Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 01:52 PM EST

PDB ID	:	3JBQ
EMDB ID	:	EMD-6258
Title	:	Domain Organization and Conformational Plasticity of the G Protein Effector, PDE6
Authors	:	Zhang, Z.; He, F.; Constantine, R.; Baker, M.L.; Baehr, W.; Schmid, M.F.; Wensel, T.G.; Agosto, M.A.
Deposited on	:	2015-09-17
Resolution	:	11.00 Å(reported)
Based on initial models	:	3IBJ, 12E8, 3DBA, 3JWR

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 (i) 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 (i)) were used in the production of this report:

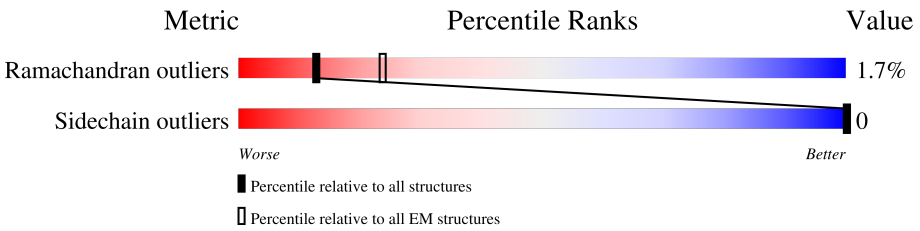
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 11.00 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)
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	L	214	11% 100%
1	l	214	11% 100%
2	H	220	6% 95%
2	h	220	6% 96%
3	B	330	13% 98%
3	F	330	13% 98%
4	D	18	22% 94% 6%
4	X	18	22% 94% 6%
5	C	185	85% 13%

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Mol	Chain	Length	Quality of chain
5	G	185	84% 13%
6	1	186	8% 89% 8%
6	2	186	6% 90% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17450 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 IgG1-kappa 2E8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	214	1649	1020	277	342	10	0	0
1	l	214	1649	1020	277	342	10	0	0

- Molecule 2 is a protein called IgG1-kappa 2E8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	214	1629	1030	266	327	6	0	0
2	h	214	1629	1030	266	327	6	0	0

- Molecule 3 is a protein called phosphodiesterase 5/6 chimera catalytic domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	328	2671	1700	465	487	19	0	0
3	F	328	2671	1700	465	487	19	0	0

- Molecule 4 is a protein called phosphodiesterase 6 gamma subunit inhibitory peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	17	141	92	23	26	0	0
4	X	17	141	92	23	26	0	0

- Molecule 5 is a protein called GafB domain of phosphodiesterase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	161	1267	805	215	240	7	0	0
5	G	161	1267	805	215	240	7	0	0

- Molecule 6 is a protein called GafA domain of cone phosphodiesterase 6C.

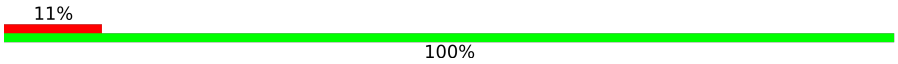
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1	171	1368	874	230	256	8	0	0
6	2	171	1368	874	230	256	8	0	0

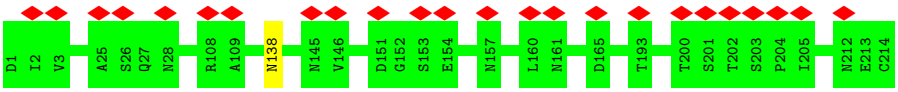
3 Residue-property plots (i)

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: IgG1-kappa 2E8 light chain

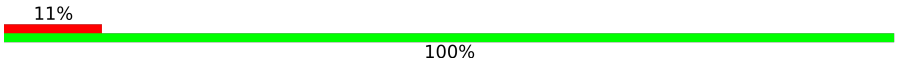
Chain L:

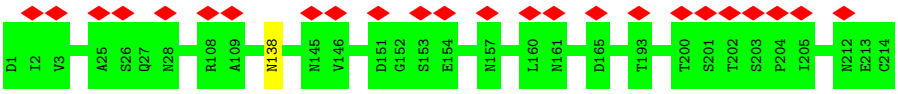




- Molecule 1: IgG1-kappa 2E8 light chain

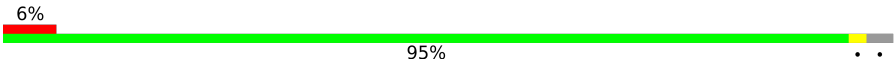
Chain l:

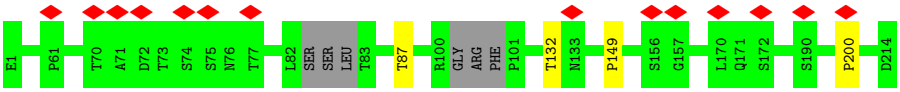




- Molecule 2: IgG1-kappa 2E8 heavy chain

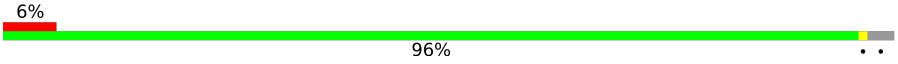
Chain H:

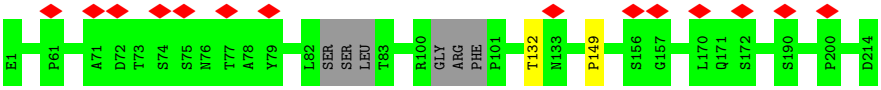




- Molecule 2: IgG1-kappa 2E8 heavy chain

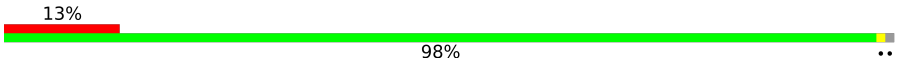
Chain h:

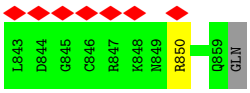




- Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

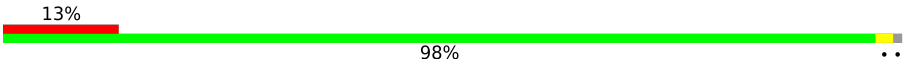
Chain B:

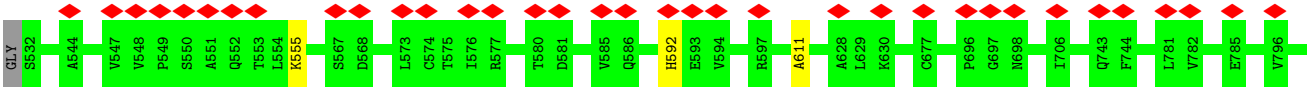


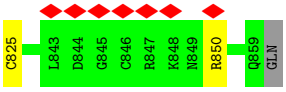


• Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

Chain F:

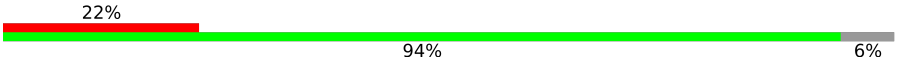


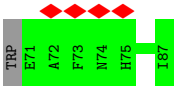




• Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide

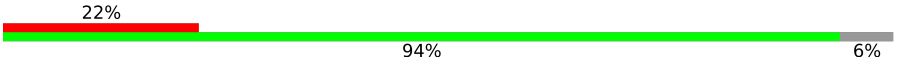
Chain D:

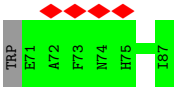




• Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide

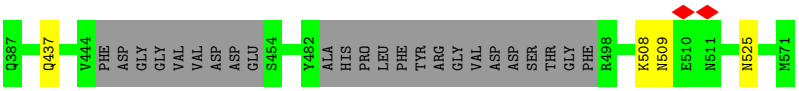
Chain X:





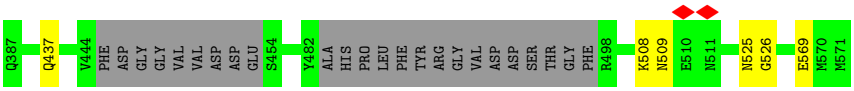
• Molecule 5: GafB domain of phosphodiesterase 2A

Chain C:



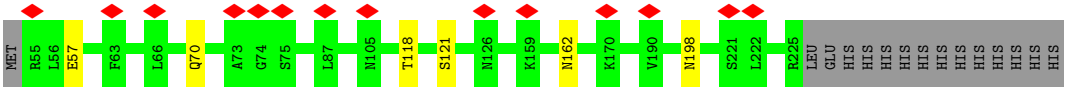
• Molecule 5: GafB domain of phosphodiesterase 2A

Chain G:



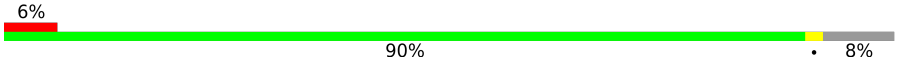
• Molecule 6: GafA domain of cone phosphodiesterase 6C

