



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 02:18 PM JST

PDB ID : 7D7E
EMDB ID : EMD-30606
Title : Structure of PKD1L3-CTD/PKD2L1 in apo state
Authors : Su, Q.; Chen, M.; Li, B.; Wang, Y.; Jing, D.; Zhan, X.; Yu, Y.; Shi, Y.
Deposited on : 2020-10-03
Resolution : 3.40 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

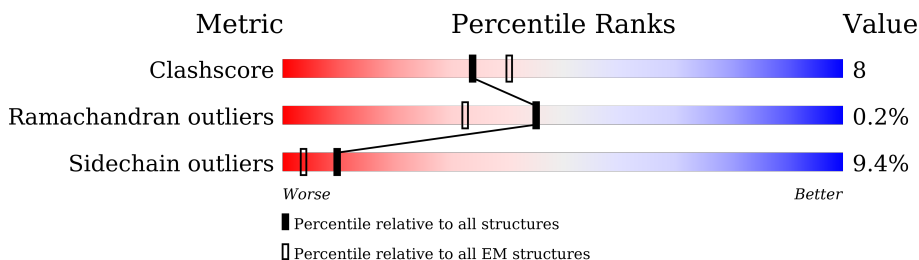
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	B	604	
1	C	604	
1	D	604	
2	A	551	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15501 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 Polycystic kidney disease 2-like 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	482	Total	C	N	O	S	0	0
			3960	2610	630	704	16		
1	C	474	Total	C	N	O	S	0	0
			3898	2572	619	691	16		
1	D	471	Total	C	N	O	S	0	0
			3862	2549	610	687	16		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MET	-	initiating methionine	UNP A2A259
B	27	GLY	-	expression tag	UNP A2A259
B	28	SER	-	expression tag	UNP A2A259
B	29	ALA	-	expression tag	UNP A2A259
B	30	GLY	-	expression tag	UNP A2A259
B	31	TRP	-	expression tag	UNP A2A259
B	32	SER	-	expression tag	UNP A2A259
B	33	HIS	-	expression tag	UNP A2A259
B	34	PRO	-	expression tag	UNP A2A259
B	35	GLN	-	expression tag	UNP A2A259
B	36	PHE	-	expression tag	UNP A2A259
B	37	GLU	-	expression tag	UNP A2A259
B	38	LYS	-	expression tag	UNP A2A259
B	39	GLY	-	expression tag	UNP A2A259
B	40	GLY	-	expression tag	UNP A2A259
B	41	GLY	-	expression tag	UNP A2A259
B	42	SER	-	expression tag	UNP A2A259
B	43	GLY	-	expression tag	UNP A2A259
B	44	GLY	-	expression tag	UNP A2A259
B	45	GLY	-	expression tag	UNP A2A259
B	46	SER	-	expression tag	UNP A2A259
B	47	GLY	-	expression tag	UNP A2A259
B	48	GLY	-	expression tag	UNP A2A259
B	49	SER	-	expression tag	UNP A2A259

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Chain	Residue	Modelled	Actual	Comment	Reference
B	50	ALA	-	expression tag	UNP A2A259
B	51	TRP	-	expression tag	UNP A2A259
B	52	SER	-	expression tag	UNP A2A259
B	53	HIS	-	expression tag	UNP A2A259
B	54	PRO	-	expression tag	UNP A2A259
B	55	GLN	-	expression tag	UNP A2A259
B	56	PHE	-	expression tag	UNP A2A259
B	57	GLU	-	expression tag	UNP A2A259
B	58	LYS	-	expression tag	UNP A2A259
B	59	GLY	-	expression tag	UNP A2A259
B	60	SER	-	expression tag	UNP A2A259
B	61	ALA	-	expression tag	UNP A2A259
B	62	ALA	-	expression tag	UNP A2A259
B	63	ALA	-	expression tag	UNP A2A259
C	26	MET	-	initiating methionine	UNP A2A259
C	27	GLY	-	expression tag	UNP A2A259
C	28	SER	-	expression tag	UNP A2A259
C	29	ALA	-	expression tag	UNP A2A259
C	30	GLY	-	expression tag	UNP A2A259
C	31	TRP	-	expression tag	UNP A2A259
C	32	SER	-	expression tag	UNP A2A259
C	33	HIS	-	expression tag	UNP A2A259
C	34	PRO	-	expression tag	UNP A2A259
C	35	GLN	-	expression tag	UNP A2A259
C	36	PHE	-	expression tag	UNP A2A259
C	37	GLU	-	expression tag	UNP A2A259
C	38	LYS	-	expression tag	UNP A2A259
C	39	GLY	-	expression tag	UNP A2A259
C	40	GLY	-	expression tag	UNP A2A259
C	41	GLY	-	expression tag	UNP A2A259
C	42	SER	-	expression tag	UNP A2A259
C	43	GLY	-	expression tag	UNP A2A259
C	44	GLY	-	expression tag	UNP A2A259
C	45	GLY	-	expression tag	UNP A2A259
C	46	SER	-	expression tag	UNP A2A259
C	47	GLY	-	expression tag	UNP A2A259
C	48	GLY	-	expression tag	UNP A2A259
C	49	SER	-	expression tag	UNP A2A259
C	50	ALA	-	expression tag	UNP A2A259
C	51	TRP	-	expression tag	UNP A2A259
C	52	SER	-	expression tag	UNP A2A259
C	53	HIS	-	expression tag	UNP A2A259

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Chain	Residue	Modelled	Actual	Comment	Reference
C	54	PRO	-	expression tag	UNP A2A259
C	55	GLN	-	expression tag	UNP A2A259
C	56	PHE	-	expression tag	UNP A2A259
C	57	GLU	-	expression tag	UNP A2A259
C	58	LYS	-	expression tag	UNP A2A259
C	59	GLY	-	expression tag	UNP A2A259
C	60	SER	-	expression tag	UNP A2A259
C	61	ALA	-	expression tag	UNP A2A259
C	62	ALA	-	expression tag	UNP A2A259
C	63	ALA	-	expression tag	UNP A2A259
D	26	MET	-	initiating methionine	UNP A2A259
D	27	GLY	-	expression tag	UNP A2A259
D	28	SER	-	expression tag	UNP A2A259
D	29	ALA	-	expression tag	UNP A2A259
D	30	GLY	-	expression tag	UNP A2A259
D	31	TRP	-	expression tag	UNP A2A259
D	32	SER	-	expression tag	UNP A2A259
D	33	HIS	-	expression tag	UNP A2A259
D	34	PRO	-	expression tag	UNP A2A259
D	35	GLN	-	expression tag	UNP A2A259
D	36	PHE	-	expression tag	UNP A2A259
D	37	GLU	-	expression tag	UNP A2A259
D	38	LYS	-	expression tag	UNP A2A259
D	39	GLY	-	expression tag	UNP A2A259
D	40	GLY	-	expression tag	UNP A2A259
D	41	GLY	-	expression tag	UNP A2A259
D	42	SER	-	expression tag	UNP A2A259
D	43	GLY	-	expression tag	UNP A2A259
D	44	GLY	-	expression tag	UNP A2A259
D	45	GLY	-	expression tag	UNP A2A259
D	46	SER	-	expression tag	UNP A2A259
D	47	GLY	-	expression tag	UNP A2A259
D	48	GLY	-	expression tag	UNP A2A259
D	49	SER	-	expression tag	UNP A2A259
D	50	ALA	-	expression tag	UNP A2A259
D	51	TRP	-	expression tag	UNP A2A259
D	52	SER	-	expression tag	UNP A2A259
D	53	HIS	-	expression tag	UNP A2A259
D	54	PRO	-	expression tag	UNP A2A259
D	55	GLN	-	expression tag	UNP A2A259
D	56	PHE	-	expression tag	UNP A2A259
D	57	GLU	-	expression tag	UNP A2A259

