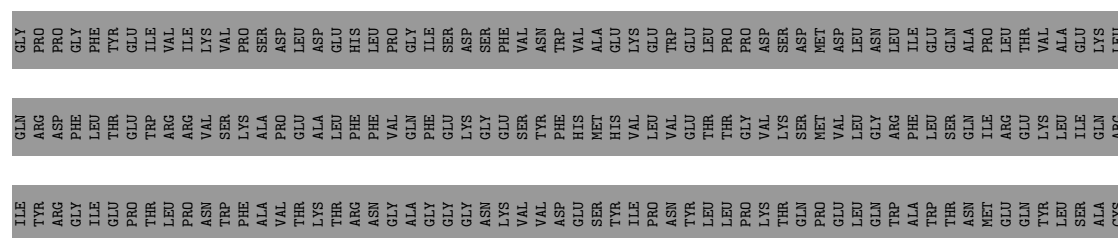
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	17	Total	C	N	O	P	0	0
			340	170	34	119	17		

- Molecule 1: Protein Rep68

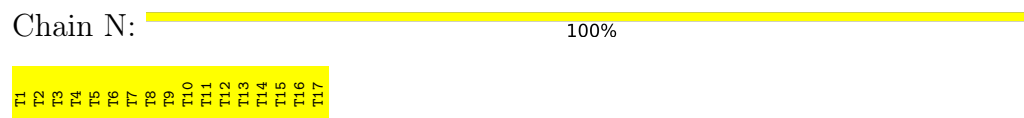


- Molecule 1: Protein Rep68





- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78701	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.815	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.223	Depositor
Map size (Å)	321.9, 321.9, 321.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.073, 1.073, 1.073	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/1087	0.44	0/1357
1	B	0.22	0/1087	0.42	0/1357
1	C	0.22	0/1087	0.43	0/1357
1	D	0.22	0/1087	0.43	0/1357
1	E	0.23	0/1087	0.41	0/1357
1	F	0.23	0/1087	0.43	0/1357
1	G	0.23	0/1087	0.42	0/1357
2	N	0.42	0/373	1.24	0/574
All	All	0.24	0/7982	0.51	0/10073

There are no bond length outliers.

There are no bond angle outliers.

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	A	1088	0	296	3	0
1	B	1088	0	296	1	0
1	C	1088	0	296	4	0
1	D	1088	0	296	3	0
1	E	1088	0	296	3	0
1	F	1088	0	296	5	0
1	G	1088	0	296	4	0
2	N	340	0	205	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7956	0	2277	58	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 6.

