



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 8, 2017 – 12:16 PM EST

PDB ID : 5MKE  
EMDB ID: : EMD-3523  
Title : cryoEM Structure of Polycystin-2 in complex with cations and lipids  
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.  
Deposited on : 2016-12-04  
Resolution : 4.30 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](mailto: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.

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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

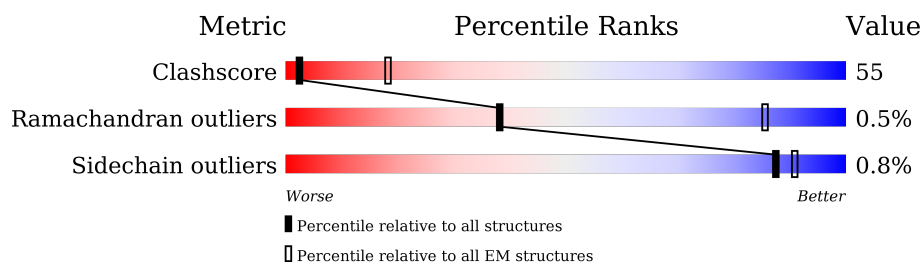
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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  $\geq 3$ , 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](#)

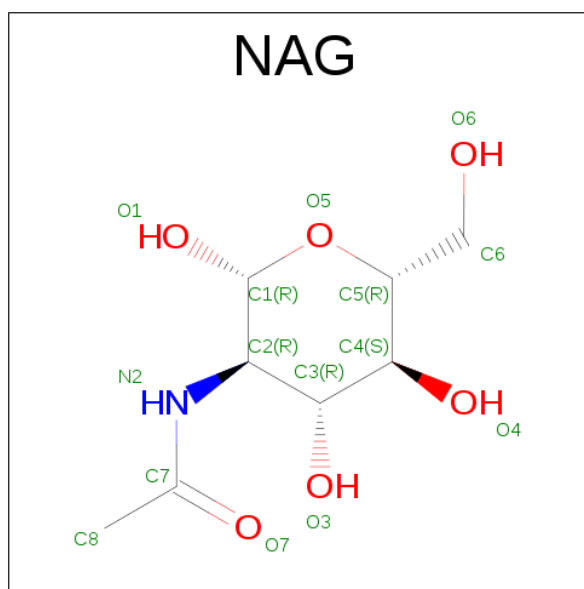
There are 6 unique types of molecules in this entry. The entry contains 16426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	B	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	C	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	D	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



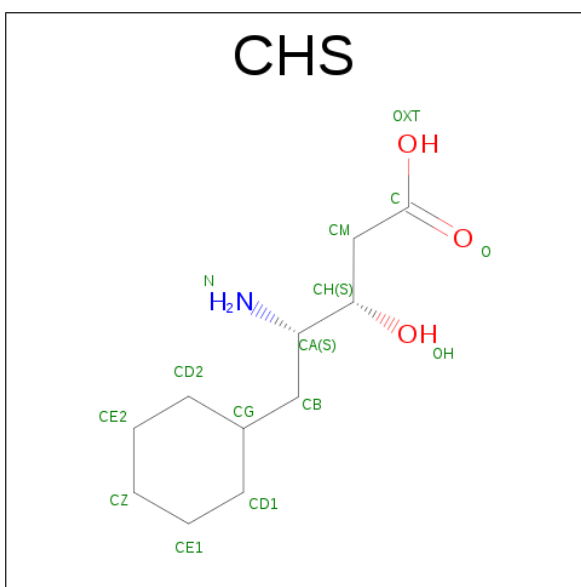
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	A	1	Total	C	N	O	0
			56	32	4	20	

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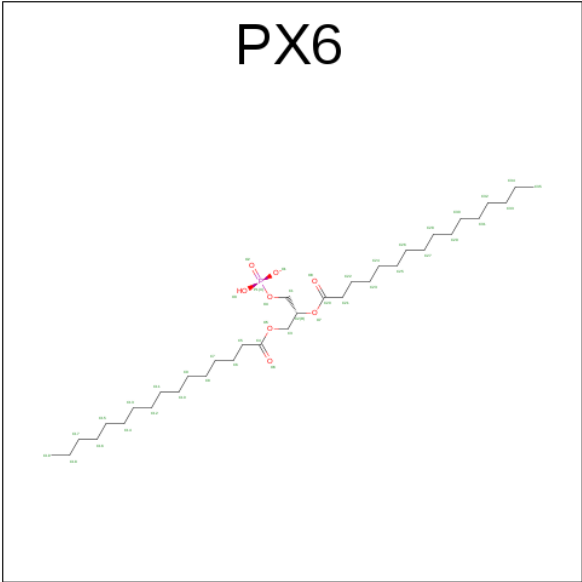
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	D	1	Total	C	N	O	0
			56	32	4	20	
2	D	1	Total	C	N	O	0
			56	32	4	20	
2	D	1	Total	C	N	O	0
			56	32	4	20	
2	D	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 3 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: C<sub>11</sub>H<sub>21</sub>NO<sub>3</sub>).