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Chain	Residue	Modelled	Actual	Comment	Reference
D	58	LYS	-	expression tag	UNP A2A259
D	59	GLY	-	expression tag	UNP A2A259
D	60	SER	-	expression tag	UNP A2A259
D	61	ALA	-	expression tag	UNP A2A259
D	62	ALA	-	expression tag	UNP A2A259
D	63	ALA	-	expression tag	UNP A2A259

- Molecule 2 is a protein called Polycystic kidney disease protein 1-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	451	Total	C	N	O	S	0	0
			3638	2375	620	631	12		

There are 32 discrepancies between the modelled and reference sequences:

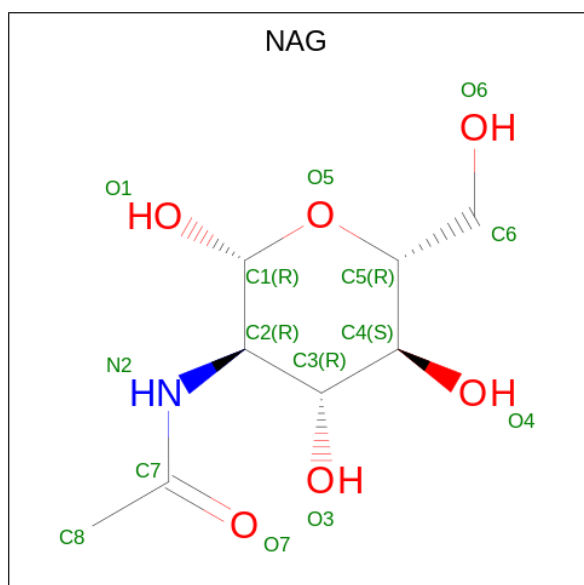
Chain	Residue	Modelled	Actual	Comment	Reference
A	1600	MET	-	initiating methionine	UNP Q2EG98
A	1601	GLY	-	expression tag	UNP Q2EG98
A	1602	SER	-	expression tag	UNP Q2EG98
A	1603	ALA	-	expression tag	UNP Q2EG98
A	1604	GLY	-	expression tag	UNP Q2EG98
A	1605	ASP	-	expression tag	UNP Q2EG98
A	1606	TYR	-	expression tag	UNP Q2EG98
A	1607	LYS	-	expression tag	UNP Q2EG98
A	1608	ASP	-	expression tag	UNP Q2EG98
A	1609	HIS	-	expression tag	UNP Q2EG98
A	1610	ASP	-	expression tag	UNP Q2EG98
A	1611	GLY	-	expression tag	UNP Q2EG98
A	1612	ASP	-	expression tag	UNP Q2EG98
A	1613	TYR	-	expression tag	UNP Q2EG98
A	1614	LYS	-	expression tag	UNP Q2EG98
A	1615	ASP	-	expression tag	UNP Q2EG98
A	1616	HIS	-	expression tag	UNP Q2EG98
A	1617	ASP	-	expression tag	UNP Q2EG98
A	1618	ILE	-	expression tag	UNP Q2EG98
A	1619	ASP	-	expression tag	UNP Q2EG98
A	1620	TYR	-	expression tag	UNP Q2EG98
A	1621	LYS	-	expression tag	UNP Q2EG98
A	1622	ASP	-	expression tag	UNP Q2EG98
A	1623	ASP	-	expression tag	UNP Q2EG98
A	1624	ASP	-	expression tag	UNP Q2EG98
A	1625	ASP	-	expression tag	UNP Q2EG98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1626	LYS	-	expression tag	UNP Q2EG98
A	1627	GLY	-	expression tag	UNP Q2EG98
A	1628	SER	-	expression tag	UNP Q2EG98
A	1629	ALA	-	expression tag	UNP Q2EG98
A	1630	ALA	-	expression tag	UNP Q2EG98
A	1631	ALA	-	expression tag	UNP Q2EG98

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

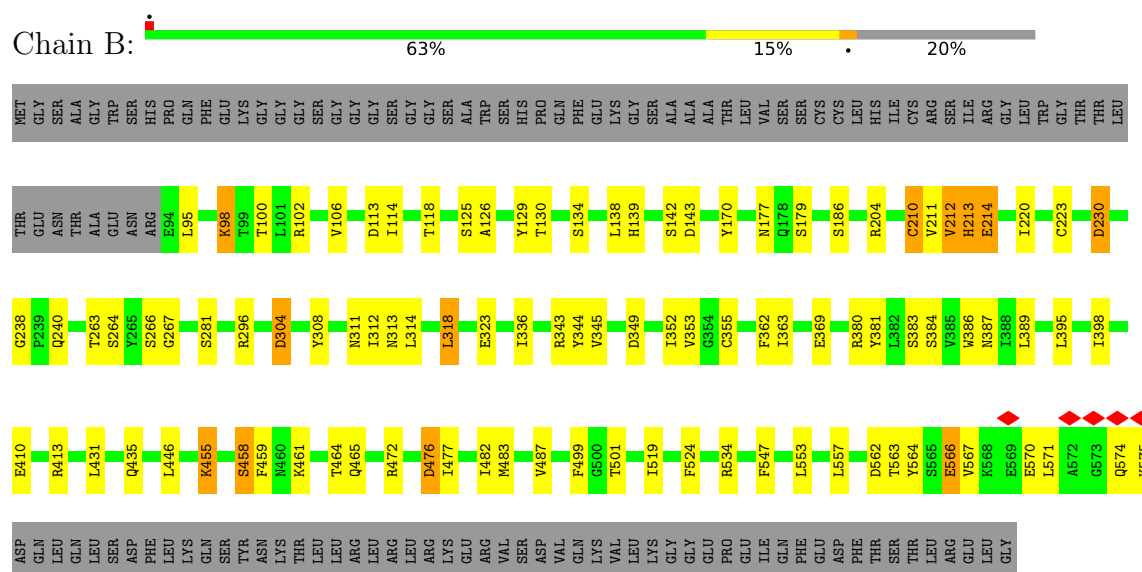
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