All (58) 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:N:1:DT:H2''	2:N:2:DT:H5'	1.43	1.01
2:N:8:DT:H3'	2:N:9:DT:H4'	1.68	0.74
2:N:12:DT:H2'	2:N:13:DT:H71	1.74	0.68
2:N:8:DT:C3'	2:N:9:DT:H4'	2.25	0.67
2:N:4:DT:H4'	2:N:5:DT:O4'	1.95	0.66
2:N:2:DT:H2''	2:N:3:DT:C5	2.32	0.65
2:N:10:DT:H3'	2:N:11:DT:H5''	1.79	0.65
2:N:15:DT:H3'	2:N:15:DT:OP2	1.98	0.63
1:C:384:ALA:N	1:C:428:ILE:O	2.29	0.61
2:N:8:DT:C2'	2:N:9:DT:H4'	2.31	0.61
1:C:377:TRP:O	1:C:419:THR:N	2.25	0.60
2:N:16:DT:OP2	2:N:16:DT:H3'	2.01	0.60
1:G:392:ALA:O	1:G:397:SER:N	2.34	0.59
2:N:6:DT:H2''	2:N:7:DT:C4'	2.34	0.58
1:D:333:PHE:O	1:D:450:LEU:N	2.31	0.58
2:N:6:DT:H2''	2:N:7:DT:C5'	2.34	0.58
1:F:382:MET:O	1:F:428:ILE:N	2.25	0.57
2:N:11:DT:H1'	2:N:12:DT:H5''	1.84	0.57
2:N:8:DT:H3'	2:N:8:DT:OP1	2.04	0.57
2:N:10:DT:C3'	2:N:11:DT:H5''	2.34	0.57
1:F:326:LYS:O	1:F:395:GLY:HA2	2.06	0.55
1:A:384:ALA:N	1:A:428:ILE:O	2.39	0.55
1:F:355:GLY:HA3	1:F:368:ASP:O	2.06	0.54
1:D:334:GLY:HA3	1:D:450:LEU:O	2.08	0.54
2:N:1:DT:C2'	2:N:2:DT:H5'	2.28	0.54
2:N:7:DT:H2''	2:N:8:DT:OP2	2.08	0.54
2:N:11:DT:H2''	2:N:12:DT:H5'	1.91	0.53
2:N:6:DT:H72	2:N:8:DT:O4'	2.09	0.52
1:G:326:LYS:O	1:G:395:GLY:HA2	2.10	0.50
1:G:429:ASP:O	1:G:431:ASN:N	2.46	0.48
2:N:1:DT:C2	2:N:2:DT:H72	2.50	0.47
2:N:2:DT:H2''	2:N:3:DT:C6	2.50	0.47
2:N:4:DT:H3'	2:N:4:DT:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:PHE:O	1:F:373:MET:N	2.38	0.46
1:B:329:THR:O	1:B:445:MET:CA	2.64	0.46
2:N:2:DT:H2''	2:N:3:DT:C4	2.51	0.46
2:N:16:DT:H3'	2:N:16:DT:P	2.56	0.46
1:D:429:ASP:O	1:D:431:ASN:N	2.49	0.46
2:N:7:DT:H1'	2:N:8:DT:C5'	2.46	0.45
2:N:4:DT:C3'	2:N:5:DT:H5'	2.47	0.44
1:E:333:PHE:O	1:E:450:LEU:N	2.49	0.44
1:E:429:ASP:O	1:E:431:ASN:N	2.50	0.43
2:N:4:DT:H5''	2:N:5:DT:H5'	2.01	0.43
2:N:16:DT:H2''	2:N:17:DT:H5'	2.00	0.42
1:A:290:VAL:O	1:A:292:ASP:N	2.52	0.42
2:N:16:DT:OP2	2:N:17:DT:H71	2.19	0.42
2:N:6:DT:H2''	2:N:7:DT:H5'	2.01	0.42
1:A:412:ASP:O	1:A:414:THR:N	2.53	0.42
2:N:16:DT:H2''	2:N:17:DT:C5'	2.50	0.41
1:F:429:ASP:O	1:F:431:ASN:N	2.53	0.41
1:C:412:ASP:O	1:C:414:THR:N	2.54	0.41
2:N:6:DT:H6	2:N:6:DT:H2'	1.71	0.41
2:N:8:DT:OP1	2:N:9:DT:H5''	2.21	0.41
1:E:392:ALA:O	1:E:397:SER:N	2.52	0.41
1:C:356:CYS:O	1:C:358:ASN:N	2.54	0.40
2:N:4:DT:C4'	2:N:5:DT:H5'	2.51	0.40
1:G:333:PHE:O	1:G:450:LEU:N	2.34	0.40
2:N:13:DT:H2''	2:N:14:DT:H5'	2.02	0.40

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	270/537 (50%)	235 (87%)	24 (9%)	11 (4%)	3 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	270/537 (50%)	219 (81%)	42 (16%)	9 (3%)	4	29
1	C	270/537 (50%)	221 (82%)	37 (14%)	12 (4%)	2	24
1	D	270/537 (50%)	225 (83%)	38 (14%)	7 (3%)	5	33
1	E	270/537 (50%)	222 (82%)	42 (16%)	6 (2%)	6	36
1	F	270/537 (50%)	227 (84%)	35 (13%)	8 (3%)	4	30
1	G	270/537 (50%)	233 (86%)	27 (10%)	10 (4%)	3	27
All	All	1890/3759 (50%)	1582 (84%)	245 (13%)	63 (3%)	6	29

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	THR
1	A	378	GLU
1	C	335	PRO
1	D	403	GLN
1	F	245	GLU
1	F	403	GLN
1	G	378	GLU
1	A	245	GLU
1	A	276	LEU
1	A	365	PRO
1	A	369	CYS
1	A	430	GLY
1	B	238	SER
1	B	365	PRO
1	B	369	CYS
1	B	385	LYS
1	B	430	GLY
1	C	279	THR
1	C	295	SER
1	C	369	CYS
1	D	352	PRO
1	E	245	GLU
1	E	430	GLY
1	F	430	GLY
1	F	478	VAL
1	G	323	LYS
1	G	404	LYS
1	G	430	GLY
1	A	280	ALA

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Mol	Chain	Res	Type
1	B	277	THR
1	C	365	PRO
1	C	430	GLY
1	C	444	ARG
1	D	245	GLU
1	D	430	GLY
1	E	291	GLU
1	E	369	CYS
1	G	245	GLU
1	G	256	ALA
1	G	280	ALA
1	G	423	ASN
1	A	291	GLU
1	B	484	PHE
1	D	291	GLU
1	F	408	SER
1	B	413	PRO
1	C	357	VAL
1	C	413	PRO
1	C	488	LYS
1	D	413	PRO
1	E	365	PRO
1	E	404	LYS
1	G	309	PRO
1	G	322	LYS
1	A	309	PRO
1	A	413	PRO
1	D	478	VAL
1	F	357	VAL
1	B	478	VAL
1	C	280	ALA
1	C	293	ILE
1	F	280	ALA
1	F	325	GLY

