



## wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 09:30 PM UTC

PDB ID : 6AP1 / pdb\_00006ap1  
EMDB ID : EMD-8887  
Title : Vps4p-Vta1p complex with peptide binding to the central pore of Vps4p  
Authors : Han, H.; Monroe, N.; Shen, P.; Sundquist, W.I.; Hill, C.P.  
Deposited on : 2017-08-16  
Resolution : 3.20 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

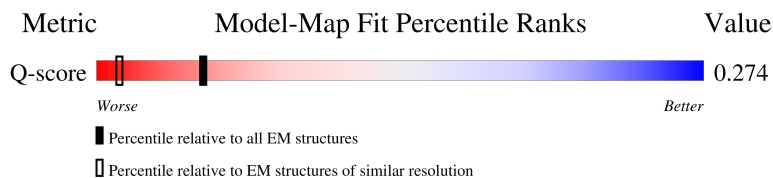
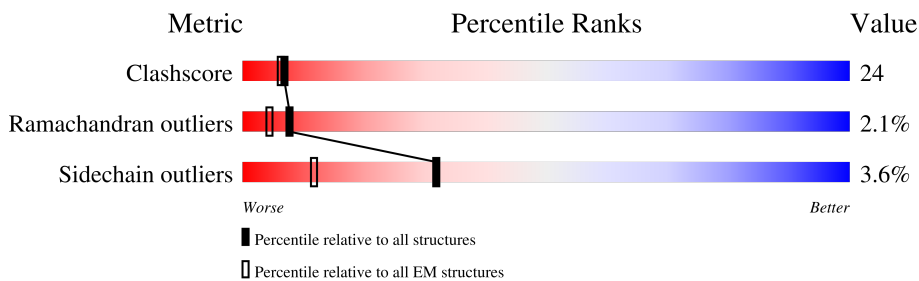
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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

Mol	Chain	Length	Quality of chain
1	A	519	<p>33% (Poor fit), 48% (0 outliers), 10% (1 outlier), 39% (Not modelled)</p>
1	B	519	<p>18% (Poor fit), 50% (0 outliers), 11% (1 outlier), 38% (Not modelled)</p>
1	C	519	<p>18% (Poor fit), 50% (0 outliers), 10% (1 outlier), 38% (Not modelled)</p>
1	D	519	<p>23% (Poor fit), 51% (0 outliers), 9% (1 outlier), 38% (Not modelled)</p>

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Mol	Chain	Length	Quality of chain
1	E	519	 41% 45% 12% 41%
1	F	519	 59% 34% 22% 41%
2	G	10	 60% 90% 10%
3	H	330	 13% 8% 87%
3	I	330	 13% 7% 5% 87%
3	J	330	 13% 8% 87%
3	K	330	 13% 7% 87%
3	L	330	 13% 7% 87%
3	M	330	 13% 7% 5% 87%
3	N	330	 13% 8% 87%
3	O	330	 13% 7% 5% 87%
3	P	330	 13% 7% 87%
3	Q	330	 13% 7% 5% 87%
3	R	330	 13% 8% 87%
3	S	330	 13% 7% 87%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18838 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 Vacuolar protein sorting-associated protein 4, Protein hcp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	314	2427	1530	414	474	9	0	0
1	B	322	2491	1568	427	487	9	0	0
1	C	322	2491	1568	427	487	9	0	0
1	D	322	2491	1568	427	487	9	0	0
1	E	304	2360	1489	401	461	9	0	0
1	F	308	2387	1507	405	466	9	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP P52917
A	438	GLY	-	linker	UNP P52917
A	439	GLY	-	linker	UNP P52917
A	440	GLY	-	linker	UNP P52917
A	441	GLY	-	linker	UNP P52917
A	442	SER	-	linker	UNP P52917
A	443	GLY	-	linker	UNP P52917
A	444	GLY	-	linker	UNP P52917
A	445	GLY	-	linker	UNP P52917
A	446	GLY	-	linker	UNP P52917
A	447	SER	-	linker	UNP P52917
A	448	GLY	-	linker	UNP P52917
A	449	GLY	-	linker	UNP P52917
A	450	GLY	-	linker	UNP P52917
A	451	GLY	-	linker	UNP P52917
A	452	SER	-	linker	UNP P52917
A	453	GLY	-	linker	UNP P52917
A	454	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	linker	UNP P52917
A	618	GLY	-	expression tag	UNP Q9I747
B	100	GLY	-	expression tag	UNP P52917
B	438	GLY	-	linker	UNP P52917
B	439	GLY	-	linker	UNP P52917
B	440	GLY	-	linker	UNP P52917
B	441	GLY	-	linker	UNP P52917
B	442	SER	-	linker	UNP P52917
B	443	GLY	-	linker	UNP P52917
B	444	GLY	-	linker	UNP P52917
B	445	GLY	-	linker	UNP P52917
B	446	GLY	-	linker	UNP P52917
B	447	SER	-	linker	UNP P52917
B	448	GLY	-	linker	UNP P52917
B	449	GLY	-	linker	UNP P52917
B	450	GLY	-	linker	UNP P52917
B	451	GLY	-	linker	UNP P52917
B	452	SER	-	linker	UNP P52917
B	453	GLY	-	linker	UNP P52917
B	454	GLY	-	linker	UNP P52917
B	455	GLY	-	linker	UNP P52917
B	618	GLY	-	expression tag	UNP Q9I747
C	100	GLY	-	expression tag	UNP P52917
C	438	GLY	-	linker	UNP P52917
C	439	GLY	-	linker	UNP P52917
C	440	GLY	-	linker	UNP P52917
C	441	GLY	-	linker	UNP P52917
C	442	SER	-	linker	UNP P52917
C	443	GLY	-	linker	UNP P52917
C	444	GLY	-	linker	UNP P52917
C	445	GLY	-	linker	UNP P52917
C	446	GLY	-	linker	UNP P52917
C	447	SER	-	linker	UNP P52917
C	448	GLY	-	linker	UNP P52917
C	449	GLY	-	linker	UNP P52917
C	450	GLY	-	linker	UNP P52917
C	451	GLY	-	linker	UNP P52917
C	452	SER	-	linker	UNP P52917
C	453	GLY	-	linker	UNP P52917
C	454	GLY	-	linker	UNP P52917
C	455	GLY	-	linker	UNP P52917
C	618	GLY	-	expression tag	UNP Q9I747

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	GLY	-	expression tag	UNP P52917
D	438	GLY	-	linker	UNP P52917
D	439	GLY	-	linker	UNP P52917
D	440	GLY	-	linker	UNP P52917
D	441	GLY	-	linker	UNP P52917
D	442	SER	-	linker	UNP P52917
D	443	GLY	-	linker	UNP P52917
D	444	GLY	-	linker	UNP P52917
D	445	GLY	-	linker	UNP P52917
D	446	GLY	-	linker	UNP P52917
D	447	SER	-	linker	UNP P52917
D	448	GLY	-	linker	UNP P52917
D	449	GLY	-	linker	UNP P52917
D	450	GLY	-	linker	UNP P52917
D	451	GLY	-	linker	UNP P52917
D	452	SER	-	linker	UNP P52917
D	453	GLY	-	linker	UNP P52917
D	454	GLY	-	linker	UNP P52917
D	455	GLY	-	linker	UNP P52917
D	618	GLY	-	expression tag	UNP Q9I747
E	100	GLY	-	expression tag	UNP P52917
E	438	GLY	-	linker	UNP P52917
E	439	GLY	-	linker	UNP P52917
E	440	GLY	-	linker	UNP P52917
E	441	GLY	-	linker	UNP P52917
E	442	SER	-	linker	UNP P52917
E	443	GLY	-	linker	UNP P52917
E	444	GLY	-	linker	UNP P52917
E	445	GLY	-	linker	UNP P52917
E	446	GLY	-	linker	UNP P52917
E	447	SER	-	linker	UNP P52917
E	448	GLY	-	linker	UNP P52917
E	449	GLY	-	linker	UNP P52917
E	450	GLY	-	linker	UNP P52917
E	451	GLY	-	linker	UNP P52917
E	452	SER	-	linker	UNP P52917
E	453	GLY	-	linker	UNP P52917
E	454	GLY	-	linker	UNP P52917
E	455	GLY	-	linker	UNP P52917
E	618	GLY	-	expression tag	UNP Q9I747
F	100	GLY	-	expression tag	UNP P52917
F	438	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
F	439	GLY	-	linker	UNP P52917
F	440	GLY	-	linker	UNP P52917
F	441	GLY	-	linker	UNP P52917
F	442	SER	-	linker	UNP P52917
F	443	GLY	-	linker	UNP P52917
F	444	GLY	-	linker	UNP P52917
F	445	GLY	-	linker	UNP P52917
F	446	GLY	-	linker	UNP P52917
F	447	SER	-	linker	UNP P52917
F	448	GLY	-	linker	UNP P52917
F	449	GLY	-	linker	UNP P52917
F	450	GLY	-	linker	UNP P52917
F	451	GLY	-	linker	UNP P52917
F	452	SER	-	linker	UNP P52917
F	453	GLY	-	linker	UNP P52917
F	454	GLY	-	linker	UNP P52917
F	455	GLY	-	linker	UNP P52917
F	618	GLY	-	expression tag	UNP Q9I747

- Molecule 2 is a protein called ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	10	68	43	11	14	1	1

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

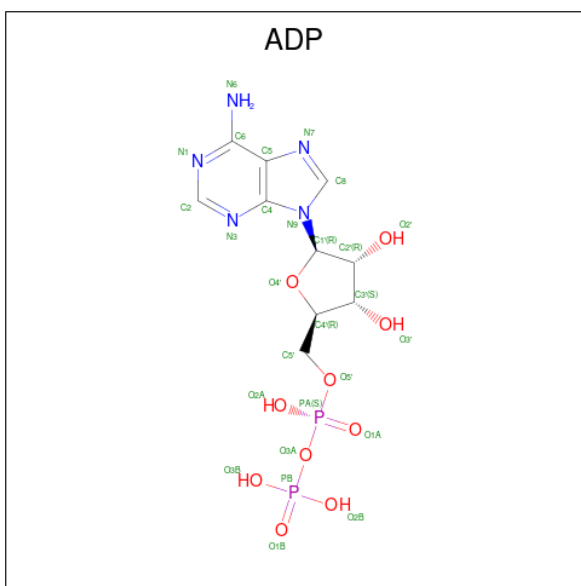
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	42	331	209	54	68	0	0
3	I	42	331	209	54	68	0	0
3	J	42	331	209	54	68	0	0
3	K	42	331	209	54	68	0	0
3	L	42	331	209	54	68	0	0
3	M	42	331	209	54	68	0	0
3	N	42	331	209	54	68	0	0