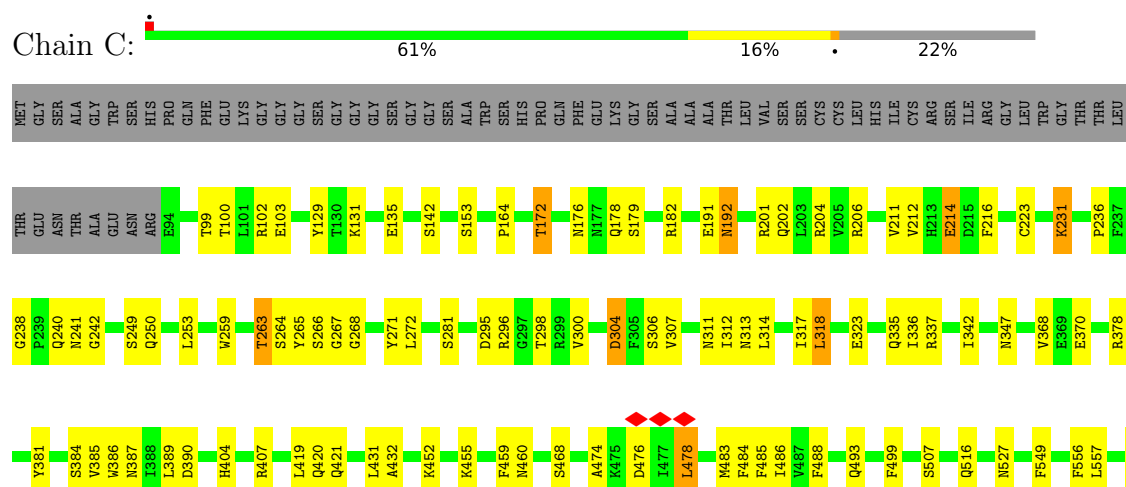
3 Residue-property plots

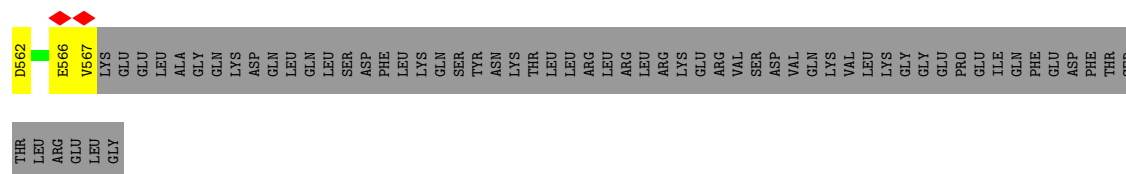
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Polycystic kidney disease 2-like 1 protein

