



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

Feb 19, 2018 – 04:02 PM EST

PDB ID : 6BAA  
EMDB ID: : EMD-7073  
Title : Cryo-EM structure of the pancreatic beta-cell KATP channel bound to ATP and glibenclamide  
Authors : Martin, G.M.; Yoshioka, C.; Shyng, S.L.  
Deposited on : 2017-10-12  
Resolution : 3.63 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 : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

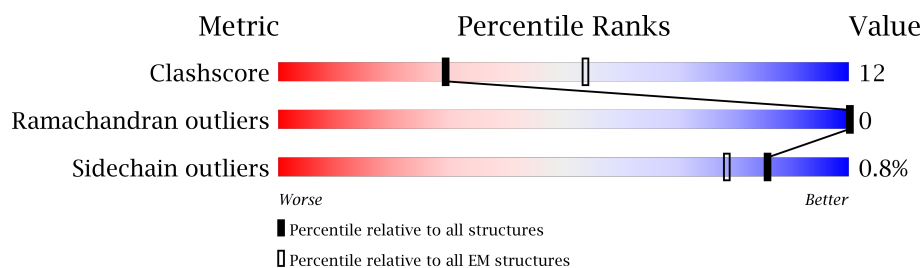
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.63 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	390	57% 25% . 18%
1	B	390	57% 25% . 18%
1	C	390	57% 25% . 18%
1	D	390	57% 25% . 18%
2	E	1582	72% 11% 17%
2	F	1582	72% 11% 17%
2	G	1582	72% 11% 17%
2	H	1582	72% 11% 17%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44852 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2507	1615	431	444	17		
1	B	321	Total	C	N	O	S	0	0
			2507	1615	431	444	17		
1	C	321	Total	C	N	O	S	0	0
			2507	1615	431	444	17		
1	D	321	Total	C	N	O	S	0	0
			2507	1615	431	444	17		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	PRO	LEU	conflict	UNP P70673
B	191	PRO	LEU	conflict	UNP P70673
C	191	PRO	LEU	conflict	UNP P70673
D	191	PRO	LEU	conflict	UNP P70673

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

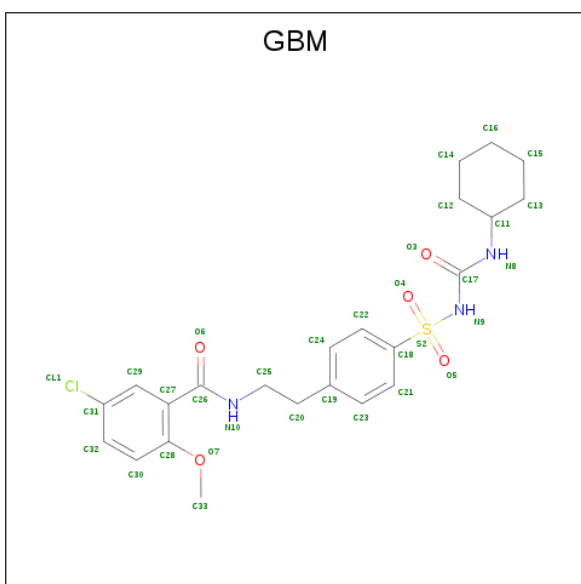
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1317	Total	C	N	O	S	0	0
			8642	5534	1532	1547	29		
2	F	1317	Total	C	N	O	S	0	0
			8642	5534	1532	1547	29		
2	G	1317	Total	C	N	O	S	0	0
			8642	5534	1532	1547	29		
2	H	1317	Total	C	N	O	S	0	0
			8642	5534	1532	1547	29		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula:  $C_{23}H_{28}ClN_3O_5S$ ).