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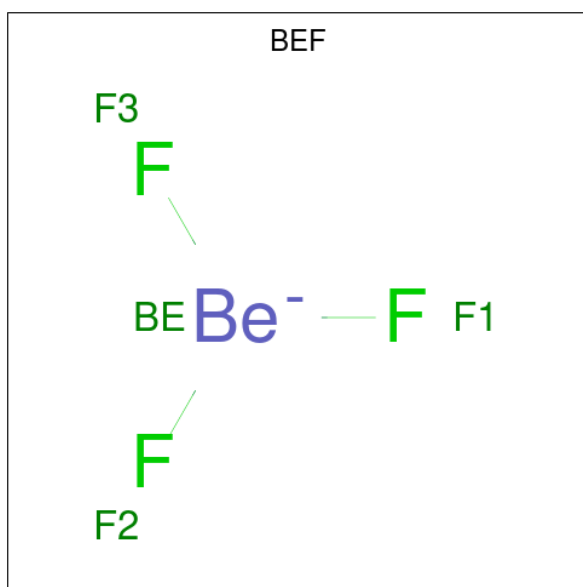
Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $BeF_3$ ).

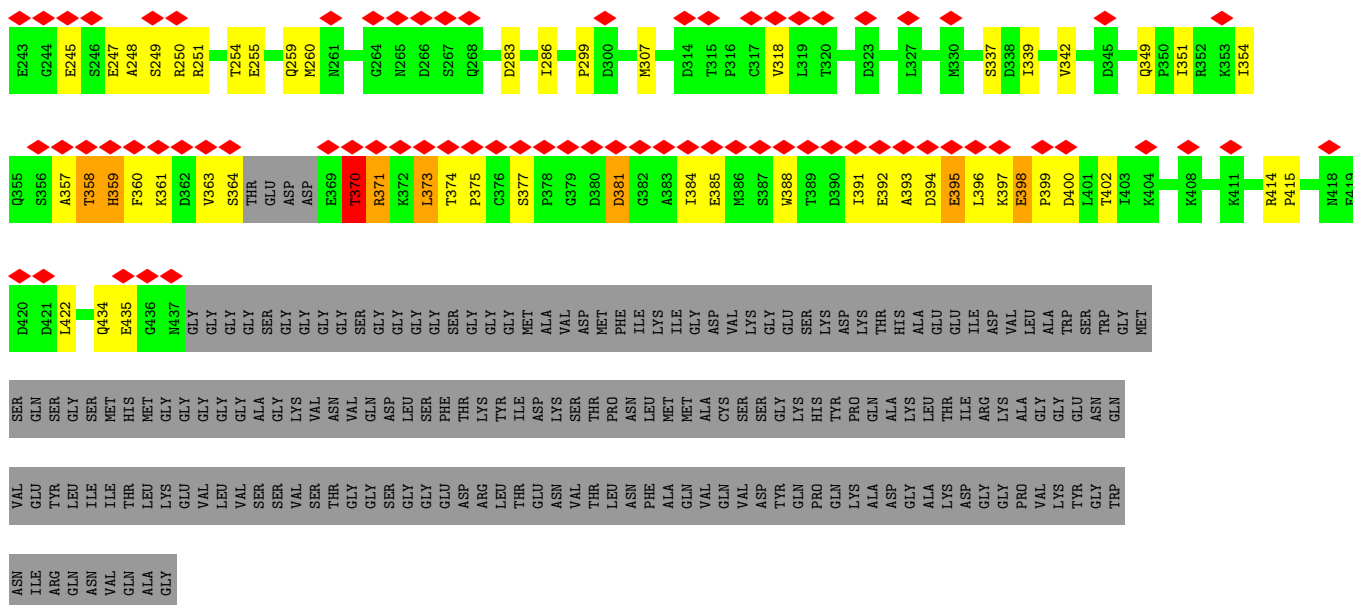


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
5	A	1	4	1	3	0
5	B	1	4	1	3	0
5	C	1	4	1	3	0

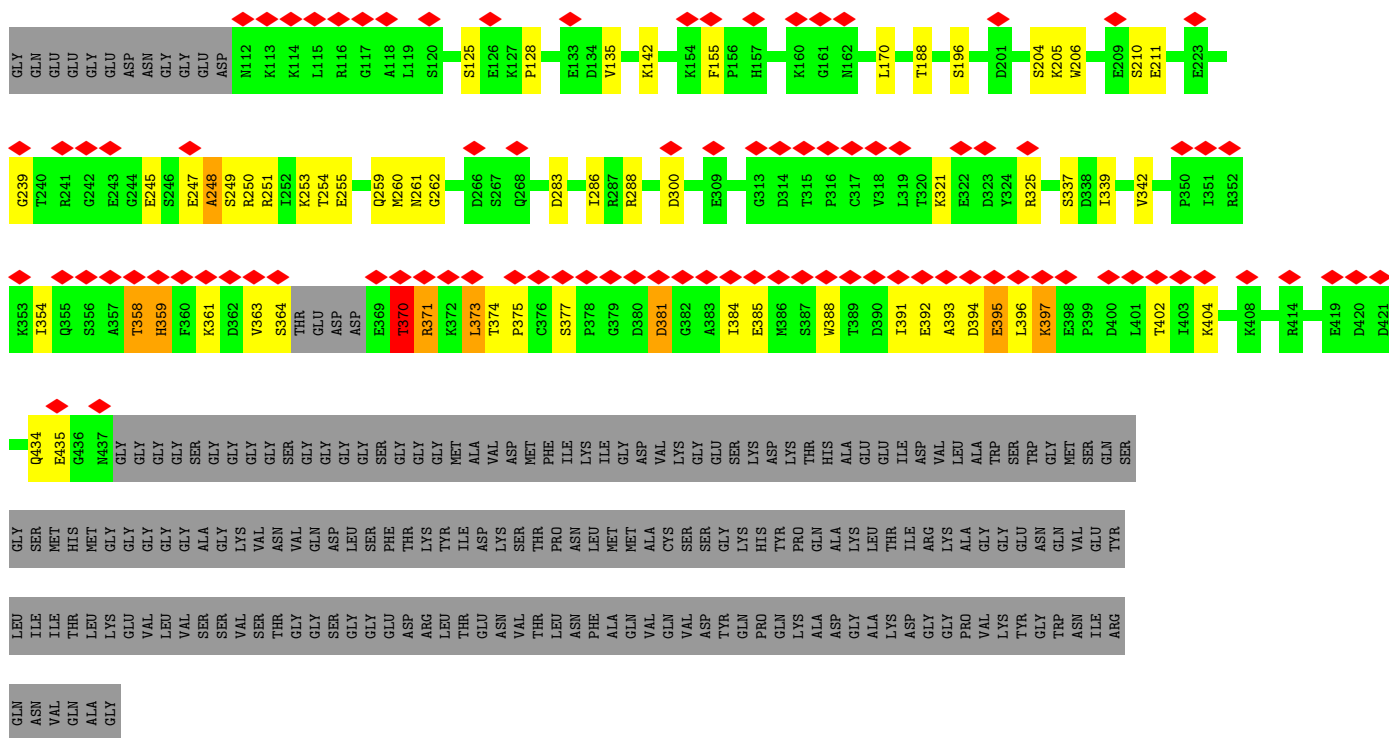
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	B	1	1	1	0
6	C	1	1	1	0
6	D	1	1	1	0