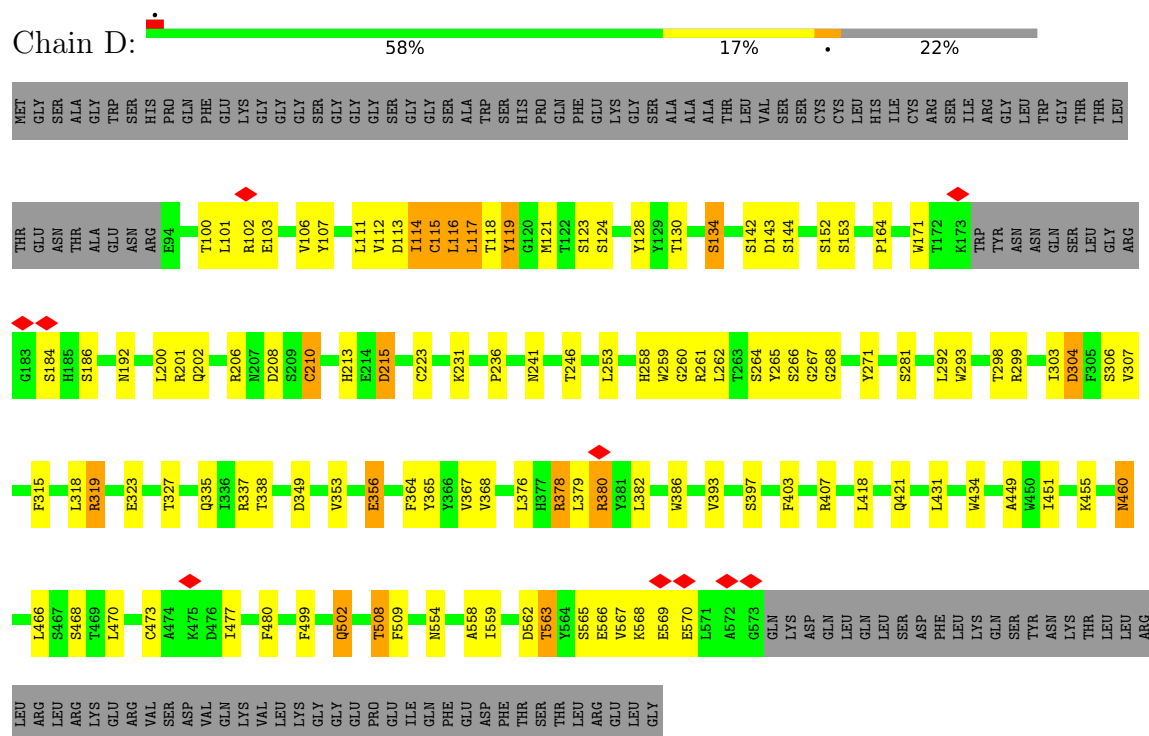


- Molecule 1: Polycystic kidney disease 2-like 1 protein

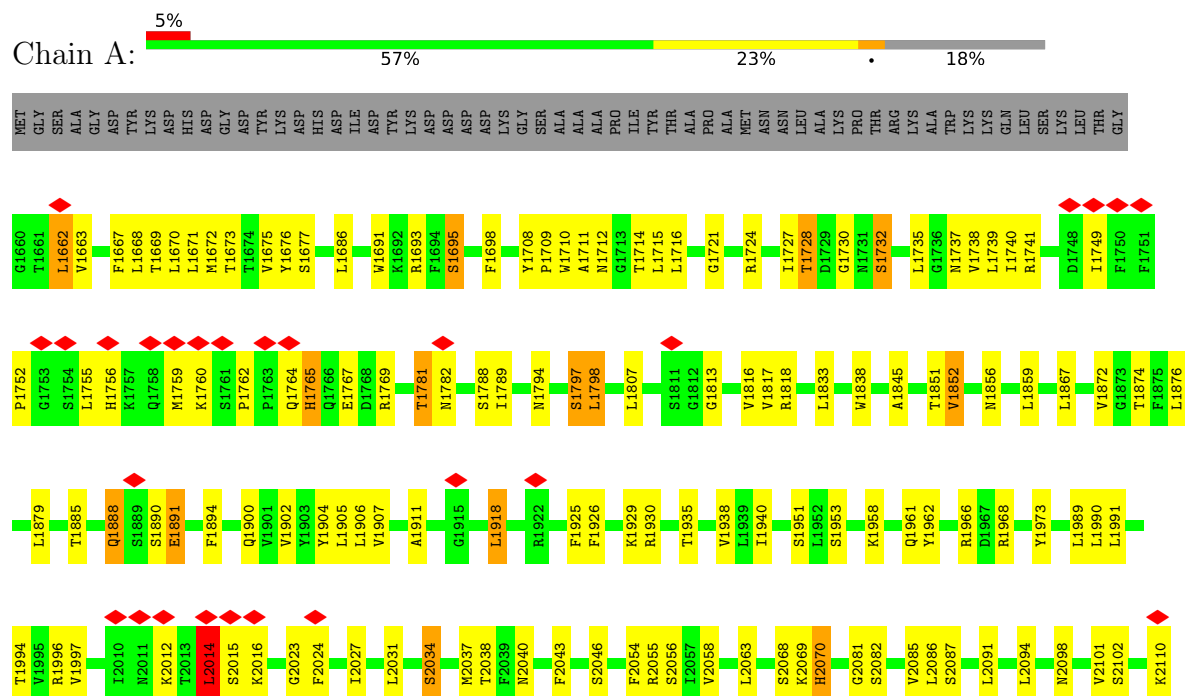




• Molecule 1: Polycystic kidney disease 2-like 1 protein



• Molecule 2: Polycystic kidney disease protein 1-like 3



GLU	ARG	LYS	ALA	CYS	GLU	LYS	GLU	ALA	THR	LEU	THR	ASP	MET	LEU	LEU	GLN	LYS	LEU	SER	SER	LEU	LEU	GLY	ILE	ARG	LEU	HIS	GLN	ASN	PRO	SER	GLU	GLU	HIS	ALA	ASP	ASN	THR	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	549716	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.43	0/4073	0.48	0/5540
1	C	0.44	0/4011	0.47	0/5459
1	D	0.40	0/3971	0.46	0/5401
2	A	0.36	0/3727	0.49	1/5056 (0.0%)
All	All	0.41	0/15782	0.48	1/21456 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2014	LEU	CA-CB-CG	5.89	128.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	HIS	Peptide

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	B	3960	0	3864	56	0
1	C	3898	0	3799	56	0
1	D	3862	0	3774	70	0
2	A	3638	0	3696	89	0
3	A	28	0	26	0	0
3	B	42	0	39	2	0
3	C	42	0	39	1	0
3	D	28	0	26	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	15501	0	15263	245	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 8.

The worst 5 of 245 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:128:TYR:CZ	2:A:1876:LEU:HD21	1.83	1.12
1:C:474:ALA:O	1:C:478:LEU:HB2	1.65	0.95
2:A:1888:GLN:HB2	2:A:1891:GLU:HG2	1.61	0.82
1:B:212:VAL:O	1:B:213:HIS:ND1	2.13	0.81
1:D:119:TYR:OH	2:A:2040:ASN:ND2	2.13	0.81

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	B	480/604 (80%)	442 (92%)	37 (8%)	1 (0%)	44	72
1	C	472/604 (78%)	436 (92%)	35 (7%)	1 (0%)	44	72
1	D	467/604 (77%)	427 (91%)	40 (9%)	0	100	100
2	A	449/551 (82%)	395 (88%)	52 (12%)	2 (0%)	30	60
All	All	1868/2363 (79%)	1700 (91%)	164 (9%)	4 (0%)	45	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1721	GLY
2	A	1727	ILE
1	B	214	GLU
1	C	385	VAL

5.3.2 Protein sidechains ⓘ

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	B	430/530 (81%)	399 (93%)	31 (7%)	12	37
1	C	424/530 (80%)	389 (92%)	35 (8%)	9	30
1	D	420/530 (79%)	372 (89%)	48 (11%)	4	17
2	A	400/482 (83%)	357 (89%)	43 (11%)	5	20
All	All	1674/2072 (81%)	1517 (91%)	157 (9%)	10	25

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1677	SER
2	A	1991	LEU
2	A	1732	SER
2	A	1879	LEU

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Mol	Chain	Res	Type
2	A	2056	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1823	HIS
2	A	1856	ASN
2	A	1961	GLN
1	C	258	HIS
1	C	222	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 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
3	NAG	A	2501	2	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	B	703	1	14,14,15	0.45	0	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	703	1	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	C	701	1	14,14,15	0.37	0	17,19,21	1.26	1 (5%)
3	NAG	D	802	1	14,14,15	0.45	0	17,19,21	1.22	1 (5%)
3	NAG	D	801	1	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	A	2500	2	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	C	702	1	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	B	701	1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	B	702	1	14,14,15	0.22	0	17,19,21	0.39	0

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	NAG	A	2501	2	-	2/6/23/26	0/1/1/1
3	NAG	B	703	1	-	4/6/23/26	0/1/1/1
3	NAG	C	703	1	-	2/6/23/26	0/1/1/1
3	NAG	C	701	1	-	3/6/23/26	0/1/1/1
3	NAG	D	802	1	-	3/6/23/26	0/1/1/1
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2500	2	-	2/6/23/26	0/1/1/1
3	NAG	C	702	1	-	3/6/23/26	0/1/1/1
3	NAG	B	701	1	-	4/6/23/26	0/1/1/1
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	NAG	C2-N2-C7	4.33	129.07	122.90
3	D	802	NAG	C2-N2-C7	4.29	129.01	122.90
3	B	703	NAG	C2-N2-C7	4.28	129.00	122.90
3	B	703	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NAG	C4-C5-C6-O6
3	A	2501	NAG	O5-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
3	C	702	NAG	C4-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	NAG	1	0
3	C	701	NAG	1	0
3	D	802	NAG	1	0
3	B	701	NAG	1	0

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.

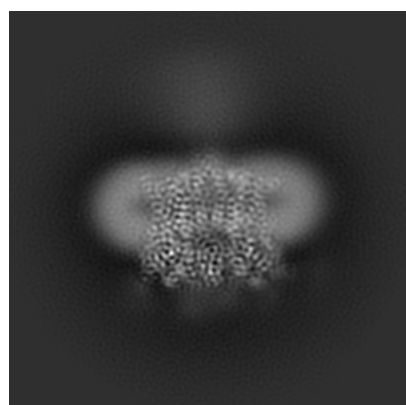
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30606. These allow visual inspection of the internal detail of the map and identification of artifacts.

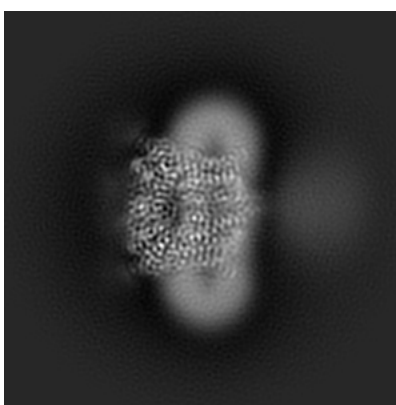
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