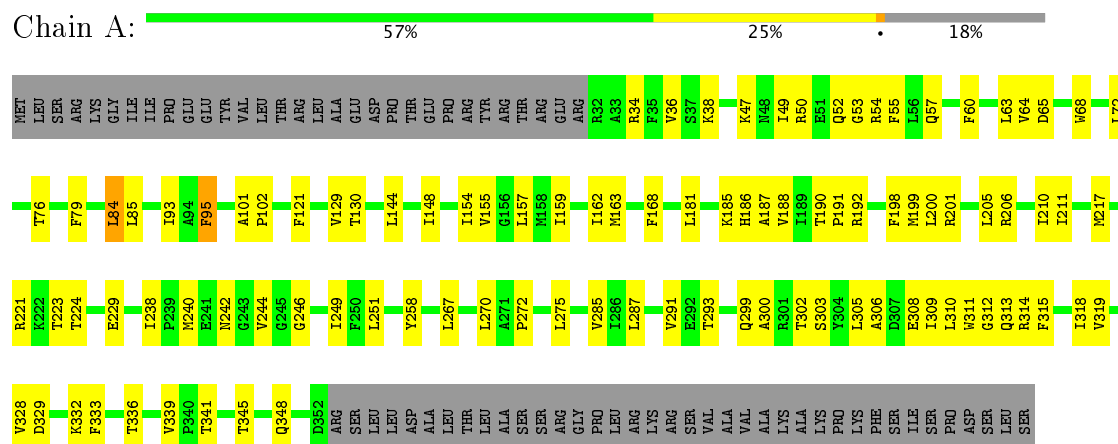


Mol	Chain	Residues	Atoms						AltConf
4	E	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	F	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	G	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	H	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0

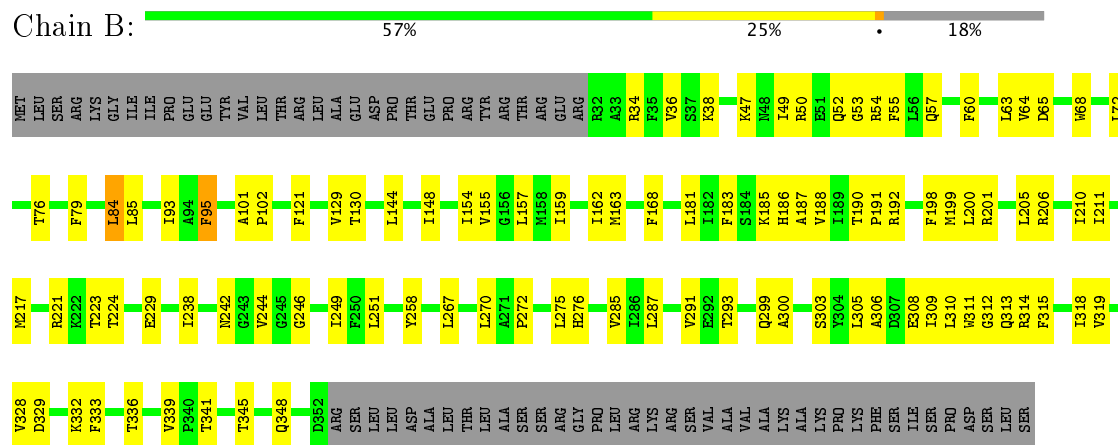
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

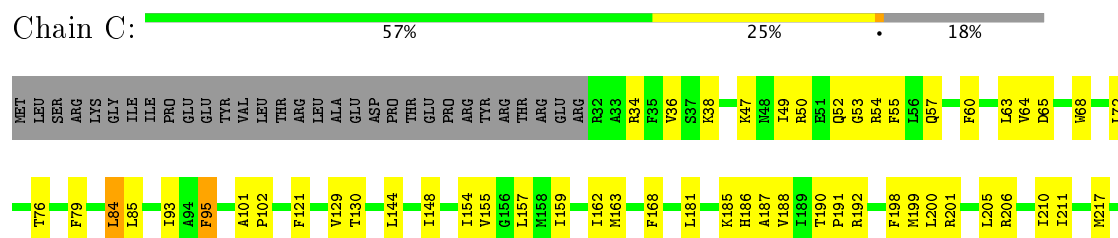
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

