



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 02:39 PM JST

PDB ID : 7D7F
EMDB ID : EMD-30607
Title : Structure of PKD1L3-CTD/PKD2L1 in calcium-bound state
Authors : Su, Q.; Shi, Y.G.
Deposited on : 2020-10-03
Resolution : 3.10 Å(reported)

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 ⓘ 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

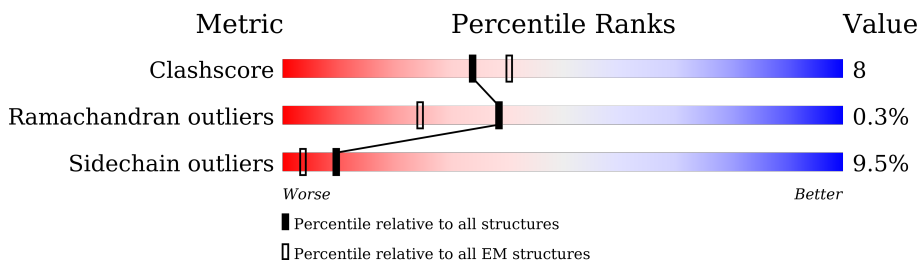
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 15468 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	446	Total	C	N	O	S	0	0
			3603	2352	614	625	12		

There are 32 discrepancies between the modelled and reference sequences:

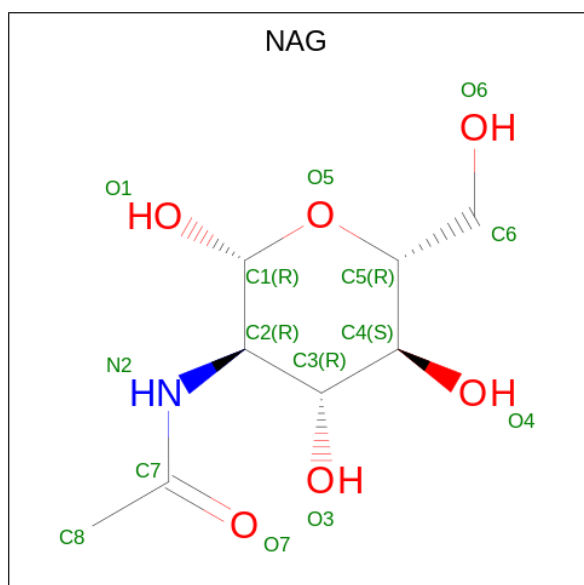
Chain	Residue	Modelled	Actual	Comment	Reference
A	1600	MET	-	initiating methionine	UNP Q2EG98
A	1601	GLY	-	expression tag	UNP Q2EG98
A	1602	SER	-	expression tag	UNP Q2EG98
A	1603	ALA	-	expression tag	UNP Q2EG98
A	1604	GLY	-	expression tag	UNP Q2EG98
A	1605	ASP	-	expression tag	UNP Q2EG98
A	1606	TYR	-	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	

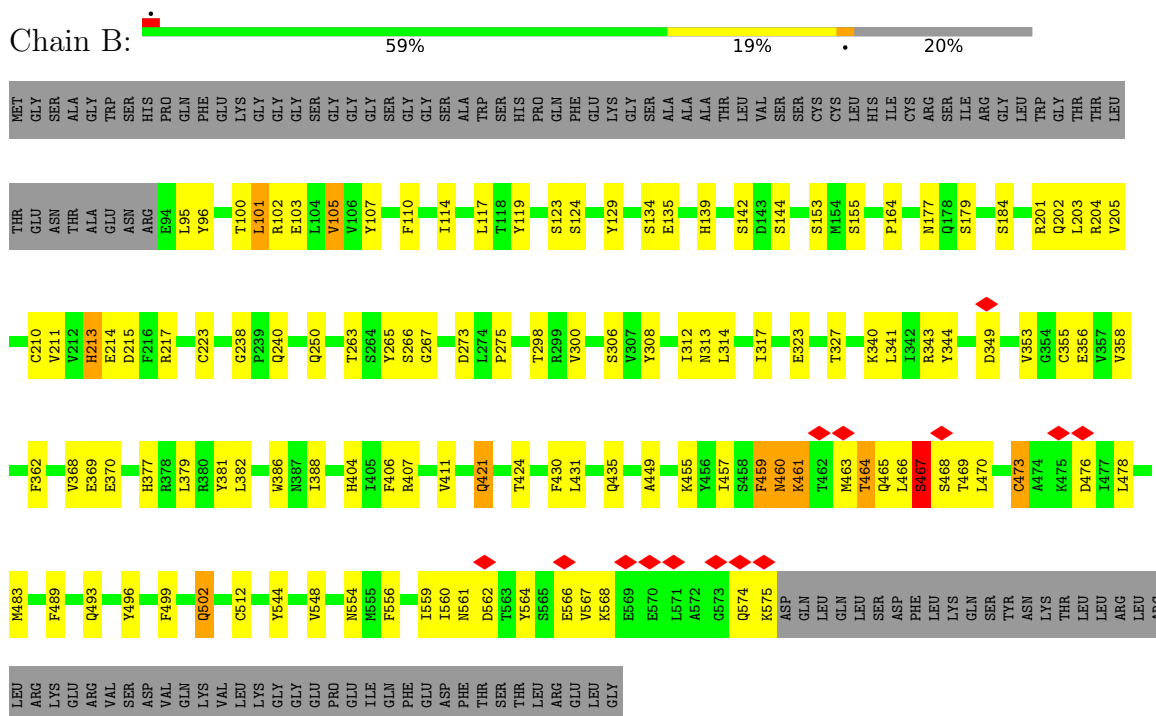
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	3	Total	Ca	0
			3	3	

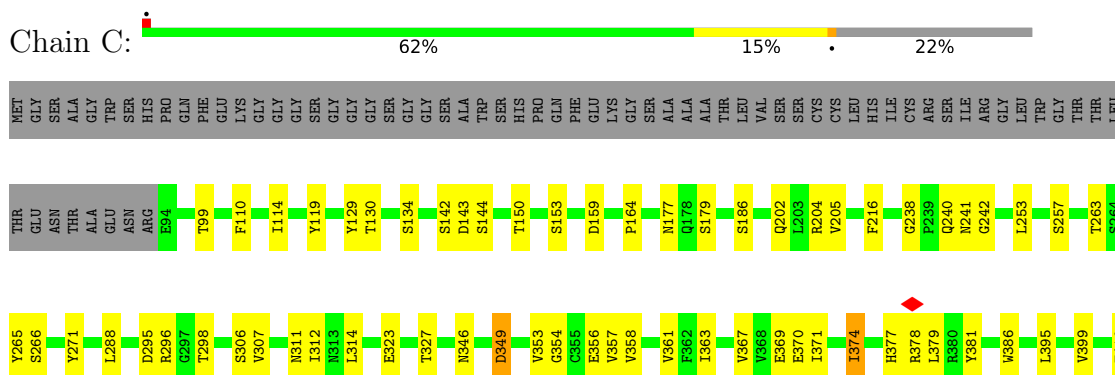
3 Residue-property plots

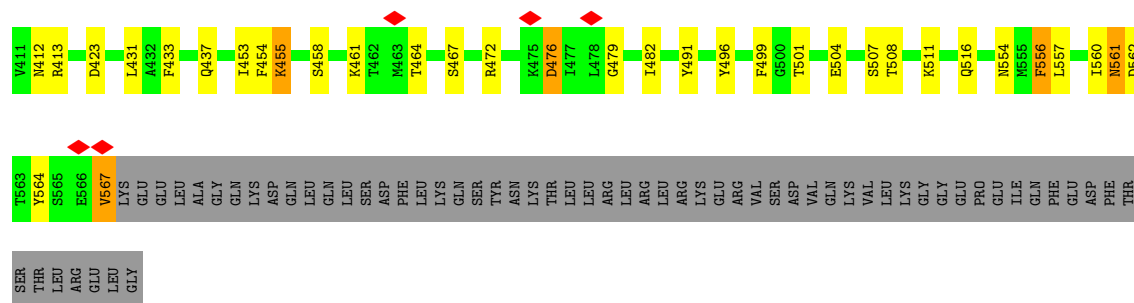
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