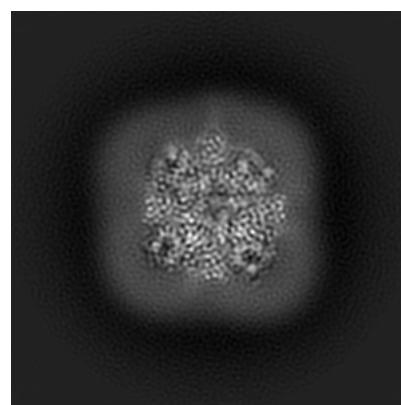
6.1.1 Primary map



X



Y

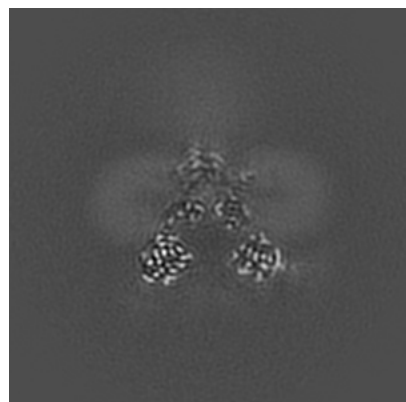


Z

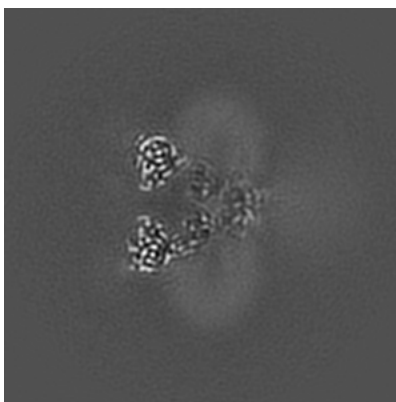
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

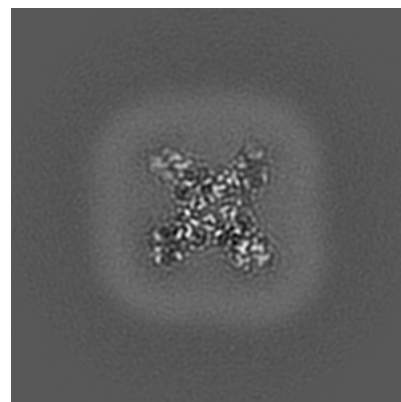
6.2.1 Primary map



X Index: 120



Y Index: 120

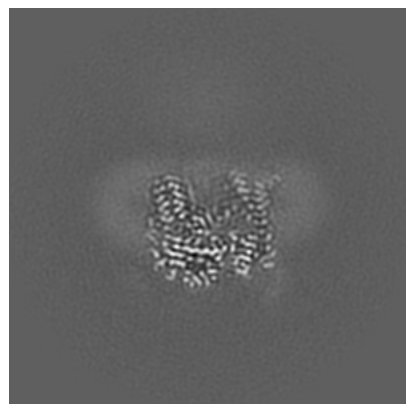


Z Index: 120

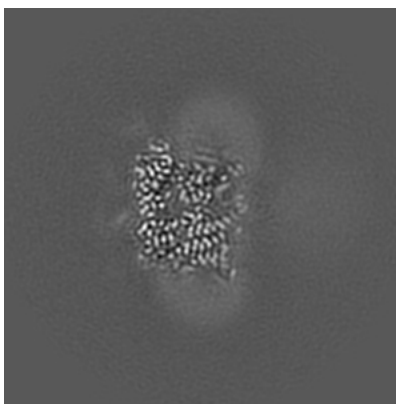
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

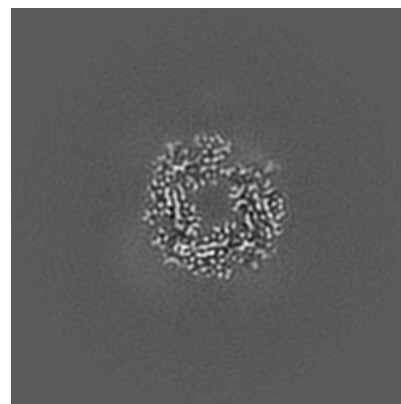
6.3.1 Primary map



X Index: 99



Y Index: 103

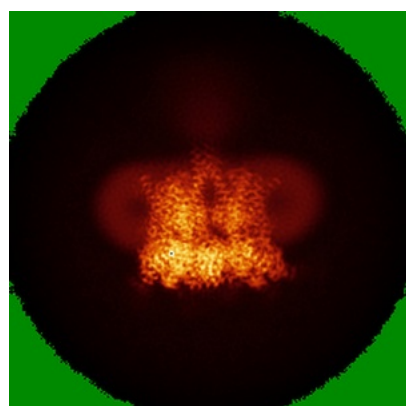


Z Index: 93

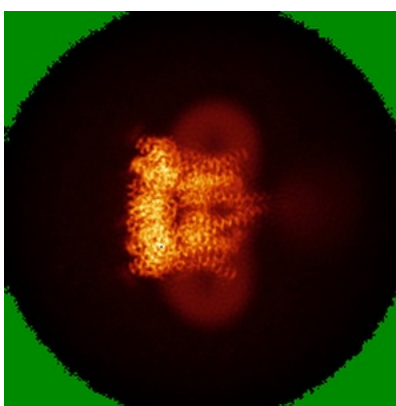
The images above show the largest variance slices of the map in three orthogonal directions.

