wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 12:38 pm GMT

PDB ID	:	4UQK
EMDB ID	:	EMD-2689
Title	:	Electron density map of GluA2em in complex with quisqualate and LY451646
Authors	:	Meyerson, J.R.; Kumar, J.; Chittori, S.; Rao, P.; Pierson, J.; Bartesaghi, A.; Mayer, M.L.; Subramaniam, S.
Deposited on	:	2014-06-24
Resolution	:	16.40 Å(reported)
Based on initial model	:	1MM7

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 (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:

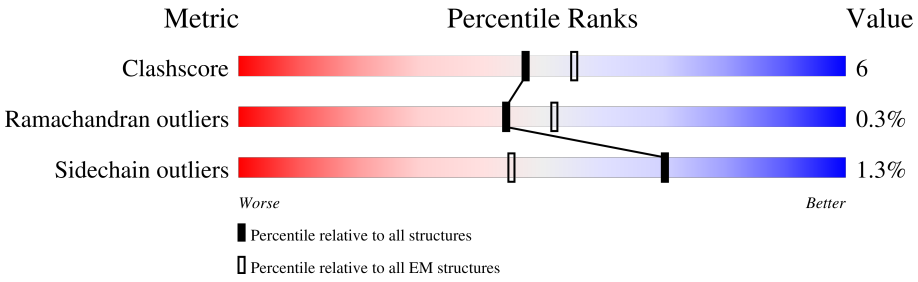
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 16.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	831	66% 10% 24%
1	B	831	66% 10% 24%
1	C	831	64% 12% 24%
1	D	831	63% 12% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18784 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 GLUTAMATE RECEPTOR 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	631	Total	C	N	O	S	0	0
			4694	3001	759	911	23		
1	B	632	Total	C	N	O	S	0	0
			4699	3004	760	912	23		
1	C	632	Total	C	N	O	S	0	0
			4672	2984	758	908	22		
1	D	631	Total	C	N	O	S	0	0
			4667	2981	757	907	22		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	384	GLU	LEU	conflict	UNP P19491
A	385	ASP	THR	conflict	UNP P19491
A	589	ALA	CYS	conflict	UNP P19491
A	631	THR	SER	conflict	UNP P19491
A	744	ASN	THR	variant	UNP P19491
A	745	ALA	PRO	variant	UNP P19491
A	754	ASN	SER	variant	UNP P19491
A	758	LEU	VAL	variant	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	384	GLU	LEU	conflict	UNP P19491
B	385	ASP	THR	conflict	UNP P19491
B	589	ALA	CYS	conflict	UNP P19491
B	631	THR	SER	conflict	UNP P19491
B	744	ASN	THR	variant	UNP P19491

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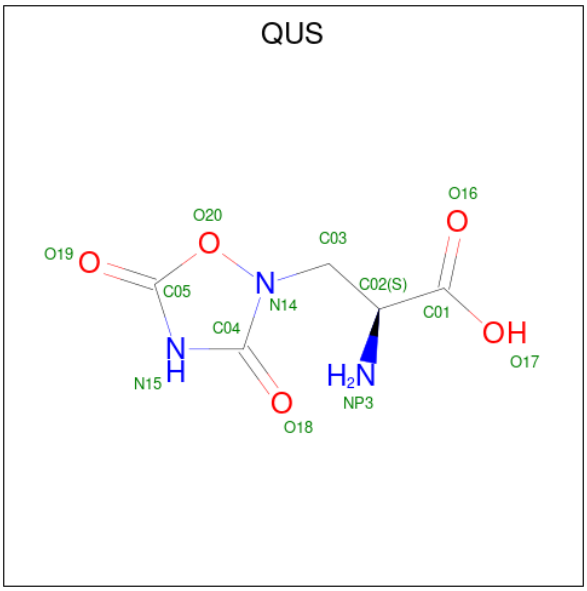
Chain	Residue	Modelled	Actual	Comment	Reference
B	745	ALA	PRO	variant	UNP P19491
B	754	ASN	SER	variant	UNP P19491
B	758	LEU	VAL	variant	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	384	GLU	LEU	conflict	UNP P19491
C	385	ASP	THR	conflict	UNP P19491
C	589	ALA	CYS	conflict	UNP P19491
C	631	THR	SER	conflict	UNP P19491
C	744	ASN	THR	variant	UNP P19491
C	745	ALA	PRO	variant	UNP P19491
C	754	ASN	SER	variant	UNP P19491
C	758	LEU	VAL	variant	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	384	GLU	LEU	conflict	UNP P19491
D	385	ASP	THR	conflict	UNP P19491
D	589	ALA	CYS	conflict	UNP P19491
D	631	THR	SER	conflict	UNP P19491
D	744	ASN	THR	variant	UNP P19491
D	745	ALA	PRO	variant	UNP P19491
D	754	ASN	SER	variant	UNP P19491
D	758	LEU	VAL	variant	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: $C_5H_7N_3O_5$).