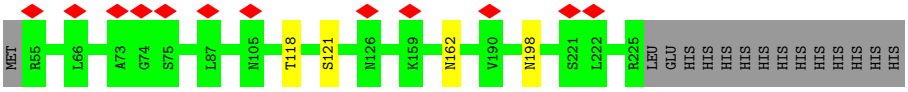
Chain 1:



• Molecule 6: GafA domain of cone phosphodiesterase 6C

Chain 2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	12373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	by particle using CtFit	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	60000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	1.835	Depositor
Minimum map value	-0.758	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	434.4, 434.4, 434.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.81, 1.81, 1.81	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	L	0.24	0/1682	0.47	0/2278
1	l	0.24	0/1682	0.47	0/2278
2	H	0.25	0/1671	0.52	0/2285
2	h	0.26	0/1671	0.53	0/2285
3	B	0.26	0/2726	0.50	0/3685
3	F	0.26	0/2726	0.50	0/3685
4	D	0.24	0/144	0.44	0/194
4	X	0.24	0/144	0.47	0/194
5	C	0.24	0/1285	0.47	0/1738
5	G	0.24	0/1285	0.47	0/1738
6	1	0.28	0/1391	0.56	0/1877
6	2	0.28	0/1391	0.56	0/1877
All	All	0.26	0/17798	0.50	0/24114

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	L	212/214 (99%)	189 (89%)	22 (10%)	1 (0%)	29	69
1	l	212/214 (99%)	191 (90%)	20 (9%)	1 (0%)	29	69
2	H	208/220 (94%)	190 (91%)	14 (7%)	4 (2%)	8	38
2	h	208/220 (94%)	190 (91%)	16 (8%)	2 (1%)	15	55
3	B	326/330 (99%)	301 (92%)	21 (6%)	4 (1%)	13	50
3	F	326/330 (99%)	301 (92%)	20 (6%)	5 (2%)	10	46
4	D	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
4	X	15/18 (83%)	15 (100%)	0	0	100	100
5	C	155/185 (84%)	142 (92%)	9 (6%)	4 (3%)	5	31
5	G	155/185 (84%)	141 (91%)	8 (5%)	6 (4%)	3	23
6	1	169/186 (91%)	148 (88%)	15 (9%)	6 (4%)	3	25
6	2	169/186 (91%)	151 (89%)	14 (8%)	4 (2%)	6	33
All	All	2170/2306 (94%)	1973 (91%)	160 (7%)	37 (2%)	13	42

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	149	PRO
5	C	508	LYS
5	G	508	LYS
5	G	509	ASN
2	h	149	PRO
6	1	198	ASN
6	2	198	ASN
5	C	509	ASN
6	2	121	SER
2	H	132	THR
5	C	437	GLN
3	F	555	LYS
3	F	611	ALA
3	F	850	ARG
5	G	437	GLN
5	G	569	GLU
6	1	70	GLN
6	1	162	ASN
6	2	162	ASN

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Mol	Chain	Res	Type
1	L	138	ASN
2	H	200	PRO
3	B	592	HIS
3	B	613	HIS
3	B	825	CYS
3	B	850	ARG
5	C	525	ASN
3	F	592	HIS
5	G	525	ASN
1	l	138	ASN
2	h	132	THR
6	1	118	THR
6	1	121	SER
2	H	87	THR
3	F	825	CYS
6	1	57	GLU
6	2	118	THR
5	G	526	GLY

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	L	189/189 (100%)	189 (100%)	0	100	100
1	l	189/189 (100%)	189 (100%)	0	100	100
2	H	183/188 (97%)	183 (100%)	0	100	100
2	h	183/188 (97%)	183 (100%)	0	100	100
3	B	294/295 (100%)	294 (100%)	0	100	100
3	F	294/295 (100%)	294 (100%)	0	100	100
4	D	14/15 (93%)	14 (100%)	0	100	100
4	X	14/15 (93%)	14 (100%)	0	100	100
5	C	140/159 (88%)	140 (100%)	0	100	100
5	G	140/159 (88%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	1	155/170 (91%)	155 (100%)	0	100	100
6	2	155/170 (91%)	155 (100%)	0	100	100
All	All	1950/2032 (96%)	1950 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	124	GLN
1	L	138	ASN
2	H	5	GLN
2	H	6	GLN
2	H	39	GLN
2	H	64	GLN
2	H	96	HIS
2	H	164	HIS
2	H	196	ASN
3	B	552	GLN
3	B	620	ASN
3	B	623	GLN
3	B	635	GLN
3	B	678	HIS
3	B	684	HIS
3	B	685	HIS
3	B	698	ASN
3	B	789	GLN
3	B	798	GLN
3	B	849	ASN
5	C	394	GLN
5	C	398	GLN
5	C	406	HIS
5	C	426	ASN
5	C	511	ASN
5	C	568	ASN
3	F	533	HIS
3	F	552	GLN
3	F	620	ASN
3	F	635	GLN
3	F	678	HIS