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

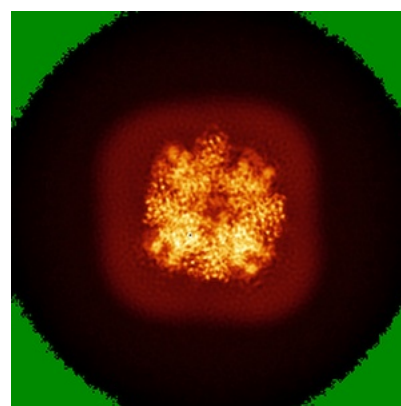
6.4.1 Primary map



X



Y

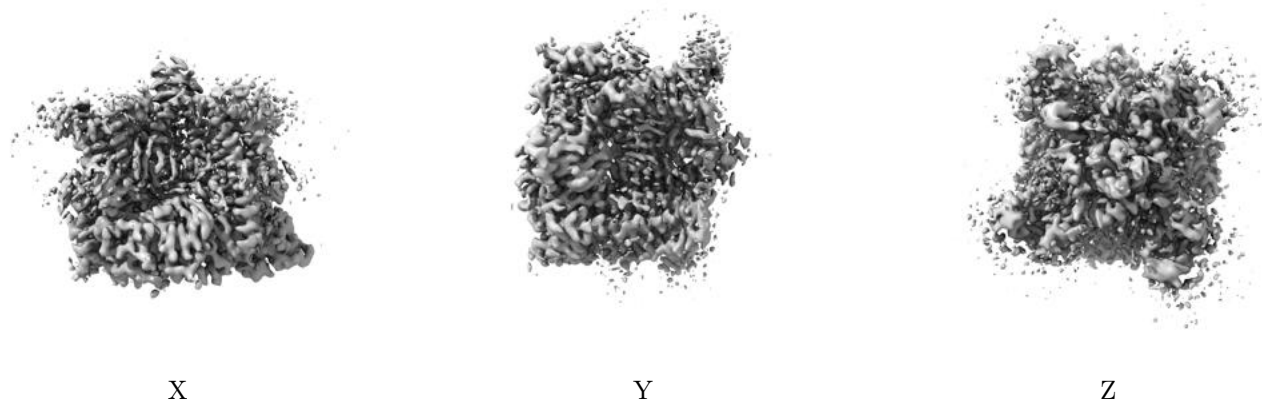


Z

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

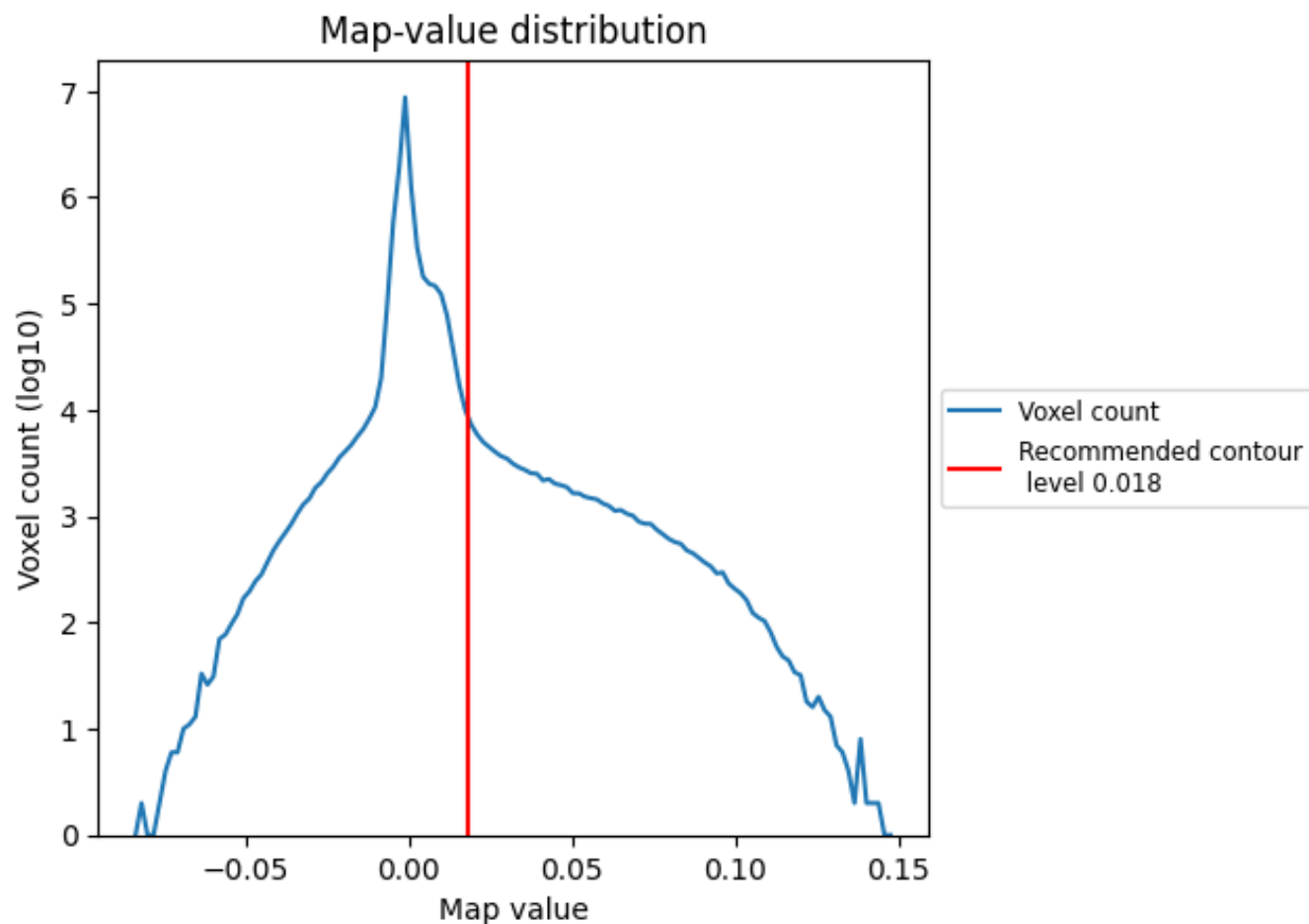
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

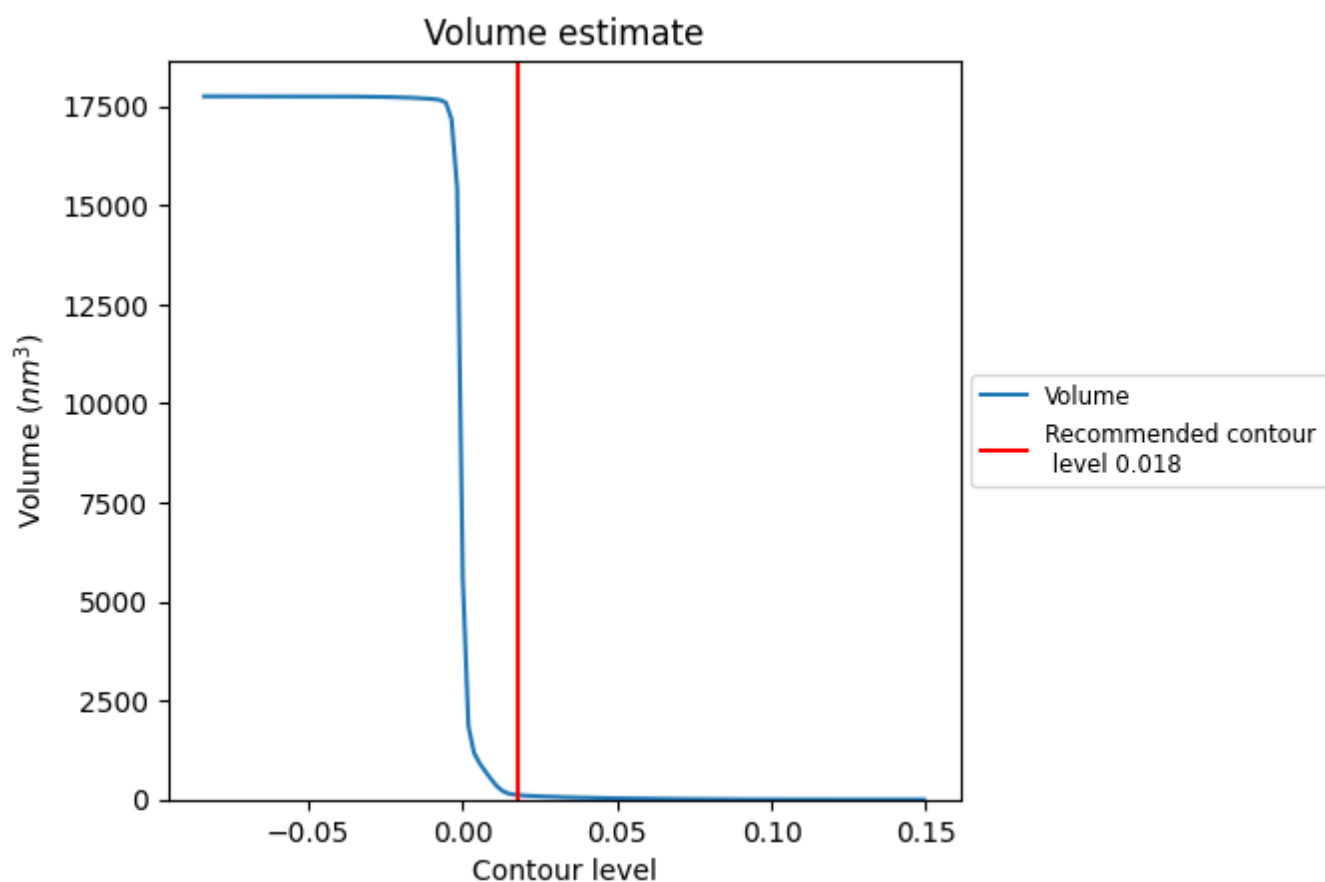
This section contains the results of statistical analysis of the map.