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

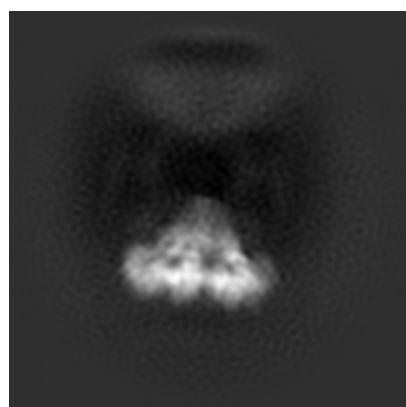
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22453. These allow visual inspection of the internal detail of the map and identification of artifacts.

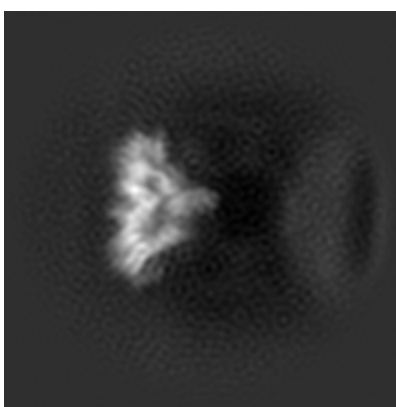
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

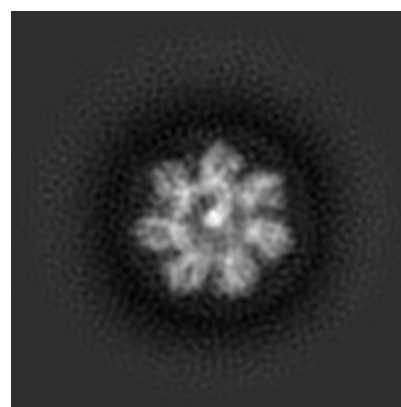
6.1.1 Primary map



X



Y

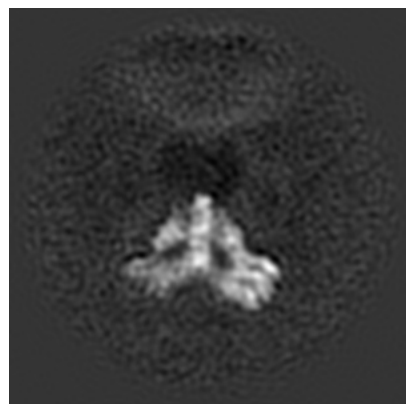


Z

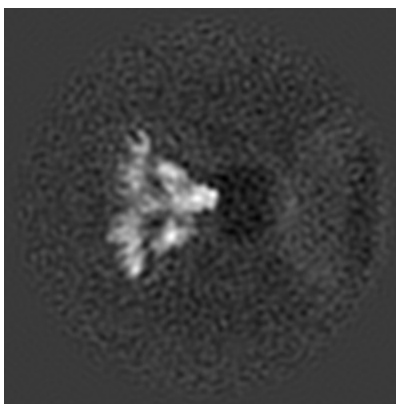
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

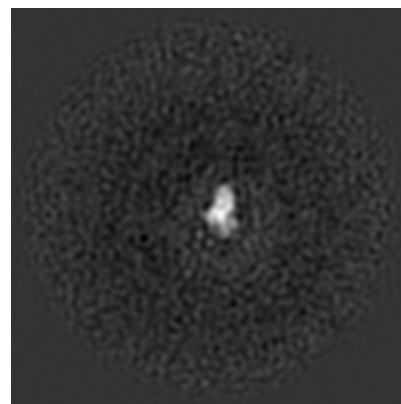
6.2.1 Primary map



X Index: 150



Y Index: 150

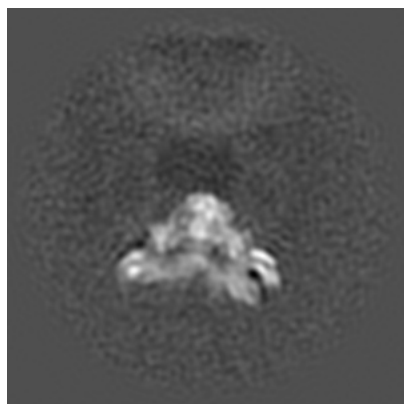


Z Index: 150

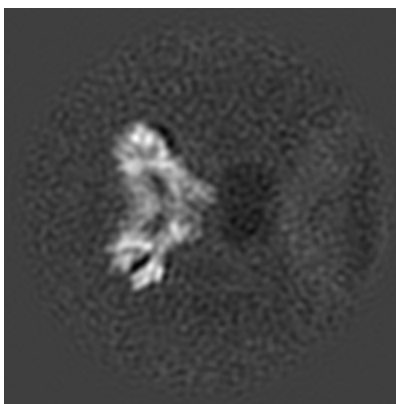
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