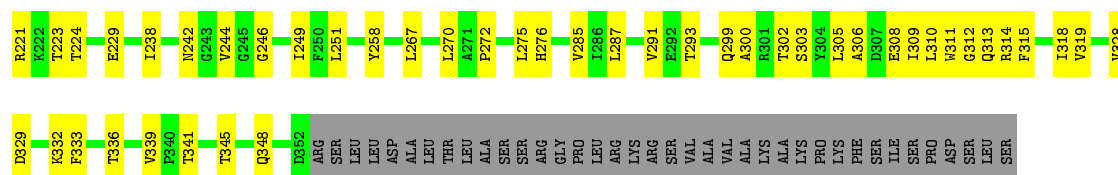


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



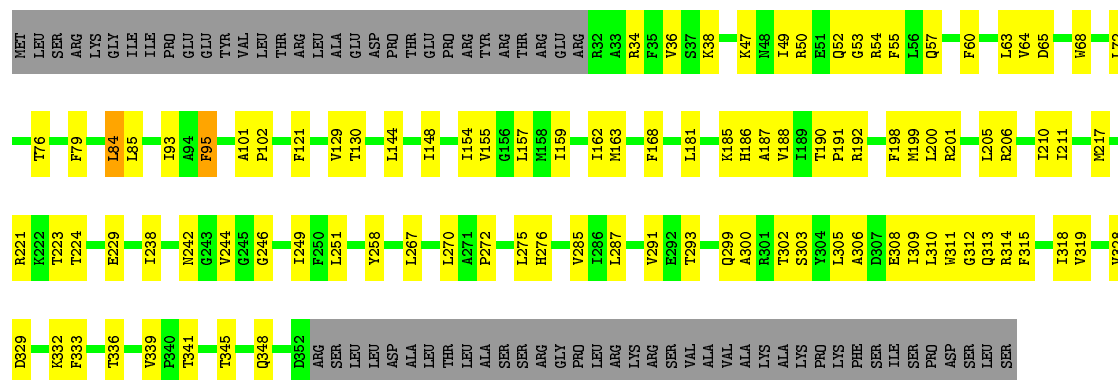
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





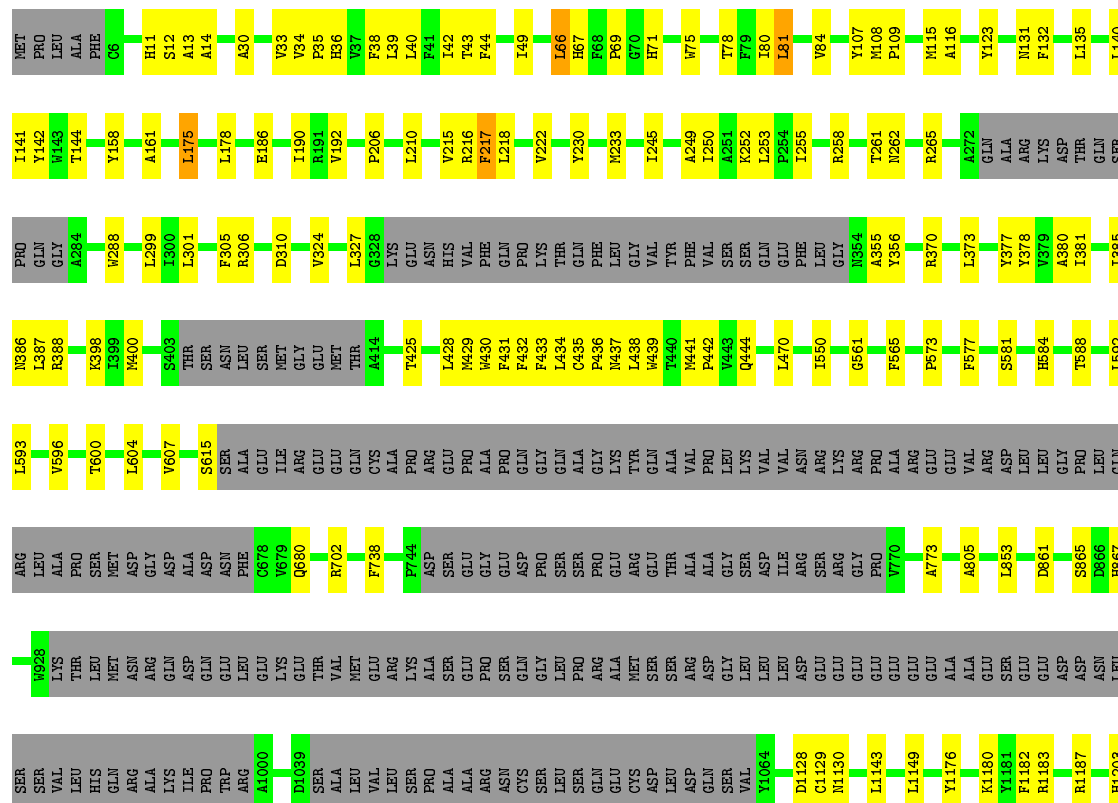
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

