



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 8, 2017 – 02:05 PM EST

PDB ID : 5MKF
EMDB ID: : EMD-3524
Title : cryoEM Structure of Polycystin-2 in complex with calcium and lipids
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.
Deposited on : 2016-12-04
Resolution : 4.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

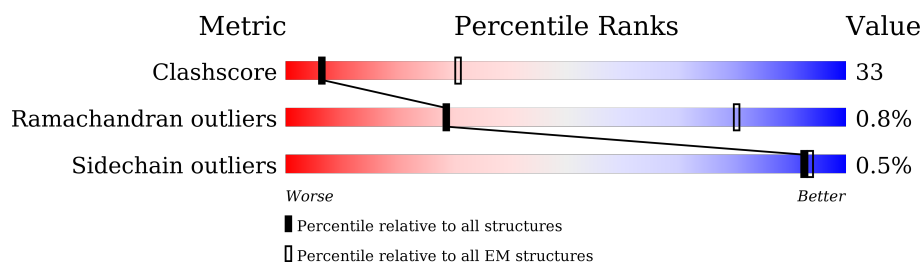
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	968	
1	B	968	
1	C	968	
1	D	968	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1002	-	-	X	-
2	NAG	B	1002	-	-	X	-
2	NAG	C	1002	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1002	-	-	X	-

2 Entry composition [i](#)

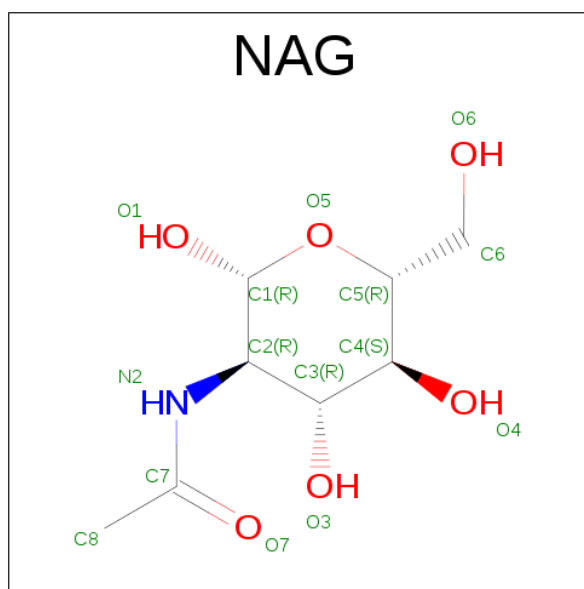
There are 6 unique types of molecules in this entry. The entry contains 16620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	481	Total	C	N	O	S	0	0
			3962	2612	629	702	19		
1	B	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		
1	C	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		
1	D	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



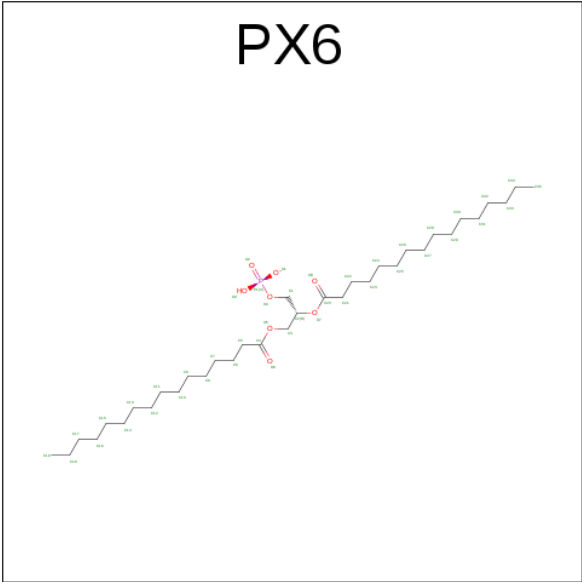
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	

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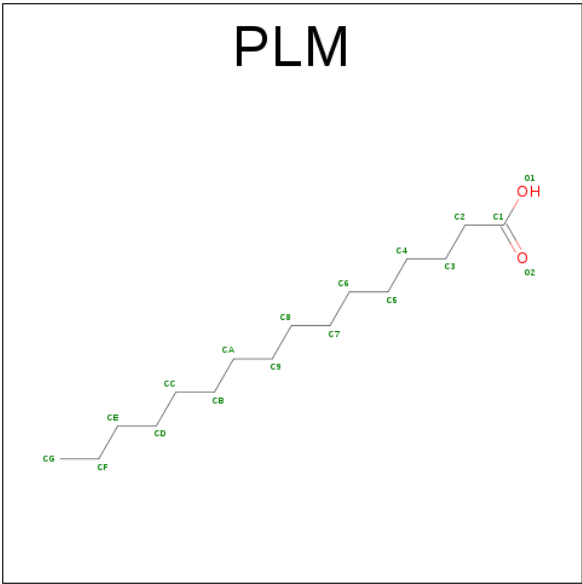
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	

- Molecule 3 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C₃₅H₆₈O₈P).