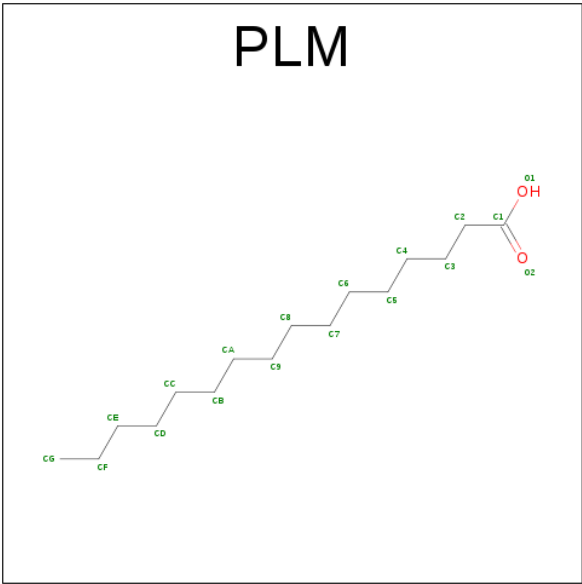
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			30	22	2	6	
3	A	1	Total	C	N	O	0
			30	22	2	6	
3	B	1	Total	C	N	O	0
			30	22	2	6	
3	B	1	Total	C	N	O	0
			30	22	2	6	
3	C	1	Total	C	N	O	0
			30	22	2	6	
3	C	1	Total	C	N	O	0
			30	22	2	6	
3	D	1	Total	C	N	O	0
			30	22	2	6	
3	D	1	Total	C	N	O	0
			30	22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

- Molecule 4 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>8</sub>P).



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

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



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

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

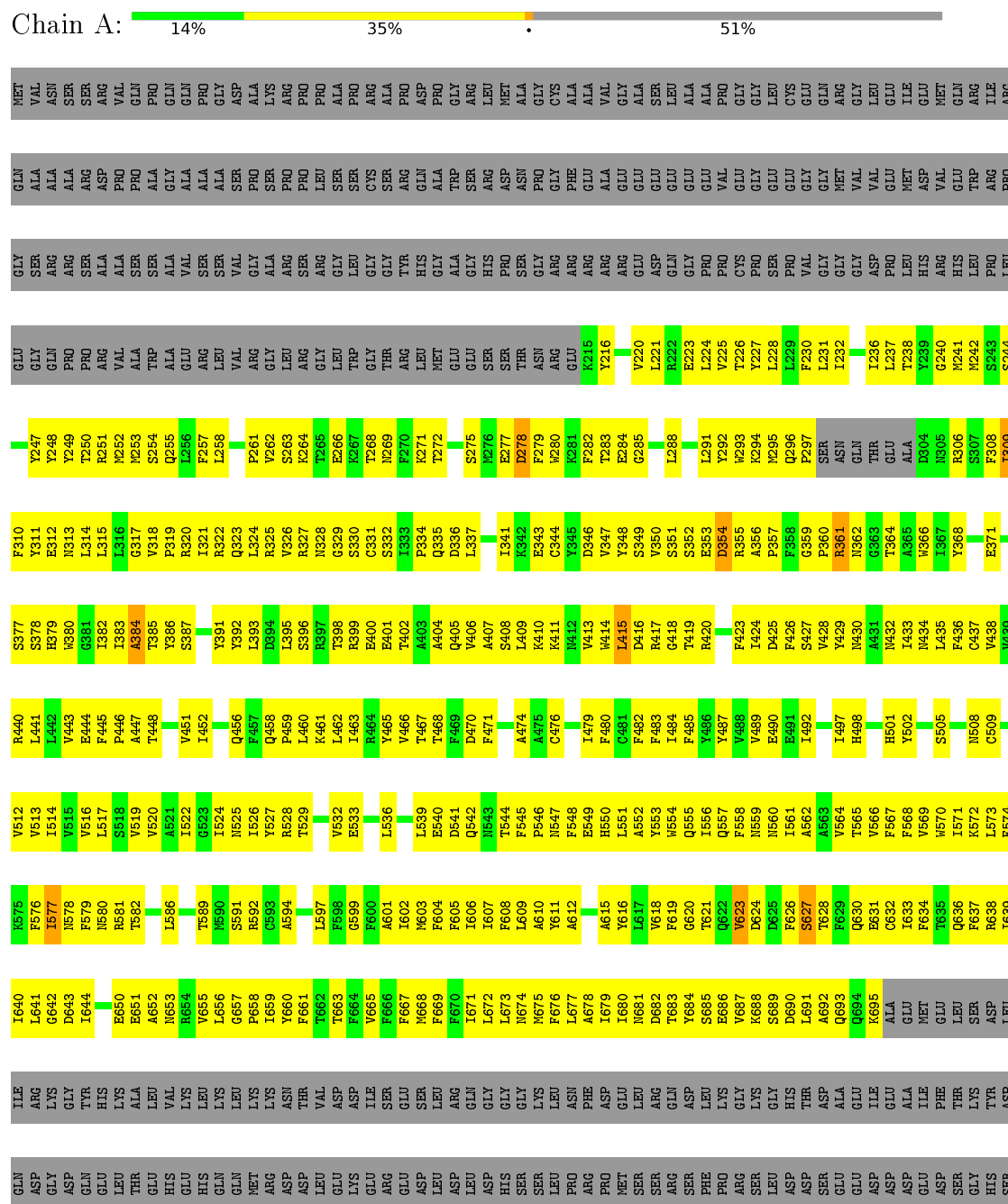
Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Ca	0
			2	2	