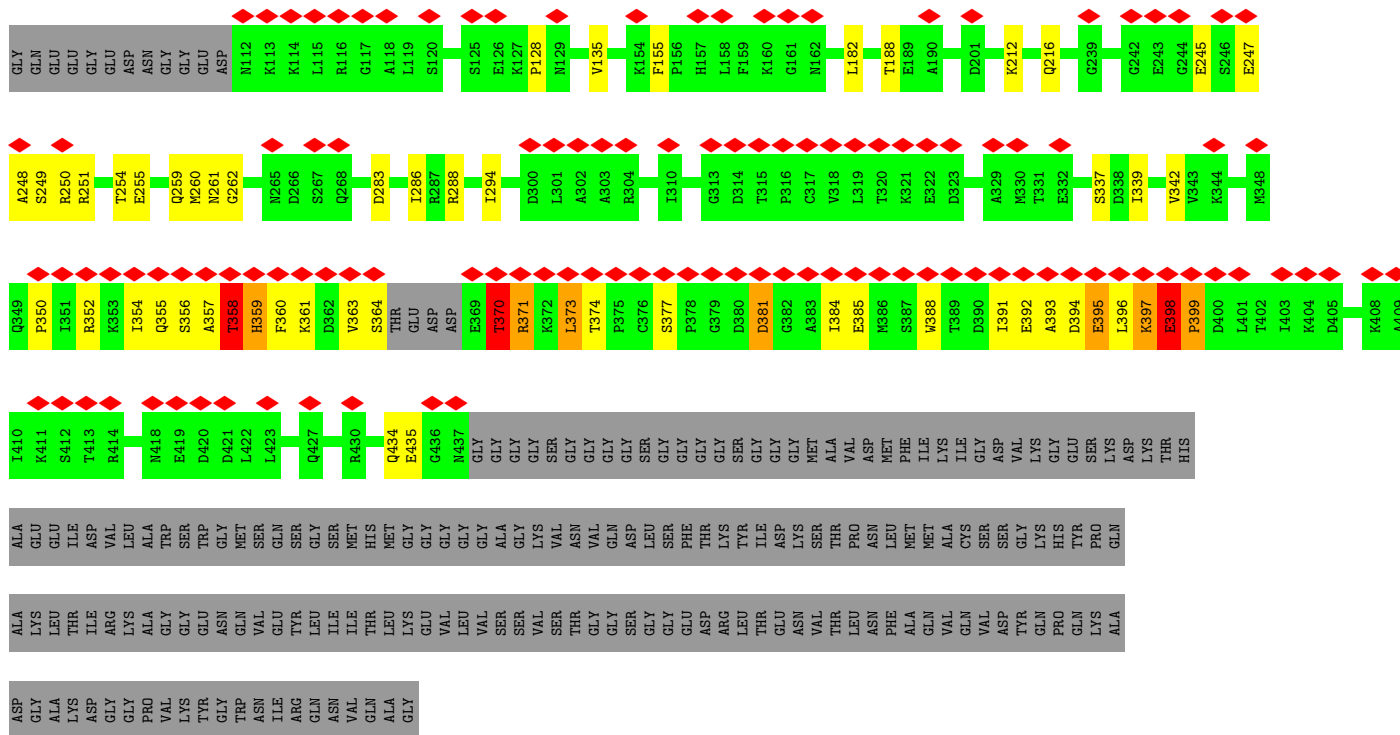


• Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

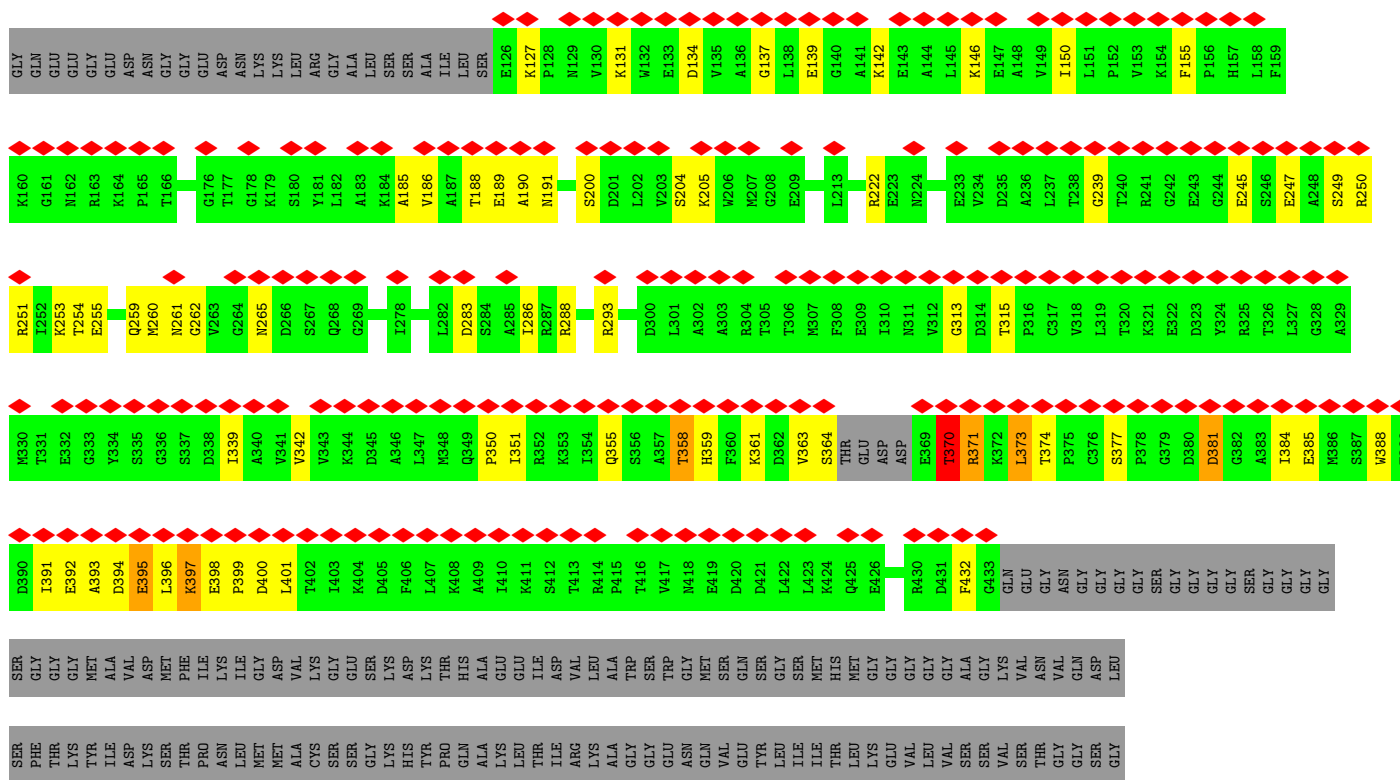
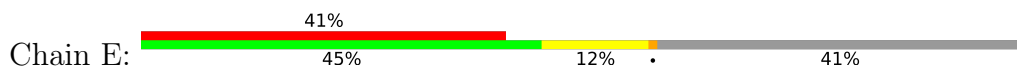


• Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



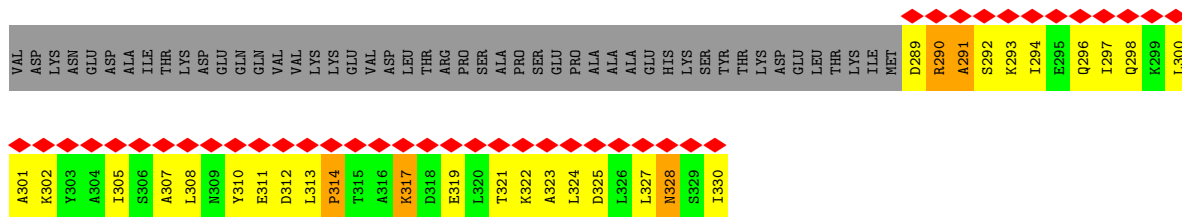


● Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1

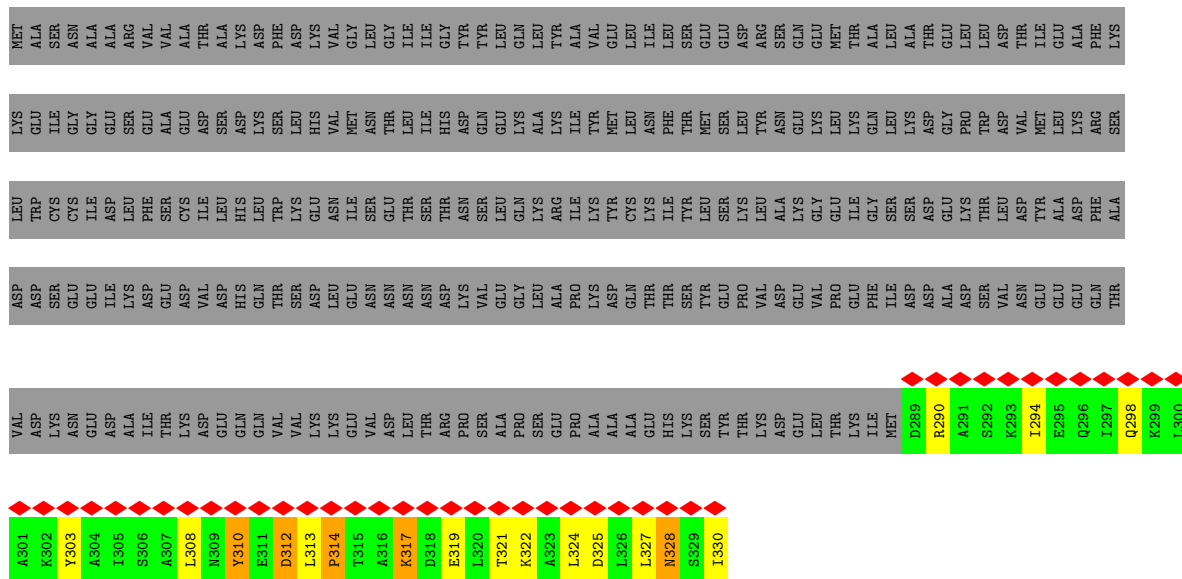




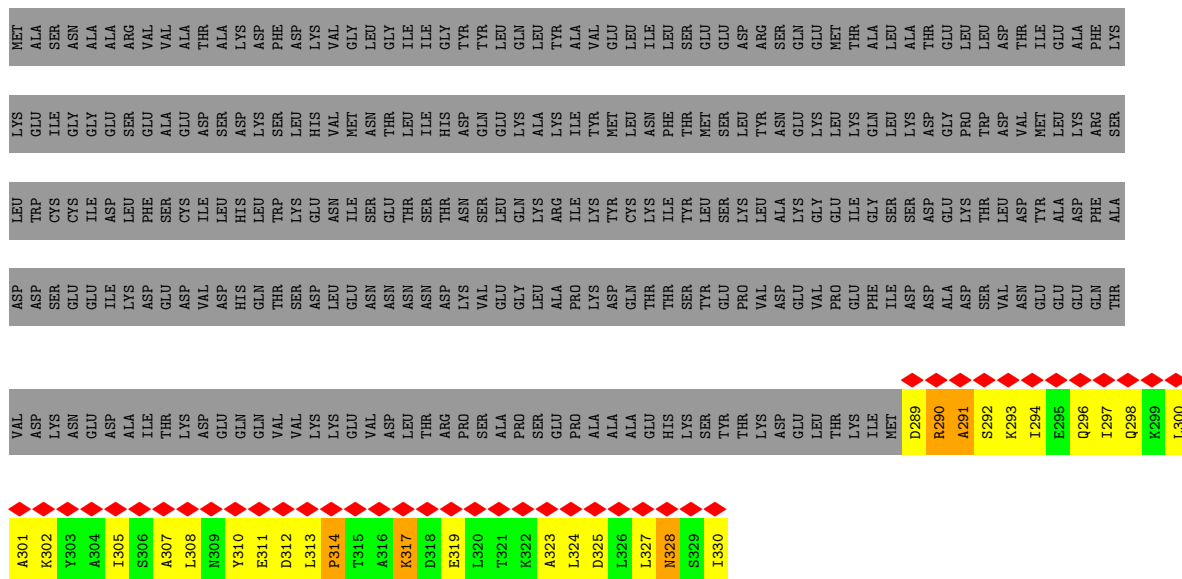




• Molecule 3: Vacuolar protein sorting-associated protein VTA1



• Molecule 3: Vacuolar protein sorting-associated protein VTA1



• Molecule 3: Vacuolar protein sorting-associated protein VTA1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82225	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 ( $e^-/\text{\AA}^2$ )	1.55	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	0.388	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0749	Depositor
Map size (Å)	280.6016, 280.6016, 280.6016	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0961, 1.0961, 1.0961	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: BEF, NH2, ADP, MG, ACE