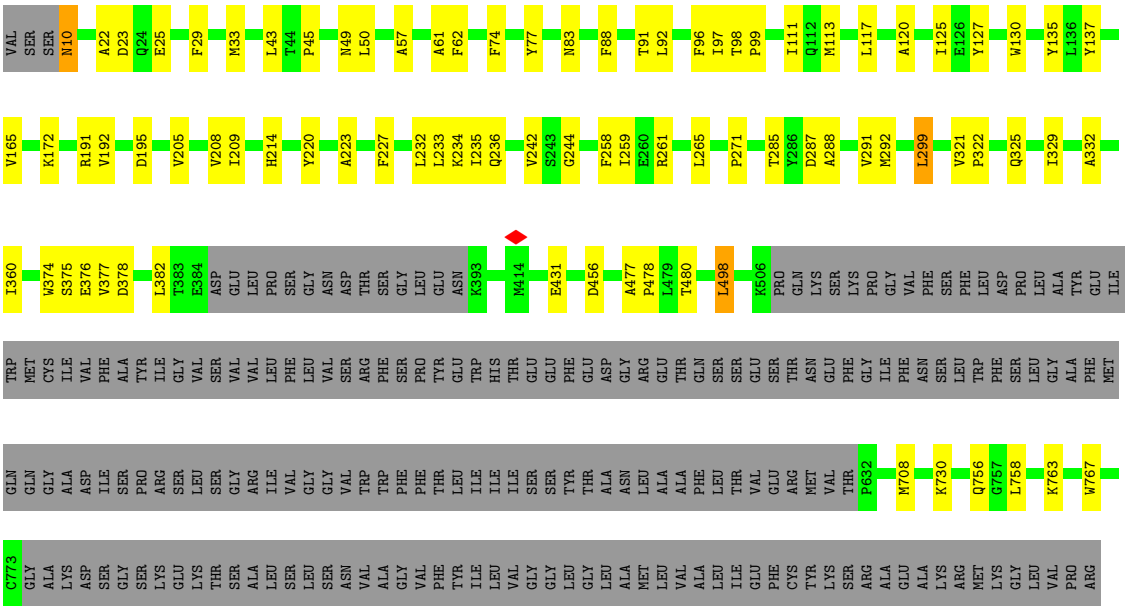
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O 13 5 3 5	0
2	B	1	Total C N O 13 5 3 5	0
2	C	1	Total C N O 13 5 3 5	0
2	D	1	Total C N O 13 5 3 5	0

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.

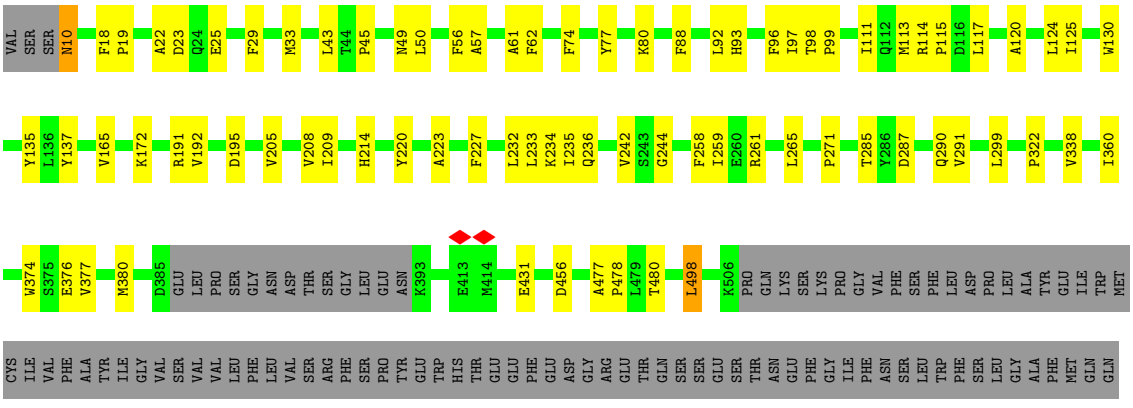
• Molecule 1: GLUTAMATE RECEPTOR 2

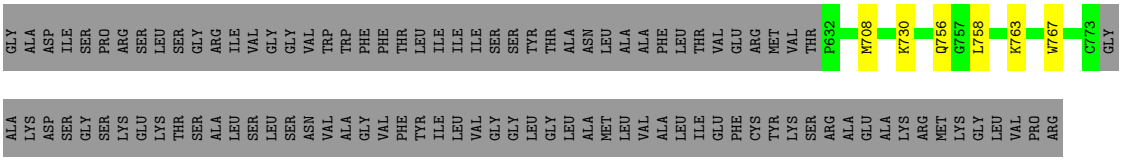
Chain A:



