wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 01:11 PM JST

PDB ID	:	7CR7
EMDB ID	:	EMD-30448
Title	:	human KCNQ2-CaM in complex with retigabine
Authors	:	Li, X.; Lv, D.; Wang, J.; Ye, S.; Guo, J.
Deposited on	:	2020-08-12
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

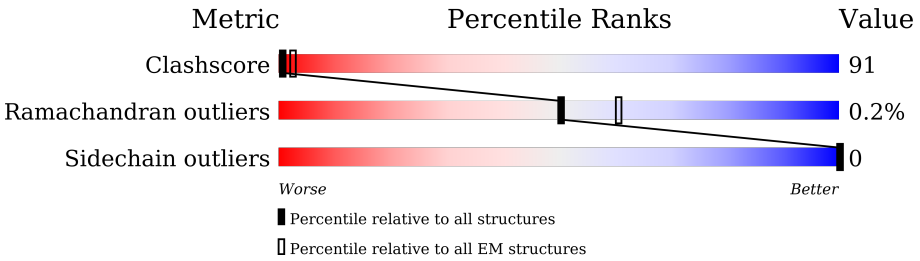
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.70 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	656	12%; 14%; 40%; 46%
1	B	656	13%; 14%; 40%; 46%
1	D	656	13%; 14%; 39%; 46%
1	G	656	12%; 14%; 40%; 46%
2	C	149	64%; 21%; 74%; .
2	E	149	63%; 20%; 76%; .
2	F	149	62%; 20%; 76%; .
2	H	149	63%; 21%; 75%; .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16208 atoms, of which 72 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 Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	354	2886	1890	503	480	13	0	0
1	B	354	2886	1890	503	480	13	0	0
1	D	354	2886	1890	503	480	13	0	0
1	G	354	2886	1890	503	480	13	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP O43526
A	703	VAL	-	expression tag	UNP O43526
A	704	GLU	-	expression tag	UNP O43526
A	705	GLY	-	expression tag	UNP O43526
A	706	GLY	-	expression tag	UNP O43526
A	707	SER	-	expression tag	UNP O43526
A	708	SER	-	expression tag	UNP O43526
A	709	GLY	-	expression tag	UNP O43526
A	710	GLY	-	expression tag	UNP O43526
A	711	TRP	-	expression tag	UNP O43526
A	712	SER	-	expression tag	UNP O43526
A	713	HIS	-	expression tag	UNP O43526
A	714	PRO	-	expression tag	UNP O43526
A	715	GLN	-	expression tag	UNP O43526
A	716	PHE	-	expression tag	UNP O43526
A	717	GLU	-	expression tag	UNP O43526
A	718	LYS	-	expression tag	UNP O43526
B	63	MET	-	initiating methionine	UNP O43526
B	703	VAL	-	expression tag	UNP O43526
B	704	GLU	-	expression tag	UNP O43526
B	705	GLY	-	expression tag	UNP O43526
B	706	GLY	-	expression tag	UNP O43526

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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	SER	-	expression tag	UNP O43526
B	708	SER	-	expression tag	UNP O43526
B	709	GLY	-	expression tag	UNP O43526
B	710	GLY	-	expression tag	UNP O43526
B	711	TRP	-	expression tag	UNP O43526
B	712	SER	-	expression tag	UNP O43526
B	713	HIS	-	expression tag	UNP O43526
B	714	PRO	-	expression tag	UNP O43526
B	715	GLN	-	expression tag	UNP O43526
B	716	PHE	-	expression tag	UNP O43526
B	717	GLU	-	expression tag	UNP O43526
B	718	LYS	-	expression tag	UNP O43526
D	63	MET	-	initiating methionine	UNP O43526
D	703	VAL	-	expression tag	UNP O43526
D	704	GLU	-	expression tag	UNP O43526
D	705	GLY	-	expression tag	UNP O43526
D	706	GLY	-	expression tag	UNP O43526
D	707	SER	-	expression tag	UNP O43526
D	708	SER	-	expression tag	UNP O43526
D	709	GLY	-	expression tag	UNP O43526
D	710	GLY	-	expression tag	UNP O43526
D	711	TRP	-	expression tag	UNP O43526
D	712	SER	-	expression tag	UNP O43526
D	713	HIS	-	expression tag	UNP O43526
D	714	PRO	-	expression tag	UNP O43526
D	715	GLN	-	expression tag	UNP O43526
D	716	PHE	-	expression tag	UNP O43526
D	717	GLU	-	expression tag	UNP O43526
D	718	LYS	-	expression tag	UNP O43526
G	63	MET	-	initiating methionine	UNP O43526
G	703	VAL	-	expression tag	UNP O43526
G	704	GLU	-	expression tag	UNP O43526
G	705	GLY	-	expression tag	UNP O43526
G	706	GLY	-	expression tag	UNP O43526
G	707	SER	-	expression tag	UNP O43526
G	708	SER	-	expression tag	UNP O43526
G	709	GLY	-	expression tag	UNP O43526
G	710	GLY	-	expression tag	UNP O43526
G	711	TRP	-	expression tag	UNP O43526
G	712	SER	-	expression tag	UNP O43526
G	713	HIS	-	expression tag	UNP O43526
G	714	PRO	-	expression tag	UNP O43526

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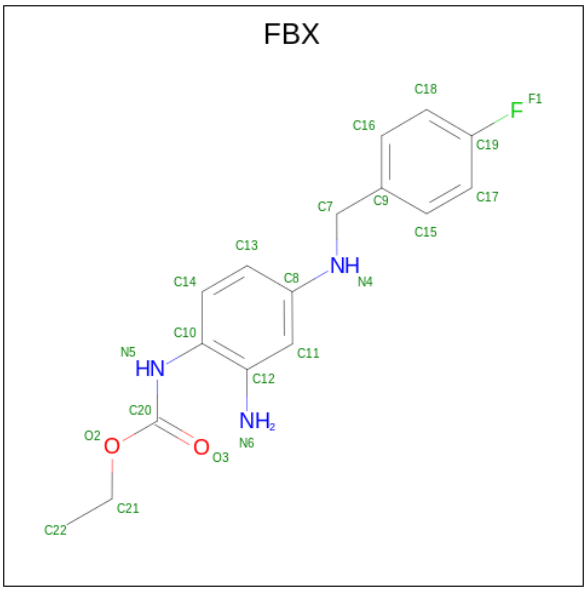
Chain	Residue	Modelled	Actual	Comment	Reference
G	715	GLN	-	expression tag	UNP O43526
G	716	PHE	-	expression tag	UNP O43526
G	717	GLU	-	expression tag	UNP O43526
G	718	LYS	-	expression tag	UNP O43526

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	143	1126	690	181	246	9	0	0
2	C	143	1126	690	181	246	9	0	0
2	E	143	1126	690	181	246	9	0	0
2	H	143	1126	690	181	246	9	0	0

- Molecule 3 is ethyl N-[2-azanyl-4-[(4-fluorophenyl)methylamino]phenyl]carbamate (three-letter code: FBX) (formula: $C_{16}H_{18}FN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
3	A	1	40	16	1	18	3	2	0
3	B	1	40	16	1	18	3	2	0
3	D	1	40	16	1	18	3	2	0