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Mol	Chain	Res	Type
3	F	684	HIS
3	F	685	HIS
3	F	698	ASN
3	F	789	GLN
3	F	798	GLN
3	F	849	ASN
3	F	854	GLN
5	G	387	GLN
5	G	398	GLN
5	G	406	HIS
5	G	426	ASN
5	G	511	ASN
5	G	512	GLN
5	G	558	ASN
5	G	568	ASN
1	l	38	GLN
1	l	124	GLN
1	l	138	ASN
2	h	5	GLN
2	h	64	GLN
2	h	96	HIS
2	h	164	HIS
6	2	70	GLN
6	2	85	GLN
6	2	126	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 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)

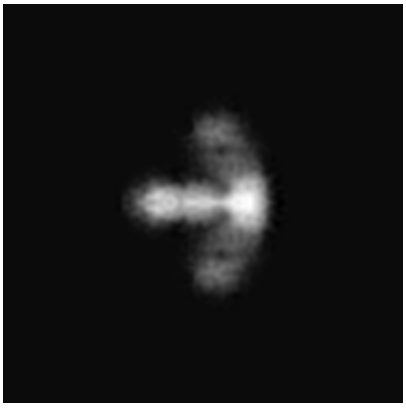
This section contains visualisations of the EMDB entry EMD-6258. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

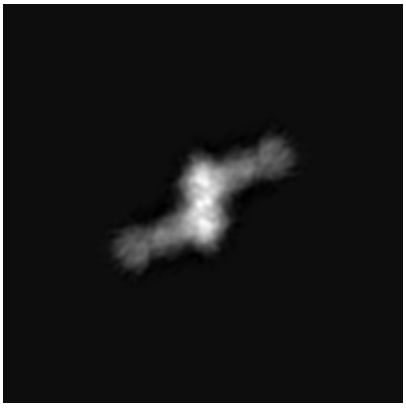
6.1 Orthogonal projections (i)

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: 120

Y Index: 120

Z Index: 120

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: 120

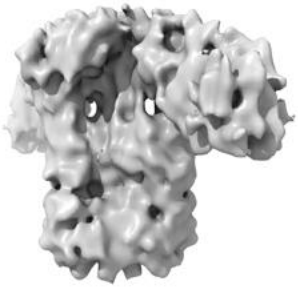
Y Index: 102

Z Index: 139

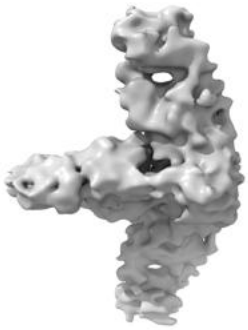
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

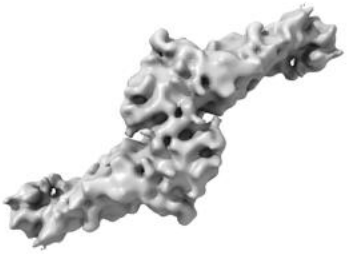
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