• Molecule 1: GLUTAMATE RECEPTOR 2

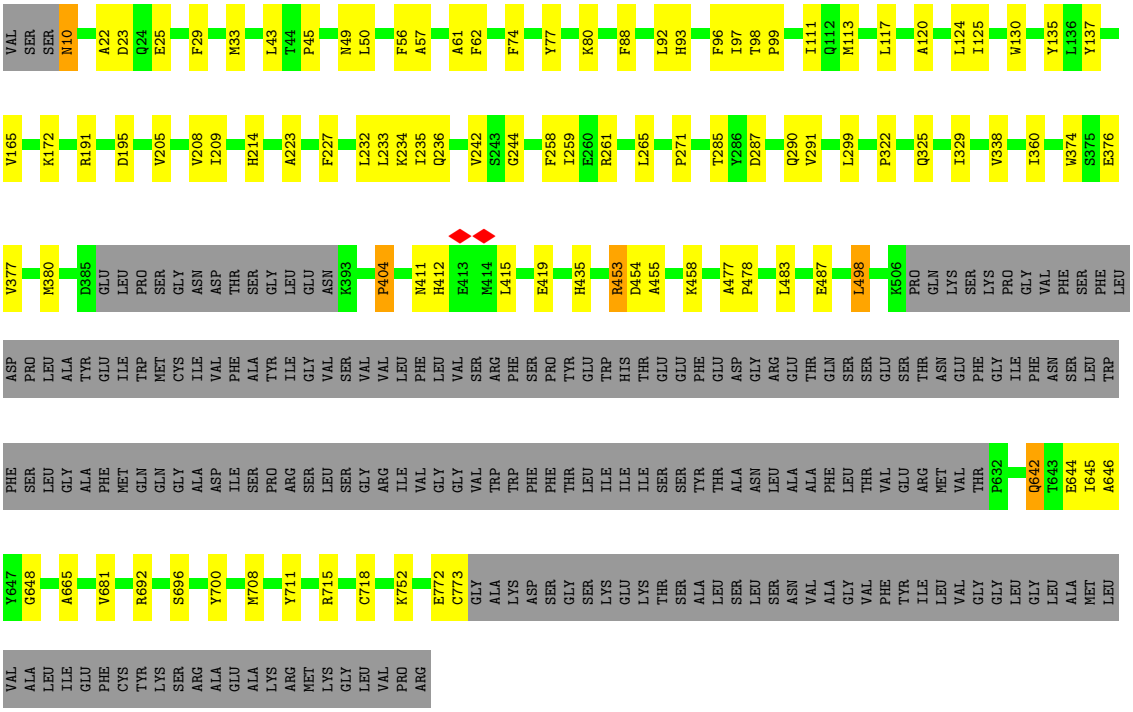
Chain B:





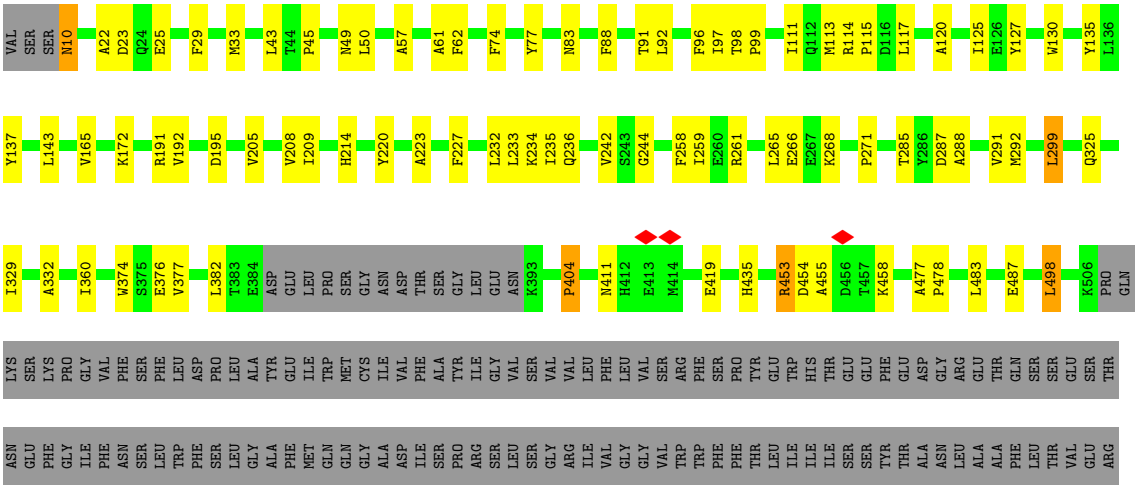
• Molecule 1: GLUTAMATE RECEPTOR 2

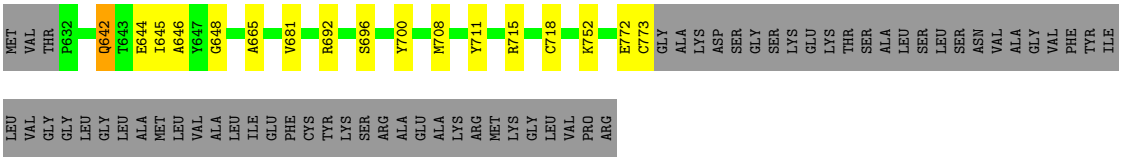
Chain C:



• Molecule 1: GLUTAMATE RECEPTOR 2

Chain D:




MET VAL THR P632 Q642 T643 E644 I645 A646 Y647 G648 A665 V681 R692 S696 Y700 M708 Y711 R715 C718 K752 E772 C773 GLY ALA LYS ASP SER GLY SER LYS GLU LYS THR SER ALA LEU SER LEU SER ASN VAL ALA GLY VAL PHE TYR ILE
LEU VAL GLY GLY LEU GLY LEU ALA MET LEU VAL ALA LEU ILE GLU PHE CYS TYR LYS SER ARG ALA GLU ALA LYS ARG MET LYS GLY LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	4795	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0361	Depositor
Map size (Å)	281.2, 281.2, 281.2	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.406, 1.406, 1.406	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUS