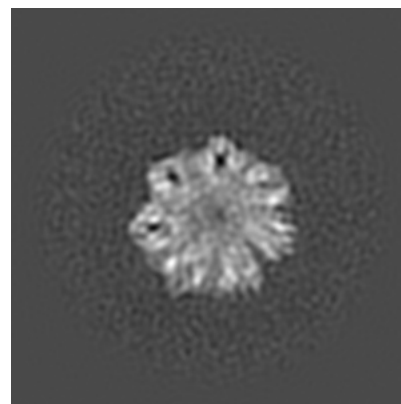
6.3.1 Primary map



X Index: 157



Y Index: 134

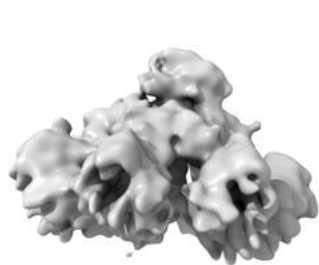


Z Index: 99

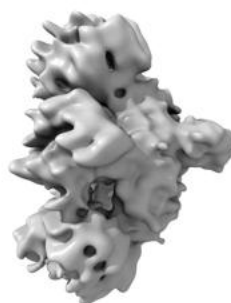
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

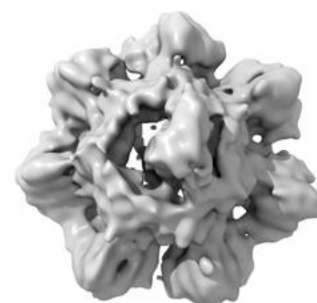
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.223. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