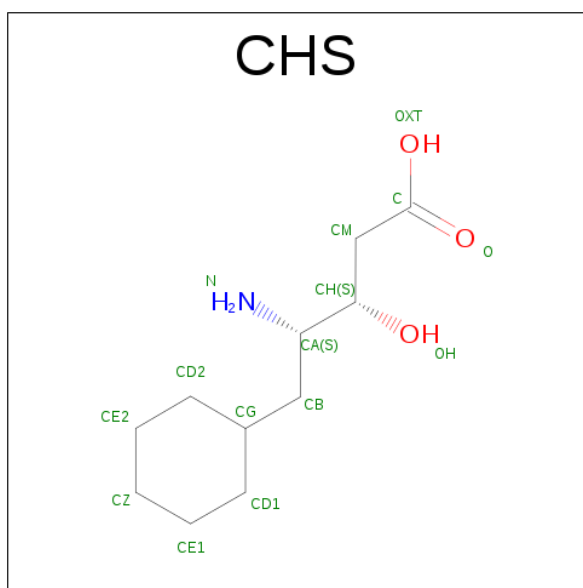
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			54	48	6	
4	A	1	Total	C	O	0
			54	48	6	
4	A	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	

- Molecule 5 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: $C_{11}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			30	22	2	6	
5	A	1	Total	C	N	O	0
			30	22	2	6	
5	B	1	Total	C	N	O	0
			30	22	2	6	
5	B	1	Total	C	N	O	0
			30	22	2	6	
5	C	1	Total	C	N	O	0
			30	22	2	6	
5	C	1	Total	C	N	O	0
			30	22	2	6	
5	D	1	Total	C	N	O	0
			30	22	2	6	
5	D	1	Total	C	N	O	0
			30	22	2	6	

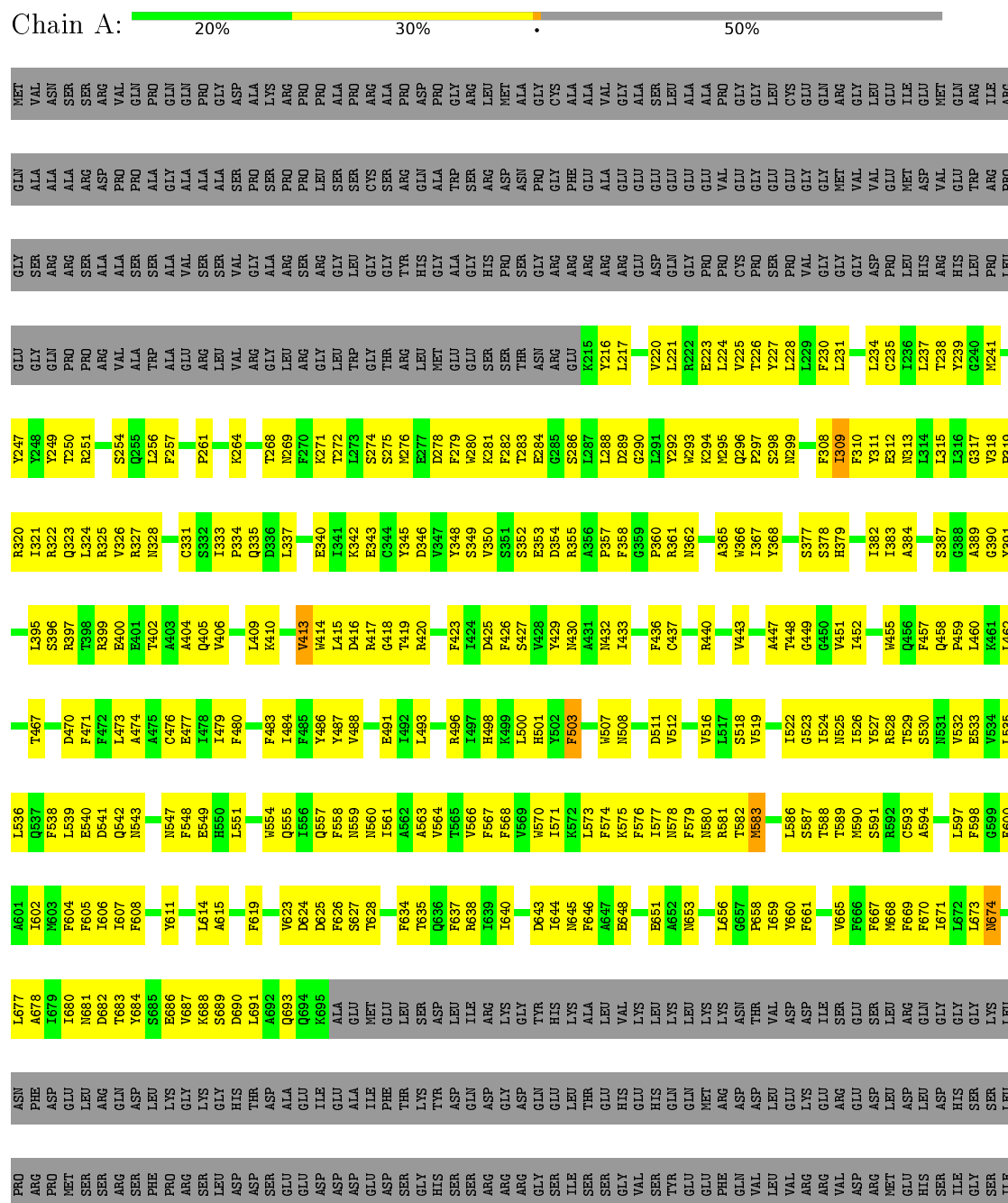
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	A	4	Total	Ca	0
			4	4	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Polycystin-2