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	0.36	0/4790	0.51	1/6520 (0.0%)
1	B	0.36	0/4795	0.51	1/6527 (0.0%)
1	C	0.34	1/4767 (0.0%)	0.50	1/6489 (0.0%)
1	D	0.34	1/4762 (0.0%)	0.50	1/6482 (0.0%)
All	All	0.35	2/19114 (0.0%)	0.50	4/26018 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	419	GLU	CB-CG	-5.41	1.41	1.52
1	C	419	GLU	CB-CG	-5.40	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	498	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	498	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	498	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	498	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4694	0	4378	55	0
1	B	4699	0	4380	51	0
1	C	4672	0	4346	61	0
1	D	4667	0	4344	66	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
2	D	13	0	6	0	0
All	All	18784	0	17472	229	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.

The worst 5 of 229 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:C:453:ARG:HH12	1:C:455:ALA:HA	1.39	0.87
1:D:453:ARG:HH12	1:D:455:ALA:HA	1.39	0.85
1:C:711:TYR:CZ	1:C:715:ARG:HD2	2.28	0.68
1:D:711:TYR:CZ	1:D:715:ARG:HD2	2.28	0.68
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.83	0.61

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	625/831 (75%)	594 (95%)	29 (5%)	2 (0%)	41 77
1	B	626/831 (75%)	596 (95%)	28 (4%)	2 (0%)	41 77
1	C	626/831 (75%)	592 (95%)	32 (5%)	2 (0%)	41 77
1	D	625/831 (75%)	590 (94%)	33 (5%)	2 (0%)	41 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2502/3324 (75%)	2372 (95%)	122 (5%)	8 (0%)	44 77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	456	ASP
1	B	172	LYS
1	B	456	ASP
1	C	172	LYS

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	470/708 (66%)	466 (99%)	4 (1%)	78 87
1	B	470/708 (66%)	466 (99%)	4 (1%)	78 87
1	C	467/708 (66%)	459 (98%)	8 (2%)	60 78
1	D	467/708 (66%)	459 (98%)	8 (2%)	60 78
All	All	1874/2832 (66%)	1850 (99%)	24 (1%)	70 81

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	642	GLN
1	D	299	LEU
1	D	10	ASN
1	D	404	PRO
1	B	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	435	HIS
1	B	435	HIS
1	D	83	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)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	QUS	D	1803	-	6,13,13	1.23	1 (16%)	4,18,18	1.38	1 (25%)
2	QUS	B	1803	-	6,13,13	1.17	0	4,18,18	1.29	1 (25%)
2	QUS	A	1803	-	6,13,13	1.20	0	4,18,18	1.30	1 (25%)
2	QUS	C	1803	-	6,13,13	1.24	1 (16%)	4,18,18	1.37	1 (25%)

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
2	QUS	D	1803	-	-	2/6/8/8	0/1/1/1
2	QUS	B	1803	-	-	2/6/8/8	0/1/1/1
2	QUS	A	1803	-	-	2/6/8/8	0/1/1/1
2	QUS	C	1803	-	-	2/6/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1803	QUS	C04-N15	2.11	1.36	1.34
2	D	1803	QUS	C04-N15	2.07	1.36	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1803	QUS	C03-C02-C01	-2.47	103.98	108.94
2	C	1803	QUS	C03-C02-C01	-2.44	104.03	108.94
2	B	1803	QUS	C03-C02-C01	-2.11	104.69	108.94
2	A	1803	QUS	C03-C02-C01	-2.11	104.69	108.94

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1803	QUS	C01-C02-C03-N14
2	B	1803	QUS	C01-C02-C03-N14
2	C	1803	QUS	C01-C02-C03-N14
2	D	1803	QUS	C01-C02-C03-N14
2	A	1803	QUS	NP3-C02-C03-N14

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2689. These allow visual inspection of the internal detail of the map and identification of artifacts.

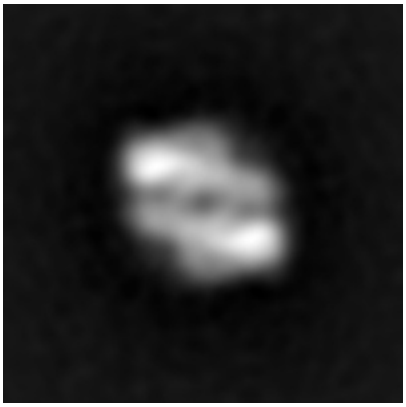
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X