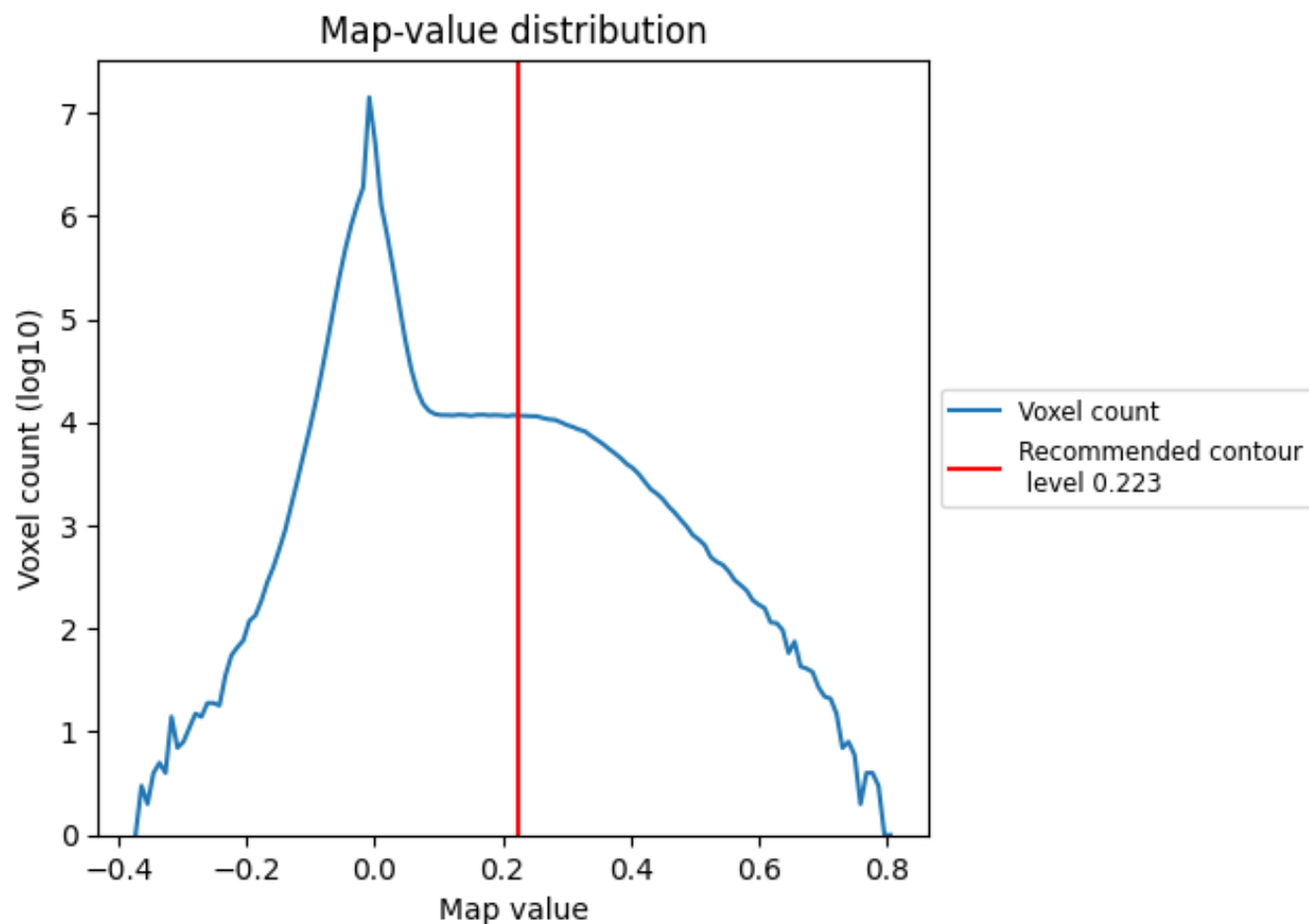
6.5 Mask visualisation

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

7 Map analysis [i](#)

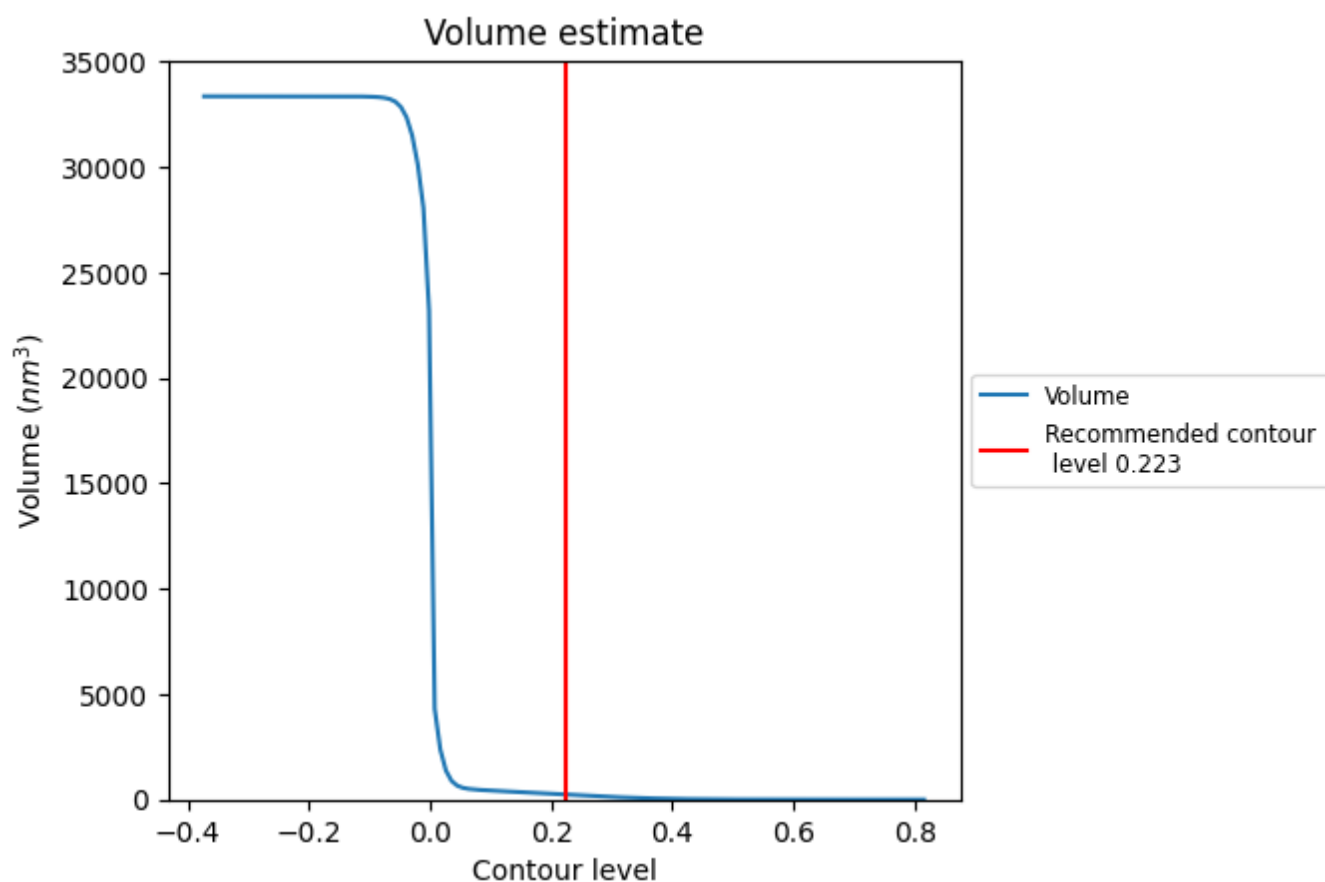
This section contains the results of statistical analysis of the map.