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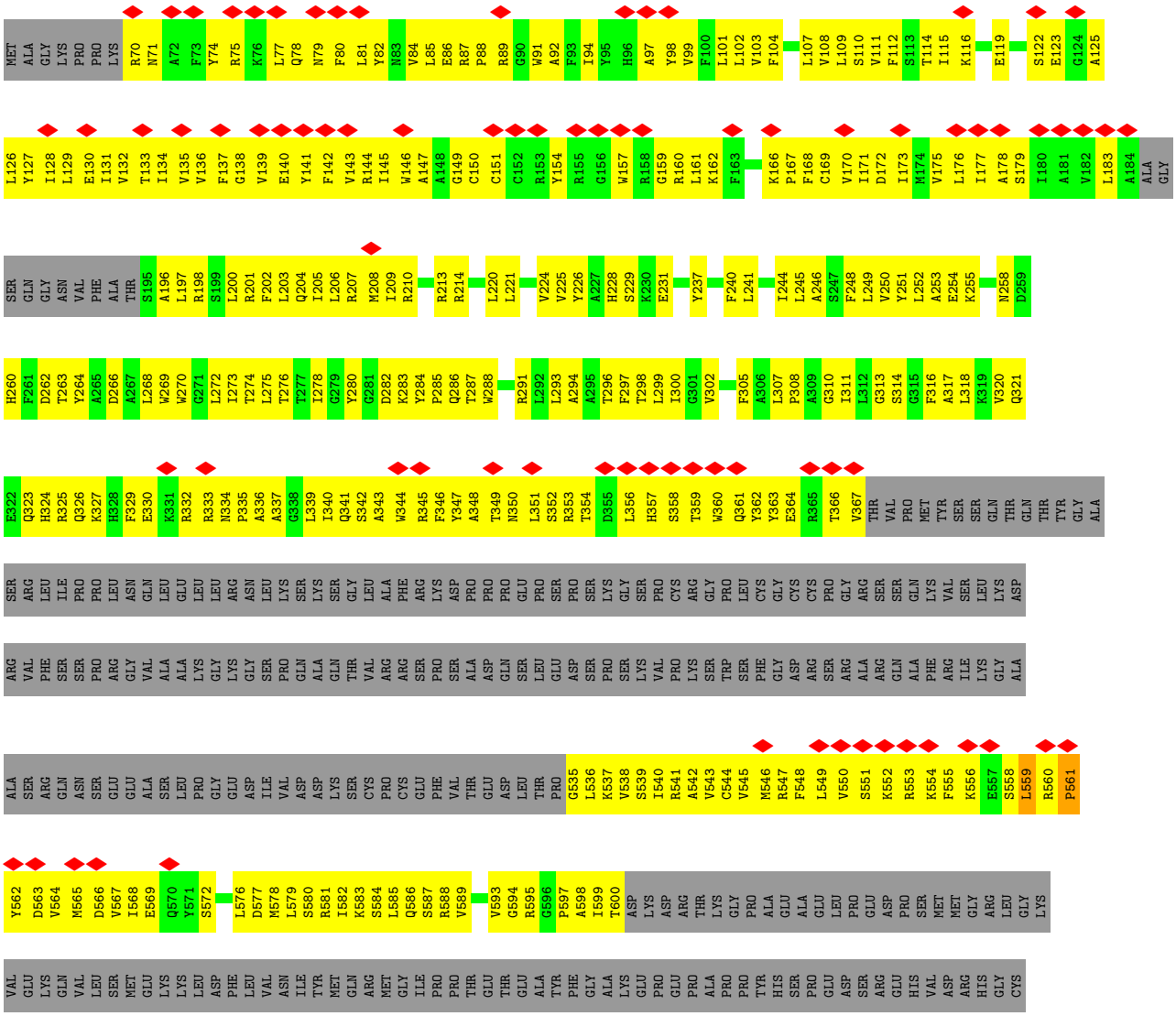
Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
3	G	1	40	16	1	18	3	2	0

3 Residue-property plots (i)

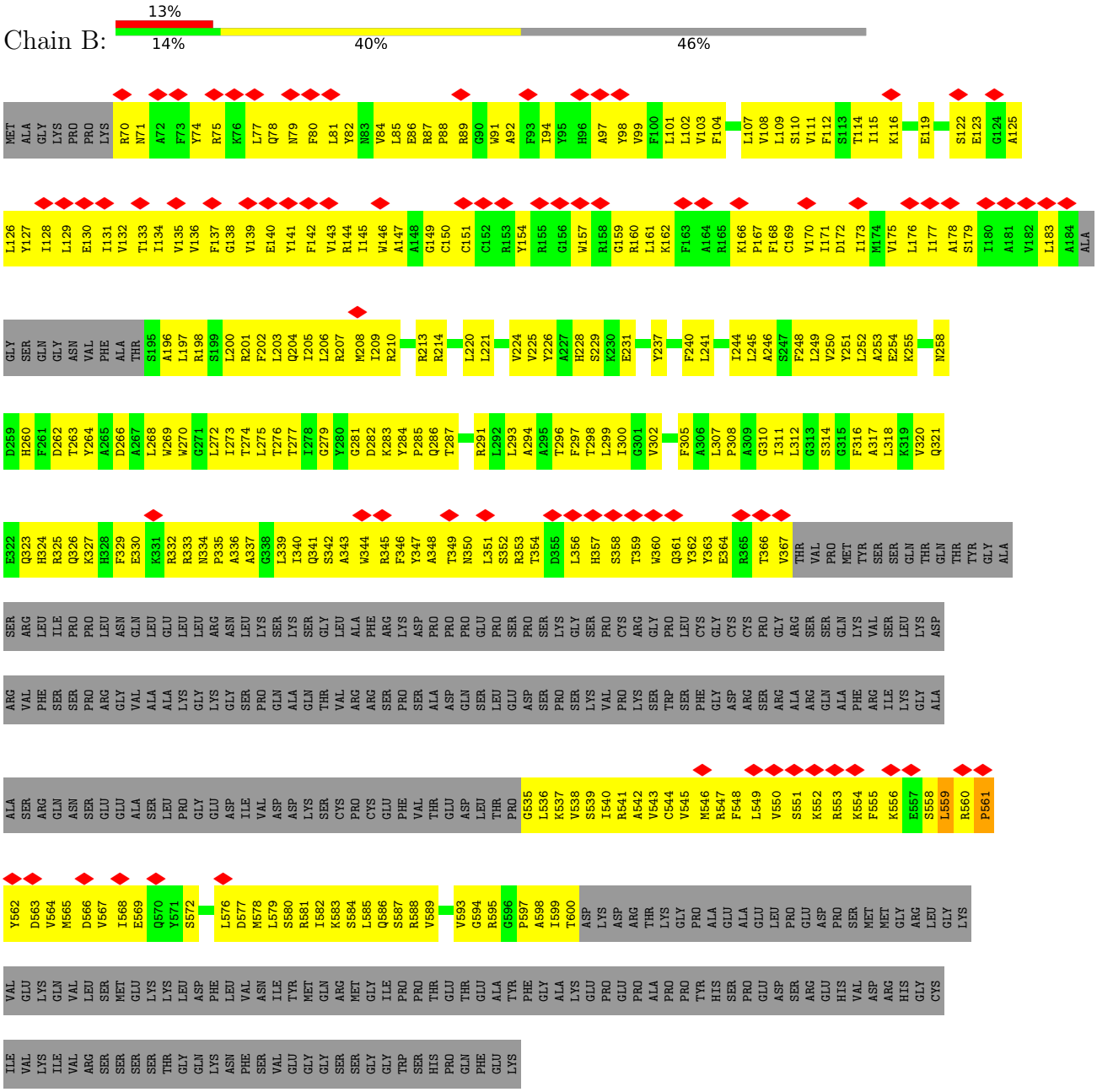
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium voltage-gated channel subfamily KQT member 2