Y



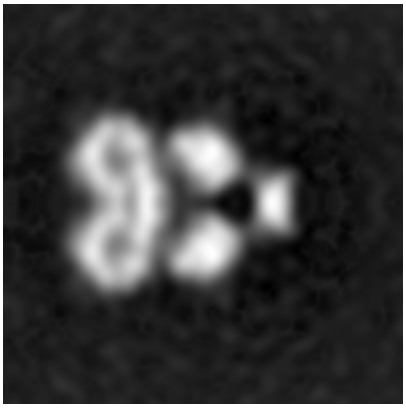
Z

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

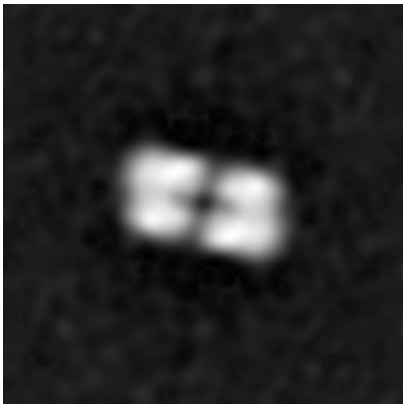
6.2 Central slices

6.2.1 Primary map

X Index: 100



Y Index: 100



Z Index: 100

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: 102

Y Index: 118

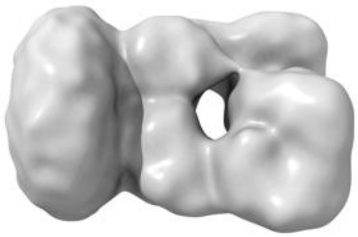
Z Index: 150

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

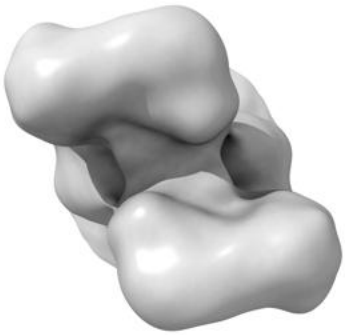
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0361. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

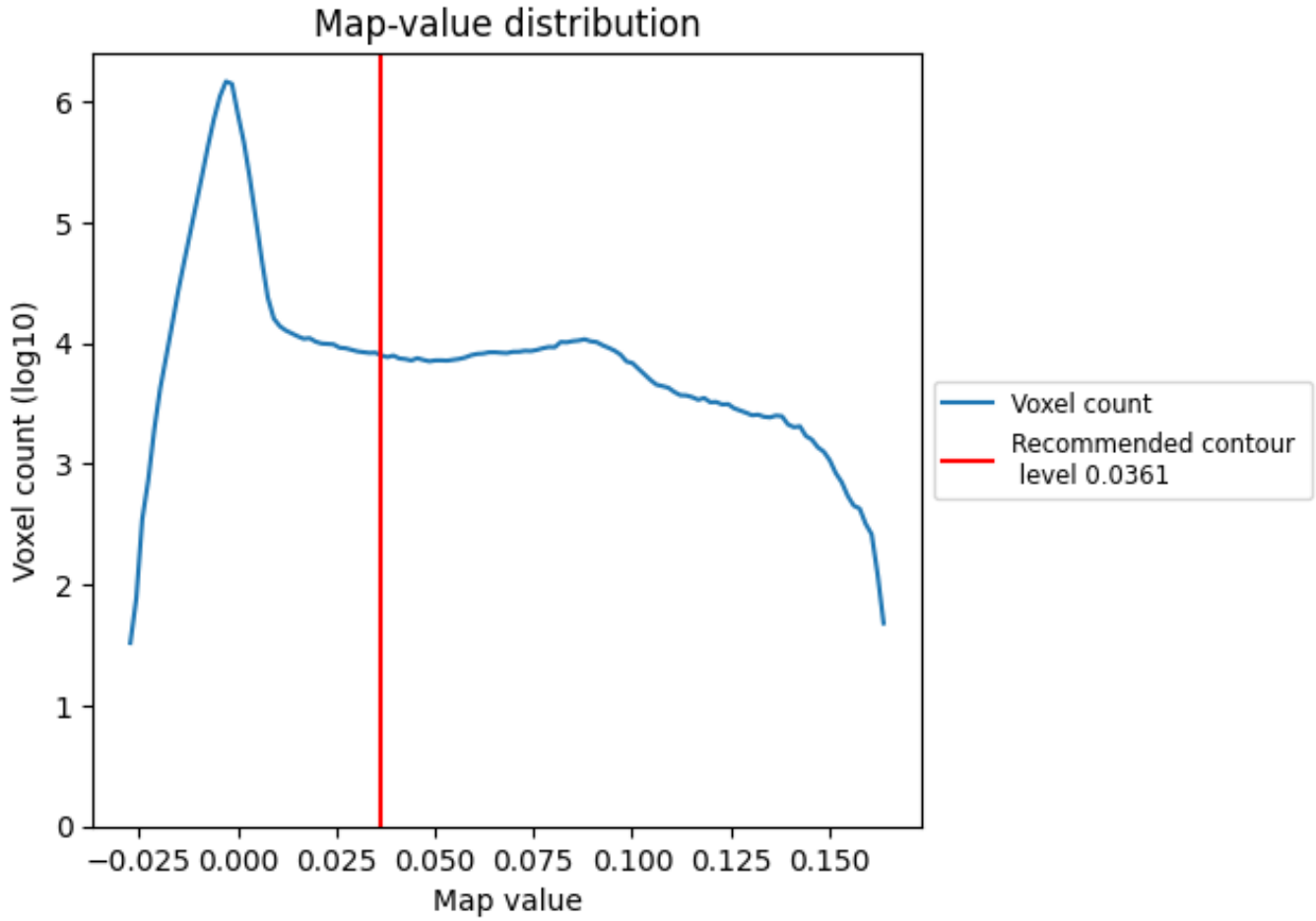
6.5 Mask visualisation (i)