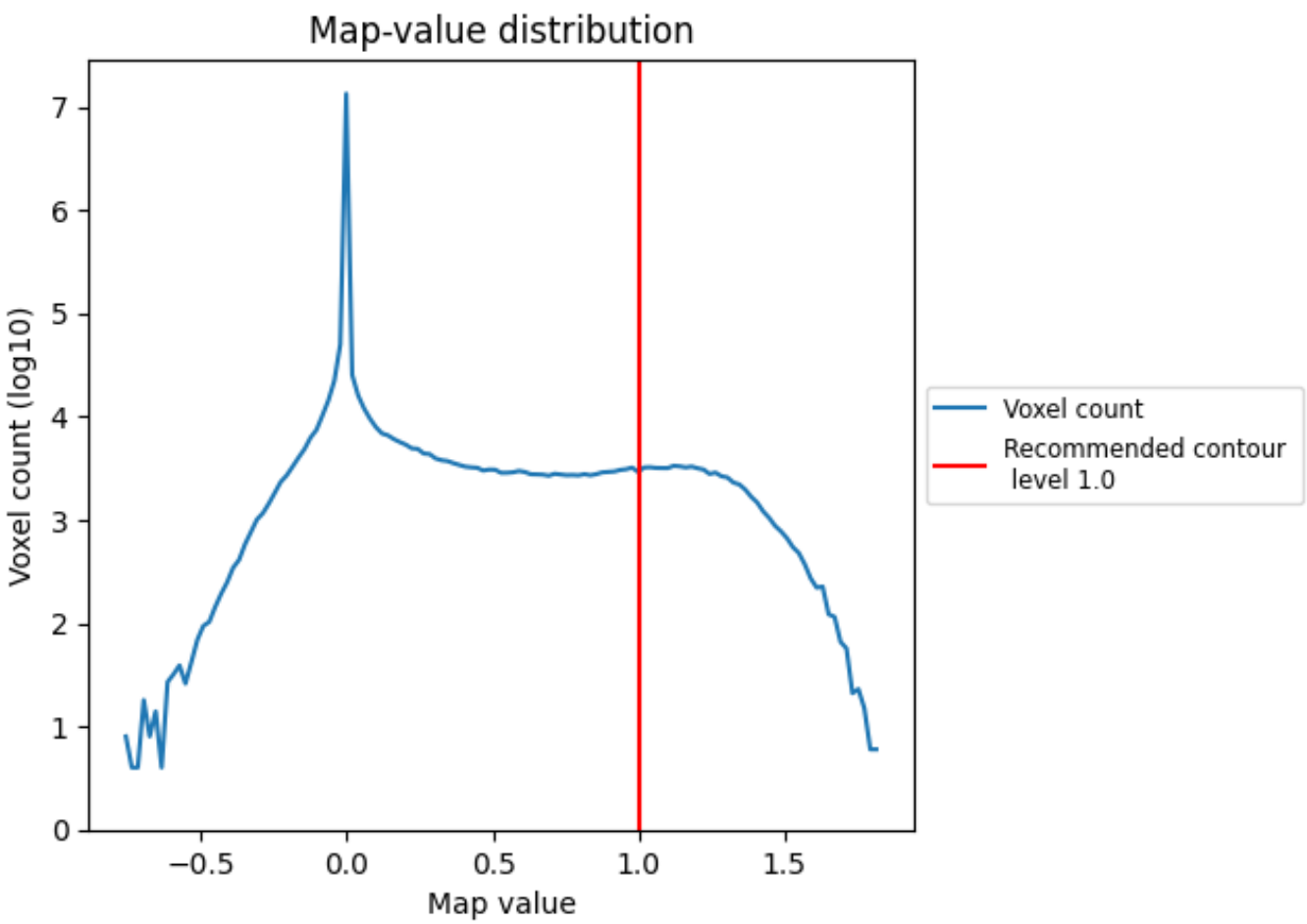
6.5 Mask visualisation (i)

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

7 Map analysis (i)

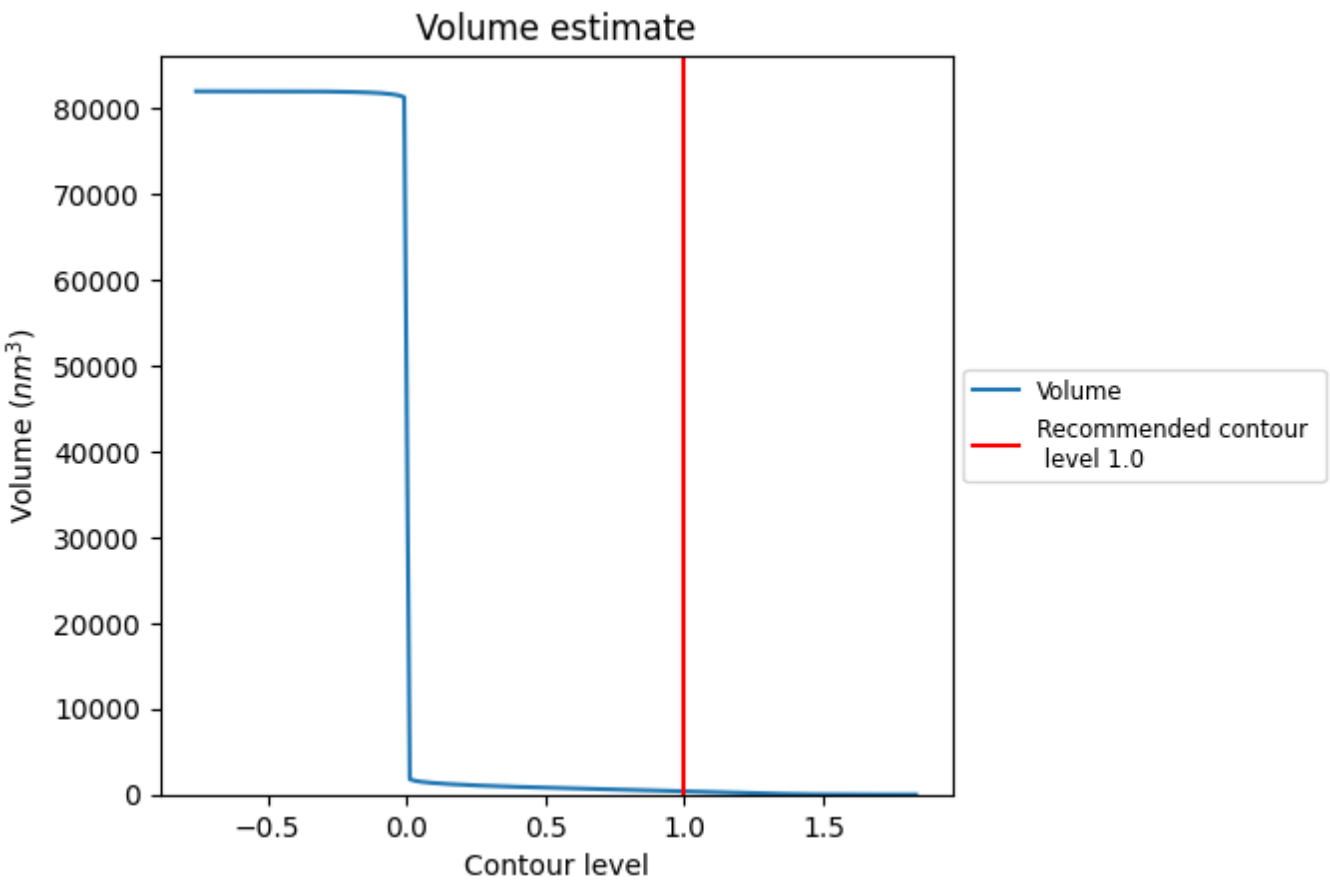
This section contains the results of statistical analysis of the map.