VAL	GLU
SER	SER
LYS	ASP
ILE	ASP
ASP	ALA
ALA	ALA
VAL	SER
ILE	GLN
VAL	ILE
LYS	ILE
LEU	HIS
GLU	GLY
ILE	LEU
MET	GLY
GLU	THR
ARG	PRO
ARG	LYS
ALA	VAL
LYS	GLY
LEU	PRO
LYS	LEU
ARG	ASN
ARG	GLY
GLU	GLN
GLU	ARG
VAL	PRO
VAL	ALA
ASP	GLY
GLY	THR
ARG	ASP
LEU	LEU
LEU	ASP
ASP	PRO
GLY	GLY
ARG	ALA
LEU	SER
LEU	SER
GLY	GLN
ASP	ASP
GLY	THR
ARG	GLU
LEU	GLY
LEU	GLY
GLY	MET
ARG	GLU
LEU	ALA
GLY	GLY
ASP	ALA
GLY	PRO
ILE	GLY
HIS	GLY
ASP	ASN
GLY	SER
GLU	SER
GLN	SER
MET	ASN
GLY	VAL
ARG	HIS
ARG	VAL
VAL	VAL
GLU	ARG
GLU	GLU
LEU	GLU
LEU	GLU
GLU	GLU
ASP	ARG
GLN	ILE
ASP	TRP