### 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




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

- Molecule 1: Polycystin-2

Chain B:  13% 34% . 51%

MET	VAL	ASN	SER	ARG	VAL	GLN	PRO	GLN	GLN	PRO	GLY	ASP	LYS	ALA	ALA	ALA	ARG	PRO	PRO	PRO	PRO	ASP	PRO	PRO	GLY	GLY	CYS	ALA	ALA	VAL	GLY	GLY	GLY	GLY	CYS	GLY	GLN	GLN	ARG	GLY	LEU	LEU	CYS	LEU	LEU	ILE	GLU	MET	GLU	GLN	GLN	ARG	ILE	ILE
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GLN  
ALA  
ALA  
ALA  
ARG  
ASP  
PRO  
PRO  
PRO  
GLY  
ALA  
ALA  
ALA  
ALA  
SER  
PRO  
SER  
PRO  
PRO  
LEU  
SER  
SER  
CYS  
ARG  
GLN  
ALA  
TRP  
PHE  
GLY  
GLU  
ALA  
GLU  
GLU  
GLU  
GLU  
GLU  
VAL  
GLU  
GLY  
GLY  
GLU  
GLU  
GLY  
MET  
VAL  
VAL  
GLU  
MET  
ASP  
VAL  
GLU  
TRP  
ARG

[illegible]