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.

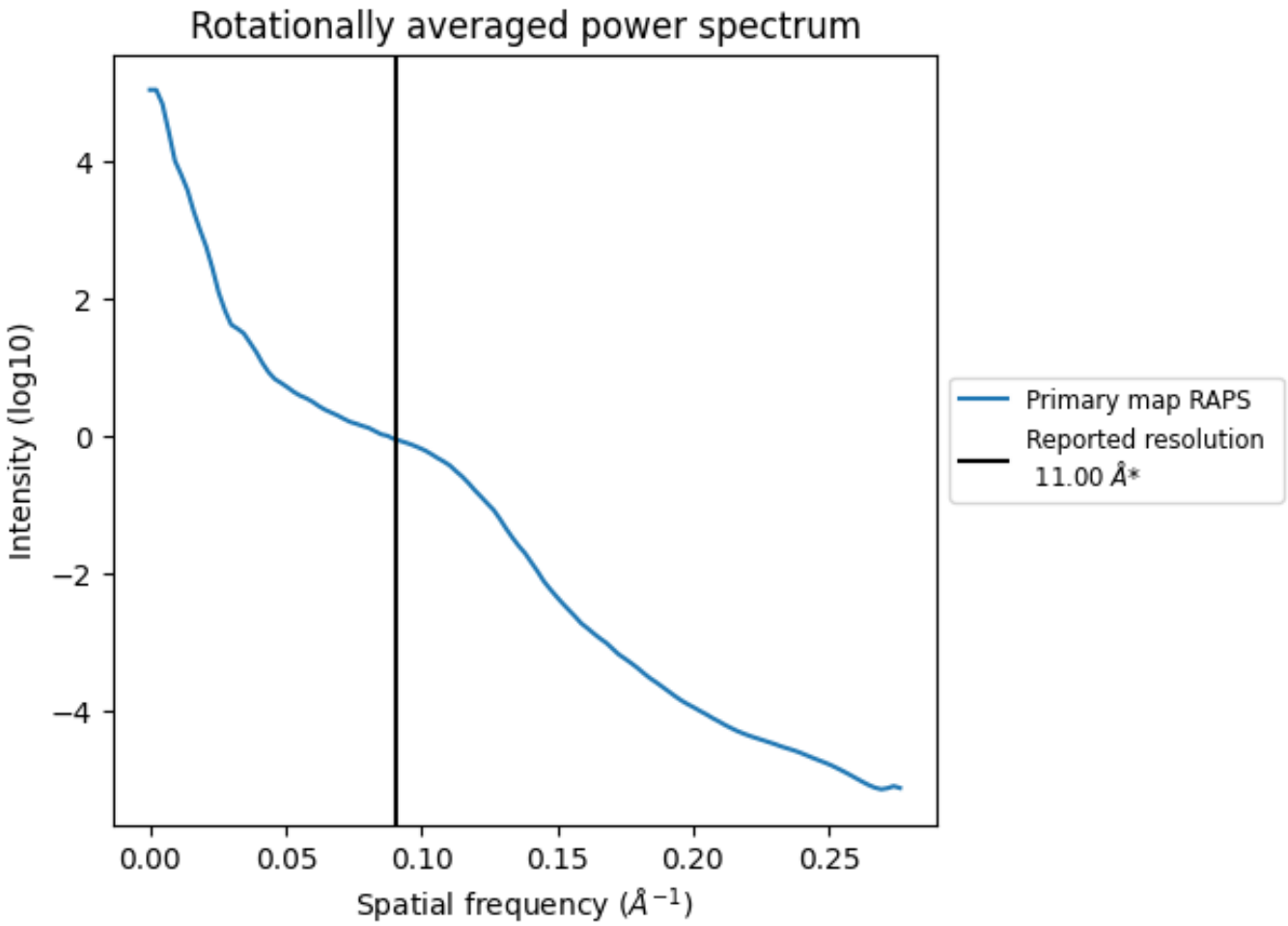
7.2 Volume estimate (i)