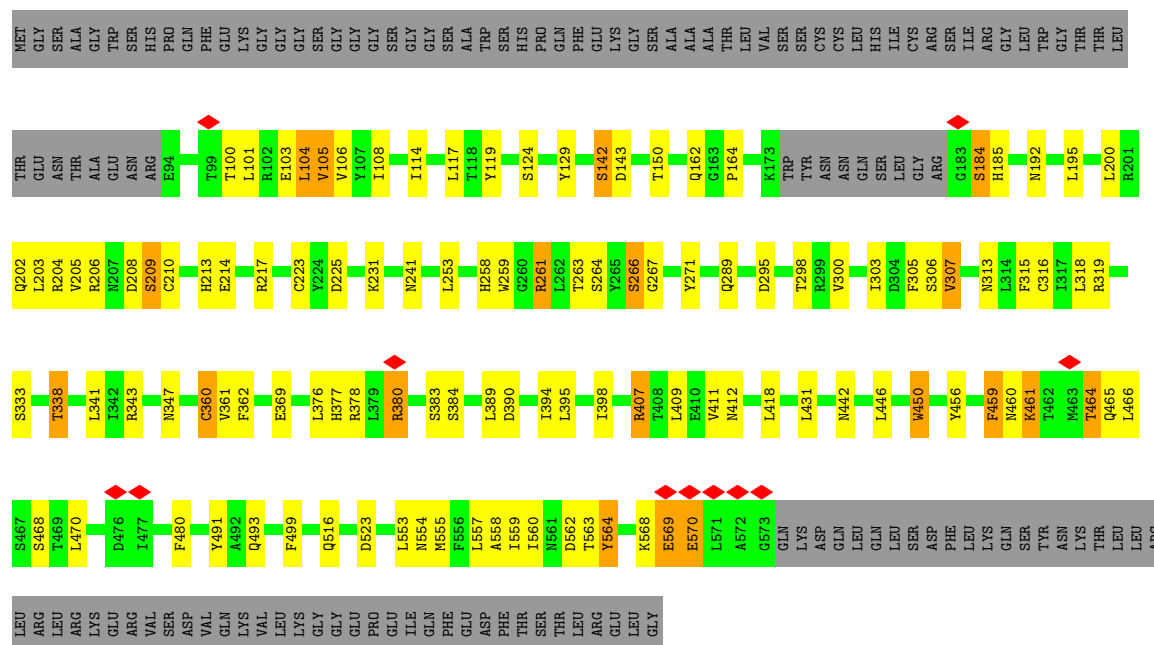


- Molecule 1: Polycystic kidney disease 2-like 1 protein

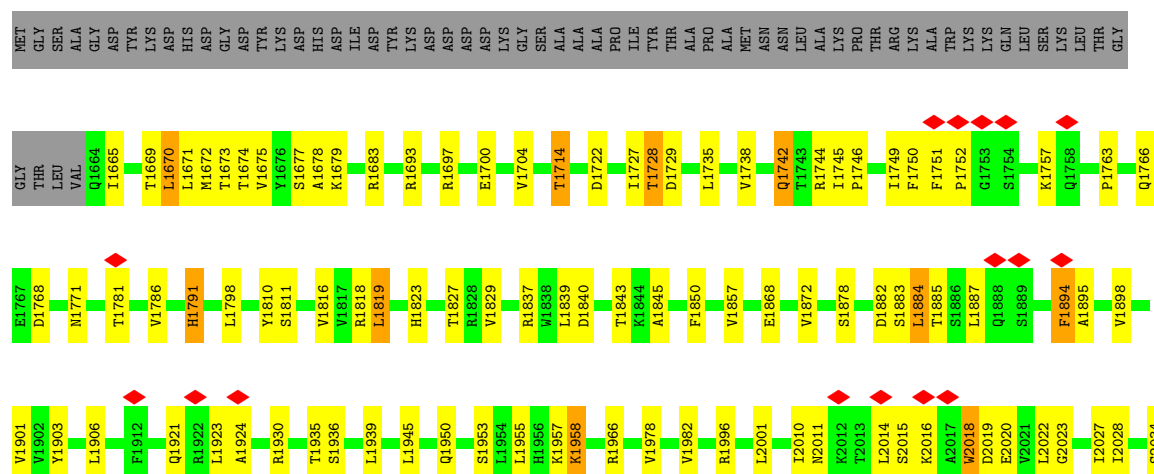


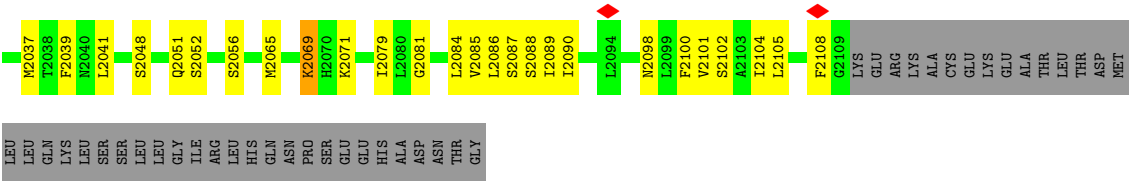


- Molecule 1: Polycystic kidney disease 2-like 1 protein



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149903	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	0.125	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.001	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/4073	0.48	0/5540
1	C	0.46	0/4011	0.48	0/5459
1	D	0.45	0/3971	0.51	0/5401
2	A	0.41	0/3692	0.51	0/5009
All	All	0.45	0/15747	0.50	0/21409

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](#)

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	72	0
1	C	3898	0	3799	47	0
1	D	3862	0	3774	74	0
2	A	3603	0	3653	77	0
3	A	28	0	26	0	0
3	B	42	0	39	2	0
3	C	42	0	39	2	0
3	D	28	0	26	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	3	0	0	0	0
All	All	15468	0	15220	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.