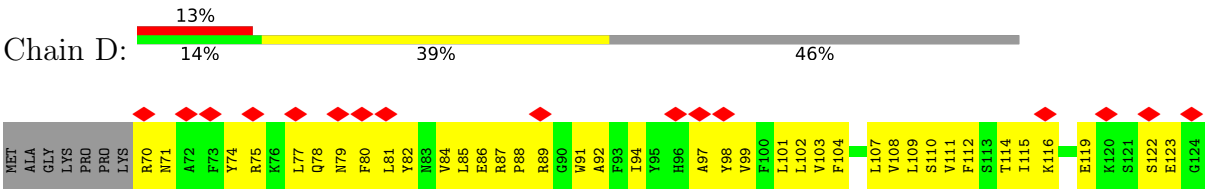
Chain A: 12% 14% 40% 46%

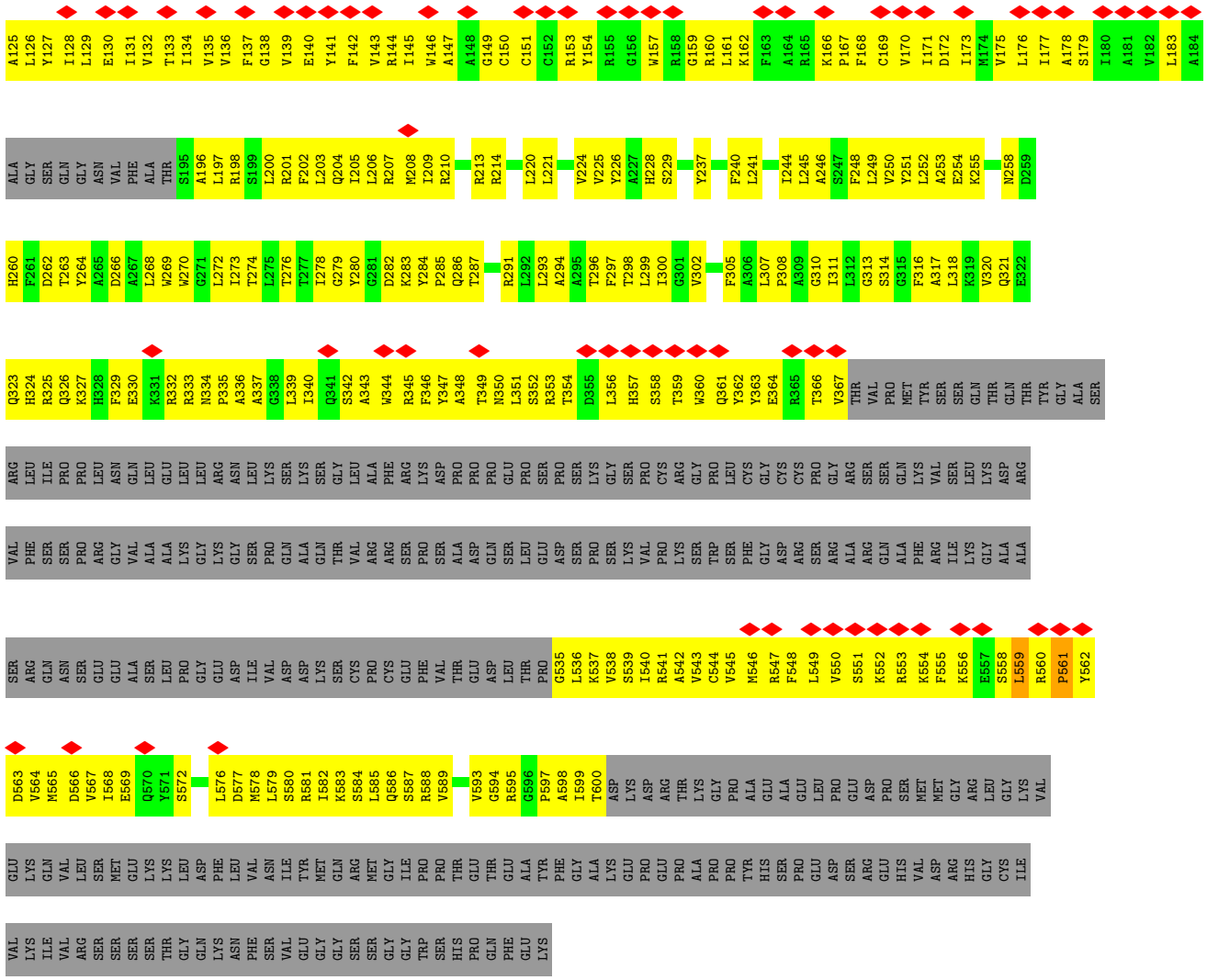


• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2



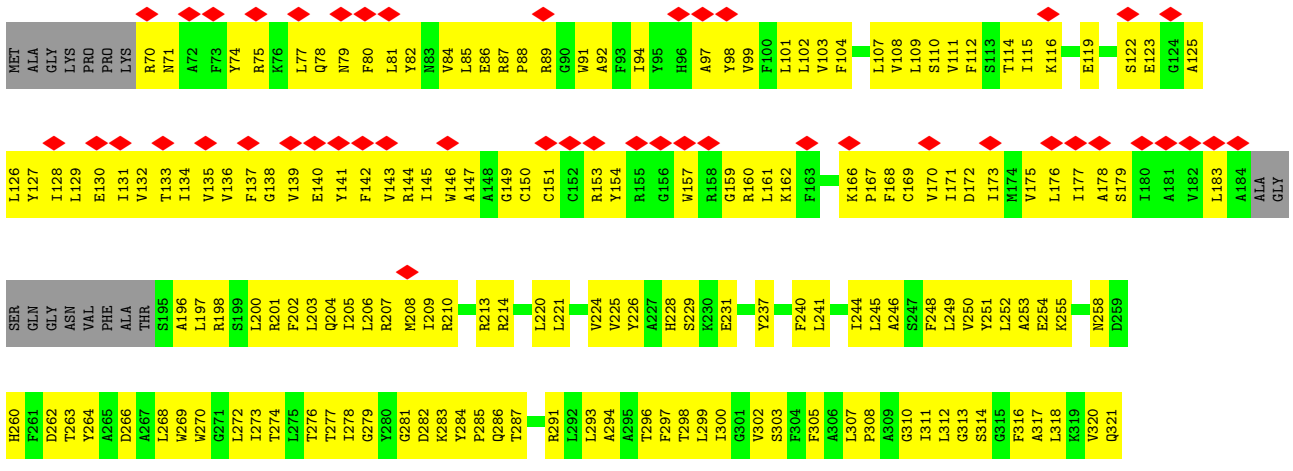
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

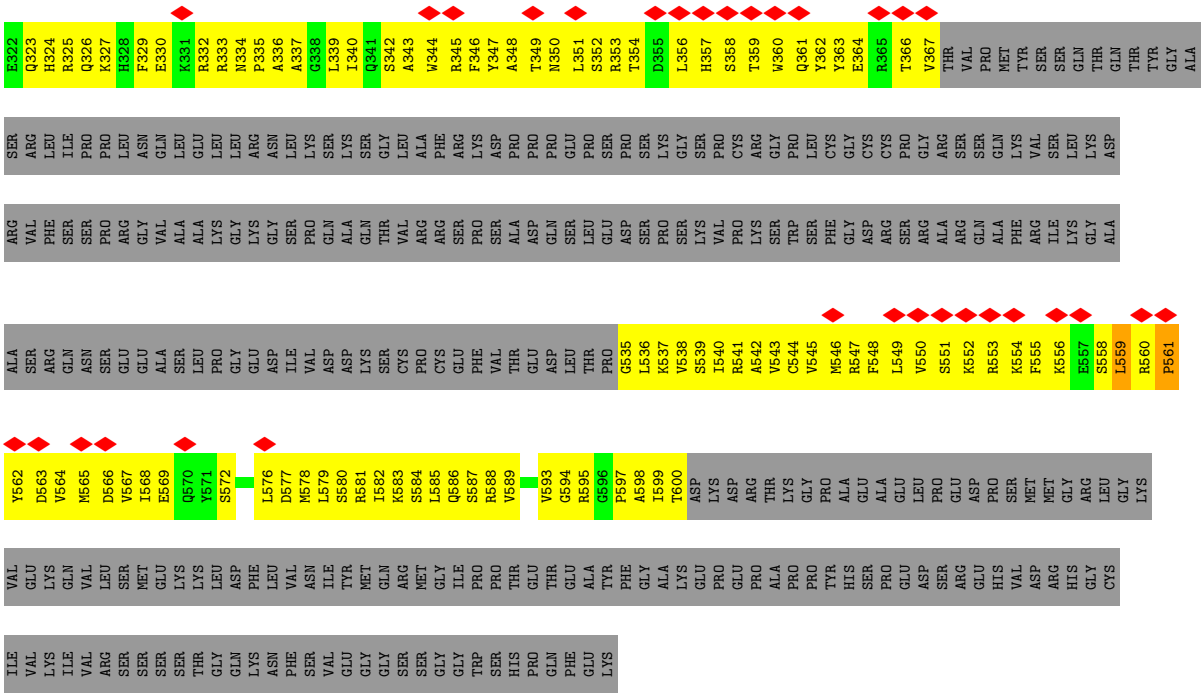




- Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

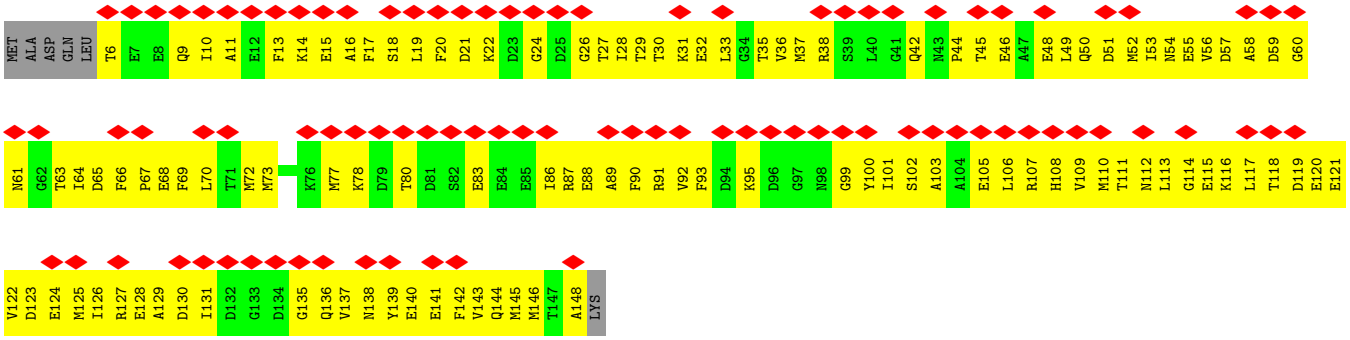
Chain G:





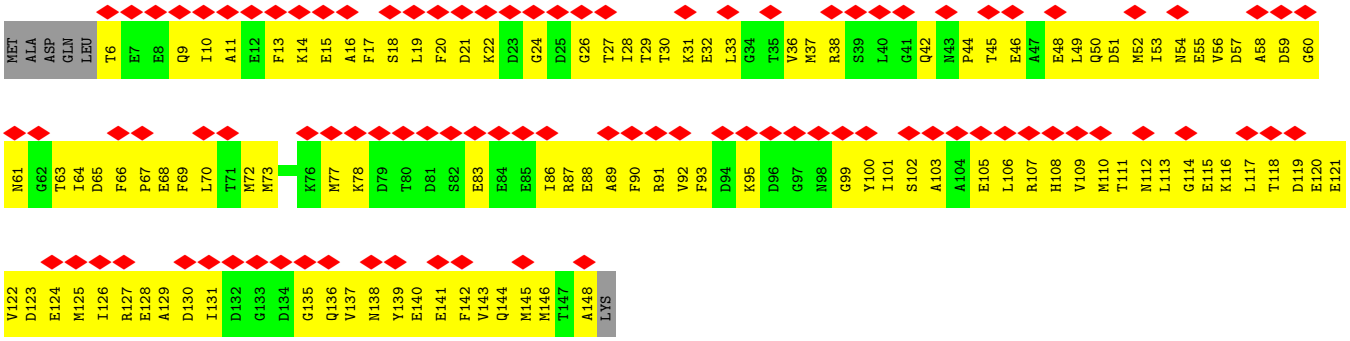
- Molecule 2: Calmodulin-3

Chain F:



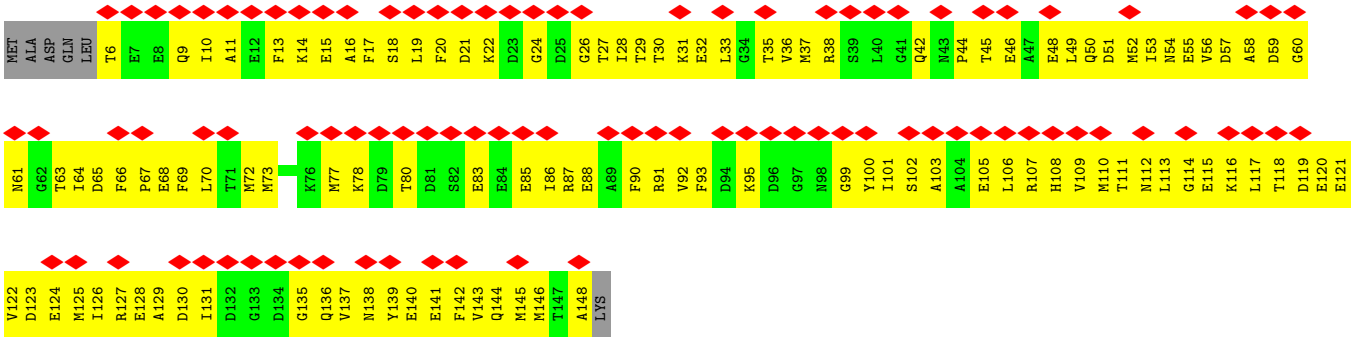
- Molecule 2: Calmodulin-3

Chain C:



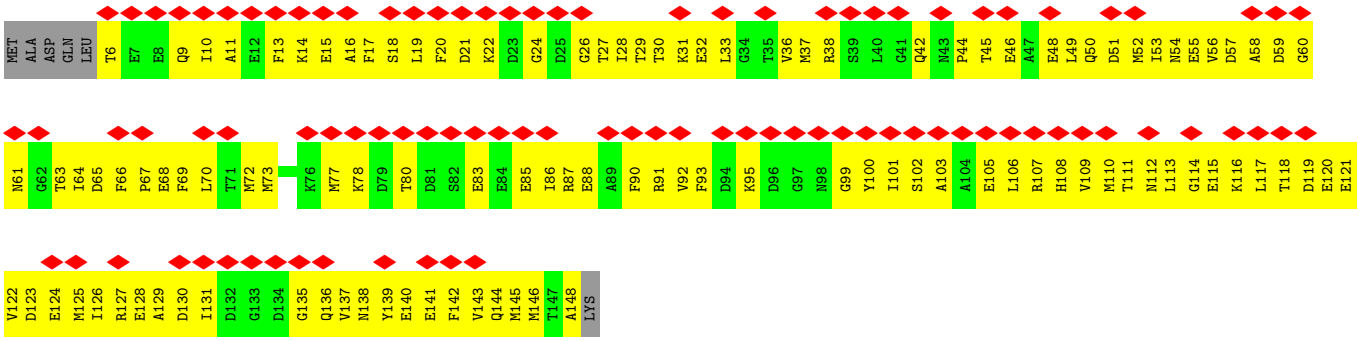
- Molecule 2: Calmodulin-3

Chain E:



- Molecule 2: Calmodulin-3

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67671	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 ($e^-/Å^2$)	1.556	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	0.060	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: FBX

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	0.35	0/2958	0.49	1/3998 (0.0%)
1	B	0.35	0/2958	0.49	1/3998 (0.0%)
1	D	0.35	0/2958	0.49	1/3998 (0.0%)
1	G	0.35	0/2958	0.49	1/3998 (0.0%)
2	C	0.28	0/1138	0.48	0/1528
2	E	0.28	0/1138	0.48	0/1528
2	F	0.28	0/1138	0.48	0/1528
2	H	0.28	0/1138	0.48	0/1528
All	All	0.33	0/16384	0.49	4/22104 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	559	LEU	C-N-CA	-5.88	106.99	121.70
1	A	559	LEU	C-N-CA	-5.88	107.00	121.70
1	G	559	LEU	C-N-CA	-5.88	107.00	121.70
1	B	559	LEU	C-N-CA	-5.87	107.04	121.70

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	2886	0	2944	542	0
1	B	2886	0	2944	559	0
1	D	2886	0	2944	556	0
1	G	2886	0	2944	540	0
2	C	1126	0	1052	283	0
2	E	1126	0	1052	289	0
2	F	1126	0	1052	280	0
2	H	1126	0	1052	276	0
3	A	22	18	0	2	0
3	B	22	18	0	1	0
3	D	22	18	0	1	0
3	G	22	18	0	1	0
All	All	16136	72	15984	2937	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 91.

The worst 5 of 2937 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:D:358:SER:HB3	2:E:121:GLU:HA	1.25	1.16
2:H:53:ILE:HA	2:H:64:ILE:HD11	1.21	1.16
1:A:347:TYR:HB2	2:F:146:MET:HE3	1.27	1.15
1:B:347:TYR:HB2	2:C:146:MET:HE3	1.23	1.13
2:C:53:ILE:HA	2:C:64:ILE:HD11	1.21	1.13

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	348/656 (53%)	328 (94%)	19 (6%)	1 (0%)	41 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	348/656 (53%)	328 (94%)	19 (6%)	1 (0%)	41	74
1	D	348/656 (53%)	327 (94%)	20 (6%)	1 (0%)	41	74
1	G	348/656 (53%)	328 (94%)	19 (6%)	1 (0%)	41	74
2	C	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
2	E	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
2	F	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
2	H	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
All	All	1956/3220 (61%)	1843 (94%)	109 (6%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	PRO
1	B	561	PRO
1	D	561	PRO
1	G	561	PRO

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	301/558 (54%)	301 (100%)	0	100	100
1	B	301/558 (54%)	301 (100%)	0	100	100
1	D	301/558 (54%)	301 (100%)	0	100	100
1	G	301/558 (54%)	301 (100%)	0	100	100
2	C	122/127 (96%)	122 (100%)	0	100	100
2	E	122/127 (96%)	122 (100%)	0	100	100
2	F	122/127 (96%)	122 (100%)	0	100	100
2	H	122/127 (96%)	122 (100%)	0	100	100
All	All	1692/2740 (62%)	1692 (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. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	78	GLN
2	E	50	GLN
2	H	54	ASN
1	G	350	ASN
2	H	50	GLN

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	$\#\|Z\| > 2$
3	FBX	G	1001	-	23,23,23	4.71	17 (73%)	30,30,30	1.63	5 (16%)
3	FBX	D	1001	-	23,23,23	4.69	17 (73%)	30,30,30	1.62	5 (16%)
3	FBX	B	1001	-	23,23,23	4.72	17 (73%)	30,30,30	1.63	5 (16%)
3	FBX	A	1001	-	23,23,23	4.71	17 (73%)	30,30,30	1.63	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBX	G	1001	-	-	1/12/12/12	0/2/2/2
3	FBX	D	1001	-	-	1/12/12/12	0/2/2/2
3	FBX	B	1001	-	-	1/12/12/12	0/2/2/2
3	FBX	A	1001	-	-	1/12/12/12	0/2/2/2