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.

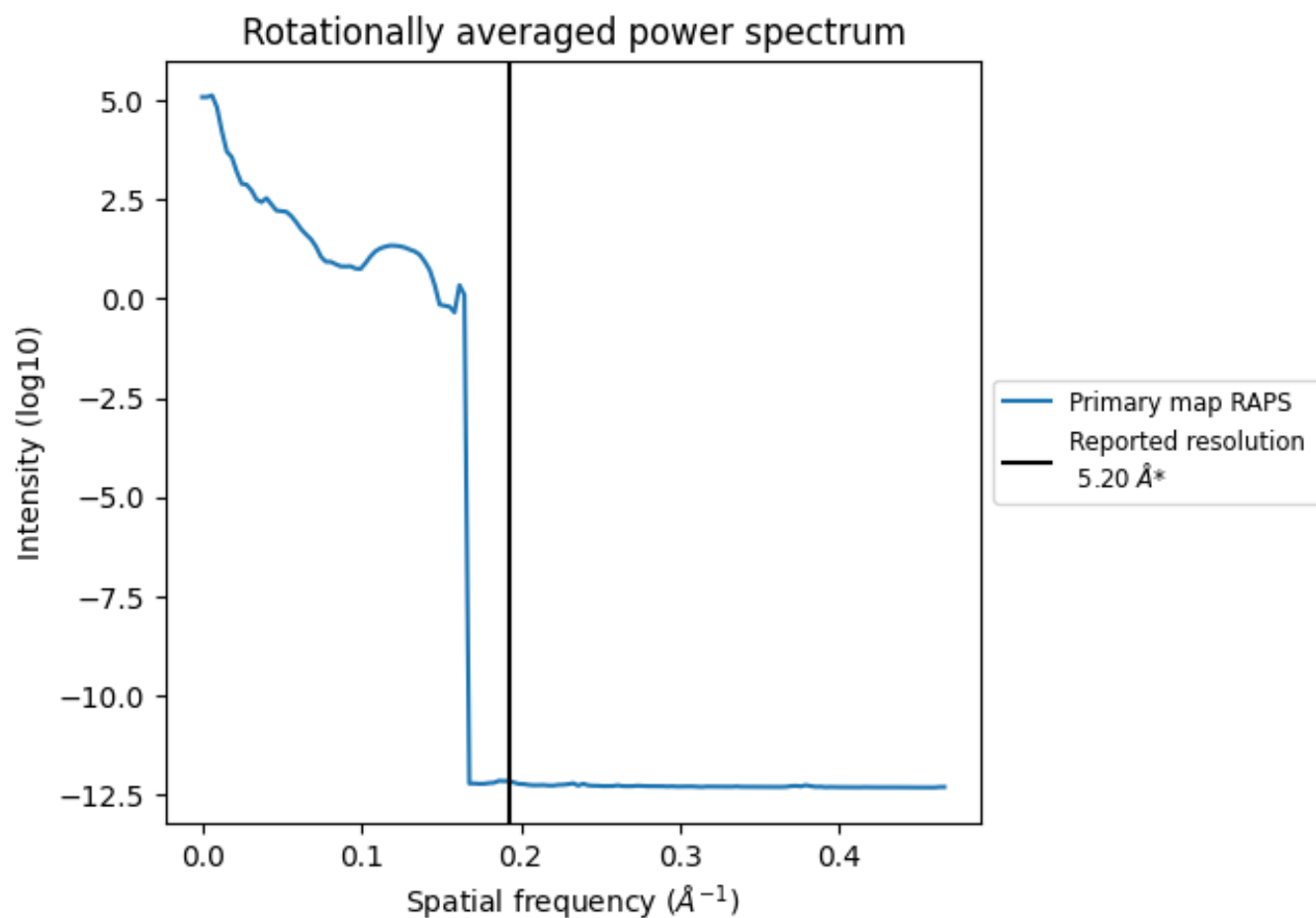
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 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 0.192 Å⁻¹