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

7 Map analysis

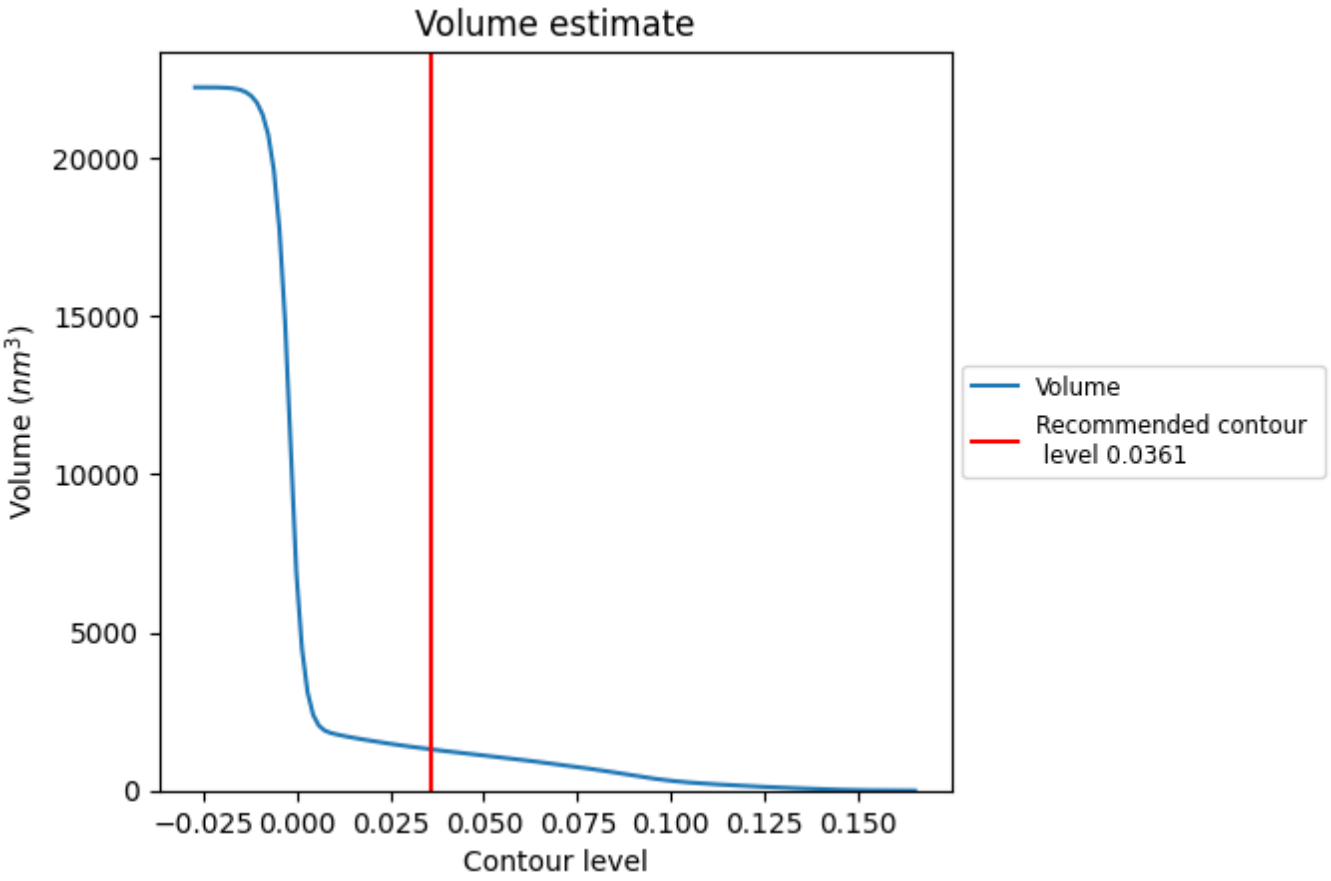
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