The volume at the recommended contour level is 390 nm^3; this corresponds to an approximate mass of 352 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 0.091 Å^{-1}

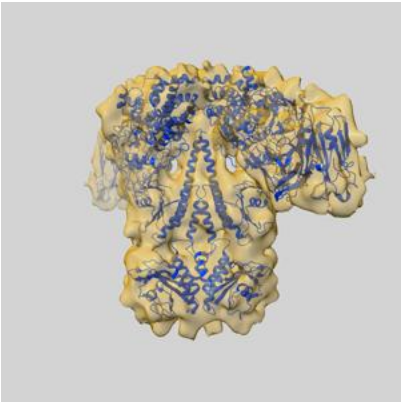
8 Fourier-Shell correlation (i)

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

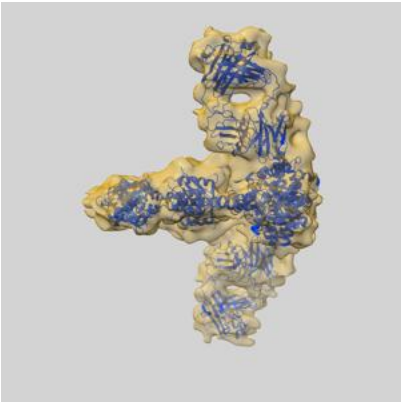
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6258 and PDB model 3JBQ. Per-residue inclusion information can be found in section 3 on page 6.

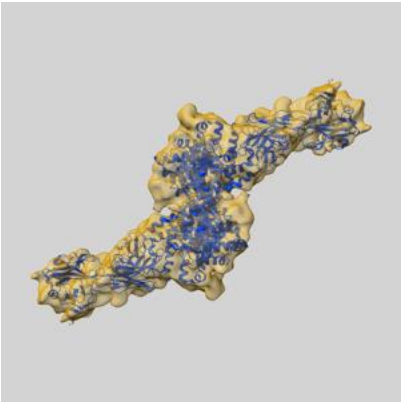
9.1 Map-model overlay (i)



X



Y



Z

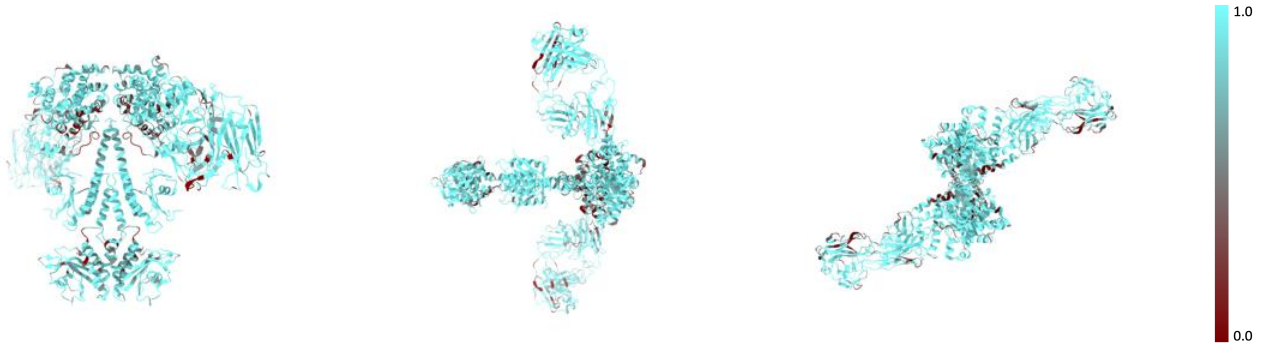
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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.