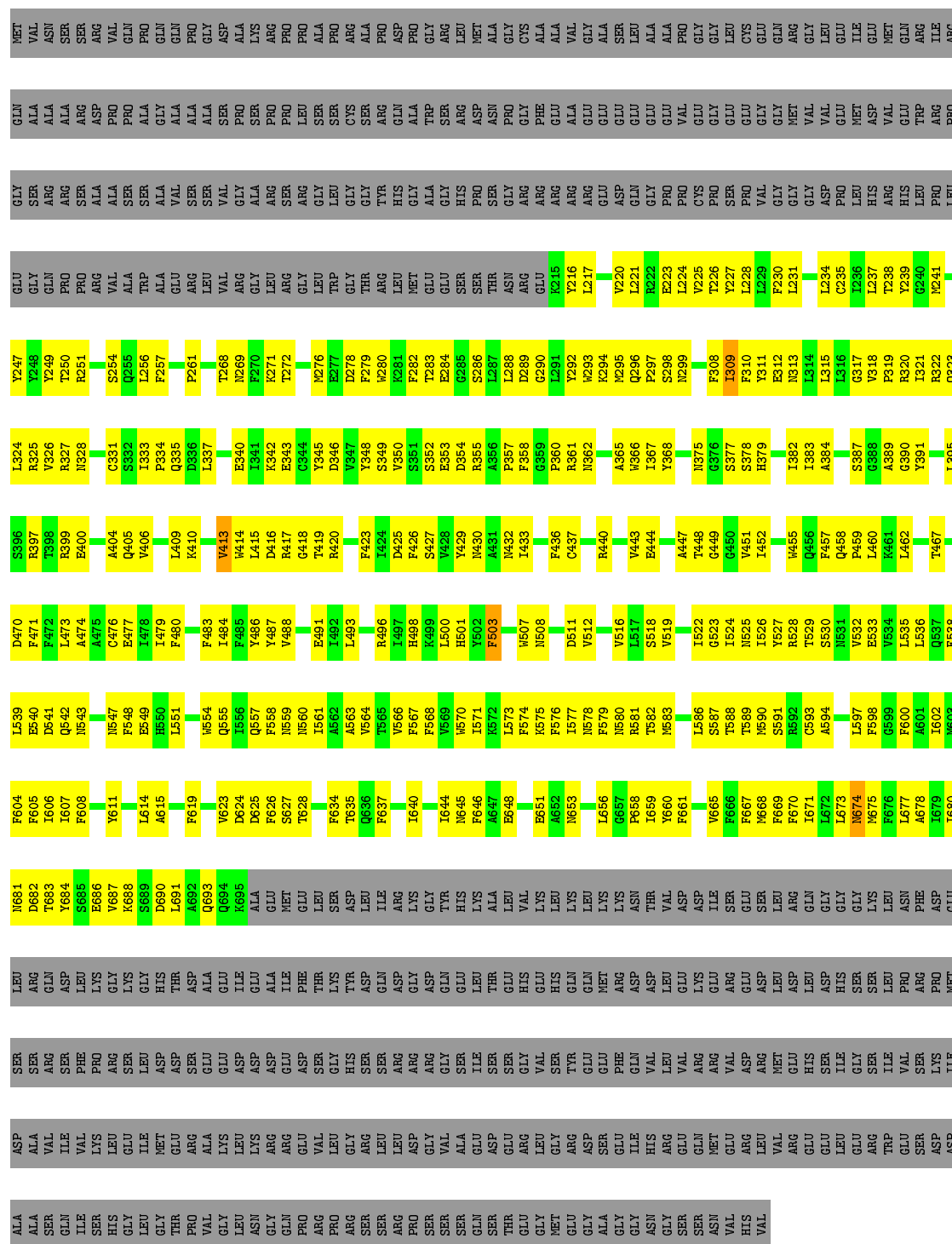
● Molecule 1: Polycystin-2



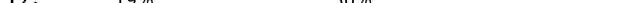
MET	GLN	GLY	GLU	Y247	R325	T398	A474	N647	Y611	E886	LYS	PRO	LYS
VAL	ALA	SER	GLY	T246	V326	R399	A475	N648	L614	V687	GLY	ARG	GLY
ASN	ALA	ARG	GLN	T249	R327	E400	E476	F548	A615	K688	LYS	SER	LYS
SER	ALA	ARG	PRO	T250	N328		E477	E549			GLY	LEU	GLY
ARG	ASP	SER	ASP	R251		A404	I478	H550	F619	D690	HIS	ASP	HIS
VAL	PRO	ALA	ARG		C331	A405	I479	L551		L691	THR	ASP	THR
GLN	PRO	ALA	VAL	S254	S332	V406	F480		V623	A692	ASP	SER	ASP
PRO	ALA	SER	ALA	Q256	I333	L409	F483	M554	D625	Q693	ALA	GLU	ALA
GLN	ALA	SER	TRP	L256	P334	K410	I484	Q555	D626	Q694	ILE	GLU	ILE
VAL	GLY	ALA	ALA	F257	Q335	K413	F485	I556	F626	K695	GLY	ASP	GLY
GLN	ALA	VAL	GLU		D336	V414	Y486	Q557	S627		ALA	ASP	GLY
PRO	ALA	SER	ARG	P261	L337	H414	Y487	F558	T628		ILE	GLU	ILE
GLY	SER	VAL	LEU		E340	L415	V488	N559			PHE	ASP	PHE
ASP	PRO	GLY	VAL	T268		D416		N560	F634		THR	ASP	THR
ALA	ALA	GLY	ARG	I269	E343	R417	E491	A563	T635		LYS	SER	LYS
PRO	GLY	ARG	GLY	T270	C344	G418	I492	V564	T636		LYS	GLY	GLY
ARG	ALA	SER	TRP	K271	G345	T419	F493	F569	D643		THR	GLY	THR
PRO	PRO	ARG	ARG	T272	Y345	T420	L493	T565	F637		GLN	SER	GLN
LEU	LEU	ARG	GLY		D346	R420	R496	V566	R638		ASP	ARG	ASP
ASN	SER	GLY	LEU	P276	V347		F497	F567	R639		ARG	ARG	ARG
PRO	SER	LEU	TRP	E277	Y348	F423	I497	F568	I640		LYS	GLY	LYS
GLY	GLY	GLY	GLY	D278	S349	I424	K498	N570	D643		GLY	GLY	GLY
ARG	GLN	TRP	GLY	F279	V350	D425	K499	F571	I644		THR	GLY	THR
VAL	ALA	ARG	ALA	K280	S351	F426	L500	I571	M645		GLU	SER	GLU
ASP	GLN	HIS	HIS	K281	S352	S427	H501	K572	M646		LEU	ILE	ILE
PRO	ALA	GLY	MET	F282	E353	V428	F502	L573	F646		THR	SER	SER
GLY	TRP	ALA	GLY	T283	D354	Y429	F503	F574	A647		GLU	ASP	GLU
SER	ALA	TRP	GLY	E284	R355	M430	F507	K575	B648		GLY	ARG	ARG