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	FBX	C12-C10	8.90	1.52	1.40
3	G	1001	FBX	C12-C10	8.88	1.52	1.40
3	A	1001	FBX	C12-C10	8.84	1.52	1.40
3	D	1001	FBX	C12-C10	8.84	1.52	1.40
3	B	1001	FBX	C11-C8	8.13	1.52	1.39

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	FBX	O2-C20-N5	6.05	119.21	109.32
3	G	1001	FBX	O2-C20-N5	6.03	119.18	109.32
3	D	1001	FBX	O2-C20-N5	6.03	119.17	109.32
3	A	1001	FBX	O2-C20-N5	6.02	119.16	109.32
3	B	1001	FBX	O3-C20-N5	-2.74	120.14	126.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	FBX	O2-C20-N5-C10
3	D	1001	FBX	O2-C20-N5-C10
3	G	1001	FBX	O2-C20-N5-C10
3	A	1001	FBX	O2-C20-N5-C10

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1001	FBX	1	0

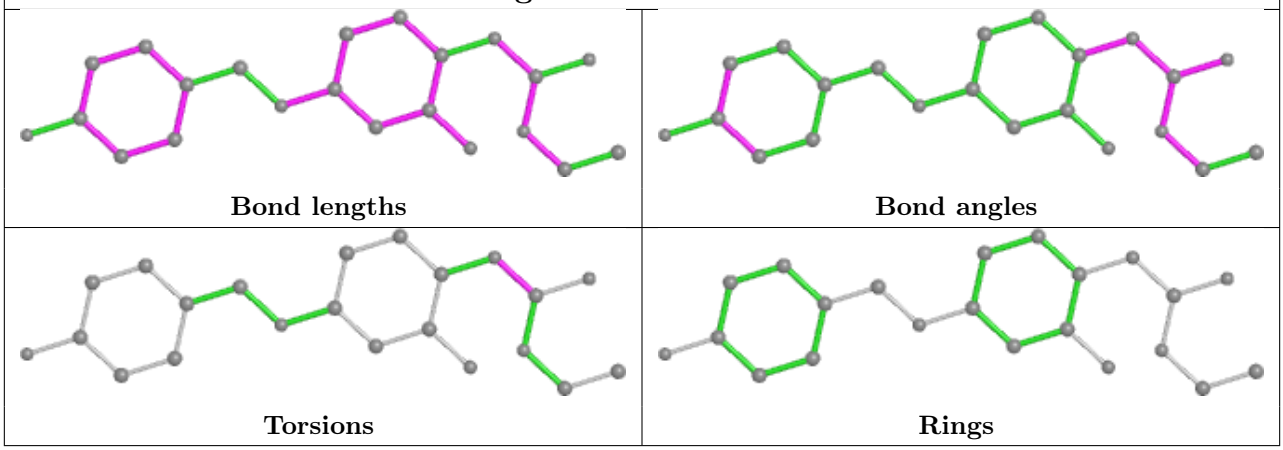
Continued on next page...

Continued from previous page...

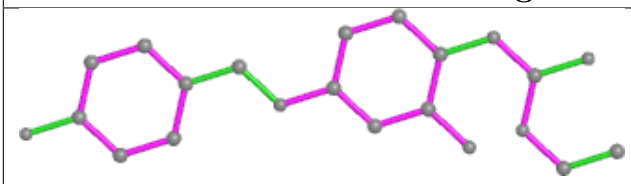
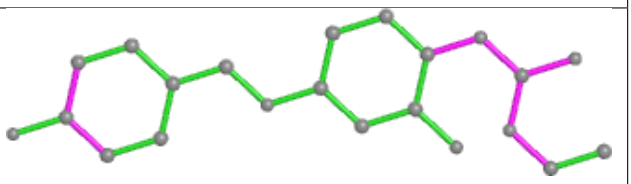
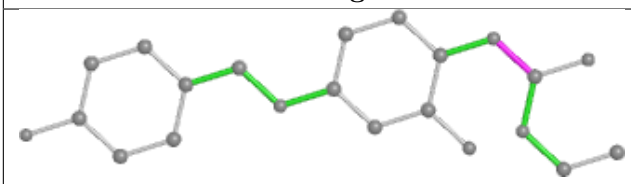
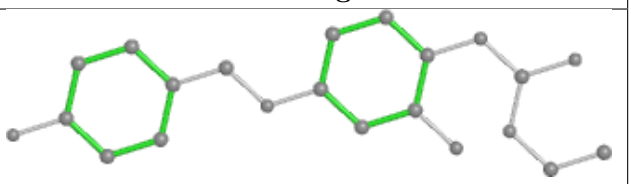
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1001	FBX	1	0
3	B	1001	FBX	1	0
3	A	1001	FBX	2	0

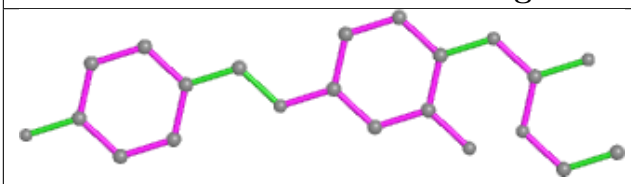
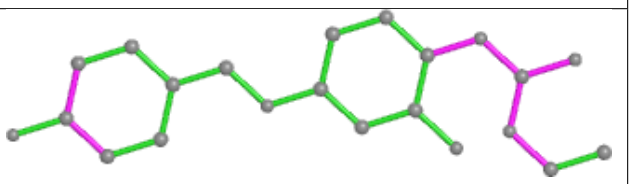
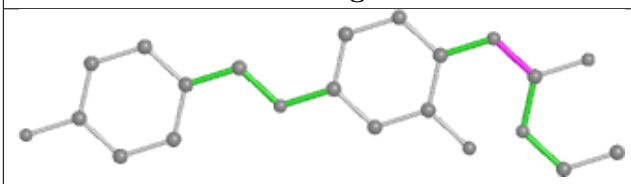
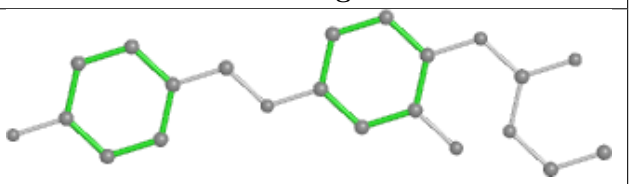
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand FBX G 1001



Ligand FBX D 1001

Ligand FBX B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FBX A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

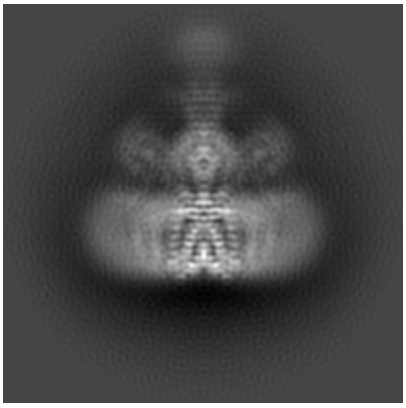
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30448. These allow visual inspection of the internal detail of the map and identification of artifacts.

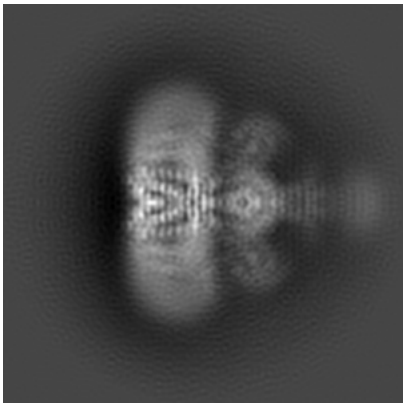
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