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	0.70	0/2468	0.90	2/3334 (0.1%)
1	B	0.77	0/2532	0.88	4/3418 (0.1%)
1	C	0.78	0/2532	0.93	6/3418 (0.2%)
1	D	0.75	0/2532	0.89	5/3418 (0.1%)
1	E	0.71	0/2401	0.91	2/3244 (0.1%)
1	F	0.77	0/2428	1.00	7/3281 (0.2%)
2	G	0.92	0/64	0.97	0/86
3	H	0.71	0/333	1.19	5/447 (1.1%)
3	I	0.71	0/333	1.13	4/447 (0.9%)
3	J	0.72	0/333	1.19	5/447 (1.1%)
3	K	0.70	0/333	1.13	4/447 (0.9%)
3	L	0.71	0/333	1.19	5/447 (1.1%)
3	M	0.72	0/333	1.13	4/447 (0.9%)
3	N	0.72	0/333	1.19	5/447 (1.1%)
3	O	0.71	0/333	1.13	4/447 (0.9%)
3	P	0.71	0/333	1.19	5/447 (1.1%)
3	Q	0.71	0/333	1.13	4/447 (0.9%)
3	R	0.71	0/333	1.20	5/447 (1.1%)
3	S	0.71	0/333	1.13	4/447 (0.9%)
All	All	0.74	0/18953	0.98	80/25563 (0.3%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	298	LEU	CA-C-N	8.25	130.15	119.84
1	F	298	LEU	C-N-CA	8.25	130.15	119.84
1	D	398	GLU	CA-C-N	8.11	129.97	119.84
1	D	398	GLU	C-N-CA	8.11	129.97	119.84
1	F	269	GLY	N-CA-C	7.78	126.06	115.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Peptide
1	B	205	LYS	Peptide
1	C	125	SER	Mainchain

## 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	2427	0	2449	109	0
1	B	2491	0	2516	71	0
1	C	2491	0	2516	85	0
1	D	2491	0	2516	78	0
1	E	2360	0	2377	124	0
1	F	2387	0	2409	343	0
2	G	68	0	71	1	0
3	H	331	0	344	35	0
3	I	331	0	344	19	0
3	J	331	0	344	34	0
3	K	331	0	344	23	0
3	L	331	0	344	33	0
3	M	331	0	344	22	0
3	N	331	0	344	36	0
3	O	331	0	344	20	0
3	P	331	0	344	32	0
3	Q	331	0	344	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	331	0	344	36	0
3	S	331	0	344	30	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	18838	0	19042	919	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 24.

The worst 5 of 919 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:F:172:TYR:CZ	1:F:428:PHE:CD2	1.78	1.63
1:F:172:TYR:CZ	1:F:428:PHE:HD2	0.93	1.57
1:F:295:TYR:CE1	1:F:425:GLN:HB3	1.37	1.54
1:F:199:SER:HB3	1:F:237:LEU:CG	1.39	1.53
1:E:388:TRP:CZ3	1:F:151:LEU:CD1	1.90	1.52

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	310/519 (60%)	274 (88%)	31 (10%)	5 (2%)	7	36
1	B	318/519 (61%)	284 (89%)	29 (9%)	5 (2%)	7	36
1	C	318/519 (61%)	280 (88%)	33 (10%)	5 (2%)	7	36
1	D	318/519 (61%)	279 (88%)	33 (10%)	6 (2%)	6	33
1	E	300/519 (58%)	260 (87%)	36 (12%)	4 (1%)	9	40
1	F	304/519 (59%)	277 (91%)	20 (7%)	7 (2%)	5	29
2	G	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	I	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	K	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	M	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	O	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	Q	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	S	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	27
All	All	2356/7084 (33%)	2050 (87%)	256 (11%)	50 (2%)	8	31

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	371	ARG
1	B	395	GLU

### 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	266/418 (64%)	258 (97%)	8 (3%)	36	66
1	B	273/418 (65%)	270 (99%)	3 (1%)	65	79
1	C	273/418 (65%)	270 (99%)	3 (1%)	65	79
1	D	273/418 (65%)	268 (98%)	5 (2%)	51	74
1	E	259/418 (62%)	255 (98%)	4 (2%)	57	76
1	F	262/418 (63%)	247 (94%)	15 (6%)	18	51
2	G	8/8 (100%)	8 (100%)	0	100	100
3	H	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	I	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	J	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	K	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	L	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	M	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	N	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	O	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	P	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	Q	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	R	36/294 (12%)	33 (92%)	3 (8%)	10	38
3	S	36/294 (12%)	33 (92%)	3 (8%)	10	38
All	All	2046/6044 (34%)	1972 (96%)	74 (4%)	32	63

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	317	LYS
3	S	314	PRO
3	O	314	PRO
3	Q	314	PRO
1	F	139	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	296	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	S	298	GLN
3	O	298	GLN
3	Q	298	GLN
1	F	191	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	ADP	D	701	6	28,29,29	1.45	4 (14%)	43,45,45	2.19	12 (27%)
4	ADP	E	701	-	28,29,29	1.33	5 (17%)	43,45,45	2.21	11 (25%)
5	BEF	A	702	4	0,3,3	-	-	-	-	-
4	ADP	A	701	5,6	28,29,29	1.45	2 (7%)	43,45,45	1.29	6 (13%)
5	BEF	B	702	4	0,3,3	-	-	-	-	-
4	ADP	B	701	5,6	28,29,29	1.76	3 (10%)	43,45,45	1.45	8 (18%)
4	ADP	C	701	5,6	28,29,29	1.84	4 (14%)	43,45,45	1.49	10 (23%)
5	BEF	C	702	4	0,3,3	-	-	-	-	-

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
4	ADP	D	701	6	-	1/16/32/32	0/3/3/3
4	ADP	E	701	-	-	3/16/32/32	0/3/3/3
4	ADP	A	701	5,6	-	6/16/32/32	0/3/3/3
4	ADP	B	701	5,6	-	4/16/32/32	0/3/3/3
4	ADP	C	701	5,6	-	2/16/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	ADP	PA-O3A	-6.64	1.52	1.59
4	B	701	ADP	PA-O3A	-6.62	1.52	1.59
4	A	701	ADP	PA-O3A	-5.15	1.53	1.59
4	D	701	ADP	C5-C4	3.60	1.45	1.39
4	E	701	ADP	C5-C4	3.49	1.45	1.39

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	ADP	C5-C4-N3	-7.08	116.97	126.72
4	E	701	ADP	C5-C4-N3	-6.34	117.99	126.72
4	D	701	ADP	N3-C4-N9	6.07	137.49	127.17
4	E	701	ADP	N3-C4-N9	5.28	136.14	127.17
4	E	701	ADP	C2'-C1'-N9	-5.10	100.62	113.30

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

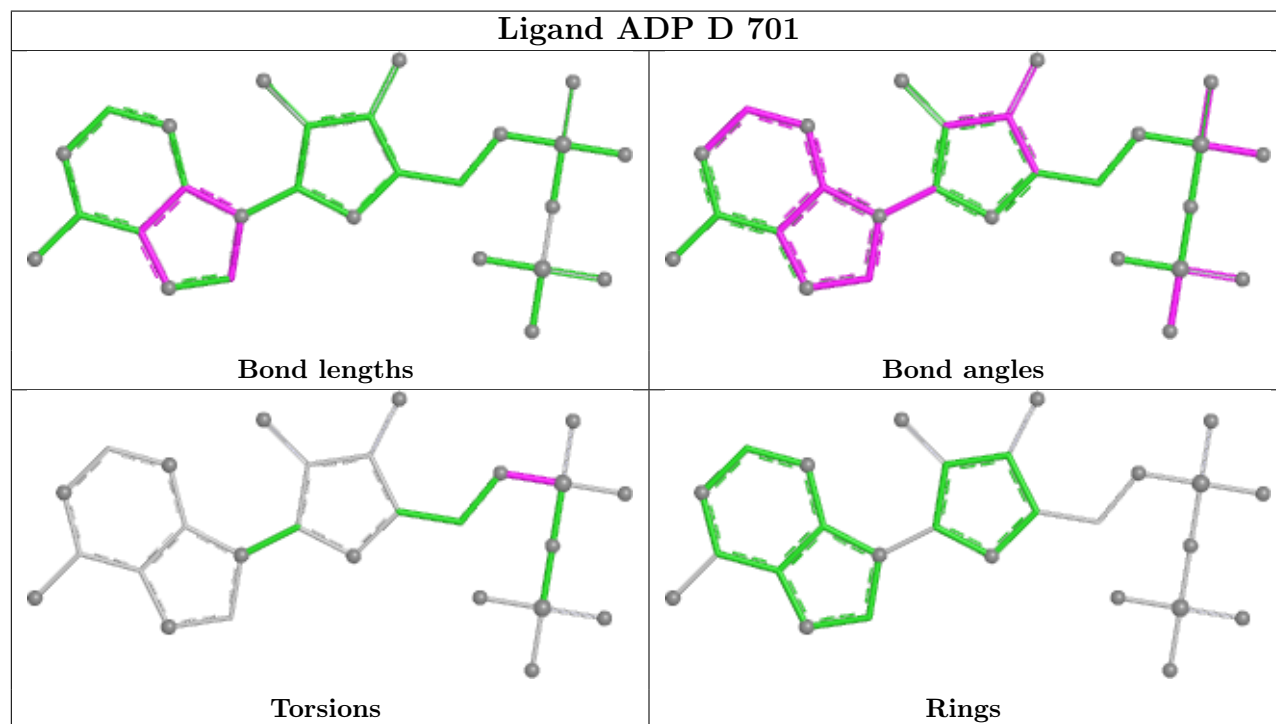
Mol	Chain	Res	Type	Atoms
4	A	701	ADP	PA-O3A-PB-O2B
4	A	701	ADP	C5'-O5'-PA-O2A
4	A	701	ADP	C5'-O5'-PA-O3A
4	B	701	ADP	PA-O3A-PB-O2B
4	E	701	ADP	C5'-O5'-PA-O2A