GLU	GLY	GLU	PRO	PRO	ARG	VAL	TRP	ALA	ALA	GLU	ARG	GLU	LEU	VAL	ARG	GLY	GLY	THR	ARG	LEU	MET	GLU	GLU	SER	SER	THR	ASU	ARG	GLU	<b>Z115</b>	<b>Z116</b>	Z220	Z221	<b>Z222</b>	<b>Z223</b>	Z224	Z225	Z226	Z227	Z228	<b>Z229</b>	Z230	Z231	Z232	<b>Z233</b>	Z236	Z237	Z238	<b>Z239</b>	Z240	M241	M242	<b>S243</b>
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	Y247	Y248	Y249	Y250	Y251	Y252	Y253	Y254	Y255	Y256	Y257	Y258		P261	Y262	S263	S264		S265	S266	S267	S268	S269	S270	S271	S272		S275		S278	S279	S280	S281	S282	S283	S284	S285		S288		S291	S292	S293	S294	S295	S296	S297	SER	ASN	GLN	THR	GLU	ALA		S304	S305	S306		S307	S308	S309
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Y311	E312	N313	L314	L315	L316	G317	V318	P319	R320	I321	R322	Q323	L324	R325	V326	R327	N328	G329	S330	C331	S332	L333	P334	Q335	D336	L337	L341	E342	E343	C344	V345	D346	V347	V348	S349	V350	S351	S352	E353	D354	R355	A356	P357	R358	G359	P360	R361	N362	G363	L364	L365	V366	L367	V368	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000
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S378	S379	S380	S381	S382	S383	S384	S385	S386	S387
S388	S389	S390	S391	S392	S393	S394	S395	S396	S397
S398	S399	S400	S401	S402	S403	S404	S405	S406	S407
S408	S409	S410	S411	S412	S413	S414	S415	S416	S417
S418	S419	S420	S421	S422	S423	S424	S425	S426	S427
S428	S429	S430	S431	S432	S433	S434	S435	S436	S437
S438	S439	S440	S441	S442	S443	S444	S445	S446	S447
S448	S449	S450	S451	S452	S453	S454	S455	S456	S457
S458	S459	S460	S461	S462	S463	S464	S465	S466	S467
S468	S469	S470	S471	S472	S473	S474	S475	S476	S477
S478	S479	S480	S481	S482	S483	S484	S485	S486	S487
S488	S489	S490	S491	S492	S493	S494	S495	S496	S497
S498	S499	S500	S501	S502	S503	S504	S505	S506	S507
S508	S509	S510	S511	S512	S513	S514	S515	S516	S517
S518	S519	S520	S521	S522	S523	S524	S525	S526	S527
S528	S529	S530	S531	S532	S533	S534	S535	S536	S537
S538	S539	S540	S541	S542	S543	S544	S545	S546	S547
S548	S549	S550	S551	S552	S553	S554	S555	S556	S557
S558	S559	S560	S561	S562	S563	S564	S565	S566	S567
S568	S569	S570	S571	S572	S573	S574	S575	S576	S577
S578	S579	S580	S581	S582	S583	S584	S585	S586	S587
S588	S589	S590	S591	S592	S593	S594	S595	S596	S597
S598	S599	S600	S601	S602	S603	S604	S605	S606	S607
S608	S609	S610	S611	S612	S613	S614	S615	S616	S617
S618	S619	S620	S621	S622	S623	S624	S625	S626	S627
S628	S629	S630	S631	S632	S633	S634	S635	S636	S637
S638	S639	S640	S641	S642	S643	S644	S645	S646	S647
S648	S649	S650	S651	S652	S653	S654	S655	S656	S657
S658	S659	S660	S661	S662	S663	S664	S665	S666	S667
S668	S669	S670	S671	S672	S673	S674	S675	S676	S677
S678	S679	S680	S681	S682	S683	S684	S685	S686	S687
S688	S689	S690	S691	S692	S693	S694	S695	S696	S697
S698	S699	S700	S701	S702	S703	S704	S705	S706	S707
S708	S709	S710	S711	S712	S713	S714	S715	S716	S717
S718	S719	S720	S721	S722	S723	S724	S725	S726	S727
S728	S729	S730	S731	S732	S733	S734	S735	S736	S737
S738	S739	S740	S741	S742	S743	S744	S745	S746	S747
S748	S749	S750	S751	S752	S753	S754	S755	S756	S757
S758	S759	S760	S761	S762	S763	S764	S765	S766	S767
S768	S769	S770	S771	S772	S773	S774	S775	S776	S777
S778	S779	S780	S781	S782	S783	S784	S785	S786	S787
S788	S789	S790	S791	S792	S793	S794	S795	S796	S797
S798	S799	S800	S801	S802	S803	S804	S805	S806	S807
S808	S809	S810	S811	S812	S813	S814	S815	S816	S817
S818	S819	S820	S821	S822	S823	S824	S825	S826	S827
S828	S829	S830	S831	S832	S833	S834	S835	S836	S837
S838	S839	S840	S841	S842	S843	S844	S845	S846	S847
S848	S849	S850	S851	S852	S853	S854	S855	S856	S857
S858	S859	S860	S861	S862	S863	S864	S865	S866	S867
S868	S869	S870	S871	S872	S873	S874	S875	S876	S877
S878	S879	S880	S881	S882	S883	S884	S885	S886	S887
S888	S889	S890	S891	S892	S893	S894	S895	S896	S897
S898	S899	S900	S901	S902	S903	S904	S905	S906	S907
S908	S909	S910	S911	S912	S913	S914	S915	S916	S917
S918	S919	S920	S921	S922	S923	S924	S925	S926	S927
S928	S929	S930	S931	S932	S933	S934	S935	S936	S937
S938	S939	S940	S941	S942	S943	S944	S945	S946	S947
S948	S949	S950	S951	S952	S953	S954	S955	S956	S957
S958	S959	S960	S961	S962	S963	S964	S965	S966	S967
S968	S969	S970	S971	S972	S973	S974	S975	S976	S977
S978	S979	S980	S981	S982	S983	S984	S985	S986	S987
S988	S989	S990	S991	S992	S993	S994	S995	S996	S997
S998	S999	S1000	S1001	S1002	S1003	S1004	S1005	S1006	S1007

L441	L442	L443	L444	L445	L446	L447	L448	L451	L452	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L474	L475	L476	L477	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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[illegible]