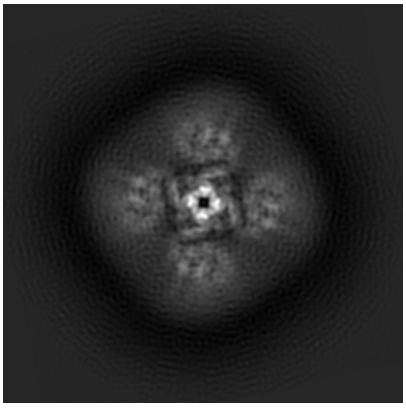
6.1.1 Primary map



X



Y

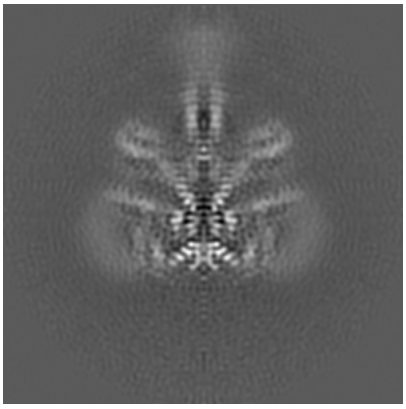


Z

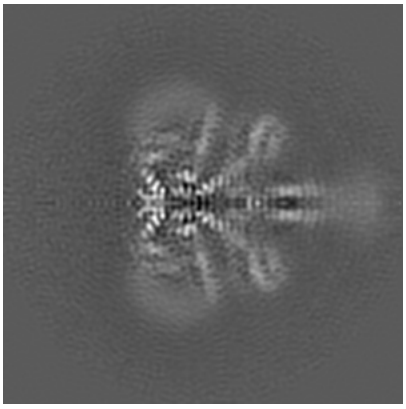
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

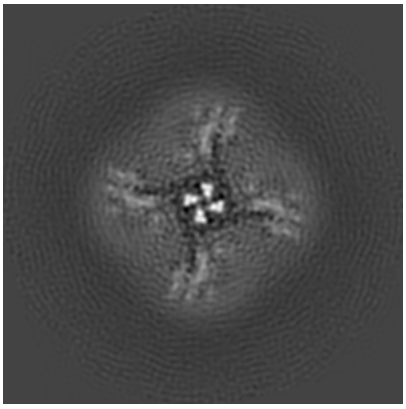
6.2.1 Primary map



X Index: 120



Y Index: 120

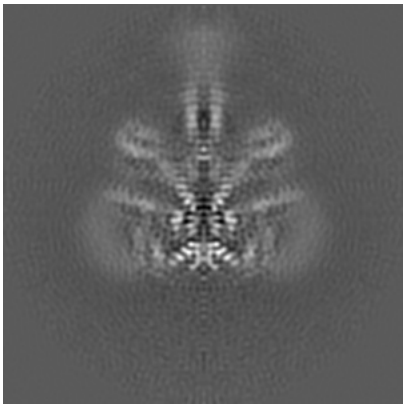


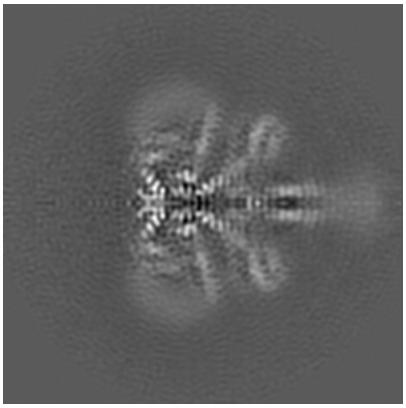
Z Index: 120

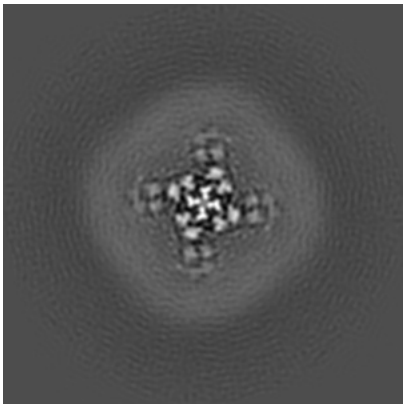
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 120

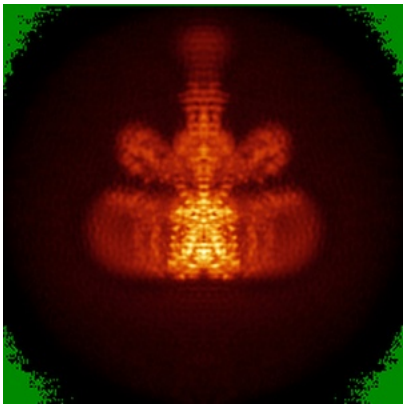

Y Index: 120

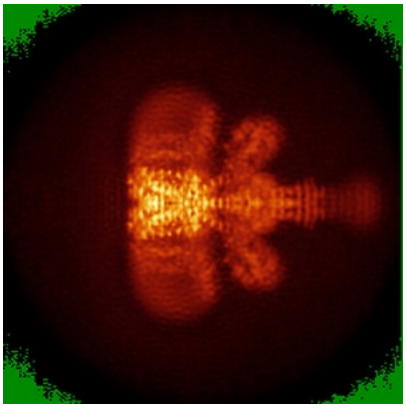

Z Index: 95

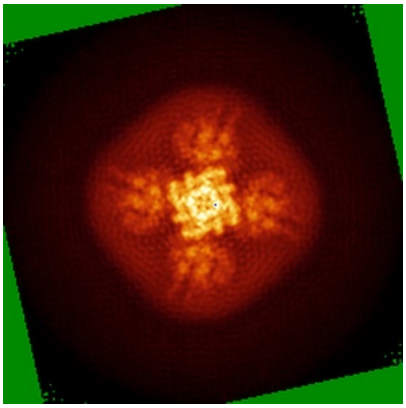
The images above show the largest variance slices of the map in three orthogonal directions.

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

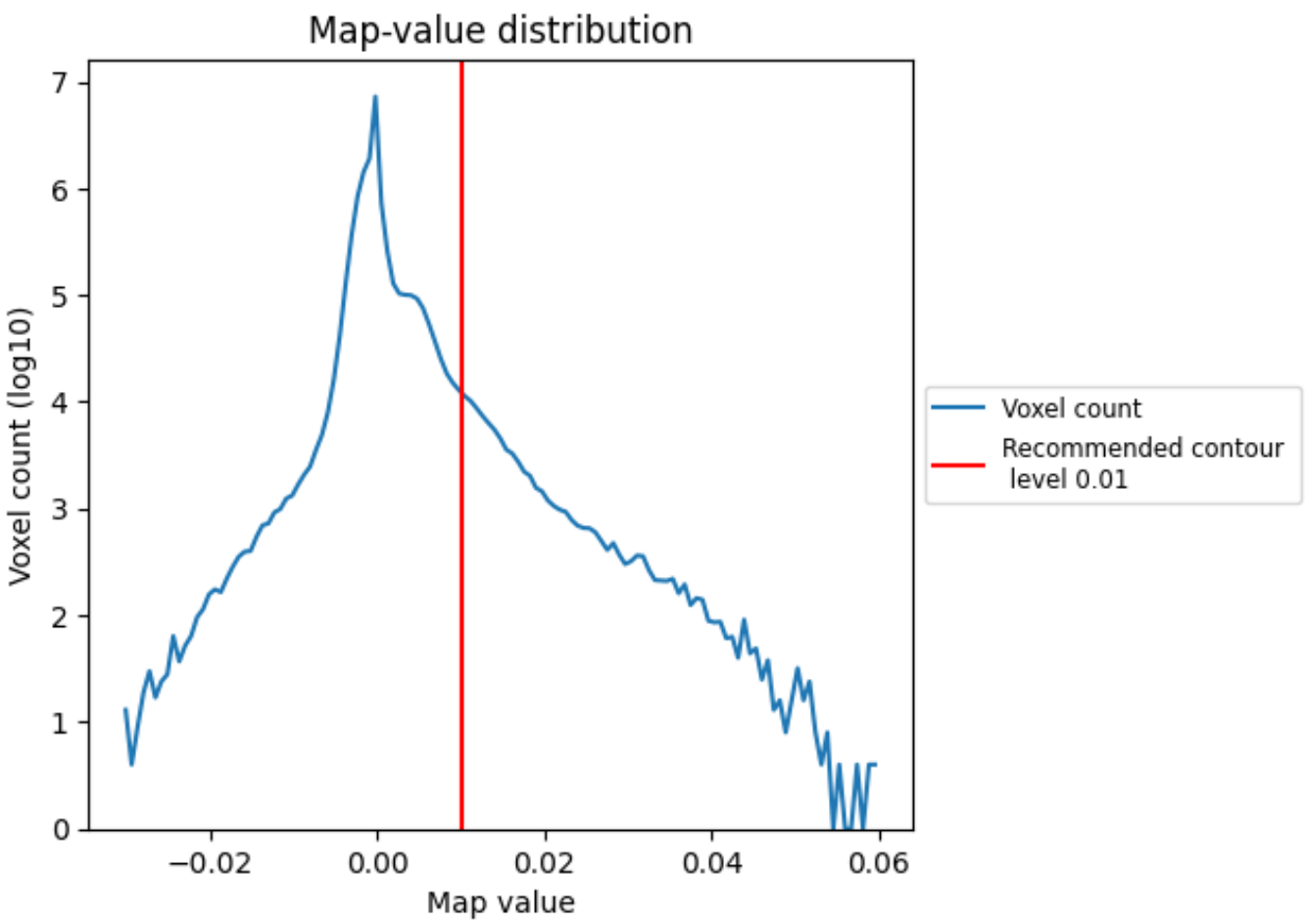
6.6 Mask visualisation (i)