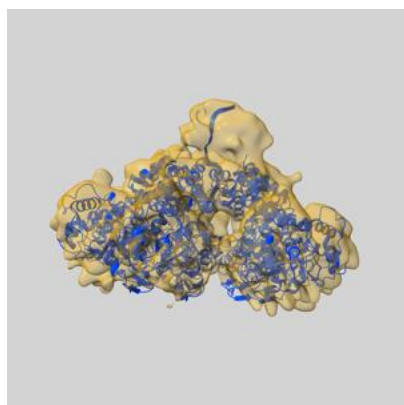
8 Fourier-Shell correlation

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

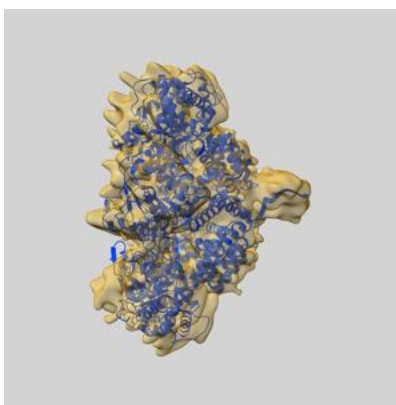
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22453 and PDB model 7JSG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

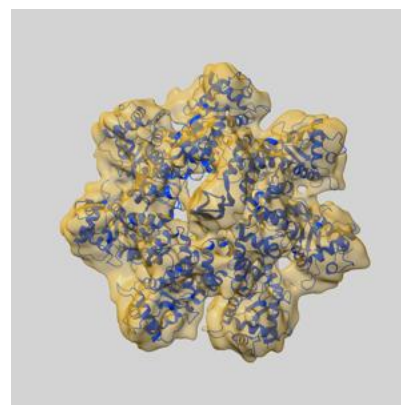
9.1 Map-model overlay [i](#)



X



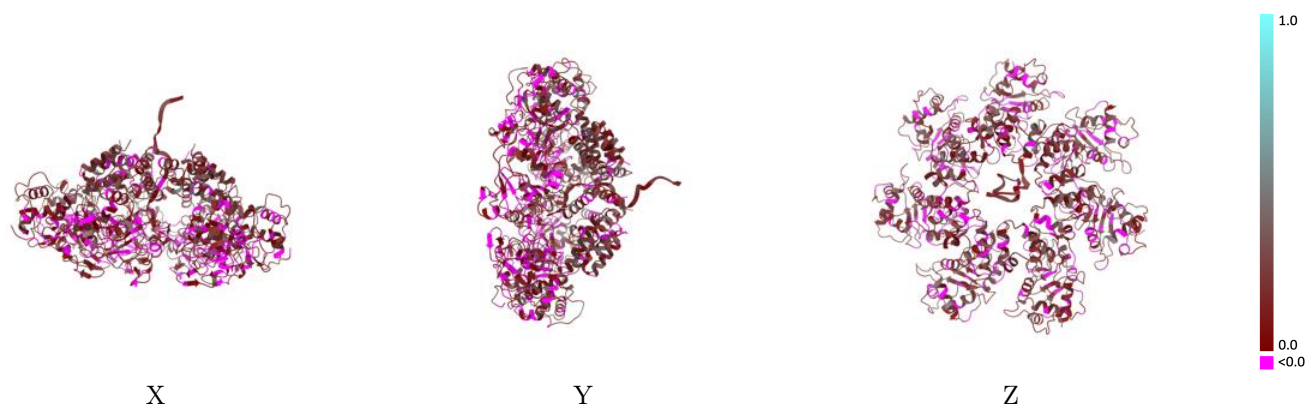
Y



Z

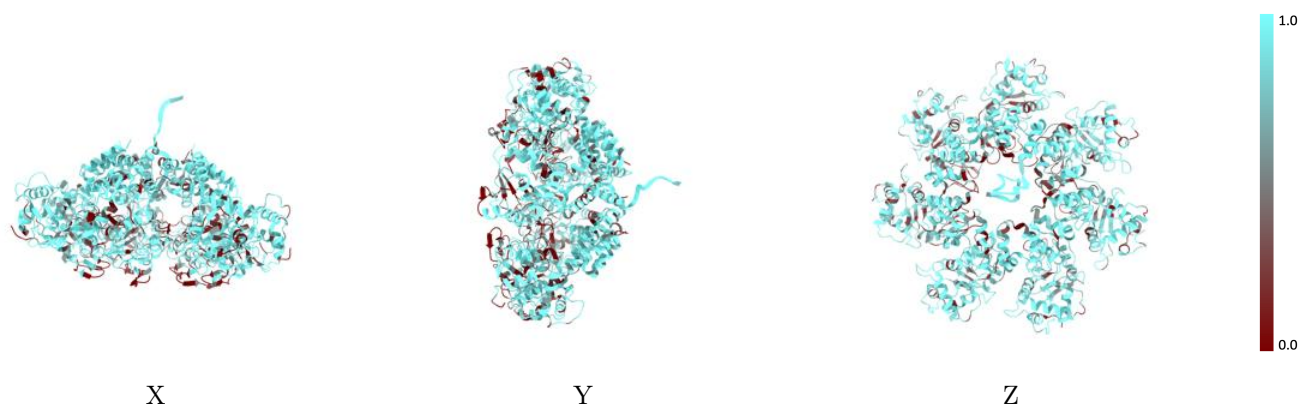
The images above show the 3D surface view of the map at the recommended contour level 0.223 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