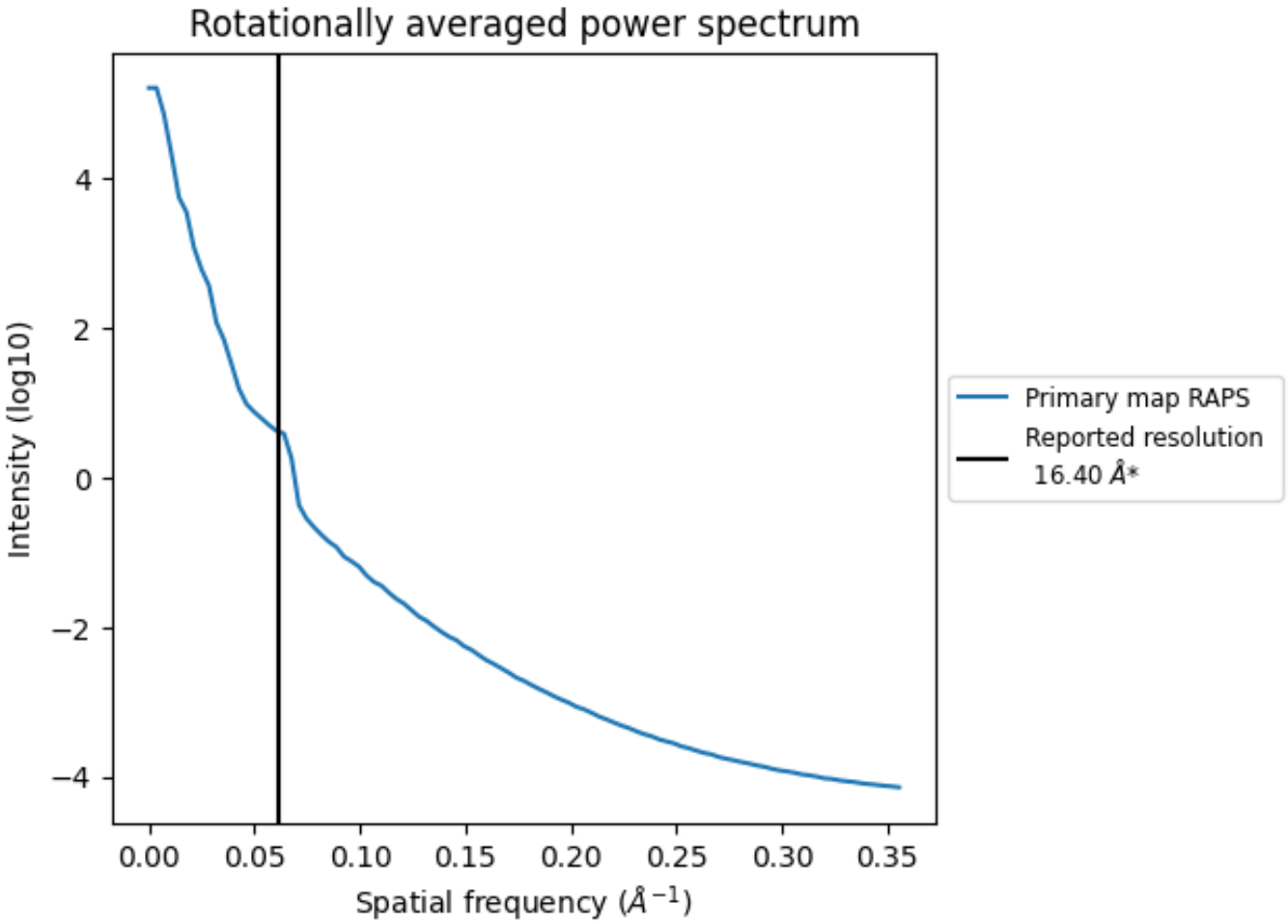
7.2 Volume estimate (i)



The volume at the recommended contour level is 1300 nm^3; this corresponds to an approximate mass of 1174 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 0.061 Å^{-1}

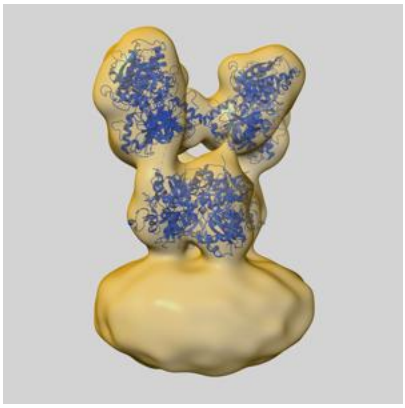
8 Fourier-Shell correlation (i)

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

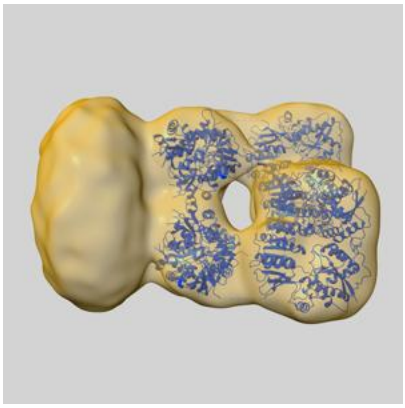
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2689 and PDB model 4UQK. Per-residue inclusion information can be found in section 3 on page 6.