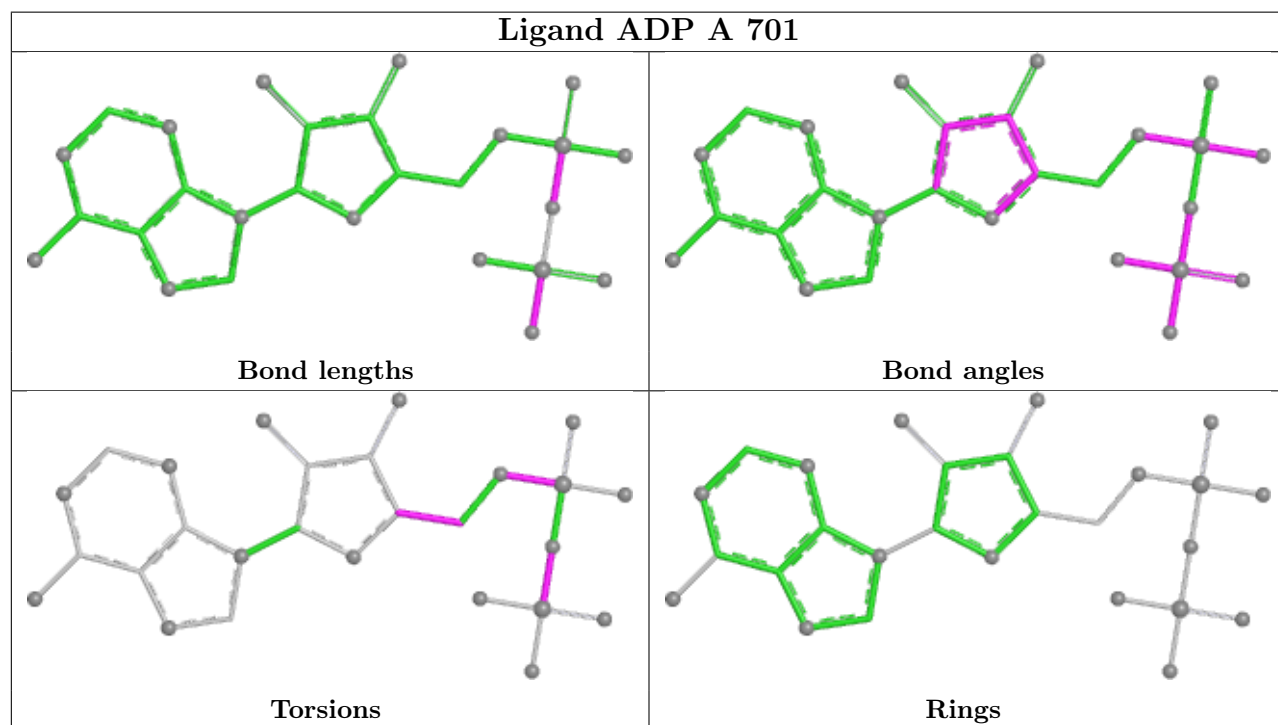
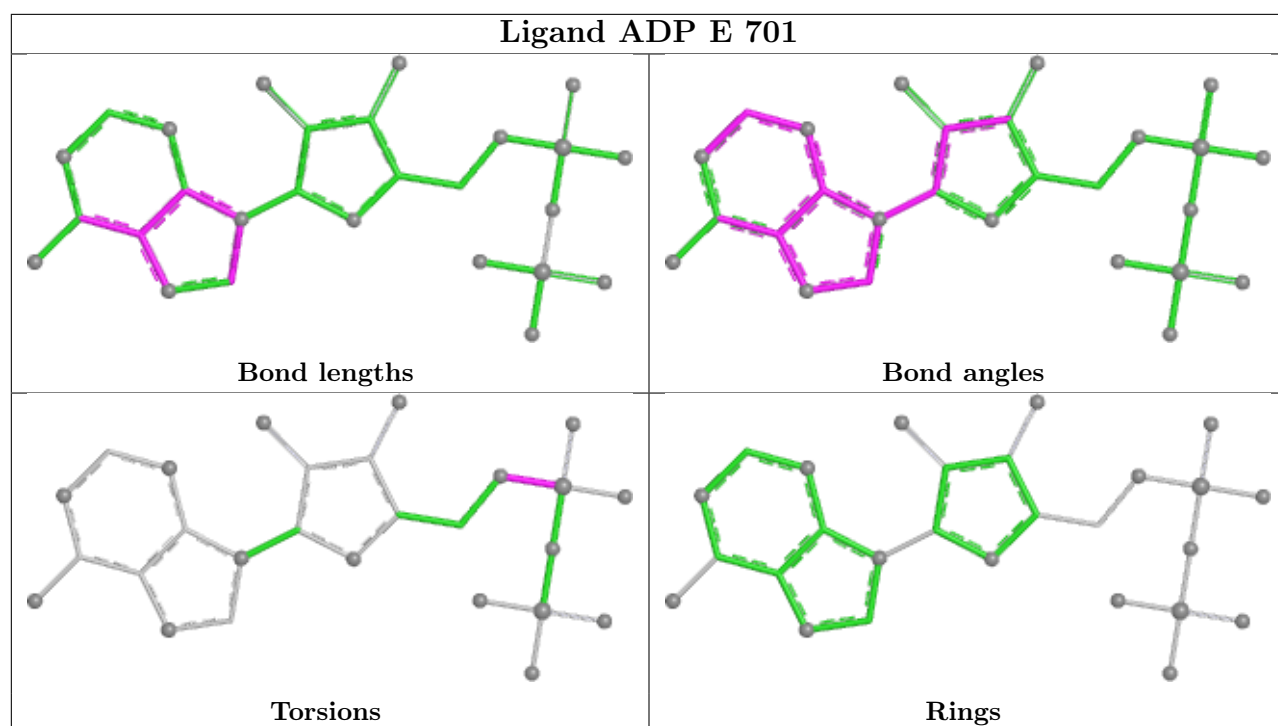
There are no ring outliers.

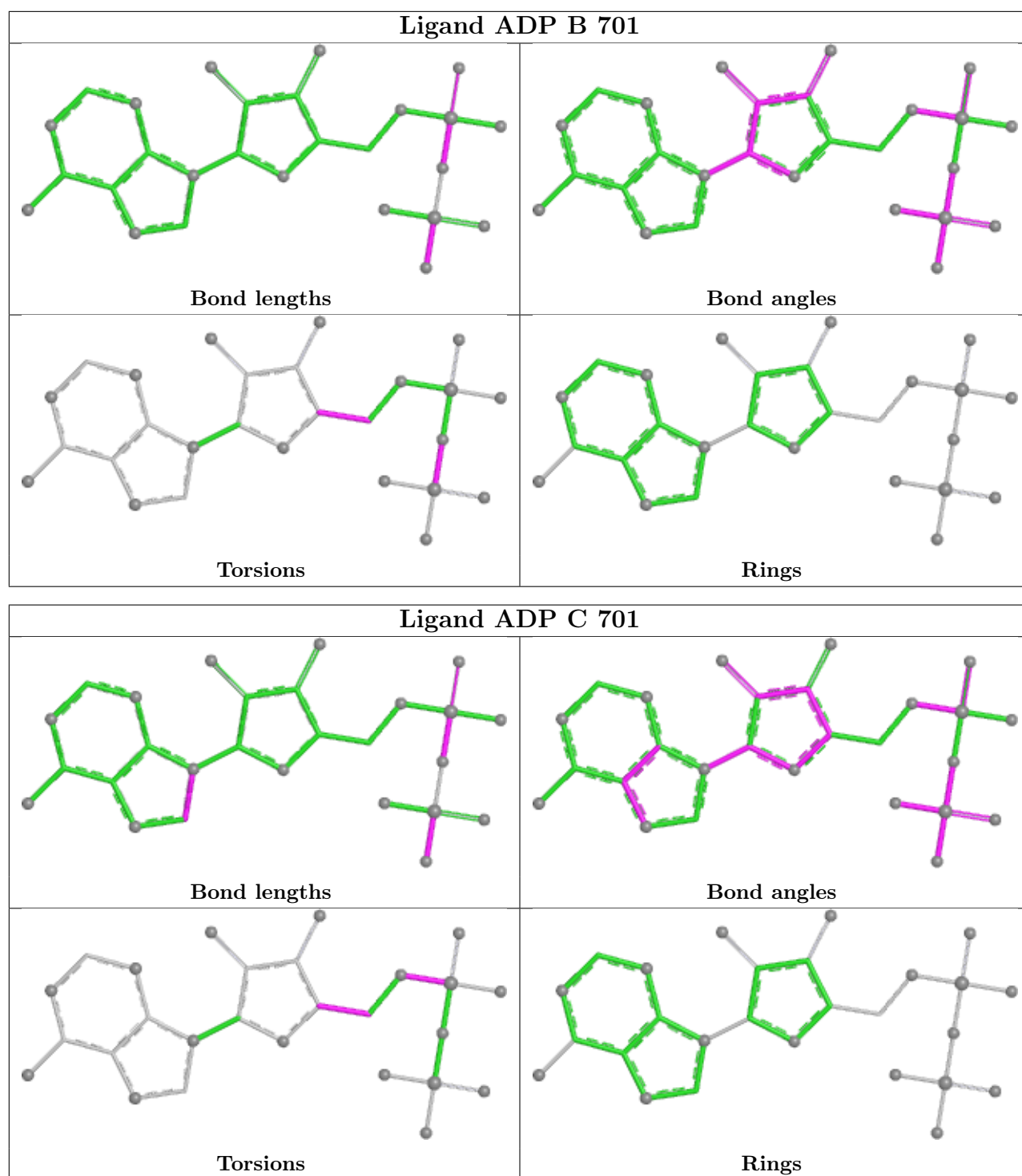
6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	BEF	1	0
4	A	701	ADP	1	0
5	B	702	BEF	1	0
4	B	701	ADP	1	0
4	C	701	ADP	1	0
5	C	702	BEF	1	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

There are no chain breaks in this entry.