All (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:563:THR:CG2	2:A:2104:ILE:HD11	1.66	1.24
1:B:265:TYR:OH	1:B:323:GLU:OE1	1.61	1.17
1:D:563:THR:HG21	2:A:2104:ILE:HD11	1.33	1.04
1:B:466:LEU:O	1:B:468:SER:N	1.93	1.01
1:D:563:THR:HG22	2:A:2104:ILE:HD11	1.38	1.01
2:A:1819:LEU:HB3	2:A:1829:VAL:HG21	1.49	0.92
1:B:465:GLN:HG2	1:D:558:ALA:HB2	1.55	0.87
1:D:259:TRP:HD1	1:D:264:SER:HB2	1.42	0.84
1:B:461:LYS:H	1:B:461:LYS:HZ2	1.27	0.80
1:D:407:ARG:O	1:D:411:VAL:HG23	1.83	0.79
1:B:461:LYS:H	1:B:461:LYS:NZ	1.80	0.78
1:B:266:SER:OG	1:B:267:GLY:N	2.16	0.78
1:B:466:LEU:HD12	1:D:554:ASN:OD1	1.84	0.78
1:D:523:ASP:OD1	2:A:2069:LYS:NZ	2.14	0.77
2:A:2010:ILE:HG21	2:A:2014:LEU:HB2	1.69	0.72
1:B:213:HIS:NE2	1:B:215:ASP:OD1	2.21	0.71
1:D:202:GLN:NE2	1:D:298:THR:OG1	2.25	0.70
2:A:1819:LEU:CB	2:A:1829:VAL:HG21	2.22	0.69
1:B:459:PHE:C	1:B:460:ASN:OD1	2.31	0.69
1:D:569:GLU:HA	1:D:569:GLU:OE2	1.92	0.69
2:A:1744:ARG:NH2	2:A:1840:ASP:OD2	2.25	0.68
1:C:142:SER:HB3	1:C:164:PRO:HD3	1.74	0.68
1:B:308:TYR:OH	1:B:313:ASN:ND2	2.27	0.68
1:D:266:SER:OG	1:D:267:GLY:N	2.25	0.68
1:D:104:LEU:HD12	1:D:456:TYR:HB3	1.77	0.67
2:A:1819:LEU:HD13	2:A:1819:LEU:O	1.95	0.67
2:A:1819:LEU:O	2:A:1819:LEU:HD22	1.95	0.66
2:A:1714:THR:O	2:A:1714:THR:OG1	2.14	0.66
1:C:241:ASN:OD1	1:C:242:GLY:N	2.29	0.65
1:D:563:THR:HG22	2:A:2104:ILE:CD1	2.22	0.65
1:C:327:THR:HG22	2:A:1857:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLN:NE2	1:D:289:GLN:OE1	2.28	0.64
1:B:466:LEU:C	1:B:468:SER:N	2.51	0.64
1:B:493:GLN:NE2	1:C:119:TYR:OH	2.30	0.64
1:B:465:GLN:HG2	1:D:558:ALA:CB	2.25	0.63
1:D:209:SER:HB3	1:D:231:LYS:HD3	1.79	0.63
2:A:1763:PRO:O	2:A:1766:GLN:NE2	2.30	0.63
1:B:312:ILE:HD12	1:B:314:LEU:HD12	1.82	0.62
1:D:192:ASN:HD21	2:A:1872:VAL:HG23	1.64	0.62
1:B:202:GLN:NE2	1:B:298:THR:OG1	2.32	0.62
1:D:563:THR:HG21	2:A:2104:ILE:CD1	2.21	0.61
1:D:105:VAL:HA	1:D:108:ILE:HG22	1.83	0.61
1:B:460:ASN:OD1	1:B:460:ASN:N	2.33	0.61
1:B:464:THR:HG23	1:B:464:THR:O	2.00	0.61
1:B:466:LEU:O	1:B:467:SER:C	2.39	0.61
1:B:564:TYR:HB2	1:D:564:TYR:OH	2.01	0.61
1:B:466:LEU:CD1	1:D:554:ASN:OD1	2.49	0.61
2:A:1750:PHE:HD1	2:A:1752:PRO:HD3	1.67	0.60
2:A:1693:ARG:NH1	2:A:1728:THR:OG1	2.35	0.60
2:A:2085:VAL:O	2:A:2089:ILE:HG13	2.01	0.60
2:A:1884:LEU:HD21	2:A:1955:LEU:HD12	1.84	0.60
2:A:1810:TYR:OH	2:A:1868:GLU:OE2	2.13	0.60
1:D:411:VAL:HG22	1:D:431:LEU:HD21	1.84	0.59
1:D:142:SER:HB2	1:D:164:PRO:HD3	1.84	0.59
1:D:203:LEU:HB2	1:D:300:VAL:HG12	1.84	0.59
1:C:204:ARG:NH1	1:C:295:ASP:OD1	2.33	0.58
2:A:1894:PHE:HD2	2:A:1895:ALA:H	1.51	0.58
1:C:508:THR:HB	1:C:511:LYS:HG3	1.85	0.58
1:D:464:THR:OG1	1:D:465:GLN:NE2	2.37	0.58
1:B:407:ARG:NH1	1:B:435:GLN:OE1	2.36	0.58
1:C:358:VAL:HA	1:C:361:VAL:HG12	1.86	0.58
1:C:472:ARG:NH2	1:C:562:ASP:OD2	2.36	0.58
2:A:1742:GLN:NE2	2:A:1843:THR:OG1	2.37	0.57
1:B:100:THR:OG1	1:B:103:GLU:OE1	2.21	0.57
1:D:209:SER:HB2	1:D:225:ASP:HB2	1.85	0.57
1:D:459:PHE:HB2	2:A:2027:ILE:HD11	1.86	0.57
1:D:491:TYR:HB3	1:D:516:GLN:HE22	1.70	0.57
1:B:327:THR:HG22	1:C:312:ILE:HD13	1.87	0.56
1:B:223:CYS:SG	1:C:311:ASN:HA	2.45	0.56
1:C:253:LEU:HD11	1:C:271:TYR:CE2	2.40	0.56
1:C:461:LYS:HG2	1:C:464:THR:HB	1.86	0.56
1:C:202:GLN:NE2	1:C:298:THR:OG1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ARG:NH2	1:D:295:ASP:OD1	2.36	0.56
3:D:703:NAG:H83	3:D:703:NAG:H3	1.86	0.56
2:A:1786:VAL:H	2:A:1791:HIS:HD2	1.53	0.56
1:D:461:LYS:HA	1:D:465:GLN:HE22	1.70	0.56
1:D:200:LEU:HD23	1:D:303:ILE:HG12	1.88	0.55
1:D:377:HIS:ND1	1:D:377:HIS:O	2.39	0.55
1:C:353:VAL:O	1:C:357:VAL:HG23	2.06	0.55
2:A:1819:LEU:H	2:A:1819:LEU:CD1	2.19	0.55
1:D:100:THR:CG2	1:D:103:GLU:HG2	2.37	0.55
2:A:2052:SER:O	2:A:2056:SER:OG	2.22	0.55
1:B:562:ASP:O	1:B:566:GLU:HG2	2.08	0.54
2:A:1665:ILE:HD12	2:A:1665:ILE:H	1.72	0.54
1:B:203:LEU:HB2	1:B:300:VAL:HG12	1.90	0.53
1:D:376:LEU:HG	1:D:377:HIS:CD2	2.43	0.53
1:B:466:LEU:C	1:B:468:SER:H	2.12	0.53
3:B:703:NAG:H83	3:B:703:NAG:H3	1.90	0.53
3:C:701:NAG:H3	3:C:701:NAG:H83	1.91	0.53
1:C:265:TYR:OH	1:C:323:GLU:OE1	2.15	0.53
1:B:100:THR:O	1:B:102:ARG:N	2.42	0.52
1:B:483:MET:HG3	1:C:454:PHE:HE2	1.75	0.52
1:D:307:VAL:HG12	1:D:316:CYS:HB3	1.91	0.52
1:B:266:SER:HG	1:B:267:GLY:H	1.55	0.52
1:B:466:LEU:O	1:B:469:THR:N	2.33	0.52
1:B:559:ILE:HD13	1:D:557:LEU:HD21	1.91	0.52
1:C:491:TYR:HB3	1:C:516:GLN:HE22	1.74	0.52
2:A:1819:LEU:CD1	2:A:1819:LEU:N	2.73	0.52
1:C:371:ILE:HA	1:C:374:ILE:HG22	1.91	0.52
1:D:460:ASN:O	1:D:461:LYS:HG2	2.09	0.52
1:D:313:ASN:ND2	1:D:341:LEU:O	2.43	0.51
1:D:376:LEU:HG	1:D:377:HIS:HD2	1.75	0.51
1:B:386:TRP:HB3	1:B:455:LYS:HD2	1.92	0.51
1:C:410:GLU:OE1	1:C:413:ARG:NH2	2.34	0.51
1:B:135:GLU:HA	1:B:139:HIS:HD2	1.75	0.51
1:C:363:ILE:O	1:C:367:VAL:HG13	2.11	0.51
2:A:1671:LEU:O	2:A:1674:THR:HG22	2.11	0.50
1:B:489:PHE:O	1:B:493:GLN:HG3	2.12	0.50
2:A:2016:LYS:HD2	2:A:2016:LYS:N	2.26	0.50
1:C:370:GLU:OE2	1:C:381:TYR:OH	2.27	0.50
1:B:273:ASP:O	1:B:275:PRO:HD3	2.12	0.50
2:A:1749:ILE:HG23	2:A:1751:PHE:HE2	1.77	0.49
2:A:1923:LEU:HD12	2:A:1924:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:O	1:B:114:ILE:HG23	2.13	0.49
1:B:238:GLY:O	1:B:240:GLN:HG3	2.13	0.49
1:D:195:LEU:HD22	1:D:418:LEU:HD21	1.94	0.49
1:B:568:LYS:HD2	1:C:567:VAL:HG23	1.95	0.49
1:C:130:THR:O	1:C:134:SER:OG	2.24	0.48
1:D:142:SER:OG	1:D:143:ASP:N	2.46	0.48
1:D:570:GLU:O	1:D:570:GLU:HG3	2.11	0.48
2:A:1935:THR:O	2:A:1939:LEU:HG	2.14	0.48
2:A:1672:MET:HA	2:A:1675:VAL:HG12	1.94	0.48
1:D:313:ASN:OD1	1:D:343:ARG:NH2	2.46	0.48
2:A:1697:ARG:NH1	2:A:1700:GLU:OE1	2.47	0.48
1:D:259:TRP:CD1	1:D:264:SER:HB2	2.34	0.48
1:C:295:ASP:OD1	1:C:295:ASP:N	2.45	0.48
2:A:1771:ASN:HD22	2:A:1791:HIS:CD2	2.32	0.48