LEU	ARG	ARG	HIS	K285	A356	M432	M507	F576	E651		LYS	VAL	LYS
ASP	ASN	SER	SER	S286	P357	L433	N508	I577	M652		GLY	THR	GLY
GLY	PRO	ALA	ASN		F358			N578	A653		GLN	GLY	GLN
SER	PRO	SER	GLY	D289	G359	F436	D511	F579	M653		GLN	GLY	GLY
ALA	CYS	SER	ARG	G290	P360	C437	V512	N580	L656		MET	GLY	GLY
GLN	ALA	GLY	PHE	L291	R361		V516	R581	G657		ARG	PHE	ARG
ALA	ALA	GLY	ALA	Y292	N362		L517	T582			ASP	GLN	ASP
VAL	VAL	ARG	ALA	K293		R440	L518	M583	P658		ASP	VAL	ASP
GLY	GLY	GLU	ALA	K294	A365	V443	S518		I659		LEU	VAL	LEU
ALA	ALA	GLY	GLY	K295	V366	E444	V519	L586	V660		GLU	VAL	GLU
SER	LEU	SER	GLY	Q296	I367			S587			LYS	ARG	LYS
ALA	ALA	GLY	ALA	F297	Y368		T522	T588	V665		ILE	ARG	ILE
PRO	ALA	PRO	ALA	S298		A447	G523	T589	F666		ARG	VAL	ARG
GLY	VAL	GLY	VAL	N299	N375	T448	I524	M590	F667		GLY	ASP	GLY
ILE	GLY	PRO	VAL		G376	G449	M525	S591	M668		ASP	ARG	ASP
GLY	GLY	GLY	PRO	F308	S377	G450	I526	R592	M669		LEU	MET	LEU
ASN	ASN	GLY	PRO	I309	S378	V451	Y527	C593	F670		GLY	GLY	GLY
GLY	LEU	LEU	GLY	F310	H379	I452	R528	A594			ASP	LEU	ASP
SER	CYS	GLY	VAL	Y311			T529		L672		ASP	SER	ASP
GLY	GLY	GLY	GLY	E312	I382	M455	S530	L597	L673		HIS	GLY	GLY
SER	GLY	GLY	GLY	F230	I383	Q456	M531	F598	M674		SER	GLY	GLY
ASN	GLY	GLY	MET	L231	A384	F457	V532	G599	M675		SER	SER	SER
VAL	VAL	GLY	GLY			Q458		F600	F676		LEU	ILE	ILE
ARG	VAL	ASP	VAL	L234	S387	P459	L535	A601	L677		PRO	VAL	VAL
LEU	GLY	LEU	ASP	C235	G388	L460	L536	F602	M678		ARG	VAL	SER
VAL	ILE	PRO	ILE	I236	V318	G317	Q537	M603	A679		ARG	SER	SER
GLU	ASP	GLY	VAL	L237	G390	P319	F538	F604	L680		PRO	ILE	ASP
GLY	VAL	ARG	VAL	T238	Y391	T467	L539	F605	M681		MET	ASP	ASP
MET	GLY	ARG	GLY	Y239	I321	D470	E540	I606	D682		SER	ALA	ALA
LEU	TRP	GLY	GLY	G240	R322	F471	D541	F607	T683		SER	ALA	ALA
ARG	ILE	PRO	PRO	M241	Q323	F472	Q542	F608	Y684		ARG	VAL	SER
TRP	ARG	LEU	LEU			L473	N543		S685		PHE	VAL	VAL