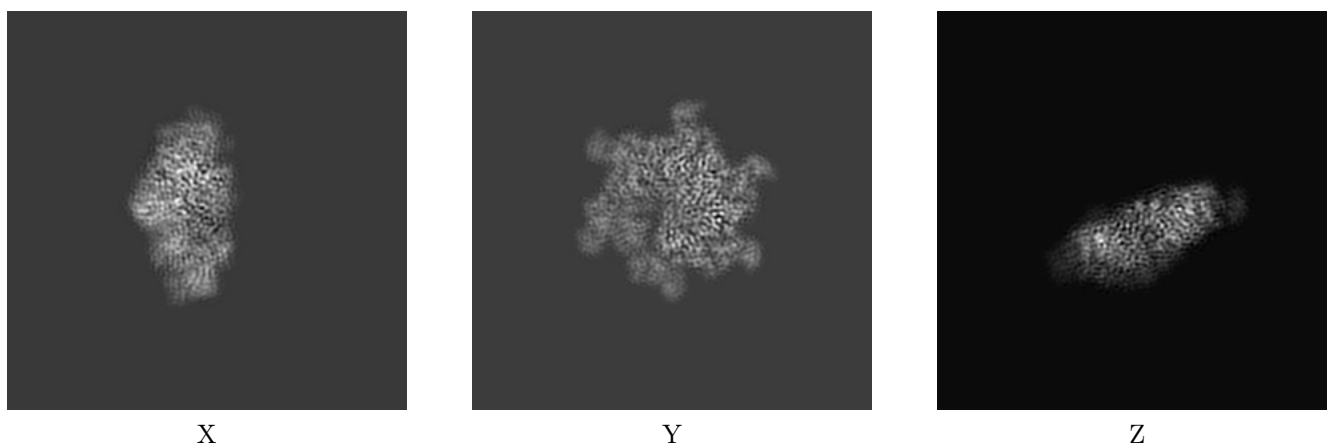
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8887. 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](#)

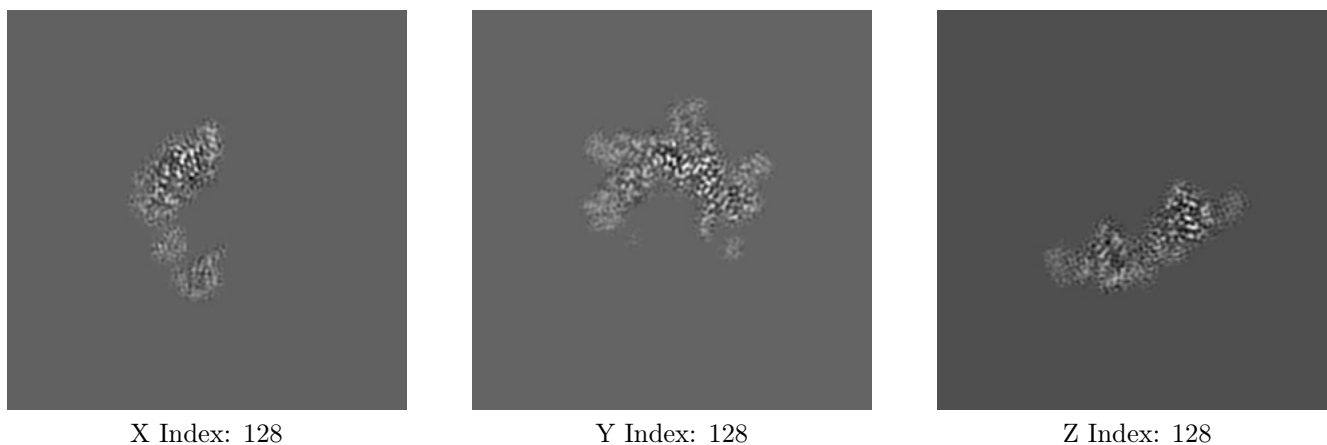
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

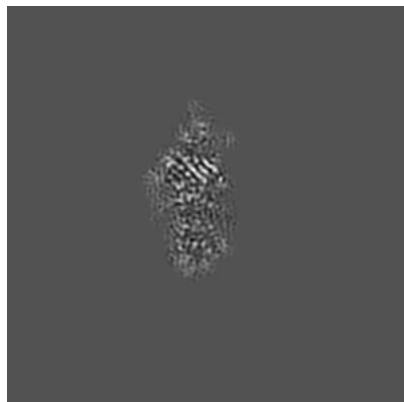
#### 6.2.1 Primary map



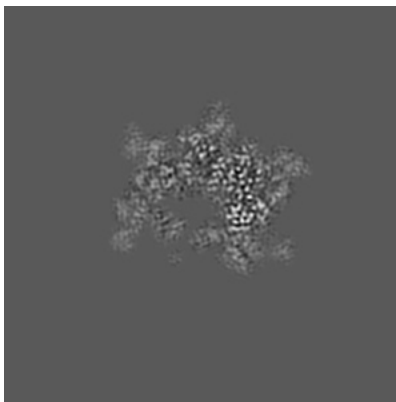
The images above show central slices of the map in three orthogonal directions.

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

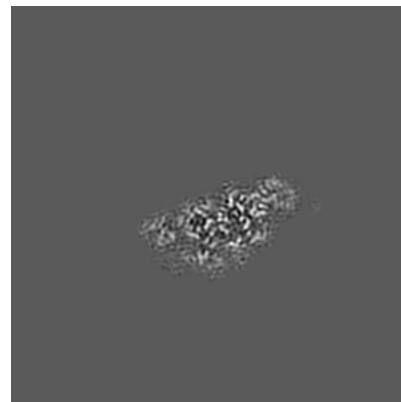
### 6.3.1 Primary map



X Index: 147



Y Index: 118

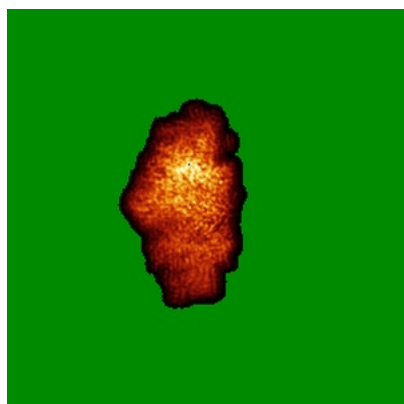


Z Index: 150

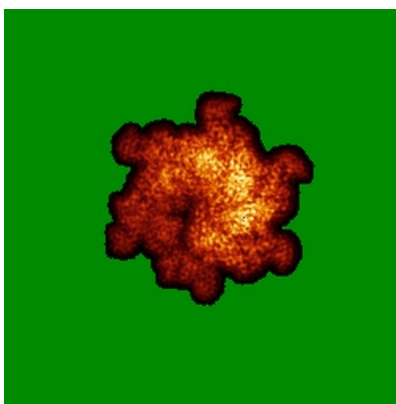
The images above show the largest variance slices of the map in three orthogonal directions.

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

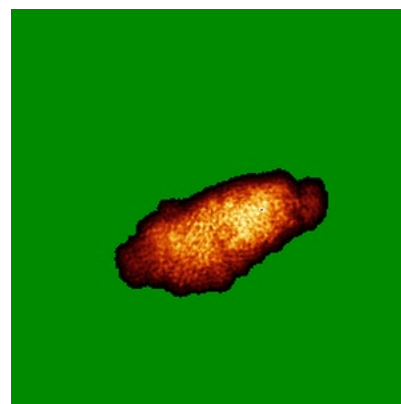
### 6.4.1 Primary map



X



Y

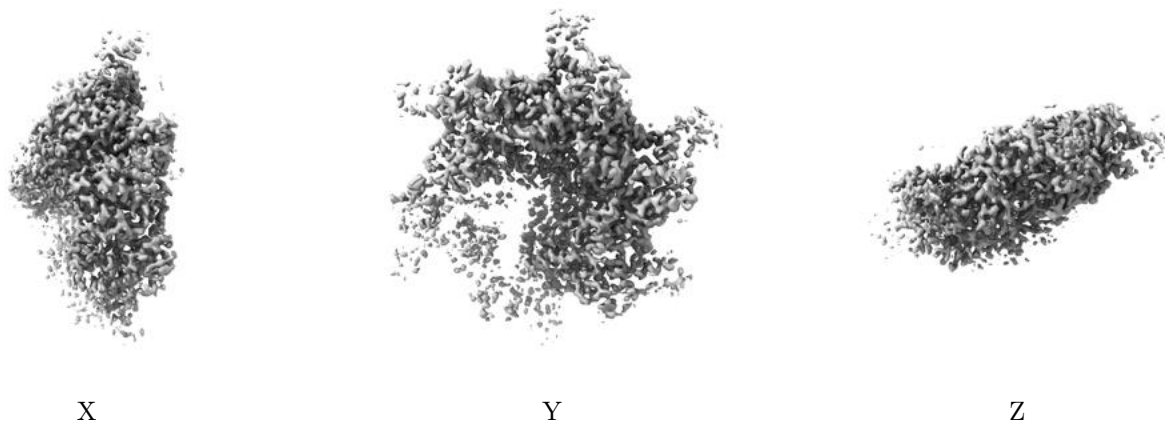


Z

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 0.0749. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