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

7 Map analysis (i)

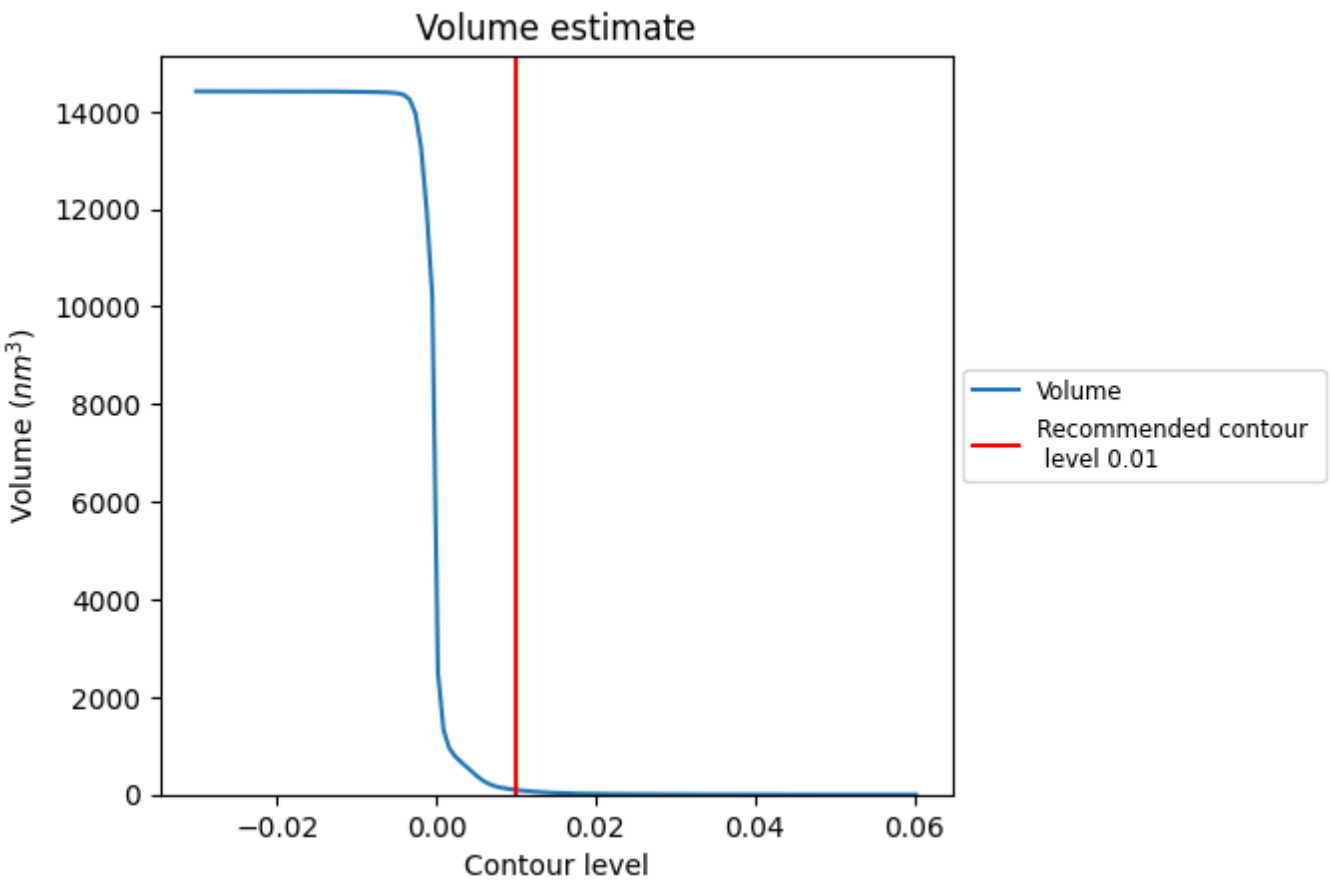
This section contains the results of statistical analysis of the map.

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.

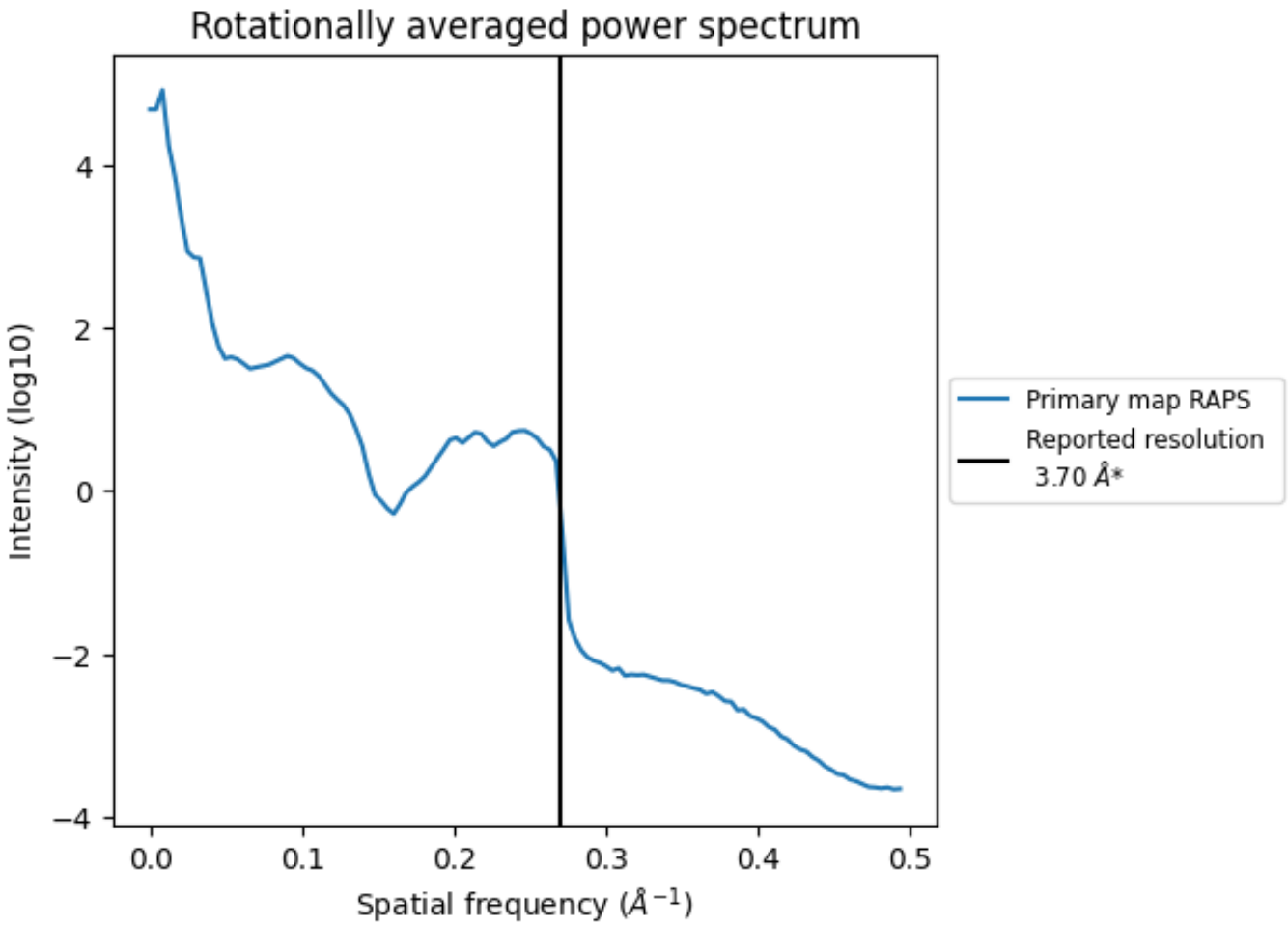
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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 0.270 Å^{-1}

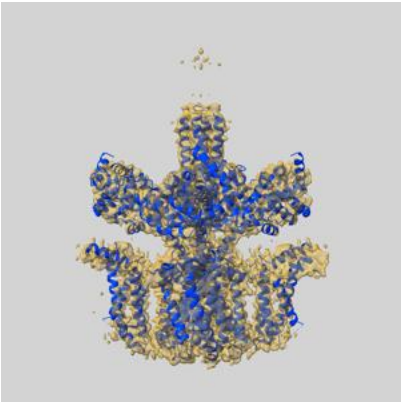
8 Fourier-Shell correlation (i)

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

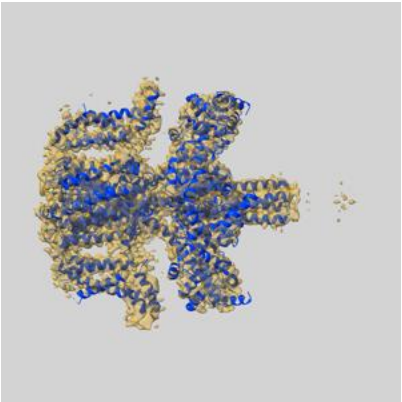
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30448 and PDB model 7CR7. Per-residue inclusion information can be found in section 3 on page 7.