- Molecule 1: Polycystin-2

Chain C:  20% 29% 50%



- Molecule 1: Polycystin-2

Chain D:  19% 30% 50%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	35318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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: PLM, CHS, CA, PX6, 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 >2	RMSZ	# Z >2
1	A	0.52	0/4068	0.57	0/5521
1	B	0.52	0/4065	0.57	0/5518
1	C	0.52	0/4065	0.57	0/5518
1	D	0.52	0/4065	0.57	0/5518
All	All	0.52	0/16263	0.57	0/22075

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PHE	Peptide
1	B	579	PHE	Peptide
1	C	579	PHE	Peptide
1	D	579	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3962	0	3898	287	0
1	B	3959	0	3891	278	0
1	C	3959	0	3891	275	0
1	D	3959	0	3891	277	0
2	A	70	0	64	15	0
2	B	70	0	64	18	0
2	C	70	0	64	18	0
2	D	70	0	64	16	0
3	A	40	0	56	2	0
3	B	40	0	56	4	0
3	C	40	0	56	5	0
3	D	40	0	56	4	0
4	A	54	0	93	5	0
4	B	54	0	93	5	0
4	C	54	0	93	4	0
4	D	54	0	93	4	0
5	A	30	0	40	2	0
5	B	30	0	40	2	0
5	C	30	0	40	1	0
5	D	30	0	40	2	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
All	All	16620	0	16583	1082	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 33.

The worst 5 of 1082 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:299:ASN:HD22	2:D:1005:NAG:C1	1.10	1.59
1:C:299:ASN:HD22	2:C:1005:NAG:C1	1.17	1.58
1:C:375:ASN:ND2	2:C:1003:NAG:C1	1.68	1.56
1:B:299:ASN:HD22	2:B:1005:NAG:C1	1.17	1.55
1:B:375:ASN:ND2	2:B:1003:NAG:C1	1.68	1.55

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	A	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	B	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	C	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	D	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
All	All	1916/3872 (50%)	1676 (88%)	224 (12%)	16 (1%)	29	69

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	THR
1	B	628	THR
1	C	628	THR
1	D	628	THR
1	A	674	ASN