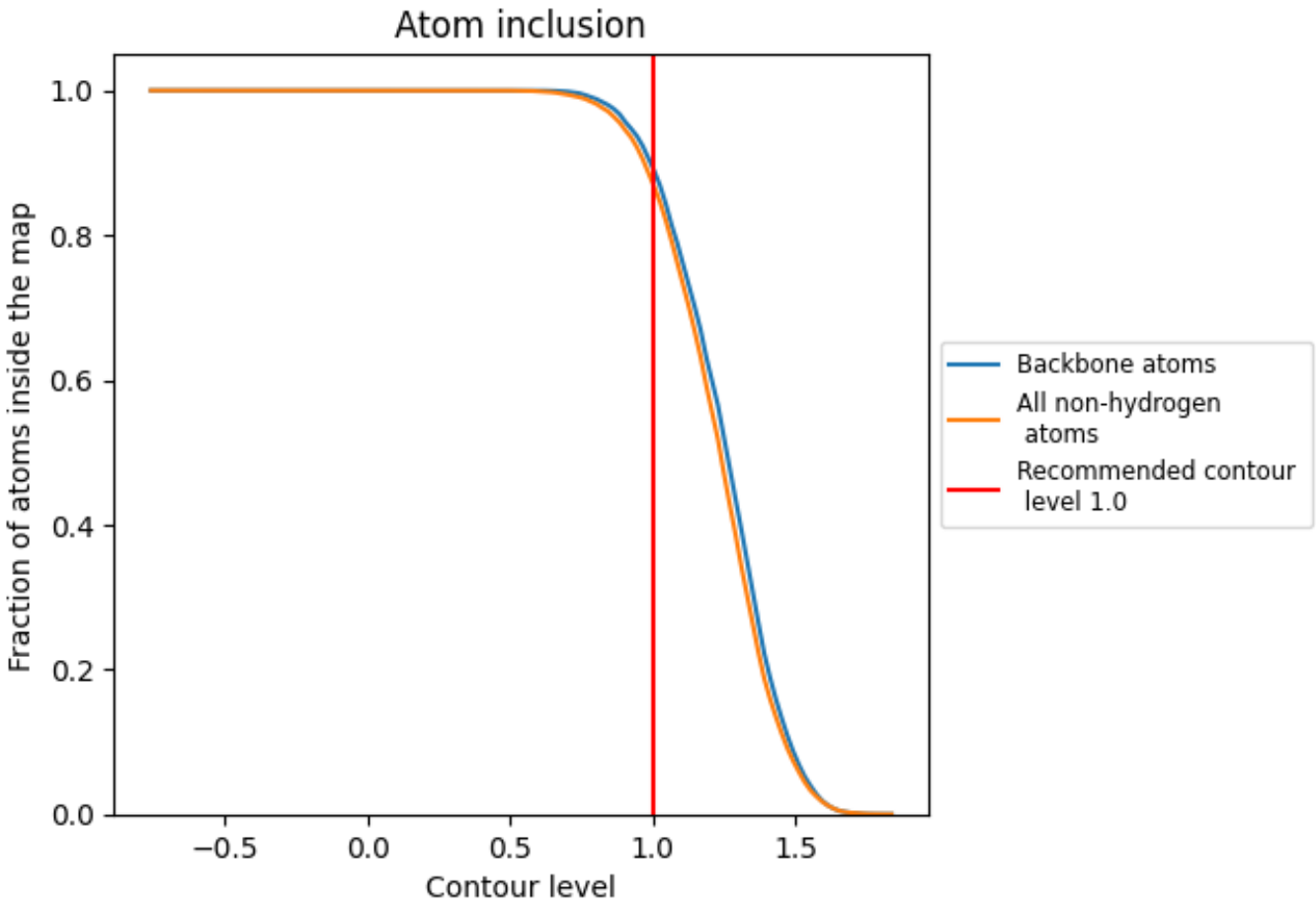
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.0800
1	0.8578	0.0640
2	0.8570	0.0650
B	0.8458	0.0640
C	0.9600	0.1240
D	0.7357	0.0160
F	0.8477	0.0680
G	0.9576	0.1230
H	0.9071	0.0960
L	0.8299	0.0720
X	0.7214	0.0210
h	0.9096	0.0970
l	0.8281	0.0720