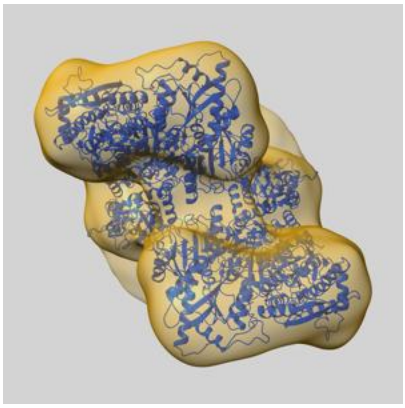
9.1 Map-model overlay



X



Y



Z

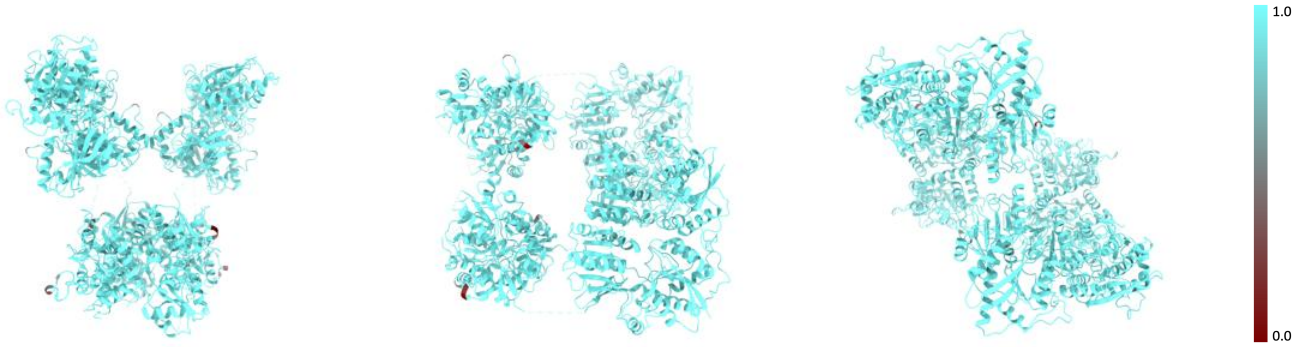
The images above show the 3D surface view of the map at the recommended contour level 0.0361 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

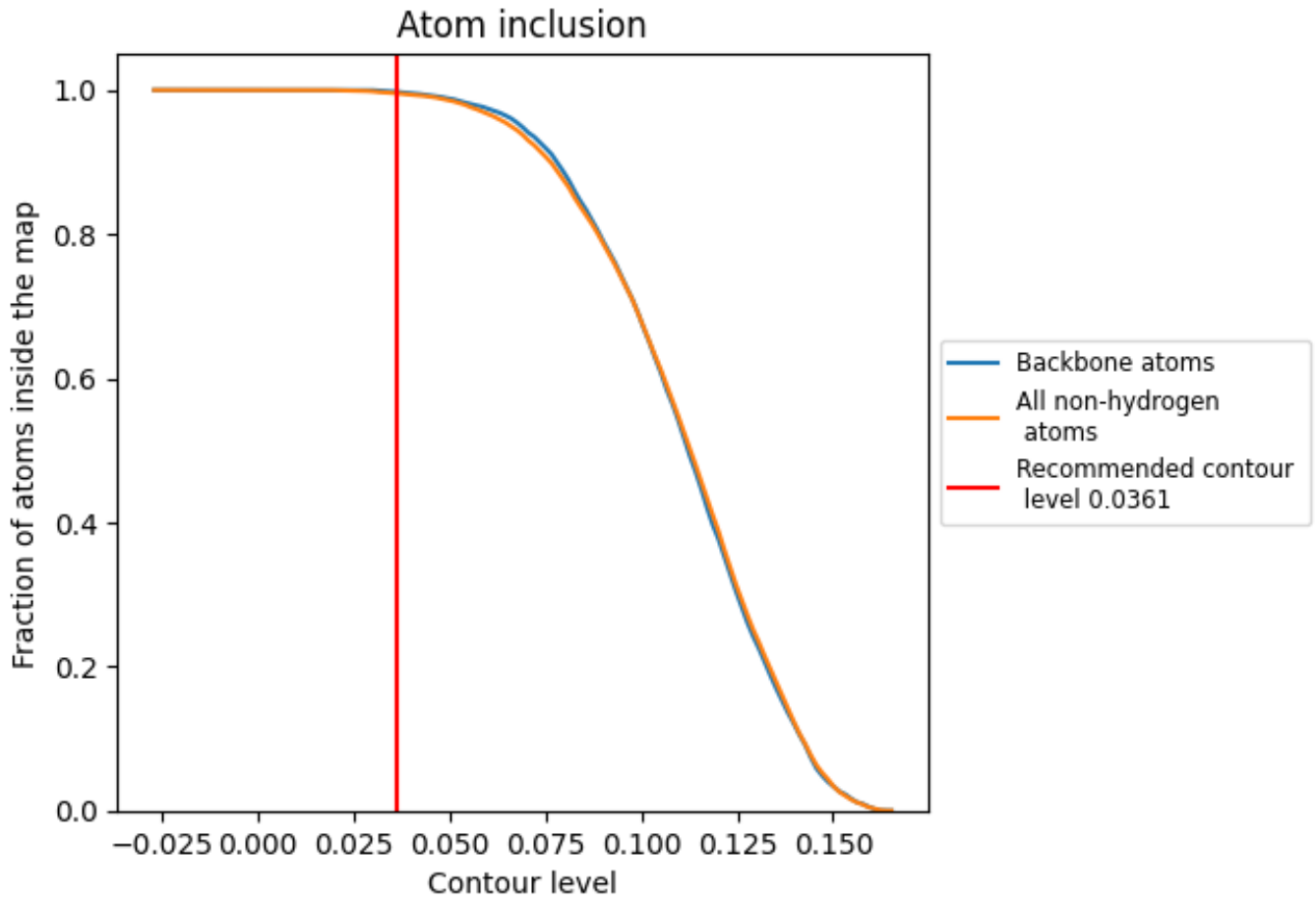
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0361).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0361) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9955	0.0760
A	0.9959	0.0740
B	0.9944	0.0770
C	0.9965	0.0740
D	0.9950	0.0800