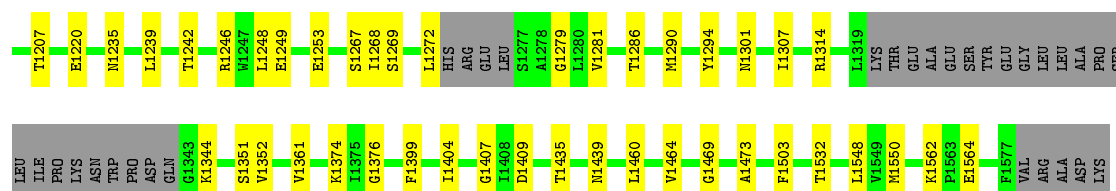
Chain D: 57% 25% 18%



- Molecule 2: ATP-binding cassette sub-family C member 8

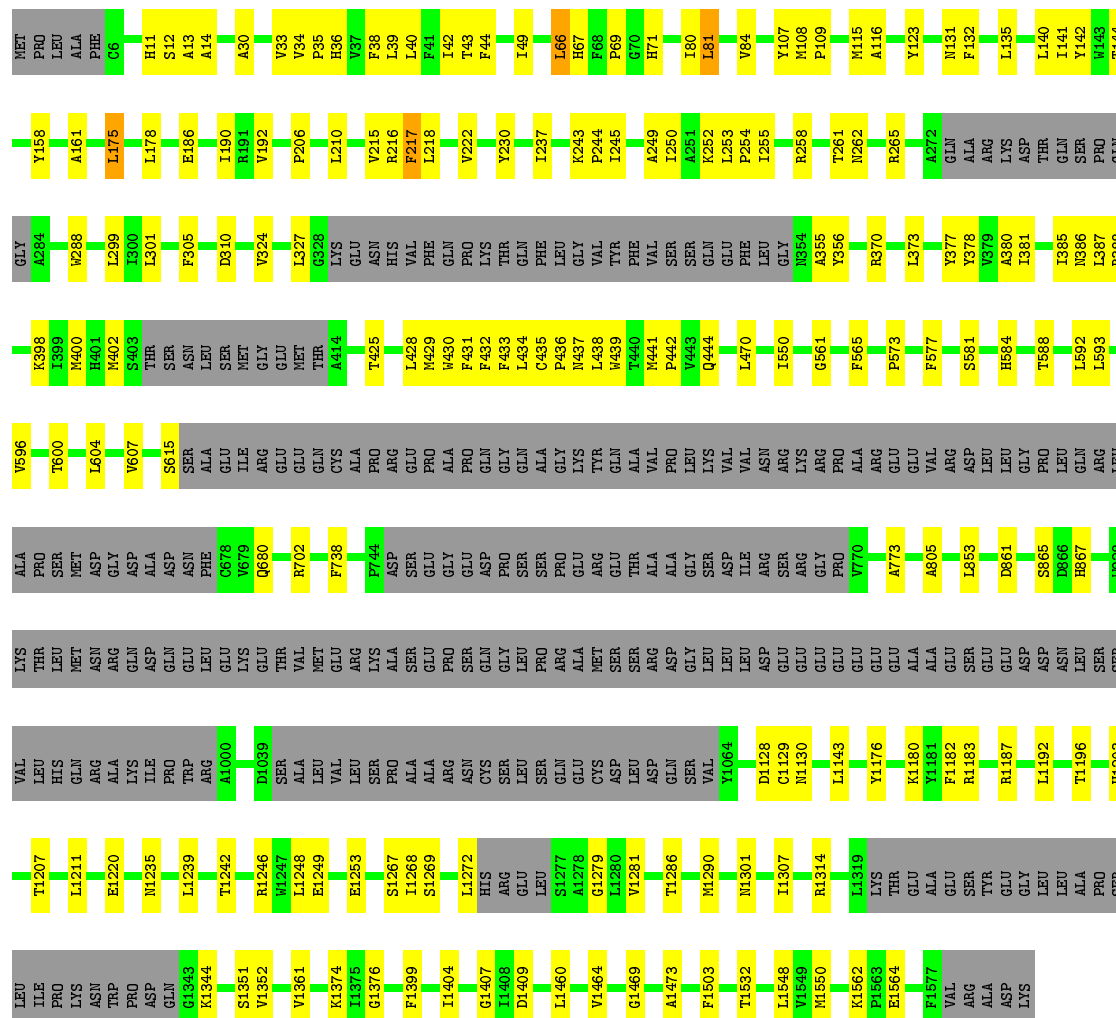
Chain E: 72% 11% 17%





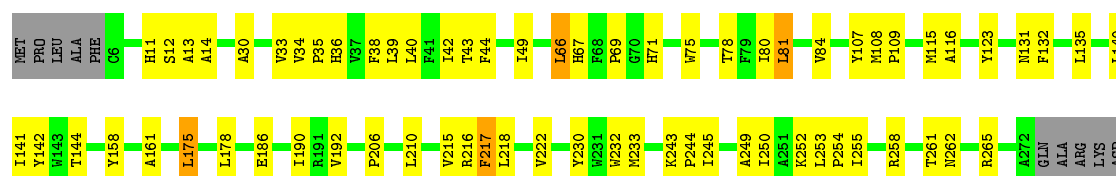
• Molecule 2: ATP-binding cassette sub-family C member 8