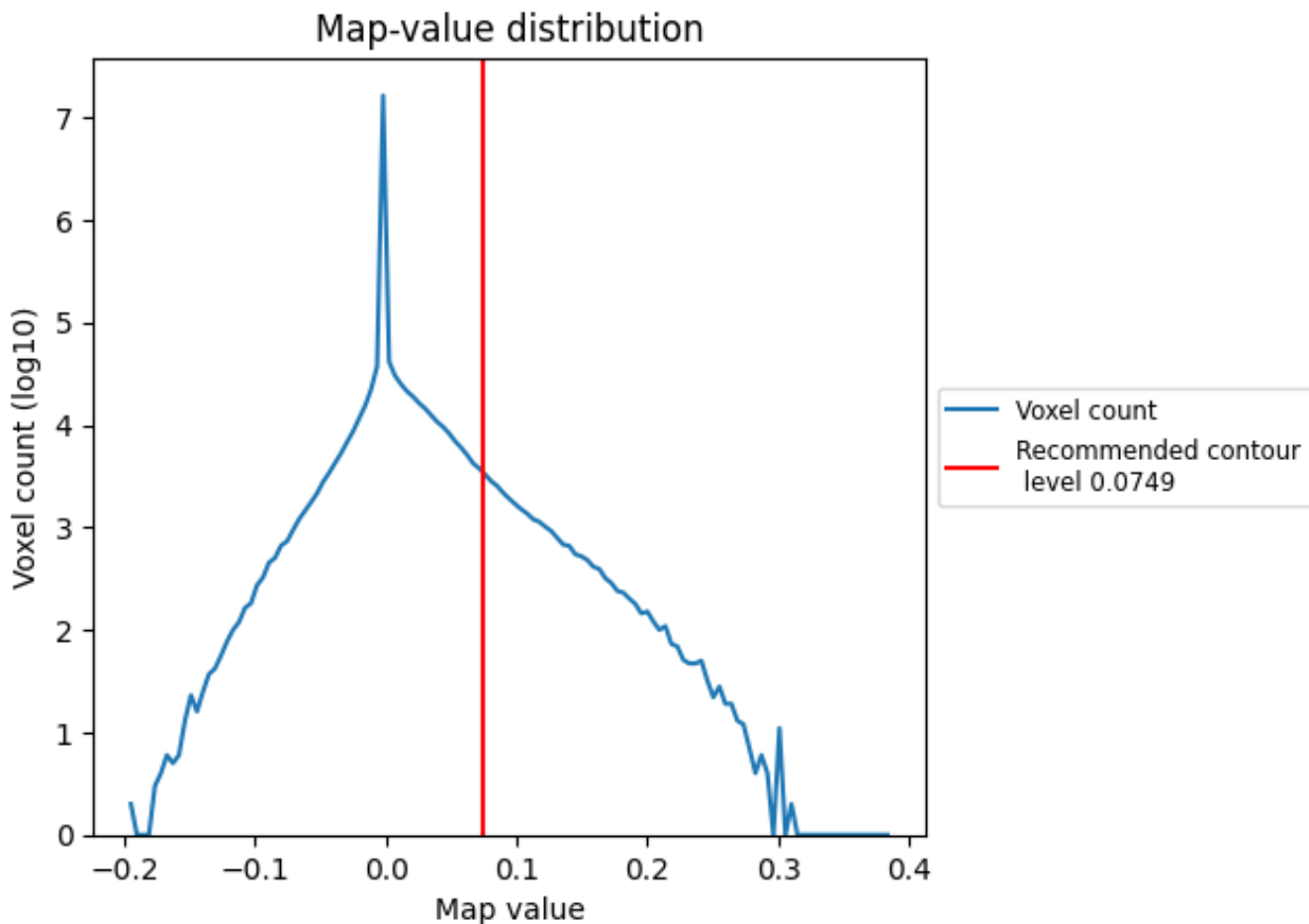
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

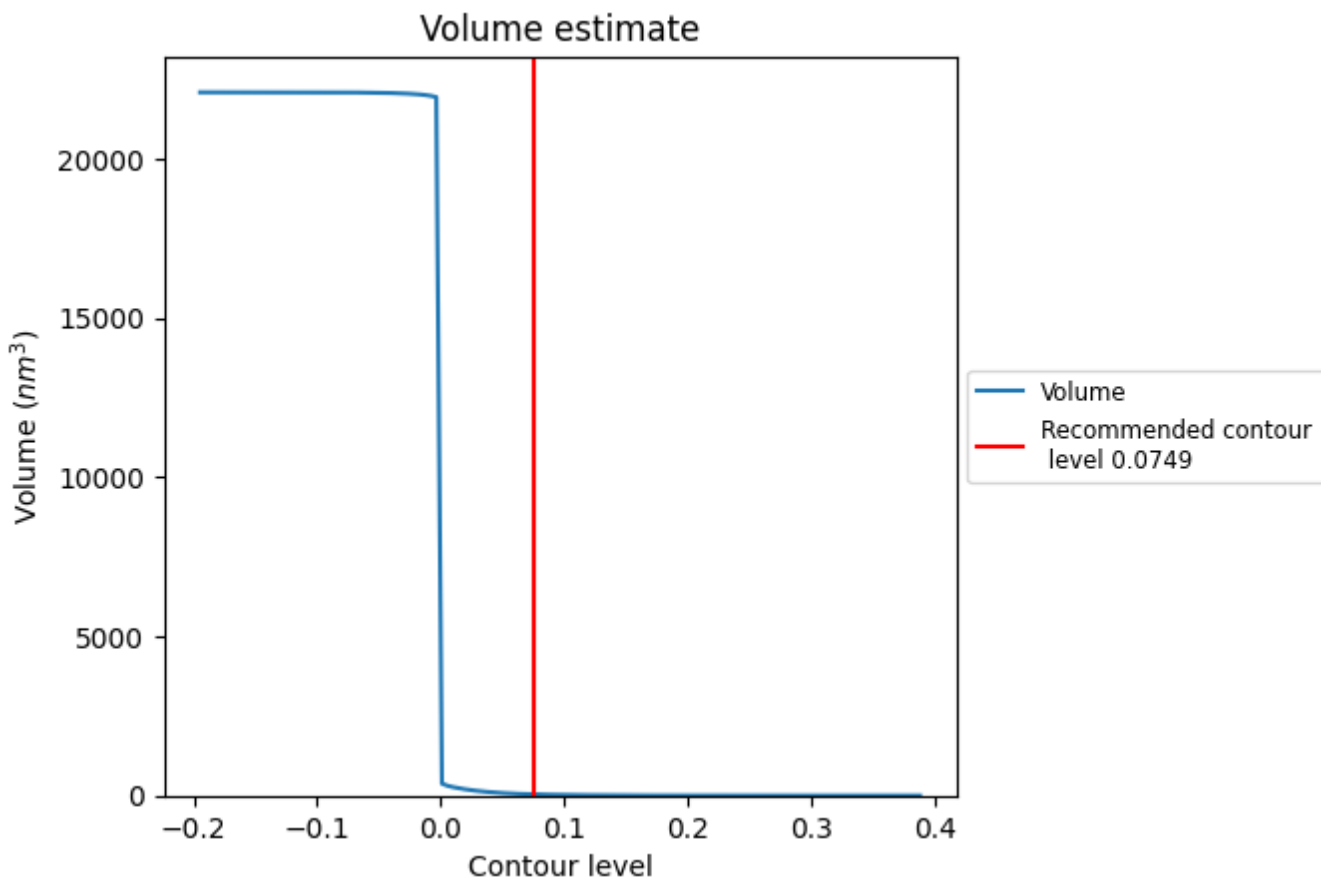
This section contains the results of statistical analysis of the map.

### 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.

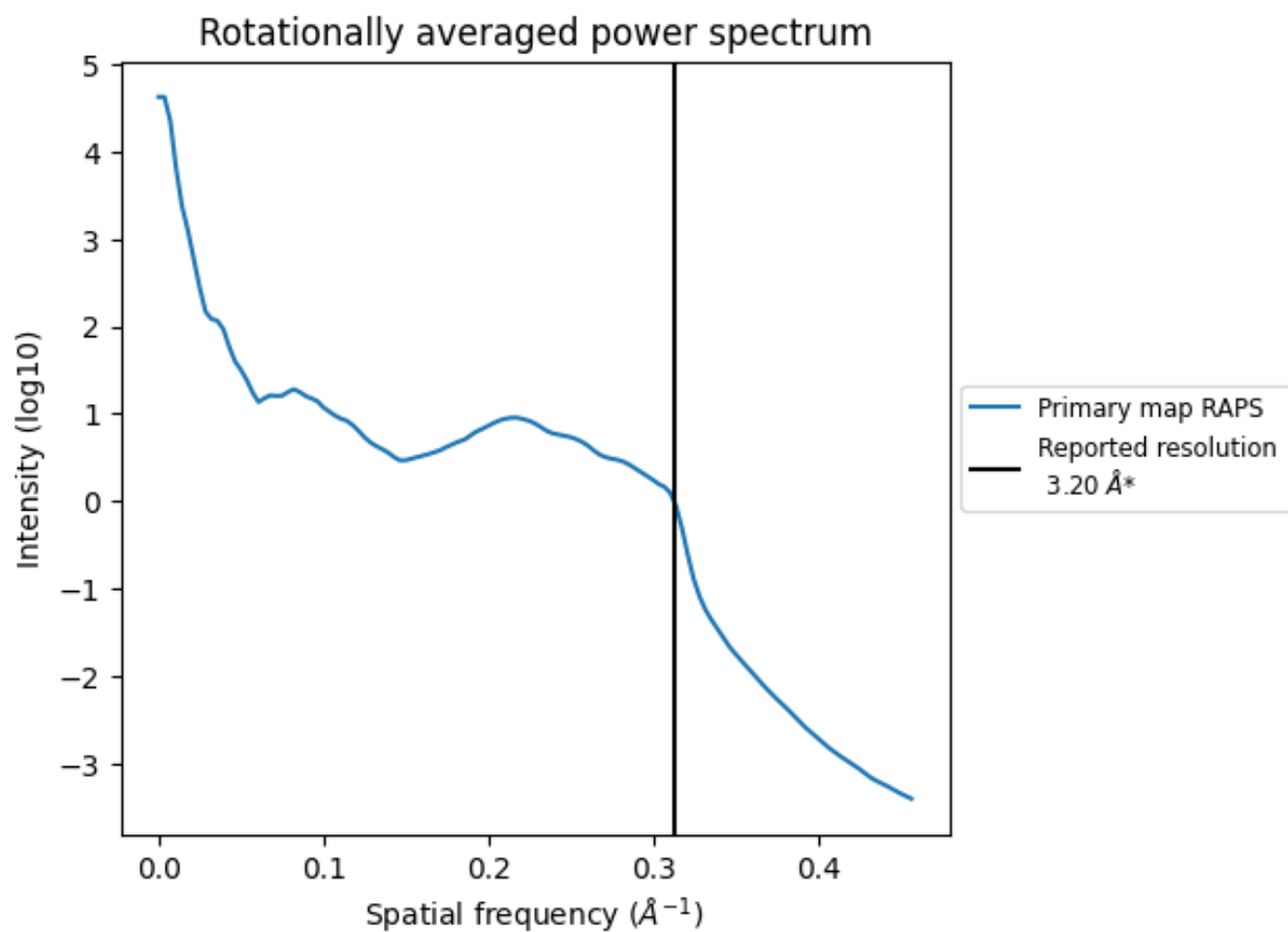
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; this corresponds to an approximate mass of 35 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 0.312 Å<sup>-1</sup>