1:C:410:GLU:HG2	1:C:431:LEU:HD13	1.96	0.48
2:A:1819:LEU:CB	2:A:1829:VAL:CG2	2.92	0.48
1:C:110:PHE:O	1:C:114:ILE:HG23	2.13	0.48
2:A:2086:LEU:O	2:A:2090:ILE:HG13	2.14	0.47
1:C:346:ASN:N	1:C:346:ASN:OD1	2.46	0.47
1:C:204:ARG:HH12	1:C:295:ASP:CG	2.16	0.47
1:D:360:CYS:SG	1:D:361:VAL:N	2.87	0.47
2:A:2019:ASP:O	2:A:2023:GLY:N	2.48	0.47
1:C:501:THR:HG22	2:A:1683:ARG:HB3	1.97	0.47
1:B:574:GLN:HB3	1:B:575:LYS:HD2	1.96	0.47
1:C:312:ILE:HD12	1:C:314:LEU:HD12	1.97	0.47
1:B:107:TYR:OH	1:B:449:ALA:O	2.28	0.47
1:D:100:THR:OG1	1:D:101:LEU:N	2.47	0.47
2:A:1729:ASP:OD1	2:A:1729:ASP:N	2.46	0.46
1:B:214:GLU:HA	1:B:217:ARG:HB2	1.97	0.46
1:D:206:ARG:NH1	1:D:231:LYS:HA	2.31	0.46
1:C:496:TYR:OH	2:A:1679:LYS:HB2	2.15	0.46
1:C:476:ASP:OD1	1:C:476:ASP:N	2.48	0.46
1:D:103:GLU:HA	1:D:106:VAL:HG22	1.97	0.46
1:D:210:CYS:HB3	1:D:223:CYS:SG	2.55	0.46
1:B:306:SER:HB3	1:B:317:ILE:HG13	1.98	0.46
1:C:556:PHE:O	1:C:560:ILE:HG23	2.16	0.46
1:C:177:ASN:HB3	3:C:701:NAG:O5	2.16	0.45
2:A:1749:ILE:HG13	2:A:1751:PHE:CD2	2.50	0.45
1:B:250:GLN:HG3	1:B:267:GLY:HA3	1.98	0.45
2:A:1727:ILE:O	2:A:1728:THR:HG22	2.16	0.45
2:A:2100:PHE:O	2:A:2104:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1823:HIS:O	2:A:1827:THR:HG23	2.16	0.45
1:C:557:LEU:O	1:C:561:ASN:HB2	2.17	0.45
2:A:1930:ARG:HG2	2:A:1996:ARG:HH22	1.80	0.45
1:B:341:LEU:HD13	1:B:431:LEU:HD23	1.98	0.45
1:D:560:ILE:HD13	1:D:560:ILE:HA	1.82	0.45
1:C:564:TYR:CE2	2:A:2104:ILE:HG22	2.52	0.45
1:D:184:SER:O	1:D:185:HIS:ND1	2.49	0.45
1:B:496:TYR:HB2	1:B:512:CYS:SG	2.57	0.45
1:D:409:LEU:HA	1:D:412:ASN:HD21	1.82	0.44
1:B:177:ASN:HB3	3:B:701:NAG:O5	2.17	0.44
2:A:1677:SER:OG	2:A:1678:ALA:N	2.48	0.44
1:B:102:ARG:O	1:B:105:VAL:HG12	2.18	0.44
2:A:1693:ARG:HD3	2:A:1728:THR:HG21	2.00	0.44
1:C:238:GLY:O	1:C:240:GLN:HG3	2.17	0.44
2:A:1819:LEU:HD13	2:A:1819:LEU:H	1.82	0.44
1:B:467:SER:HA	1:B:470:LEU:HG	2.00	0.44
1:C:412:ASN:HD22	1:C:412:ASN:HA	1.67	0.44
1:D:108:ILE:O	1:D:108:ILE:HG13	2.18	0.44
1:B:142:SER:HB3	1:B:164:PRO:HD3	2.00	0.44
1:C:349:ASP:OD1	1:C:349:ASP:N	2.51	0.44
2:A:1746:PRO:CD	2:A:1766:GLN:HB2	2.48	0.44
2:A:2098:ASN:HA	2:A:2101:VAL:HG22	2.00	0.44
1:B:502:GLN:HE21	1:B:502:GLN:HB3	1.68	0.43
2:A:1738:VAL:HG13	2:A:1850:PHE:HB3	1.99	0.43
1:D:119:TYR:CE2	2:A:2041:LEU:HD21	2.54	0.43
1:D:442:ASN:HD22	1:D:442:ASN:HA	1.57	0.43
2:A:2019:ASP:OD1	2:A:2020:GLU:N	2.51	0.43
1:B:556:PHE:O	1:B:559:ILE:HG13	2.18	0.43
1:C:504:GLU:O	1:C:507:SER:OG	2.28	0.43
2:A:1958:LYS:HE3	2:A:1958:LYS:HB2	1.71	0.43
1:D:466:LEU:O	1:D:470:LEU:HB2	2.19	0.43
1:D:380:ARG:O	1:D:383:SER:HB3	2.19	0.43
1:B:312:ILE:HG13	1:B:312:ILE:O	2.18	0.43
1:B:421:GLN:HE21	1:B:424:THR:HG21	1.84	0.43
2:A:2028:ILE:HD13	2:A:2028:ILE:HA	1.83	0.43
1:B:96:TYR:HB2	1:B:460:ASN:HD21	1.84	0.43
2:A:1930:ARG:HA	2:A:1996:ARG:HH22	1.83	0.43
1:B:406:PHE:HZ	1:B:430:PHE:HE2	1.67	0.42
1:B:465:GLN:OE1	1:D:558:ALA:HB1	2.19	0.42
2:A:1670:LEU:HG	2:A:1903:TYR:HB2	2.00	0.42
2:A:1746:PRO:HD2	2:A:1766:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1798:LEU:HD21	2:A:1816:VAL:HG21	2.00	0.42
1:D:253:LEU:HD11	1:D:271:TYR:CE2	2.54	0.42
1:B:353:VAL:O	1:B:356:GLU:HG2	2.19	0.42
1:C:386:TRP:CZ2	1:C:455:LYS:HB2	2.55	0.42
1:B:560:ILE:HG13	1:B:561:ASN:N	2.35	0.42
1:D:305:PHE:CE1	1:D:318:LEU:HD13	2.55	0.42
1:D:390:ASP:O	1:D:394:ILE:HG13	2.20	0.42
2:A:2027:ILE:H	2:A:2027:ILE:HG12	1.66	0.42
2:A:1798:LEU:HD12	2:A:1798:LEU:HA	1.76	0.42
2:A:1669:THR:O	2:A:1673:THR:HG22	2.19	0.42
1:C:433:PHE:O	1:C:437:GLN:HG2	2.20	0.42
2:A:1845:ALA:HA	2:A:1868:GLU:HA	2.01	0.42
2:A:1898:VAL:O	2:A:1901:VAL:HG12	2.20	0.42
1:D:258:HIS:CD2	1:D:319:ARG:HH11	2.38	0.41
1:B:95:LEU:HD23	1:B:457:ILE:HD11	2.02	0.41
1:B:344:TYR:HD2	1:B:349:ASP:HB3	1.85	0.41
1:B:355:CYS:O	1:B:358:VAL:HB	2.20	0.41
1:B:461:LYS:HE2	1:B:461:LYS:HB2	1.65	0.41
1:B:483:MET:O	1:B:483:MET:HG2	2.20	0.41
1:D:213:HIS:CG	1:D:214:GLU:H	2.38	0.41
2:A:1978:VAL:O	2:A:1982:VAL:HG23	2.20	0.41
2:A:2039:PHE:HE1	2:A:2084:LEU:HD13	1.86	0.41
1:C:395:LEU:O	1:C:399:VAL:HG23	2.21	0.41
1:D:315:PHE:O	1:D:338:THR:HA	2.20	0.41
1:D:394:ILE:O	1:D:398:ILE:HG23	2.20	0.41
2:A:2048:SER:O	2:A:2051:GLN:HG3	2.20	0.41
1:D:395:LEU:HD13	1:D:395:LEU:HA	1.88	0.41
1:B:340:LYS:O	1:B:343:ARG:NH2	2.54	0.41
1:C:386:TRP:CE2	1:C:455:LYS:HB2	2.55	0.41
1:C:479:GLY:O	1:C:482:ILE:HG13	2.21	0.41
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.88	0.41
1:B:119:TYR:OH	1:D:493:GLN:NE2	2.50	0.41
1:B:370:GLU:OE1	1:B:381:TYR:OH	2.22	0.41
1:B:469:THR:O	1:B:473:CYS:HB3	2.21	0.41
1:D:450:TRP:HB3	2:A:2034:SER:OG	2.21	0.41
1:C:386:TRP:CH2	1:C:455:LYS:HB2	2.56	0.41
1:D:261:ARG:HE	1:D:261:ARG:HB2	1.80	0.41
2:A:2081:GLY:O	2:A:2085:VAL:HG23	2.21	0.41
1:B:544:TYR:O	1:B:548:VAL:HG22	2.22	0.40
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.75	0.40
1:D:555:MET:O	1:D:559:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1704:VAL:HG21	2:A:1839:LEU:HB3	2.04	0.40
2:A:2015:SER:C	2:A:2016:LYS:HD2	2.42	0.40
1:B:388:ILE:HD13	1:B:388:ILE:HA	1.86	0.40
1:D:341:LEU:O	1:D:341:LEU:HG	2.20	0.40
1:B:559:ILE:HD12	1:B:560:ILE:N	2.37	0.40
1:D:101:LEU:HD13	1:D:101:LEU:O	2.22	0.40
1:D:446:LEU:HD21	2:A:2037:MET:SD	2.62	0.40
1:C:354:GLY:O	1:C:358:VAL:HG13	2.20	0.40
2:A:1921:GLN:C	2:A:1923:LEU:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	448 (93%)	28 (6%)	4 (1%)	16	48
1	C	472/604 (78%)	447 (95%)	24 (5%)	1 (0%)	44	74
1	D	467/604 (77%)	427 (91%)	40 (9%)	0	100	100
2	A	444/551 (81%)	389 (88%)	54 (12%)	1 (0%)	44	74
All	All	1863/2363 (79%)	1711 (92%)	146 (8%)	6 (0%)	38	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	467	SER
1	B	101	LEU
1	C	99	THR
1	B	213	HIS
1	B	464	THR
2	A	2018	TRP