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L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	ALA	GLU	GLU	GLU	LEU	LEU	SER
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LEU ILE ARG GLY TYR HIS LYS LEU VAL LYS LYS LYS LYS ASN THR VAL ASP ASP ILE SER GLU GLU SER SER LEU ARG GLN GLY GLY GLY LYS LEU ASN PHE ASP ASP GLU LEU ARG GLN ASP LEU LYS GLY LYS GLY HIS THR ASP ALA ALA LEU GLU LEU GLU ILE ALA ILE PHE THR LYS

ASP	GLN	ASP	GLY	ASP	GLN	LEU	THR	GLU	HIS	HIS	GLJ	GLN	GLN	GLN	NET	ARG	ASP	ASP	LEU	GLU	LYS	GLU	GLU	ARG	GLU	GLU	ASP	ASP	SER	SER	SER	SER	PRO	ARG	PRO	PRO	PRO	ARG	ARG	SER	SER	LEU	ASP	ASP	GLU	GLU	ASP	ASP	GLU	GLY
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GLN	ASP	ILE	I640	K576	V512	L441	S378	Y311	Y247	GLU	GLY	GLN	ALA	ASP	VAL	SER	SER
ASP	GLY	ARG	L641	F576	V513	L442	H379	E312	Y248	GLY	SER	ALA	ASP	ARG	ARG	ARG	ARG
GLY	ASP	LYS	G642	N577	V514	V443	G380	N313	Y249	ASP	ARG	ALA	SER	PRO	ASP	LEU	LEU
GLN	GLN	THR	I643	N578	V515	F444	G381	L314	Y250	PRO	ARG	ALA	ALA	ARG	VAL	GLY	ARG
GLU	GLY	HIS	I644	N579	V516	F445	I382	L315	Y251	PRO	SER	ALA	ASP	SER	VAL	GLY	GLY
LEU	LEU	LYS	E650	N580	S518	F446	I383	L316	Y252	VAL	ALA	ALA	PRO	SER	ALA	SER	SER
THR	LEU	ALA	E651	N581	S519	F447	O384	G317	Y253	GLN	ALA	SER	ALA	GLN	LEU	ILE	ILE
GLU	GLU	LEU	A652	T582	V520	T448	T386	P319	Y254	TRP	SER	ALA	PRO	THR	ASP	SER	SER
HIS	GLU	VAL	R653	L586	A521	V451	Y386	R320	Y255	ALA	ALA	ALA	ALA	GLY	ARG	GLY	GLY
GLU	GLU	LYS	R654	L587	I522	I452	S387	I321	Y256	GLU	VAL	ALA	GLY	THR	ARG	ARG	ARG
HIS	LEU	LYS	V655	T589	G523	Q456	Y391	I322	Y257	ARG	ALA	ALA	PRO	GLY	VAL	VAL	VAL
GLN	LYS	LYS	L656	N590	I524	F457	Y392	Q323	Y258	LEU	SER	SER	ALA	GLY	GLY	THR	THR
GLN	LEU	LEU	G657	S591	N525	F458	L393	L324		ASP	VAL	VAL	ALA	ASP	ARG	ARG	ARG
MET	GLY	LYS	P658	N592	I526	Q458	D394	R325	Y261	LYS	GLY	GLY	PRO	GLY	ASP	ASP	ASP
ASP	ARG	LYS	C593	R592	Y527	F459	S396	V326	Y262	ASP	ALA	ALA	LYS	ALA	ASP	GLY	GLY
ASP	ASP	ASN	A594	A594	R528	L460	S397	R327	Y263	PRO	ARG	PRO	PRO	ALA	ARG	GLY	GLY
ASP	THR	THR	F661	F661	T529	K461	T398	N328	Y264	PRO	ARG	PRO	PRO	ALA	VAL	GLY	GLY
LEU	LEU	VAL	T662	L597	T529	L462	T398	G329	Y265	LEU	ARG	LEU	LEU	ASN	HIS	VAL	VAL
GLU	GLU	ASP	T663	F598	V532	L463	R399	S330	Y266	ALA	GLY	SER	SER	GLY	GLY	GLY	GLY
LYS	ASP	ASP	F664	N599	E533	F464	E400	C331	Y267	TRP	LEU	SER	PRO	ASP	VAL	LEU	LEU
GLU	GLU	ILE	V665	F600	Q542	V465	E401	S332	Y268	GLY	GLY	GLY	GLN	ARG	ARG	ARG	ARG
GLU	GLU	SER	F666	A601	L536	F466	T402	I333	Y269	THR	GLY	GLY	ASP	ASN	MET	MET	MET
GLU	GLU	GLU	F667	I602	L539	T467	A403	P334	Y270	ARG	THR	THR	GLN	VAL	GLY	VAL	VAL
SER	SER	LEU	M668	M603	E540	F468	A404	Q335	Y271	LEU	HIS	GLY	GLN	ASP	ARG	ASP	ASP
LEU	LEU	LEU	F669	F604	D541	F469	Q405	S386	Y272	MET	GLY	ALA	ALA	PRO	LEU	ARG	ARG
ASP	ASP	ARG	F670	F605	Q542	F471	V406	L337	Y273	GLU	ALA	TRP	ALA	PRO	VAL	LEU	LEU
ASP	ASP	GLN	I671	I606	Q542	F471	A407	I341	Y274	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	GLY	L672	L607	N543	F472	S408	R342	Y275	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
HIS	HIS	GLY	L673	T608	T544	A474	L409	E343	Y276	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	LYS	N674	L609	F545	A475	K410	C344	Y277	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	LYS	M675	L609	F546	C476	K411	F345	Y278	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
LEU	LEU	LYS	F676	A610	N547	C476	K412	F346	Y279	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
LEU	LEU	LYS	M677	L611	F548	F477	V413	F347	Y280	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
PRO	PRO	ASN	L678	A612	E549	F478	V414	F348	Y281	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	ASP	I679	A615	H550	C481	L415	F349	Y282	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
PRO	PRO	GLY	L680	L616	L551	F482	D416	S349	Y283	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
MET	MET	LEU	N681	L617	A552	F483	R417	V350	Y284	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	ARG	D682	L618	Y553	F484	G418	S351	Y285	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ARG	ARG	GLN	T683	F619	W554	F485	T419	S352	Y286	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	LYS	Y684	G620	Q555	F486	T419	E353	Y287	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
PHE	PHE	LEU	S685	T621	I556	F487	R420	D354	Y288	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
PRO	PRO	LYS	E686	G622	Q557	F488	F423	R355	Y289	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ARG	ARG	GLY	V687	G623	F558	V489	I424	R356	Y290	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ARG	ARG	LYS	K688	D624	N559	E490	D425	A356	Y291	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
LEU	LEU	GLY	S689	D625	N560	F491	F426	P357	Y292	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	HIS	D690	F626	I561	I492	S427	F358	Y293	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	THR	L691	S627	A562	I492	V428	G359	Y294	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	ASP	A692	T628	A563	I497	Y429	P360	Y295	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
GLU	GLU	ALA	Q693	F629	V564	H498	M430	R361	Y296	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
GLU	GLU	GLU	Q694	G630	V565	H498	M431	N362	Y297	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	ILE	K695	B631	T566	H501	M432	G363	Y298	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	GLU	ALA	C632	V567	Y502	I433	T364	Y299	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	ALA	GLU	I633	F568	F503	M434	W366	Y300	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
GLU	GLU	ILE	MET	I634	F569	R504	L435	I367	Y301	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
ASP	ASP	PHE	GLY	T635	W570	S505	F436	I368	Y302	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	THR	LEU	Q636	I571	S505	C437	Y368	Y303	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
GLY	GLY	LYS	SER	F637	K572	M508	C437	E371	Y304	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
HIS	HIS	THR	ASP	R638	L573	C509	V438	I309	Y305	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
SER	SER	ASP	LEU	I639	F574		V439	S243	Y306	GLY	ALA	ALA	ALA	ASP	VAL	VAL	VAL
							R440	S244									