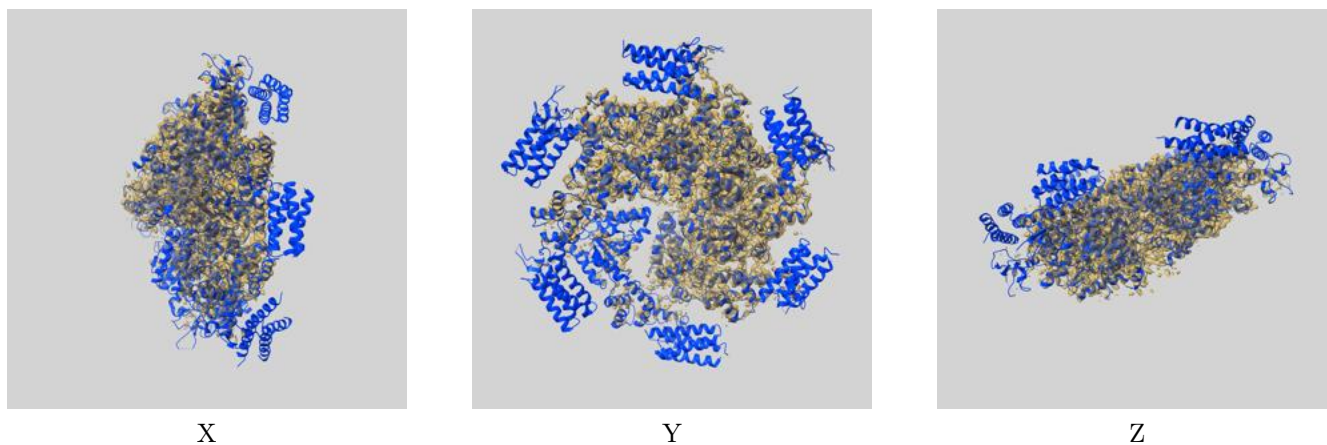
## 8 Fourier-Shell correlation

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

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

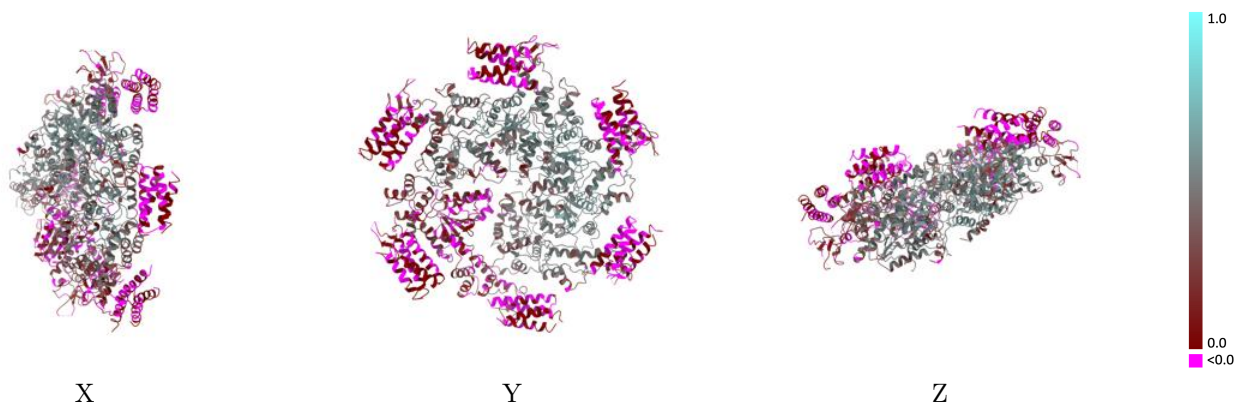
This section contains information regarding the fit between EMDB map EMD-8887 and PDB model 6AP1. Per-residue inclusion information can be found in section 3 on page 10.

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



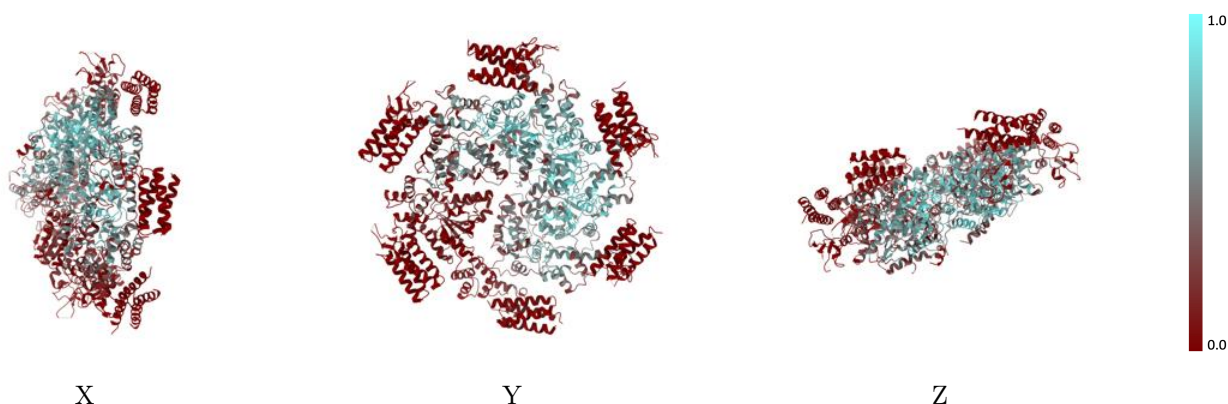
The images above show the 3D surface view of the map at the recommended contour level 0.0749 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



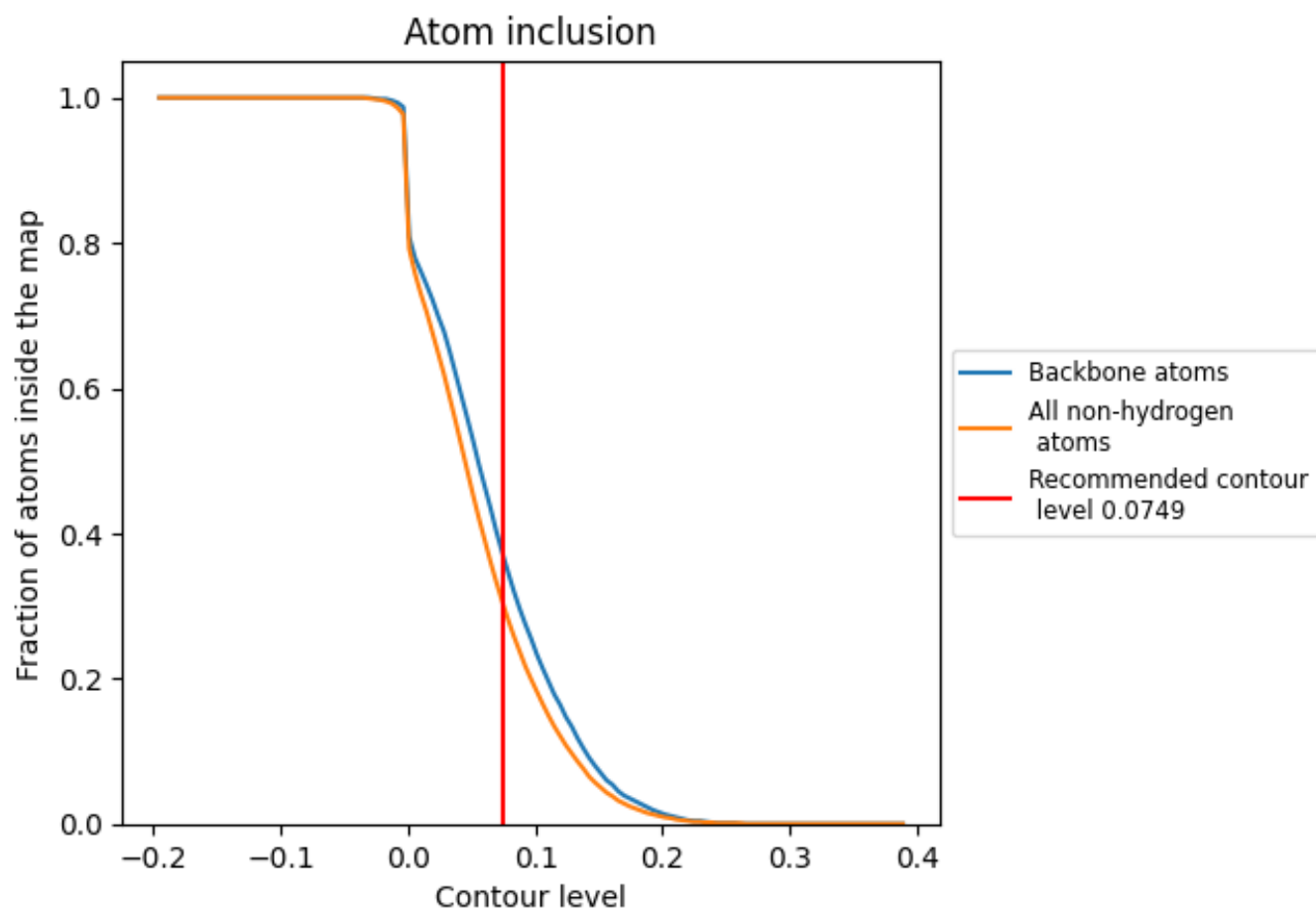
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0749).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 30% 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 (0.0749) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3020	 0.2740
A	 0.3750	 0.3850
B	 0.5540	 0.4520
C	 0.5630	 0.4620
D	 0.4950	 0.4220
E	 0.2640	 0.3250
F	 0.0250	 0.0570
G	 0.3430	 0.4940
H	 0.0000	 -0.0030
I	 0.0030	 -0.0450
J	 0.0000	 0.0020
K	 0.0000	 -0.0460
L	 0.0000	 -0.0200
M	 0.0000	 -0.0280
N	 0.0000	 -0.0130
O	 0.0000	 -0.0150
P	 0.0000	 -0.0400
Q	 0.0000	 -0.0400
R	 0.0000	 -0.0290
S	 0.0000	 -0.0310