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%)	392 (91%)	38 (9%)	8	30
1	C	424/530 (80%)	389 (92%)	35 (8%)	9	33
1	D	420/530 (79%)	378 (90%)	42 (10%)	6	24
2	A	396/482 (82%)	353 (89%)	43 (11%)	5	21
All	All	1670/2072 (81%)	1512 (90%)	158 (10%)	9	26

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	101	LEU
1	B	105	VAL
1	B	123	SER
1	B	124	SER
1	B	129	TYR
1	B	134	SER
1	B	144	SER
1	B	153	SER
1	B	155	SER
1	B	179	SER
1	B	184	SER
1	B	201	ARG
1	B	204	ARG
1	B	205	VAL
1	B	210	CYS
1	B	211	VAL
1	B	263	THR
1	B	362	PHE
1	B	368	VAL
1	B	369	GLU
1	B	377	HIS
1	B	379	LEU
1	B	382	LEU
1	B	404	HIS

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Mol	Chain	Res	Type
1	B	411	VAL
1	B	421	GLN
1	B	459	PHE
1	B	460	ASN
1	B	461	LYS
1	B	463	MET
1	B	467	SER
1	B	473	CYS
1	B	476	ASP
1	B	478	LEU
1	B	499	PHE
1	B	502	GLN
1	B	554	ASN
1	B	567	VAL
1	C	129	TYR
1	C	143	ASP
1	C	144	SER
1	C	150	THR
1	C	153	SER
1	C	159	ASP
1	C	179	SER
1	C	186	SER
1	C	205	VAL
1	C	216	PHE
1	C	257	SER
1	C	263	THR
1	C	266	SER
1	C	288	LEU
1	C	296	ARG
1	C	306	SER
1	C	307	VAL
1	C	349	ASP
1	C	356	GLU
1	C	369	GLU
1	C	374	ILE
1	C	377	HIS
1	C	378	ARG
1	C	379	LEU
1	C	423	ASP
1	C	453	ILE
1	C	455	LYS
1	C	458	SER

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Mol	Chain	Res	Type
1	C	467	SER
1	C	476	ASP
1	C	499	PHE
1	C	554	ASN
1	C	556	PHE
1	C	561	ASN
1	C	567	VAL
1	D	104	LEU
1	D	105	VAL
1	D	114	ILE
1	D	117	LEU
1	D	124	SER
1	D	129	TYR
1	D	142	SER
1	D	150	THR
1	D	184	SER
1	D	205	VAL
1	D	208	ASP
1	D	209	SER
1	D	217	ARG
1	D	241	ASN
1	D	261	ARG
1	D	263	THR
1	D	266	SER
1	D	306	SER
1	D	307	VAL
1	D	333	SER
1	D	338	THR
1	D	347	ASN
1	D	360	CYS
1	D	362	PHE
1	D	369	GLU
1	D	378	ARG
1	D	380	ARG
1	D	384	SER
1	D	407	ARG
1	D	450	TRP
1	D	459	PHE
1	D	461	LYS
1	D	464	THR
1	D	468	SER
1	D	480	PHE

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Mol	Chain	Res	Type
1	D	499	PHE
1	D	553	LEU
1	D	562	ASP
1	D	564	TYR
1	D	568	LYS
1	D	569	GLU
1	D	570	GLU
2	A	1670	LEU
2	A	1714	THR
2	A	1722	ASP
2	A	1728	THR
2	A	1735	LEU
2	A	1742	GLN
2	A	1745	ILE
2	A	1757	LYS
2	A	1768	ASP
2	A	1781	THR
2	A	1791	HIS
2	A	1811	SER
2	A	1818	ARG
2	A	1819	LEU
2	A	1837	ARG
2	A	1878	SER
2	A	1882	ASP
2	A	1883	SER
2	A	1884	LEU
2	A	1885	THR
2	A	1887	LEU
2	A	1894	PHE
2	A	1906	LEU
2	A	1936	SER
2	A	1945	LEU
2	A	1950	GLN
2	A	1953	SER
2	A	1957	LYS
2	A	1958	LYS
2	A	1966	ARG
2	A	2001	LEU
2	A	2011	ASN
2	A	2018	TRP
2	A	2022	LEU
2	A	2065	MET

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Mol	Chain	Res	Type
2	A	2069	LYS
2	A	2071	LYS
2	A	2079	ILE
2	A	2087	SER
2	A	2088	SER
2	A	2102	SER
2	A	2105	LEU
2	A	2108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	139	HIS
1	B	192	ASN
1	B	202	GLN
1	B	309	ASN
1	B	313	ASN
1	B	377	HIS
1	B	421	GLN
1	B	493	GLN
1	B	502	GLN
1	B	516	GLN
1	B	527	ASN
1	B	574	GLN
1	C	202	GLN
1	C	222	ASN
1	C	412	ASN
1	C	420	GLN
1	C	421	GLN
1	C	505	ASN
1	C	516	GLN
1	D	192	ASN
1	D	202	GLN
1	D	258	HIS
1	D	286	GLN
1	D	346	ASN
1	D	420	GLN
1	D	421	GLN
1	D	442	ASN
1	D	445	ASN
1	D	465	GLN
1	D	493	GLN

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Mol	Chain	Res	Type
1	D	516	GLN
2	A	1742	GLN
2	A	1791	HIS
2	A	1823	HIS
2	A	1856	ASN
2	A	1858	ASN
2	A	1931	ASN
2	A	2011	ASN
2	A	2040	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 15 ligands modelled in this entry, 5 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	0.20	0	17,19,21	0.63	0
3	NAG	A	2500	2	14,14,15	0.45	0	17,19,21	0.37	0
3	NAG	B	703	1	14,14,15	0.80	1 (7%)	17,19,21	1.34	2 (11%)
3	NAG	B	701	1	14,14,15	0.28	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	703	1	14,14,15	0.45	0	17,19,21	1.24	1 (5%)
3	NAG	C	701	1	14,14,15	0.29	0	17,19,21	1.24	1 (5%)
3	NAG	C	703	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	B	702	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	D	702	1	14,14,15	0.35	0	17,19,21	0.44	0
3	NAG	C	702	1	14,14,15	0.18	0	17,19,21	0.63	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	A	2500	2	-	2/6/23/26	0/1/1/1
3	NAG	B	703	1	-	5/6/23/26	0/1/1/1
3	NAG	B	701	1	-	4/6/23/26	0/1/1/1
3	NAG	D	703	1	-	3/6/23/26	0/1/1/1
3	NAG	C	701	1	-	5/6/23/26	0/1/1/1
3	NAG	C	703	1	-	2/6/23/26	0/1/1/1
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1
3	NAG	D	702	1	-	2/6/23/26	0/1/1/1
3	NAG	C	702	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	NAG	C1-C2	2.10	1.55	1.52

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	703	NAG	C2-N2-C7	4.26	128.97	122.90
3	B	703	NAG	C2-N2-C7	4.26	128.97	122.90
3	B	703	NAG	C1-O5-C5	2.40	115.45	112.19

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	NAG	O5-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	B	702	NAG	C4-C5-C6-O6
3	C	703	NAG	C4-C5-C6-O6
3	C	701	NAG	O5-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6
3	A	2500	NAG	O5-C5-C6-O6
3	C	703	NAG	O5-C5-C6-O6
3	D	702	NAG	O5-C5-C6-O6
3	B	703	NAG	C4-C5-C6-O6
3	B	702	NAG	O5-C5-C6-O6
3	A	2500	NAG	C4-C5-C6-O6
3	A	2501	NAG	O5-C5-C6-O6
3	C	701	NAG	C4-C5-C6-O6
3	B	701	NAG	C8-C7-N2-C2
3	B	701	NAG	O7-C7-N2-C2
3	B	703	NAG	C8-C7-N2-C2
3	B	703	NAG	O7-C7-N2-C2
3	C	701	NAG	C8-C7-N2-C2
3	C	701	NAG	O7-C7-N2-C2
3	D	703	NAG	C8-C7-N2-C2
3	D	703	NAG	O7-C7-N2-C2
3	D	702	NAG	C4-C5-C6-O6
3	A	2501	NAG	C4-C5-C6-O6
3	C	702	NAG	O5-C5-C6-O6
3	B	703	NAG	C3-C2-N2-C7
3	C	701	NAG	C3-C2-N2-C7
3	C	702	NAG	C3-C2-N2-C7
3	D	703	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	NAG	1	0
3	B	701	NAG	1	0
3	D	703	NAG	1	0
3	C	701	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

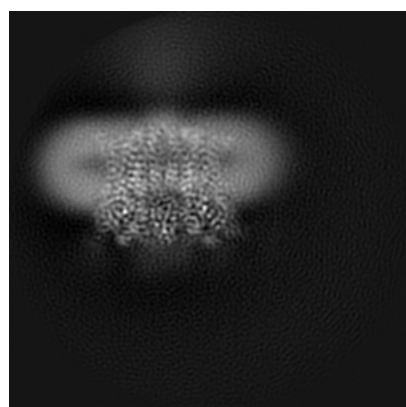
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30607. These allow visual inspection of the internal detail of the map and identification of artifacts.