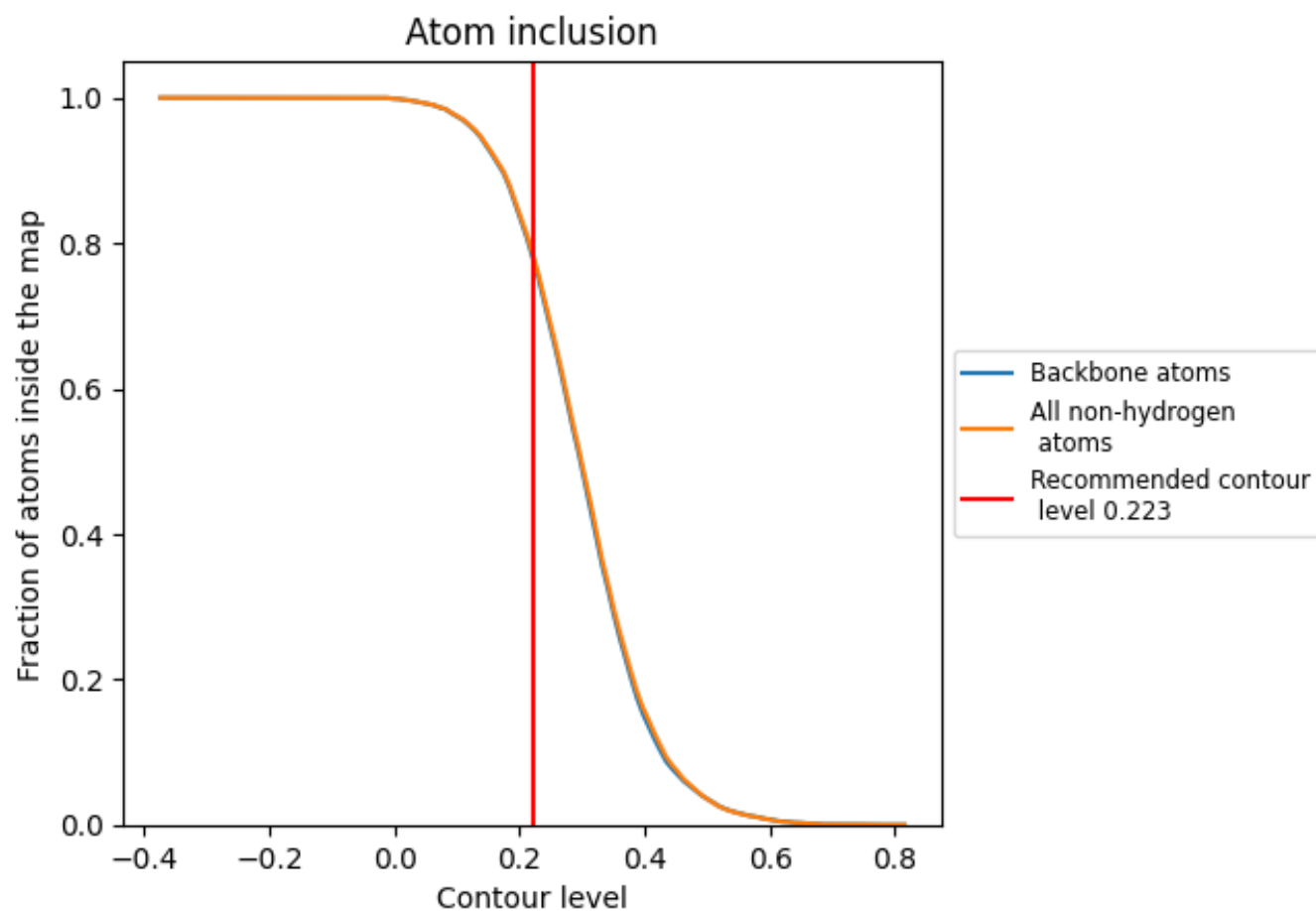
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.223).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.223) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7804	<div></div> 0.1220
A	<div></div> 0.8263	<div></div> 0.1430
B	<div></div> 0.7914	<div></div> 0.1200
C	<div></div> 0.7206	<div></div> 0.1010
D	<div></div> 0.7399	<div></div> 0.1070
E	<div></div> 0.7748	<div></div> 0.1080
F	<div></div> 0.7858	<div></div> 0.1300
G	<div></div> 0.7776	<div></div> 0.1300
N	<div></div> 0.9294	<div></div> 0.1650

1.0

0.0

<0.0