Chain F: 72% 11% 17%

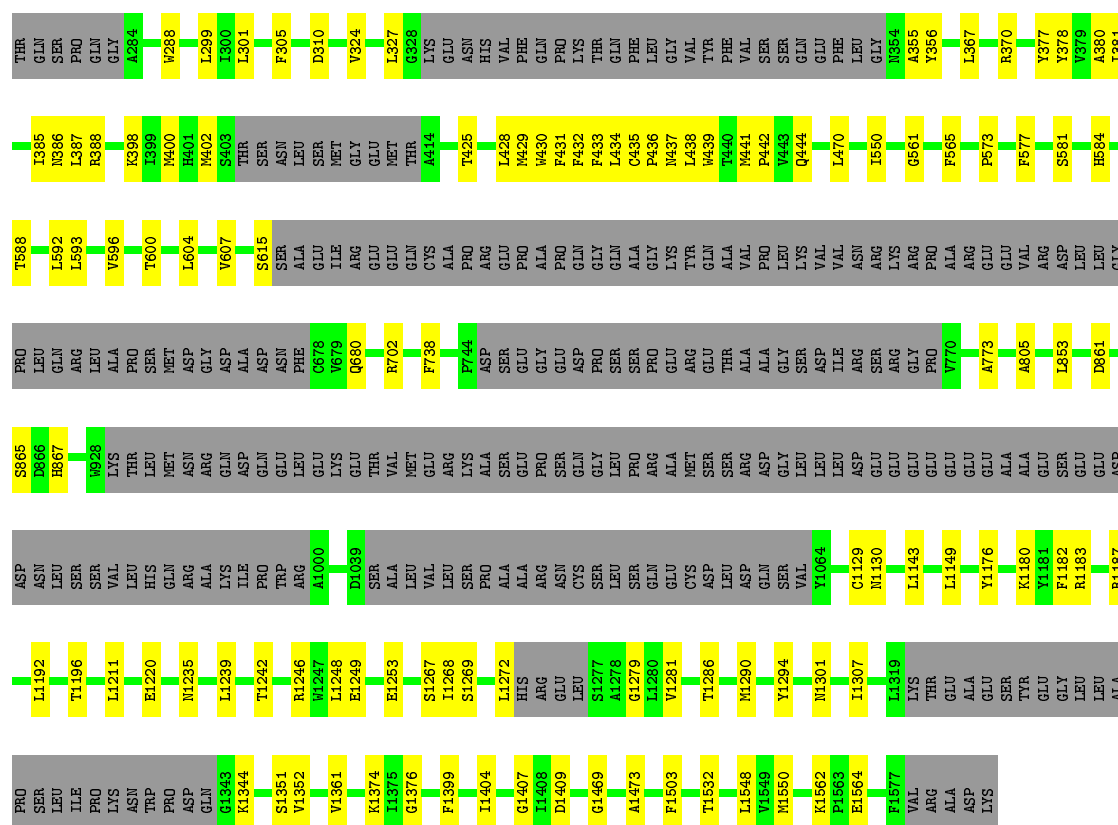


• Molecule 2: ATP-binding cassette sub-family C member 8

Chain G: 72% 11% 17%

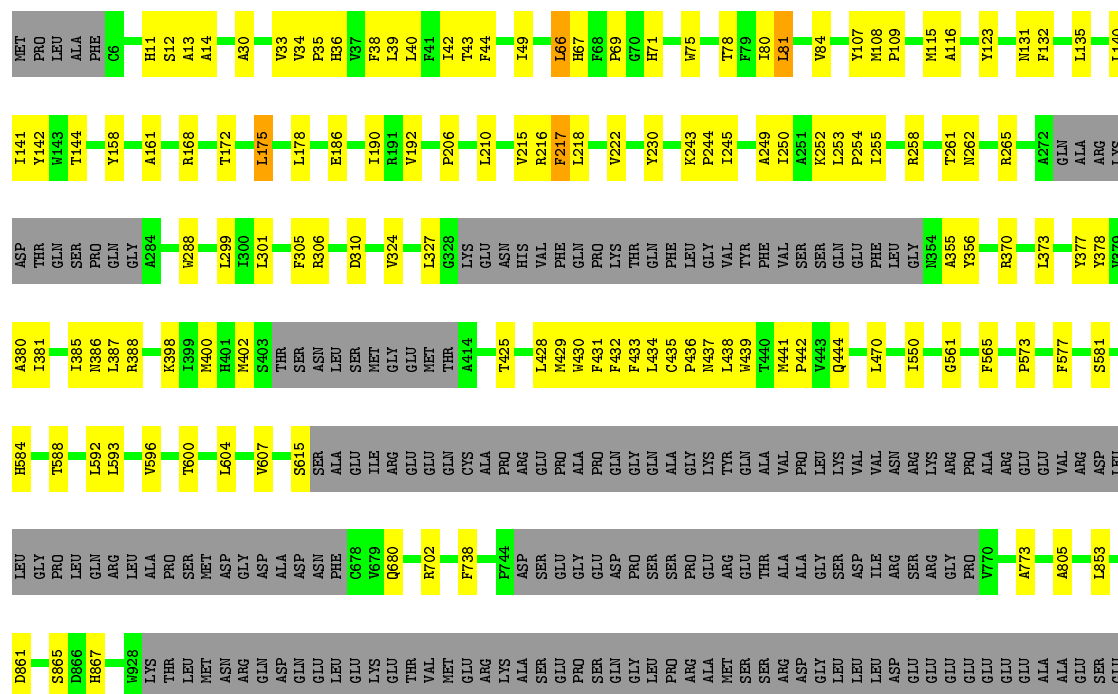






• Molecule 2: ATP-binding cassette sub-family C member 8

Chain H: 72% 11% 17%



ASP LYS	ALA	R1183	GLU
	GLU		ASP
	SER	R1187	ASP
	TTR		ASN
	GLU	L1192	LEU
	GLY		SER
	LEU	T1196	SER
	LEU		VAL
	PRO	H1203	LEU
	SER		HIS
	LEU	T1207	GLN
	ILE	L1211	ARG
	PRO		ALA
	LYS	E1220	LYS
	ASN		ILE
	TTP	M1235	PRO
	PRO		TRP
	ASP	L1239	ARG
	GLN		A1900
	K1344	T1242	D1039
	S1351	R1246	SER
	V1352	H1247	ALA
		E1248	LEU
	V1361	E1249	VAL
			LEU
	K1374	E1253	SER
	H1375		PRO
	G1376	S1267	ALA
	F1399	I1268	ALA
		S1269	ARG
	I1404	L1272	ASN
	G1407	HIS	CYS
	I1408	ARG	SER
	D1409	GLU	LEU
	G1469	LEU	SER
	A1473	S1277	LEU
	F1503	A1278	ASP
	T1532	L1279	GLN
	L1548	L1280	SER
	M1550	V1281	VAL
	K1562	T1286	
	F1563		Y1064
	E1564	M1290	
	F1577	Y1294	D1128
	VAL		C1129
	ARG	M1301	M1130
	ALA	M1307	
			L1143
		R1314	
			L1149
		L1319	Y1176
		LYS	
		TTR	K1180
		GLU	Y1181
			Y1182