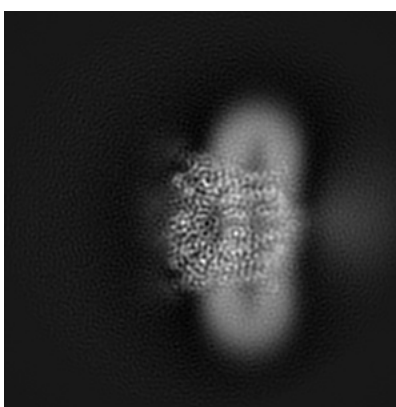
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

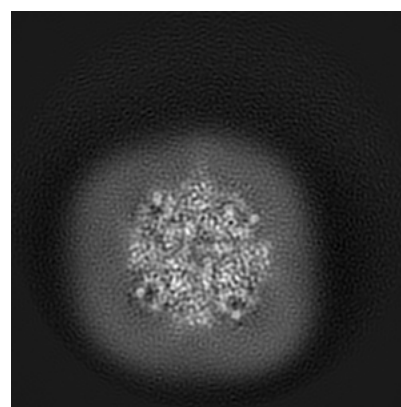
6.1.1 Primary map



X



Y

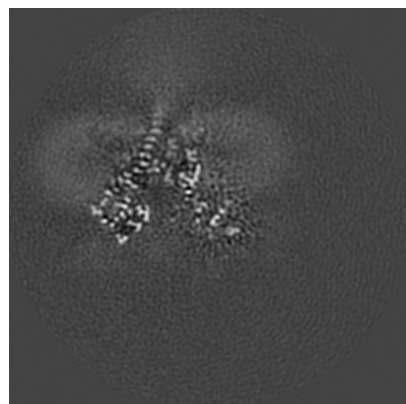


Z

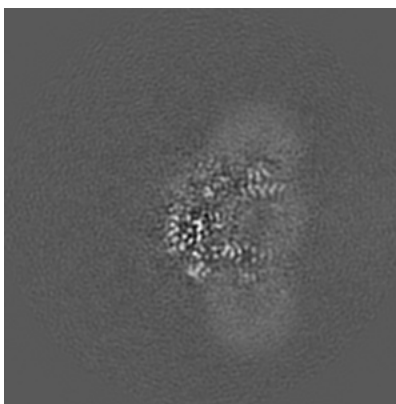
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

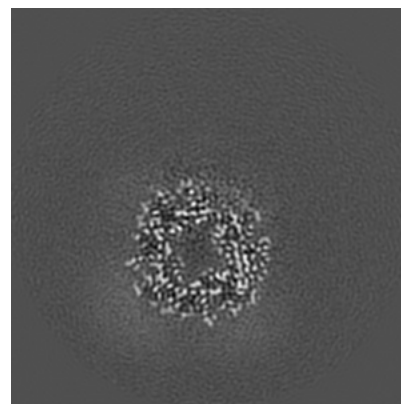
6.2.1 Primary map



X Index: 120



Y Index: 120

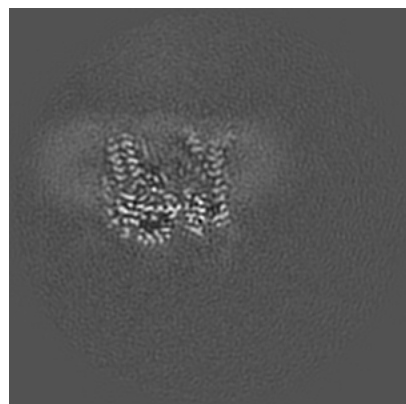


Z Index: 120

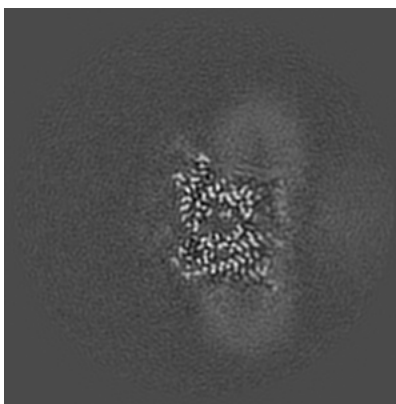
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

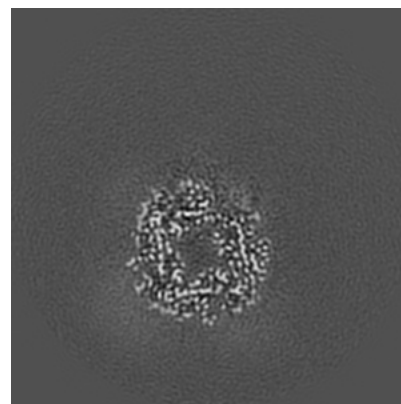
6.3.1 Primary map



X Index: 89



Y Index: 77

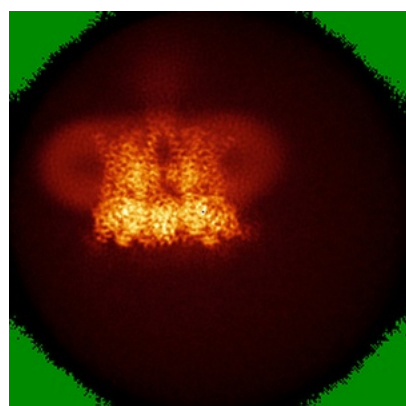


Z Index: 119

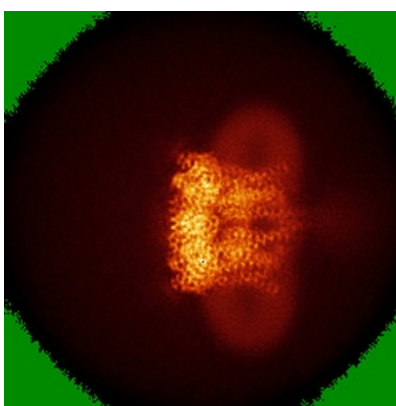
The images above show the largest variance slices of the map in three orthogonal directions.

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

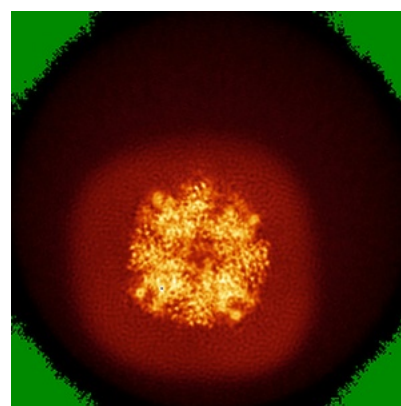
6.4.1 Primary map



X



Y

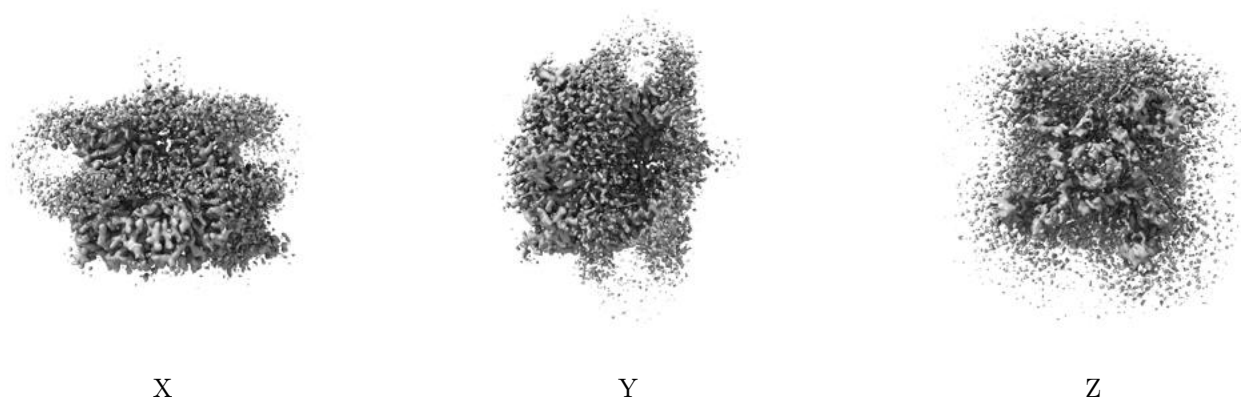


Z

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.