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.

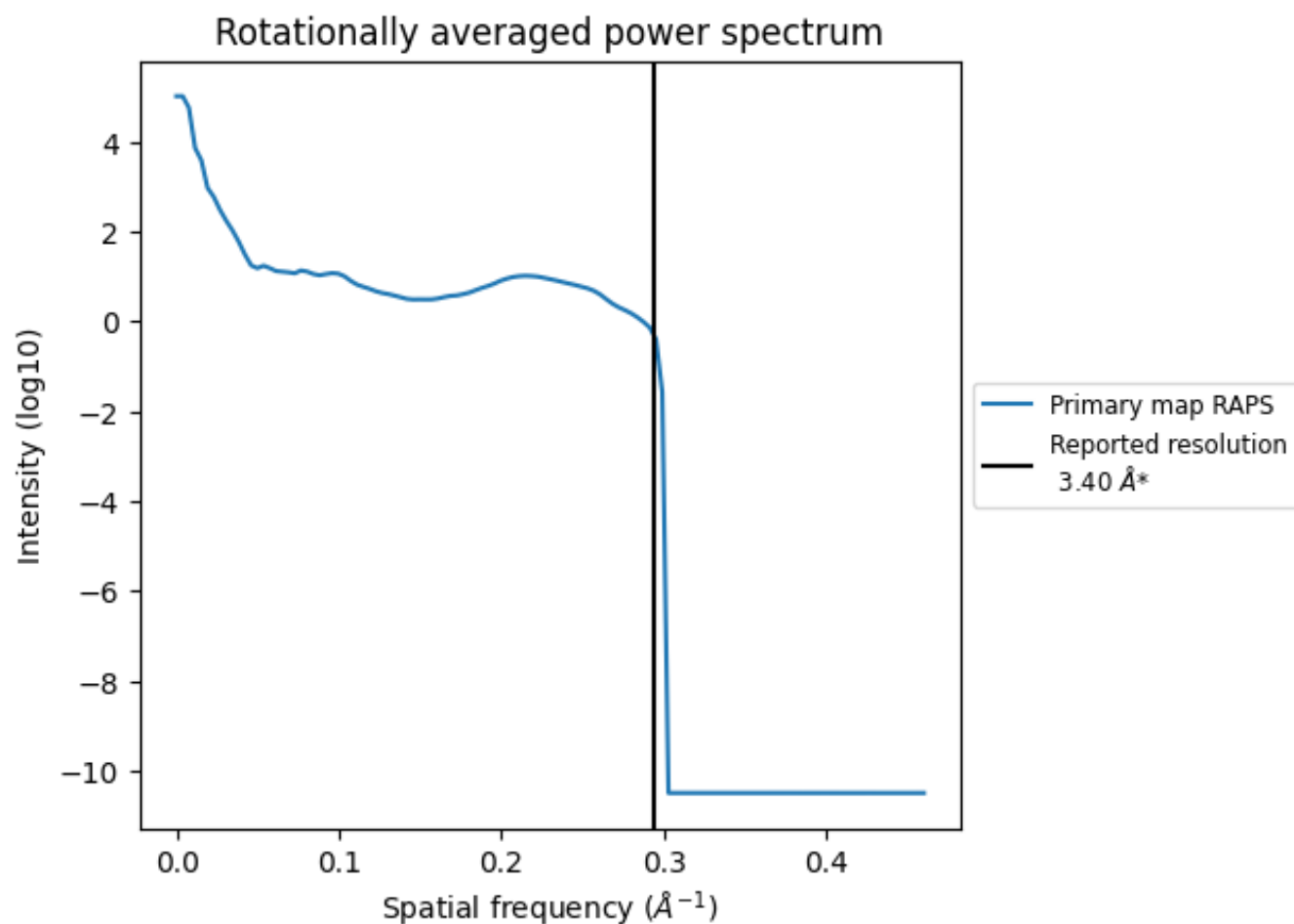
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

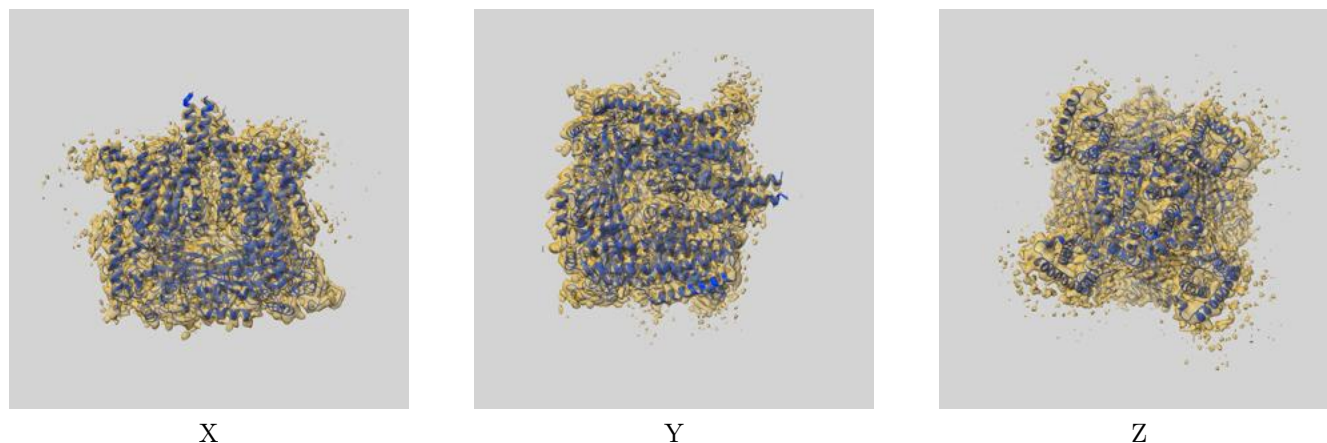
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