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	59417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.30	0/2565	0.59	0/3489
1	B	0.30	0/2565	0.59	0/3489
1	C	0.30	0/2565	0.59	0/3489
1	D	0.30	0/2565	0.59	0/3489
2	E	0.38	0/8801	0.60	5/12092 (0.0%)
2	F	0.38	0/8801	0.60	5/12092 (0.0%)
2	G	0.38	0/8801	0.60	5/12092 (0.0%)
2	H	0.38	0/8801	0.60	5/12092 (0.0%)
All	All	0.37	0/45464	0.60	20/62324 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	387	LEU	CA-CB-CG	-7.10	98.96	115.30
2	F	387	LEU	CA-CB-CG	-7.10	98.96	115.30
2	G	387	LEU	CA-CB-CG	-7.10	98.96	115.30
2	H	387	LEU	CA-CB-CG	-7.10	98.96	115.30
2	H	217	PHE	N-CA-C	-6.40	93.71	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2507	0	2533	110	0
1	B	2507	0	2533	109	0
1	C	2507	0	2533	111	0
1	D	2507	0	2533	110	0
2	E	8642	0	7143	146	0
2	F	8642	0	7143	145	0
2	G	8642	0	7143	148	0
2	H	8642	0	7143	150	0
3	A	31	0	12	4	0
3	B	31	0	12	4	0
3	C	31	0	12	4	0
3	D	31	0	12	4	0
4	E	33	0	28	12	0
4	F	33	0	28	11	0
4	G	33	0	28	11	0
4	H	33	0	28	11	0
All	All	44852	0	38864	968	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 12.