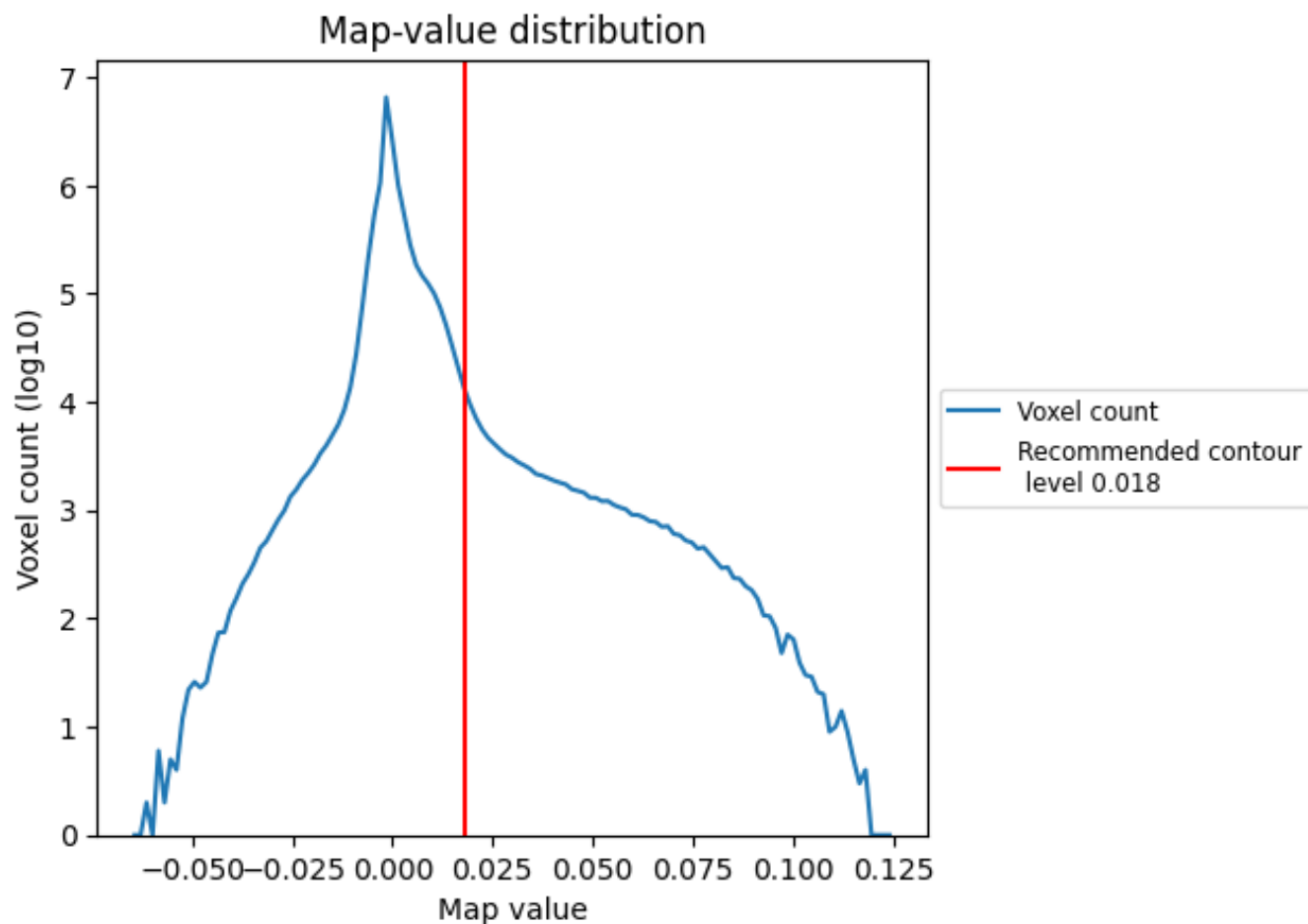
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

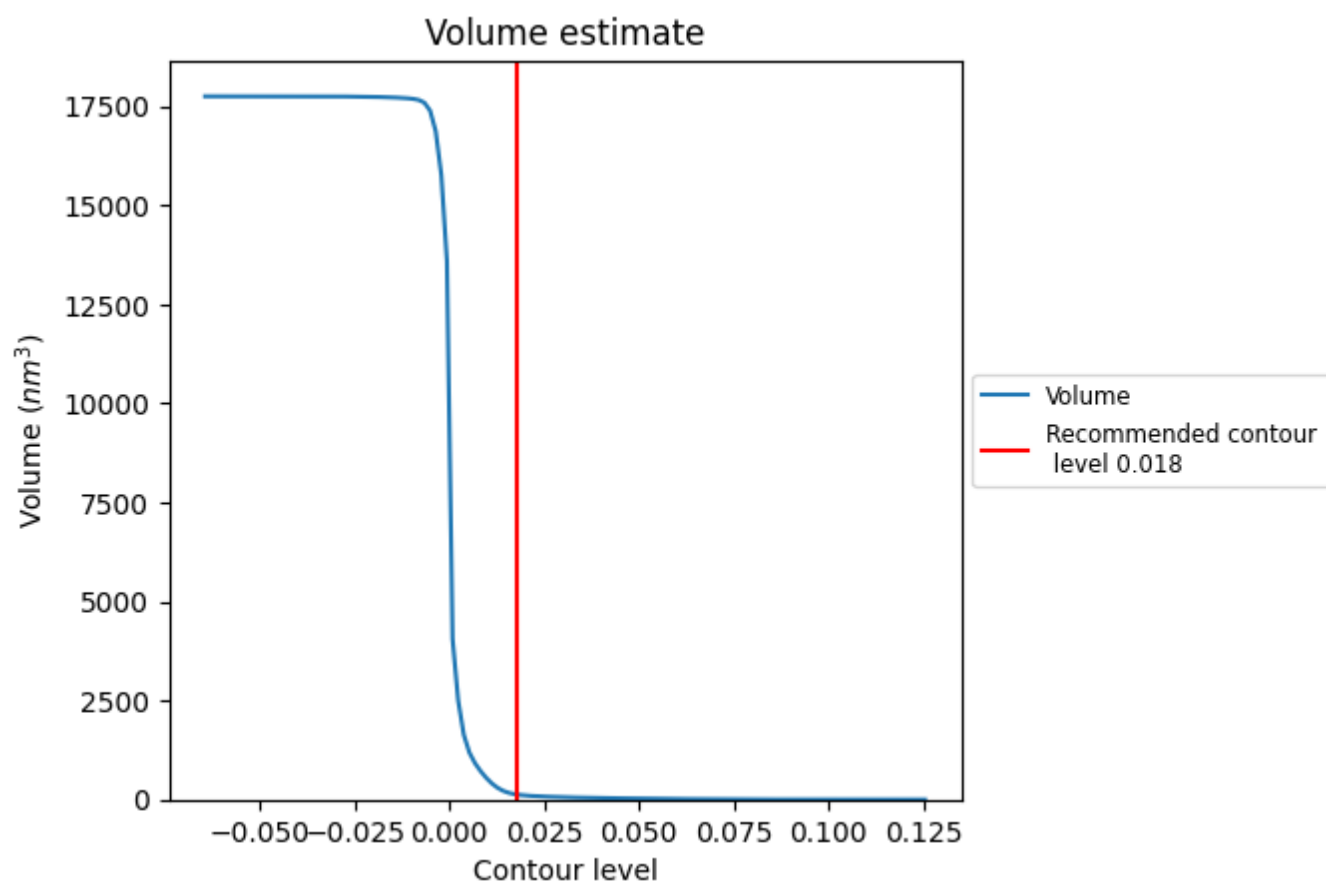
This section contains the results of statistical analysis of the map.

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.

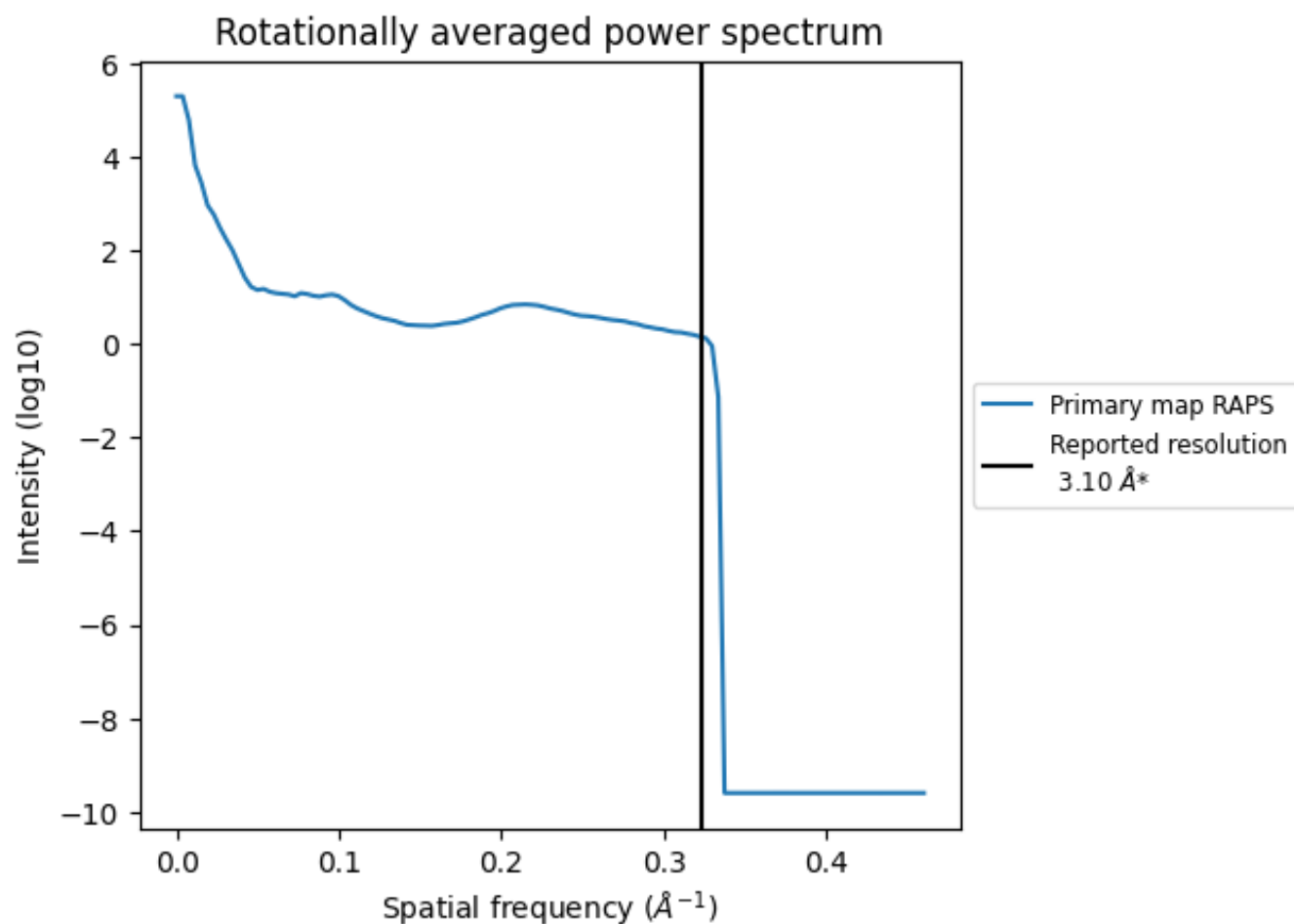
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 114 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 0.323 Å⁻¹