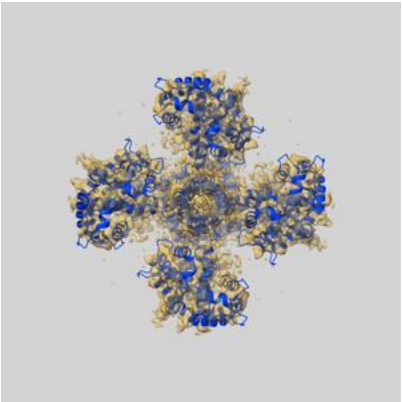
9.1 Map-model overlay (i)



X



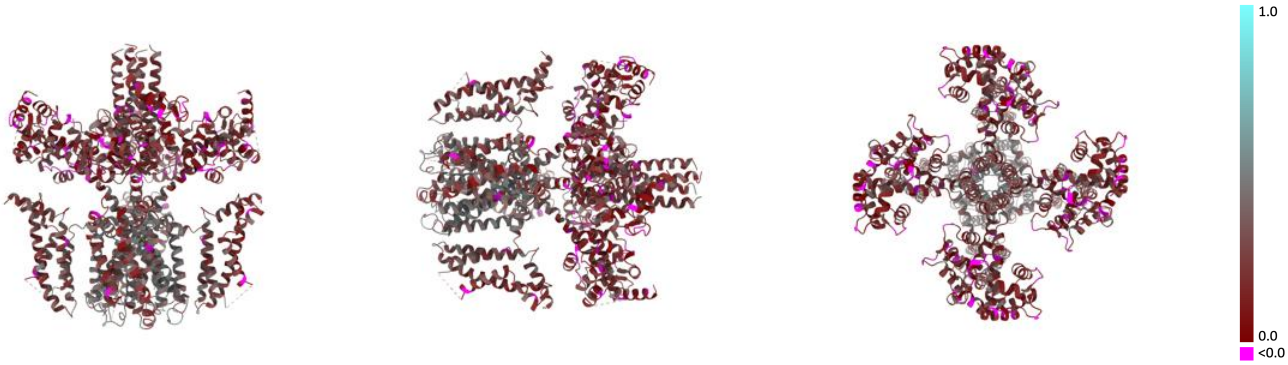
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

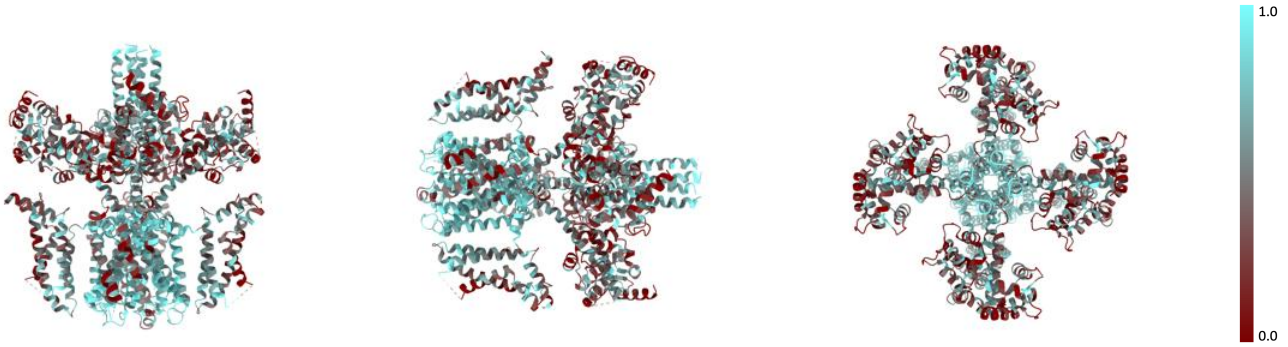
9.2 Q-score mapped to coordinate model (i)



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.

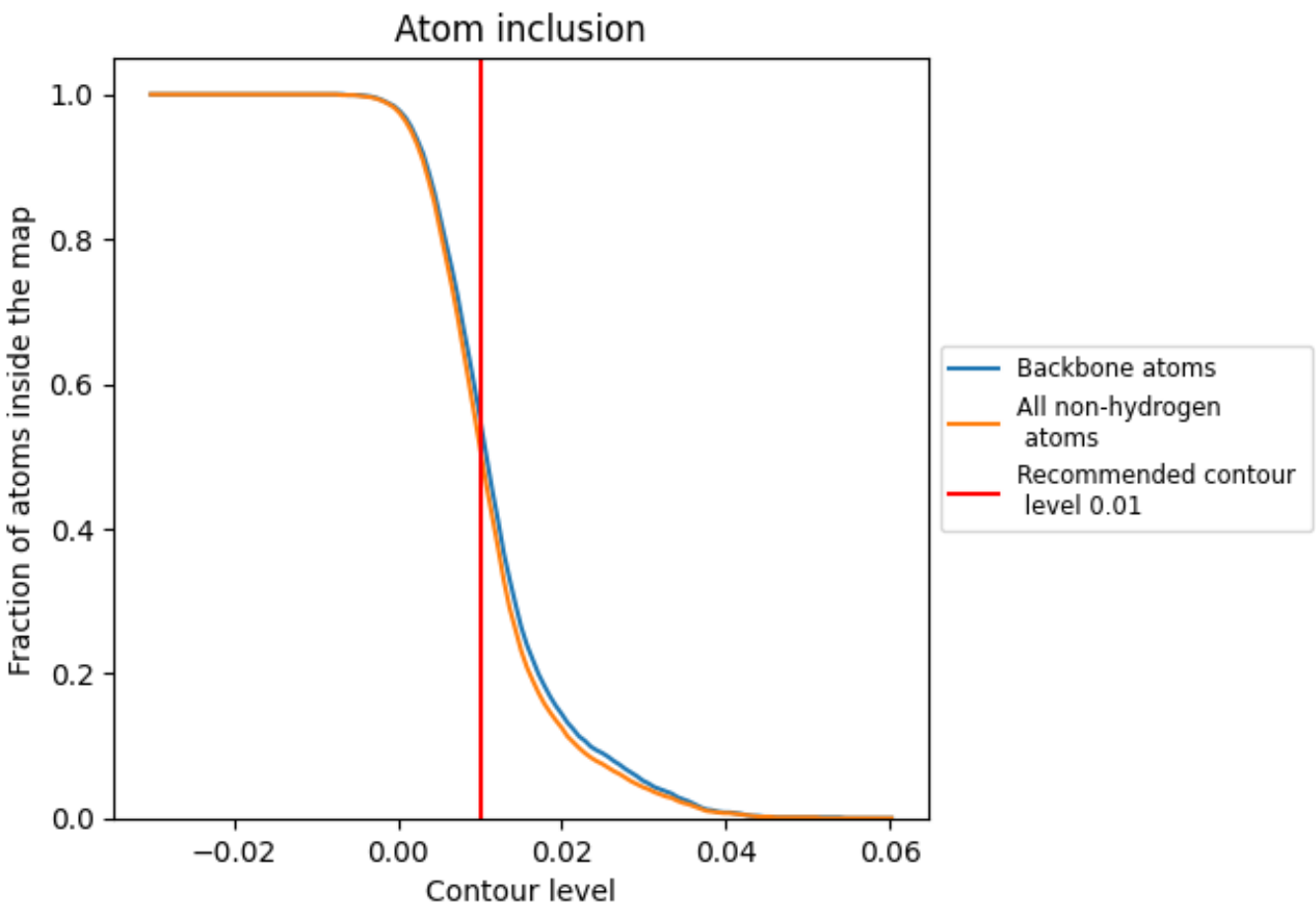
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 51% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5140	0.2680
A	0.6100	0.3050
B	0.6060	0.3050
C	0.3000	0.1700
D	0.6060	0.3050
E	0.3070	0.1740
F	0.2960	0.1710
G	0.6060	0.3060
H	0.2940	0.1700