● Molecule 1: Polycystin-2


Chain C: 14% 35% 51%

● Molecule 1: Polycystin-2

Chain D:

Position	Residue	Position	Residue	Position	Residue	Position	Residue	Position	Residue
1	ARG	21	GLY	41	GLY	61	GLY	81	GLY
2	LYS	22	GLN	42	ARG	62	GLY	82	GLY
3	GLY	23	ASP	43	ASP	63	GLY	83	GLY
4	ASP	24	ALA	44	GLY	64	GLY	84	GLY
5	GLN	25	ALA	45	GLY	65	GLY	85	GLY
6	THR	26	ARG	46	GLY	66	GLY	86	GLY
7	GLY	27	GLY	47	GLY	67	GLY	87	GLY
8	LYS	28	GLY	48	GLY	68	GLY	88	GLY
9	ALA	29	GLY	49	GLY	69	GLY	89	GLY
10	VAL	30	GLY	50	GLY	70	GLY	90	GLY
11	GLY	31	GLY	51	GLY	71	GLY	91	GLY
12	LEU	32	GLY	52	GLY	72	GLY	92	GLY
13	LEU	33	GLY	53	GLY	73	GLY	93	GLY
14	LEU	34	GLY	54	GLY	74	GLY	94	GLY
15	LEU	35	GLY	55	GLY	75	GLY	95	GLY
16	LEU	36	GLY	56	GLY	76	GLY	96	GLY
17	LEU	37	GLY	57	GLY	77	GLY	97	GLY
18	LEU	38	GLY	58	GLY	78	GLY	98	GLY
19	LEU	39	GLY	59	GLY	79	GLY	99	GLY
20	LEU	40	GLY	60	GLY	80	GLY	100	GLY