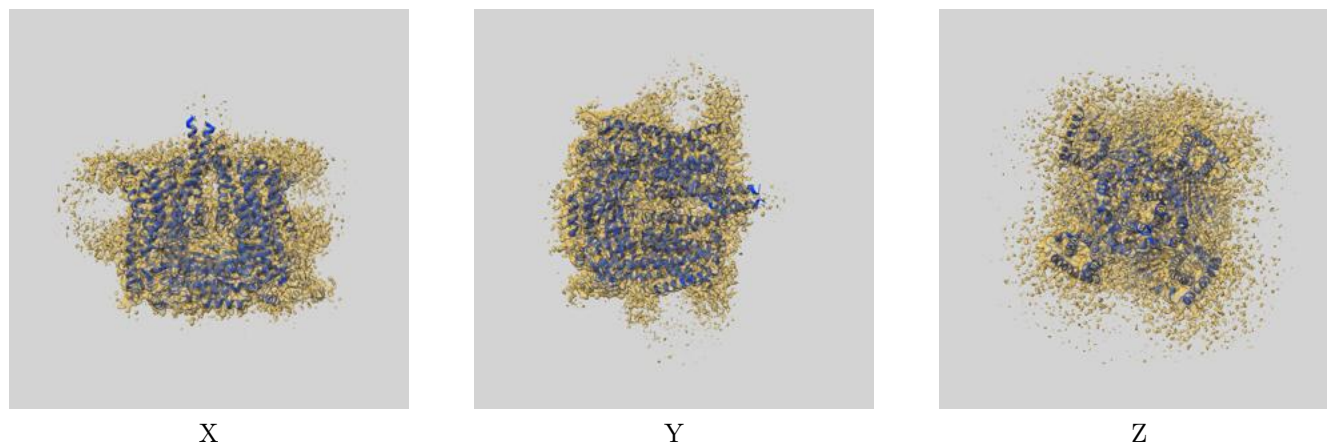
8 Fourier-Shell correlation ⓘ

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-30607 and PDB model 7D7F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



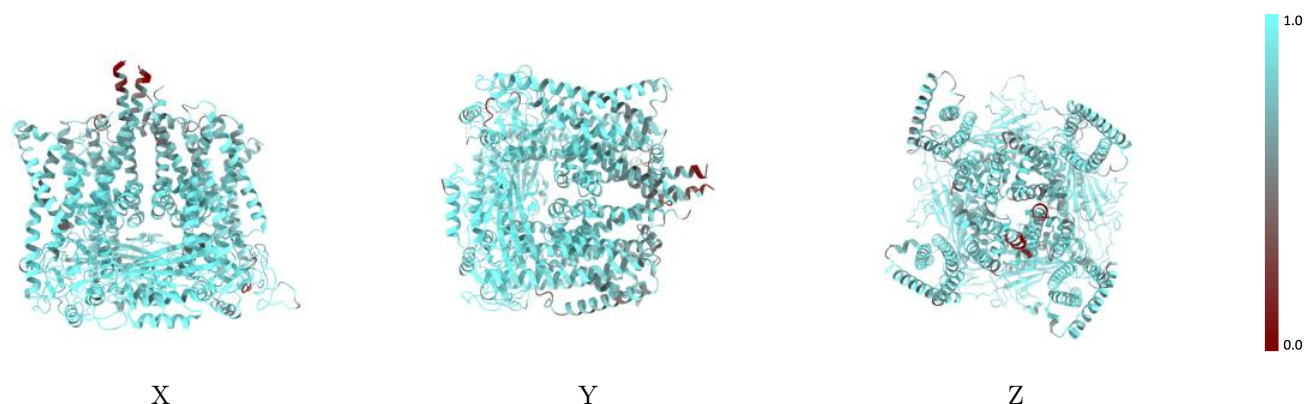
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



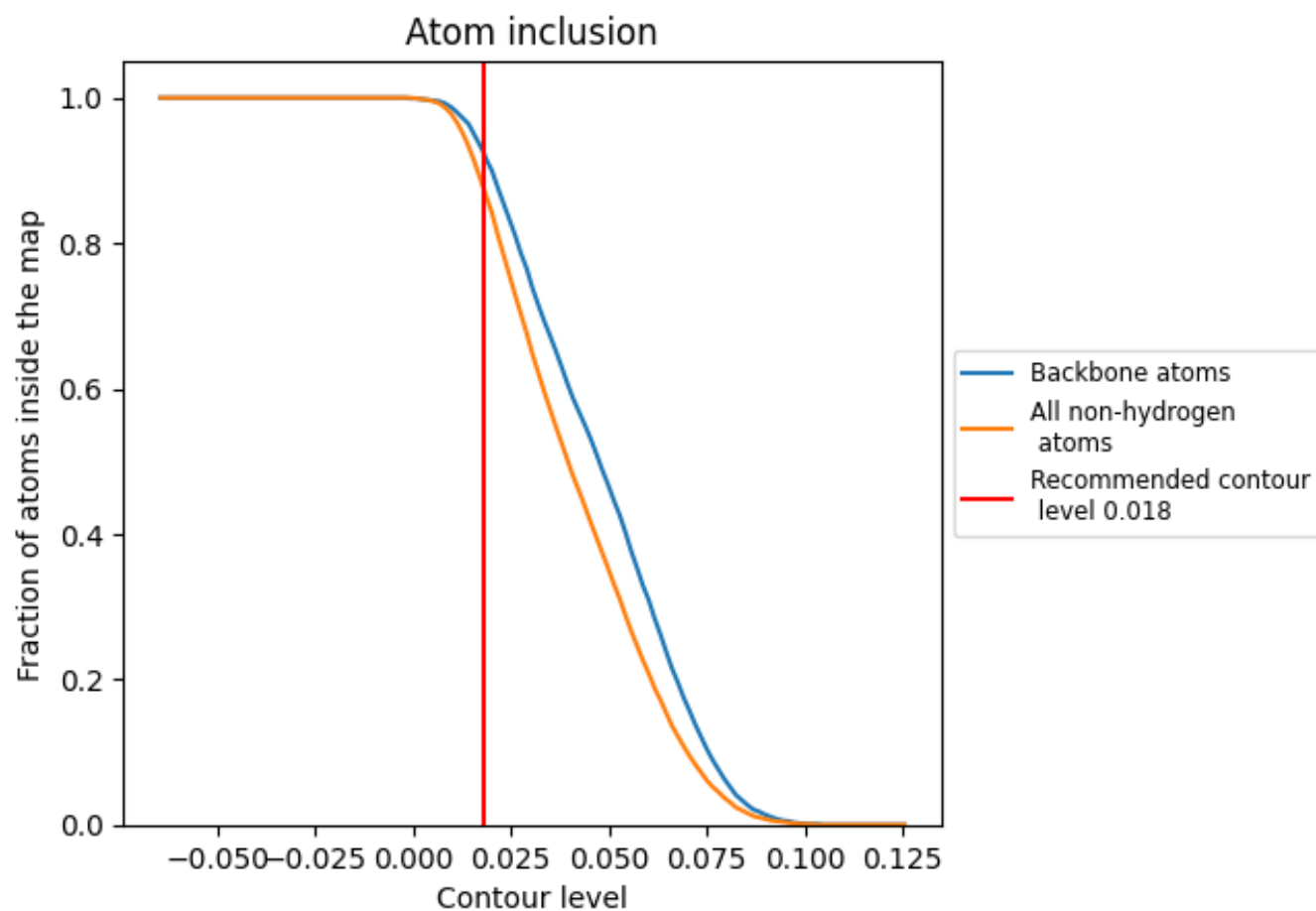
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 88% 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> 0.8770	<div></div> 0.5640
A	<div></div> 0.8410	<div></div> 0.5400
B	<div></div> 0.8880	<div></div> 0.5750
C	<div></div> 0.9010	<div></div> 0.5820
D	<div></div> 0.8760	<div></div> 0.5590