The worst 5 of 968 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:C:186:HIS:HB2	1:C:308:GLU:O	1.74	0.87
1:D:186:HIS:HB2	1:D:308:GLU:O	1.74	0.87
1:A:186:HIS:HB2	1:A:308:GLU:O	1.74	0.87
1:B:186:HIS:HB2	1:B:308:GLU:O	1.74	0.86
1:C:129:VAL:O	1:C:129:VAL:HG12	1.80	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/390 (82%)	309 (97%)	10 (3%)	0	100	100
1	B	319/390 (82%)	309 (97%)	10 (3%)	0	100	100
1	C	319/390 (82%)	309 (97%)	10 (3%)	0	100	100
1	D	319/390 (82%)	309 (97%)	10 (3%)	0	100	100
2	E	1297/1582 (82%)	1241 (96%)	56 (4%)	0	100	100
2	F	1297/1582 (82%)	1241 (96%)	56 (4%)	0	100	100
2	G	1297/1582 (82%)	1241 (96%)	56 (4%)	0	100	100
2	H	1297/1582 (82%)	1241 (96%)	56 (4%)	0	100	100
All	All	6464/7888 (82%)	6200 (96%)	264 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	277/341 (81%)	274 (99%)	3 (1%)	78	90
1	B	277/341 (81%)	274 (99%)	3 (1%)	78	90
1	C	277/341 (81%)	274 (99%)	3 (1%)	78	90
1	D	277/341 (81%)	274 (99%)	3 (1%)	78	90
2	E	614/1373 (45%)	610 (99%)	4 (1%)	87	94
2	F	614/1373 (45%)	610 (99%)	4 (1%)	87	94
2	G	614/1373 (45%)	610 (99%)	4 (1%)	87	94
2	H	614/1373 (45%)	610 (99%)	4 (1%)	87	94
All	All	3564/6856 (52%)	3536 (99%)	28 (1%)	86	93

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	44	PHE
2	E	1249	GLU

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*Continued from previous page...*

Mol	Chain	Res	Type
2	H	222	VAL
2	E	222	VAL
2	E	432	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	HIS
1	D	186	HIS
1	C	48	ASN
1	A	186	HIS
1	C	186	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	A	401	-	27,33,33	1.48	3 (11%)	25,52,52	2.07	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	B	401	-	27,33,33	1.48	3 (11%)	25,52,52	2.06	5 (20%)
3	ATP	C	401	-	27,33,33	1.48	3 (11%)	25,52,52	2.07	5 (20%)
3	ATP	D	401	-	27,33,33	1.48	3 (11%)	25,52,52	2.06	5 (20%)
4	GBM	E	2001	-	35,35,35	5.16	9 (25%)	48,48,48	1.77	10 (20%)
4	GBM	F	2001	-	35,35,35	5.16	9 (25%)	48,48,48	1.77	10 (20%)
4	GBM	G	2001	-	35,35,35	5.16	9 (25%)	48,48,48	1.77	10 (20%)
4	GBM	H	2001	-	35,35,35	5.15	9 (25%)	48,48,48	1.77	10 (20%)

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	ATP	A	401	-	-	0/18/38/38	0/3/3/3
3	ATP	B	401	-	-	0/18/38/38	0/3/3/3
3	ATP	C	401	-	-	0/18/38/38	0/3/3/3
3	ATP	D	401	-	-	0/18/38/38	0/3/3/3
4	GBM	E	2001	-	-	0/27/35/35	0/3/3/3
4	GBM	F	2001	-	-	0/27/35/35	0/3/3/3
4	GBM	G	2001	-	-	0/27/35/35	0/3/3/3
4	GBM	H	2001	-	-	0/27/35/35	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ATP	C2'-C1'	-2.94	1.49	1.53
3	B	401	ATP	C2'-C1'	-2.94	1.49	1.53
3	C	401	ATP	C2'-C1'	-2.94	1.49	1.53
3	A	401	ATP	C2'-C1'	-2.94	1.49	1.53
4	G	2001	GBM	O3-C17	-2.16	1.18	1.23

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2001	GBM	O4-S2-O5	-7.02	110.57	119.55
4	E	2001	GBM	O4-S2-O5	-7.02	110.57	119.55
4	F	2001	GBM	O4-S2-O5	-7.02	110.57	119.55
4	H	2001	GBM	O4-S2-O5	-7.02	110.57	119.55
3	D	401	ATP	C1'-N9-C4	-5.00	118.00	126.64



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	4	0
3	B	401	ATP	4	0
3	C	401	ATP	4	0
3	D	401	ATP	4	0
4	E	2001	GBM	12	0
4	F	2001	GBM	11	0
4	G	2001	GBM	11	0
4	H	2001	GBM	11	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.