- Molecule 1: Polycystin-2

Chain D:  14% 34% . 51%

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

ARG
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ALA
GLY
GLY
ASN
GLY
SER
SER
ASN
VAL
HIS
VAL

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	42268	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	0.49	0/4031	0.62	2/5469 (0.0%)
1	B	0.49	0/4031	0.62	3/5469 (0.1%)
1	C	0.49	0/4031	0.62	3/5469 (0.1%)
1	D	0.49	0/4031	0.63	2/5469 (0.0%)
All	All	0.49	0/16124	0.62	10/21876 (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	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	278	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	278	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	278	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	384	ALA	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	LEU	Peptide
1	A	354	ASP	Peptide
1	A	361	ARG	Peptide
1	A	578	ASN	Peptide
1	A	627	SER	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	3926	0	3880	489	0
1	B	3926	0	3880	496	0
1	C	3926	0	3880	476	0
1	D	3926	0	3880	490	0
2	A	56	0	51	10	0
2	B	56	0	51	10	0
2	C	56	0	51	10	0
2	D	56	0	51	16	0
3	A	30	0	40	3	0
3	B	30	0	40	4	0
3	C	30	0	40	5	0
3	D	30	0	40	4	0
4	A	40	0	56	3	0
4	B	40	0	56	6	0
4	C	40	0	56	4	0
4	D	40	0	56	4	0
5	A	54	0	93	9	0
5	B	54	0	93	8	0
5	C	54	0	93	9	0
5	D	54	0	93	6	0
6	A	2	0	0	0	0
All	All	16426	0	16480	1816	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 55.

The worst 5 of 1816 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:A:606:ILE:CD1	1:D:573:LEU:HD11	1.21	1.66
1:A:606:ILE:HD11	1:D:573:LEU:CD1	1.26	1.63
1:A:573:LEU:CD1	1:B:606:ILE:HD11	1.17	1.62
1:C:573:LEU:HD11	1:D:606:ILE:CD1	1.18	1.58
1:B:573:LEU:CD1	1:C:606:ILE:HD11	1.15	1.57

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/968 (49%)	382 (81%)	87 (18%)	2 (0%)	39	80
1	B	471/968 (49%)	383 (81%)	86 (18%)	2 (0%)	39	80
1	C	471/968 (49%)	381 (81%)	88 (19%)	2 (0%)	39	80
1	D	471/968 (49%)	381 (81%)	87 (18%)	3 (1%)	30	74
All	All	1884/3872 (49%)	1527 (81%)	348 (18%)	9 (0%)	38	77

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	TYR
1	A	258	LEU
1	B	258	LEU
1	C	258	LEU
1	D	258	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/837 (51%)	426 (99%)	3 (1%)	88	94
1	B	429/837 (51%)	426 (99%)	3 (1%)	88	94
1	C	429/837 (51%)	426 (99%)	3 (1%)	88	94
1	D	429/837 (51%)	425 (99%)	4 (1%)	84	92
All	All	1716/3348 (51%)	1703 (99%)	13 (1%)	87	93