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	A	432/837 (52%)	429 (99%)	3 (1%)	88	94
1	B	431/837 (52%)	429 (100%)	2 (0%)	92	96
1	C	431/837 (52%)	429 (100%)	2 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	431/837 (52%)	429 (100%)	2 (0%)	92	96
All	All	1725/3348 (52%)	1716 (100%)	9 (0%)	92	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	623	VAL
1	D	623	VAL
1	C	623	VAL
1	A	623	VAL
1	C	503	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	630	GLN
1	C	299	ASN
1	D	299	ASN
1	B	430	ASN
1	D	379	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 5 are monoatomic - leaving 44 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	$\# Z > 2$
2	NAG	A	1001	1	14,14,15	0.31	0	15,19,21	0.42	0
2	NAG	A	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	A	1003	2	14,14,15	0.33	0	15,19,21	0.55	0
2	NAG	A	1004	2	14,14,15	0.95	1 (7%)	15,19,21	0.50	0
2	NAG	A	1005	-	14,14,15	0.32	0	15,19,21	0.28	0
3	PX6	A	1006	-	39,39,43	1.41	5 (12%)	43,44,48	1.53	5 (11%)
4	PLM	A	1007	-	14,17,17	0.22	0	14,17,17	0.43	0
4	PLM	A	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	A	1009	-	14,17,17	0.23	0	14,17,17	0.47	0
5	CHS	A	1010	-	12,15,15	0.52	0	12,19,19	0.63	0
5	CHS	A	1011	-	12,15,15	0.34	0	12,19,19	0.76	0
2	NAG	B	1001	1	14,14,15	0.32	0	15,19,21	0.42	0
2	NAG	B	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	B	1003	2	14,14,15	0.34	0	15,19,21	0.54	0
2	NAG	B	1004	2	14,14,15	0.96	1 (7%)	15,19,21	0.51	0
2	NAG	B	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	B	1006	-	39,39,43	1.41	5 (12%)	43,44,48	1.52	5 (11%)
4	PLM	B	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	B	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	B	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	B	1010	-	12,15,15	0.50	0	12,19,19	0.63	0
5	CHS	B	1011	-	12,15,15	0.34	0	12,19,19	0.72	0
2	NAG	C	1001	1	14,14,15	0.32	0	15,19,21	0.43	0
2	NAG	C	1002	1	14,14,15	0.34	0	15,19,21	0.19	0
2	NAG	C	1003	2	14,14,15	0.34	0	15,19,21	0.54	0
2	NAG	C	1004	2	14,14,15	0.95	1 (7%)	15,19,21	0.50	0
2	NAG	C	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	C	1006	-	39,39,43	1.42	5 (12%)	43,44,48	1.52	5 (11%)
4	PLM	C	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	C	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	C	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	C	1010	-	12,15,15	0.50	0	12,19,19	0.62	0
5	CHS	C	1011	-	12,15,15	0.36	0	12,19,19	0.76	0
2	NAG	D	1001	1	14,14,15	0.32	0	15,19,21	0.42	0
2	NAG	D	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	D	1003	2	14,14,15	0.34	0	15,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1004	2	14,14,15	0.96	1 (7%)	15,19,21	0.50	0
2	NAG	D	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	D	1006	-	39,39,43	1.42	5 (12%)	43,44,48	1.52	5 (11%)
4	PLM	D	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	D	1008	-	14,17,17	0.17	0	14,17,17	0.68	0
4	PLM	D	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	D	1010	-	12,15,15	0.50	0	12,19,19	0.61	0
5	CHS	D	1011	-	12,15,15	0.36	0	12,19,19	0.74	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
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	A	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	A	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	A	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	A	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	A	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	A	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	B	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	B	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	B	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	B	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	B	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	B	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1005	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX6	C	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	C	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	C	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	C	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	C	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	C	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	D	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	D	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	D	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	D	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	D	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	D	1011	-	-	0/10/20/20	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1006	PX6	O7-C2	-2.86	1.38	1.46
3	B	1006	PX6	O7-C2	-2.86	1.38	1.46
3	D	1006	PX6	O7-C2	-2.83	1.39	1.46
3	A	1006	PX6	O7-C2	-2.82	1.39	1.46
3	D	1006	PX6	P1-O3	-2.28	1.46	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1006	PX6	O3-P1-O1	-2.42	100.95	110.60
3	B	1006	PX6	O3-P1-O1	-2.41	100.99	110.60
3	C	1006	PX6	O3-P1-O1	-2.41	100.99	110.60
3	D	1006	PX6	O3-P1-O1	-2.40	101.01	110.60
3	D	1006	PX6	O3-P1-O4	2.17	110.60	105.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	3	0
2	A	1002	NAG	10	0
2	A	1005	NAG	2	0
3	A	1006	PX6	2	0
4	A	1007	PLM	4	0
4	A	1008	PLM	1	0
5	A	1010	CHS	1	0
5	A	1011	CHS	1	0
2	B	1001	NAG	3	0
2	B	1002	NAG	10	0
2	B	1003	NAG	3	0
2	B	1005	NAG	2	0
3	B	1006	PX6	4	0
4	B	1007	PLM	4	0
4	B	1008	PLM	1	0
5	B	1010	CHS	1	0
5	B	1011	CHS	1	0
2	C	1001	NAG	3	0
2	C	1002	NAG	10	0
2	C	1003	NAG	3	0
2	C	1005	NAG	2	0
3	C	1006	PX6	5	0
4	C	1007	PLM	3	0
4	C	1008	PLM	1	0
5	C	1010	CHS	1	0
2	D	1001	NAG	3	0
2	D	1002	NAG	10	0
2	D	1003	NAG	1	0
2	D	1005	NAG	2	0
3	D	1006	PX6	4	0
4	D	1007	PLM	3	0
4	D	1009	PLM	1	0
5	D	1010	CHS	1	0
5	D	1011	CHS	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.