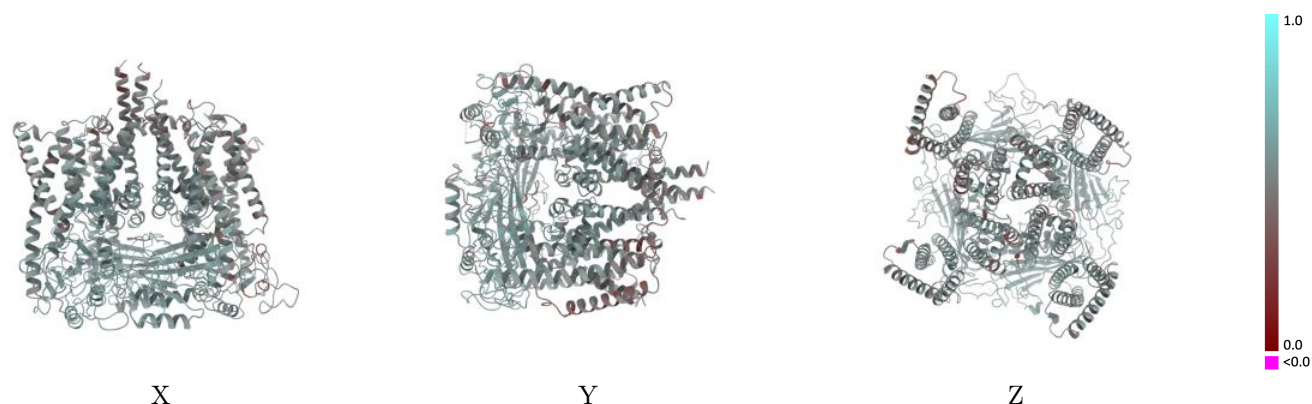
This section contains information regarding the fit between EMDB map EMD-30606 and PDB model 7D7E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



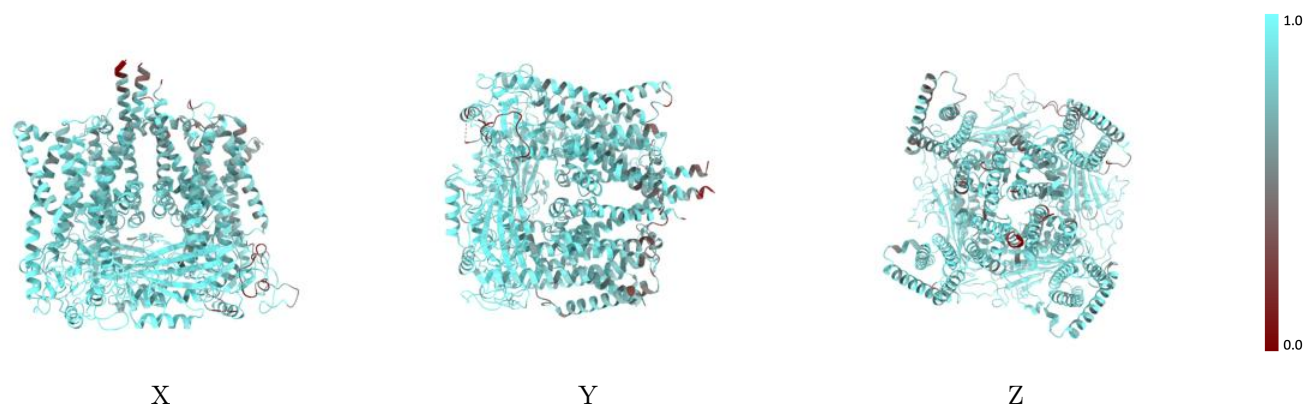
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



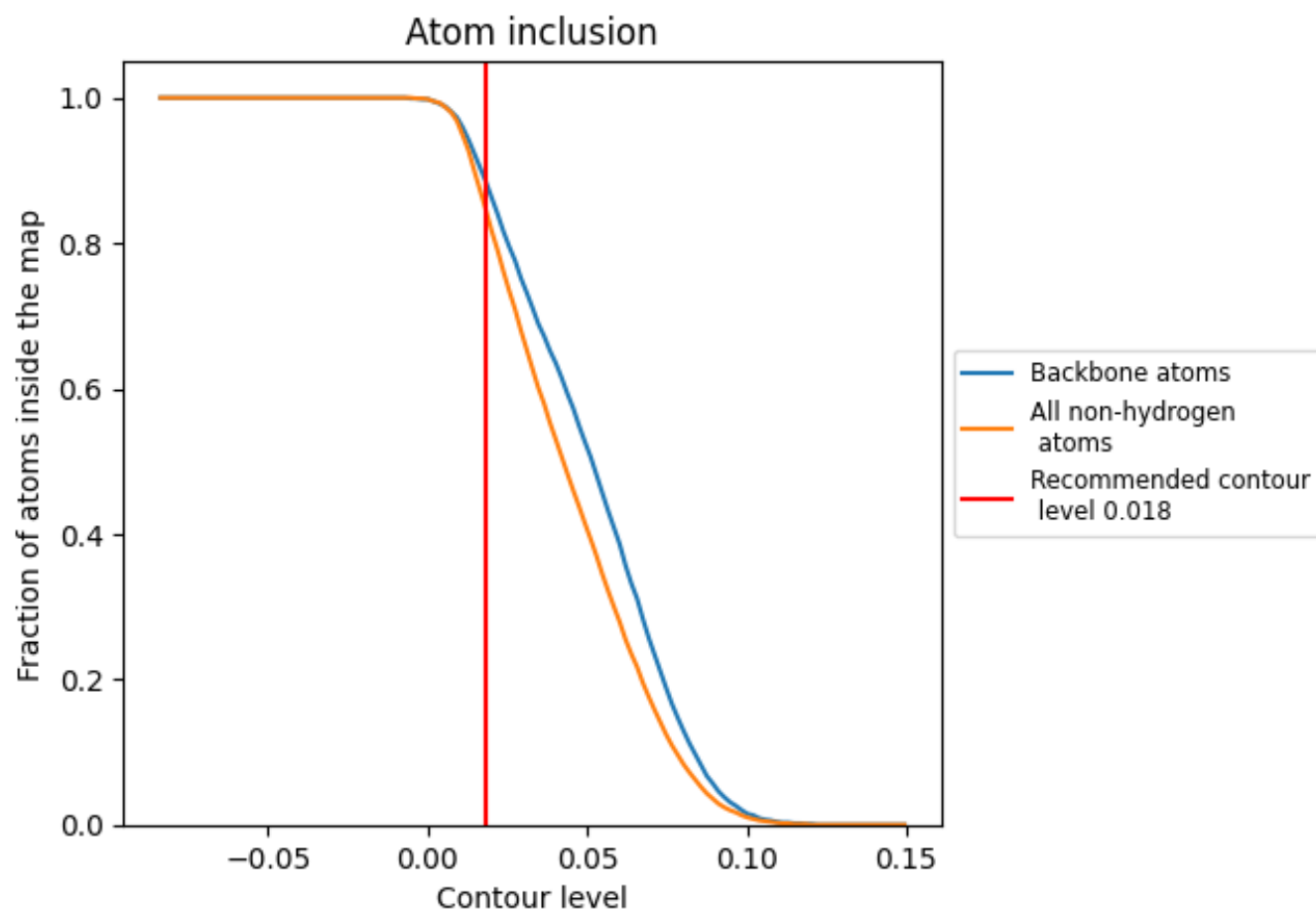
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8510	<div></div> 0.5350
A	<div></div> 0.7810	<div></div> 0.5070
B	<div></div> 0.8870	<div></div> 0.5500
C	<div></div> 0.8840	<div></div> 0.5490
D	<div></div> 0.8450	<div></div> 0.5340