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	577	ILE
1	C	308	PHE
1	D	310	PHE
1	B	415	LEU
1	D	309	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	693	GLN
1	C	501	HIS
1	D	622	GLN
1	C	458	GLN
1	C	537	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 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	0.70	1 (7%)	15,19,21	0.81	1 (6%)
2	NAG	A	1002	1	14,14,15	0.39	0	15,19,21	1.15	2 (13%)
2	NAG	A	1003	1,2	14,14,15	0.48	0	15,19,21	1.15	2 (13%)
2	NAG	A	1004	2	14,14,15	0.38	0	15,19,21	1.16	2 (13%)
3	CHS	A	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	A	1006	-	12,15,15	0.42	0	12,19,19	0.61	0
4	PX6	A	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	A	1008	-	14,17,17	0.22	0	14,17,17	0.49	0
5	PLM	A	1009	-	14,17,17	0.17	0	14,17,17	0.69	0
5	PLM	A	1010	-	14,17,17	0.22	0	14,17,17	0.53	0
2	NAG	B	1001	1	14,14,15	0.60	0	15,19,21	0.79	1 (6%)
2	NAG	B	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	B	1003	1,2	14,14,15	0.49	0	15,19,21	1.14	2 (13%)
2	NAG	B	1004	2	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
3	CHS	B	1005	-	12,15,15	0.22	0	12,19,19	0.58	0
3	CHS	B	1006	-	12,15,15	0.40	0	12,19,19	0.61	0
4	PX6	B	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	B	1008	-	14,17,17	0.22	0	14,17,17	0.50	0
5	PLM	B	1009	-	14,17,17	0.17	0	14,17,17	0.68	0
5	PLM	B	1010	-	14,17,17	0.22	0	14,17,17	0.52	0
2	NAG	C	1001	1	14,14,15	0.54	0	15,19,21	0.66	1 (6%)
2	NAG	C	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	C	1003	1,2	14,14,15	0.45	0	15,19,21	1.13	2 (13%)
2	NAG	C	1004	2	14,14,15	0.40	0	15,19,21	1.17	2 (13%)
3	CHS	C	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	C	1006	-	12,15,15	0.40	0	12,19,19	0.60	0
4	PX6	C	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.59	4 (9%)
5	PLM	C	1008	-	14,17,17	0.22	0	14,17,17	0.51	0
5	PLM	C	1009	-	14,17,17	0.17	0	14,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PLM	C	1010	-	14,17,17	0.22	0	14,17,17	0.52	0
2	NAG	D	1001	1	14,14,15	0.88	1 (7%)	15,19,21	0.77	1 (6%)
2	NAG	D	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	D	1003	1	14,14,15	0.42	0	15,19,21	1.17	2 (13%)
2	NAG	D	1004	-	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
3	CHS	D	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	D	1006	-	12,15,15	0.40	0	12,19,19	0.62	0
4	PX6	D	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	D	1008	-	14,17,17	0.22	0	14,17,17	0.49	0
5	PLM	D	1009	-	14,17,17	0.17	0	14,17,17	0.68	0
5	PLM	D	1010	-	14,17,17	0.22	0	14,17,17	0.52	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
3	CHS	A	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	A	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	A	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	A	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	A	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	A	1010	-	-	0/13/15/15	0/0/0/0
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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
3	CHS	B	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	B	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	B	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	B	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	B	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	B	1010	-	-	0/13/15/15	0/0/0/0
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	1,2	-	0/6/23/26	0/1/1/1

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

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	PX6	O7-C2	-2.91	1.38	1.46
4	D	1007	PX6	O7-C2	-2.89	1.38	1.46
4	C	1007	PX6	O7-C2	-2.88	1.38	1.46
4	B	1007	PX6	O7-C2	-2.86	1.38	1.46
4	D	1007	PX6	P1-O3	-2.36	1.45	1.55

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	PX6	O3-P1-O1	-2.59	100.26	110.60
4	D	1007	PX6	O3-P1-O1	-2.58	100.32	110.60
4	B	1007	PX6	O3-P1-O1	-2.58	100.32	110.60
4	C	1007	PX6	O3-P1-O1	-2.56	100.40	110.60
2	C	1003	NAG	C2-N2-C7	-2.42	119.96	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NAG	8	0
2	A	1004	NAG	2	0
3	A	1005	CHS	2	0
3	A	1006	CHS	2	0
4	A	1007	PX6	3	0
5	A	1008	PLM	2	0
5	A	1009	PLM	4	0
5	A	1010	PLM	3	0
2	B	1002	NAG	8	0
2	B	1004	NAG	2	0
3	B	1005	CHS	3	0
3	B	1006	CHS	3	0
4	B	1007	PX6	6	0
5	B	1008	PLM	2	0
5	B	1009	PLM	3	0
5	B	1010	PLM	3	0
2	C	1002	NAG	8	0
2	C	1004	NAG	2	0
3	C	1005	CHS	4	0
3	C	1006	CHS	3	0
4	C	1007	PX6	4	0
5	C	1008	PLM	2	0
5	C	1009	PLM	4	0
5	C	1010	PLM	3	0
2	D	1001	NAG	6	0
2	D	1002	NAG	8	0
2	D	1004	NAG	2	0
3	D	1005	CHS	3	0
3	D	1006	CHS	2	0
4	D	1007	PX6	4	0
5	D	1008	PLM	2	0
5	D	1009	PLM	1	0
5	D	1010	PLM	3	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.