



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 5, 2019 – 06:51 PM EDT

PDB ID : 6PZC
EMDB ID: : EMD-20534
Title : Cryo-EM structure of the pancreatic beta-cell SUR1 bound to carbamazepine
Authors : Shyng, S.L.; Yoshioka, C.; Martin, G.M.; Sung, M.W.
Deposited on : 2019-07-31
Resolution : 4.34 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

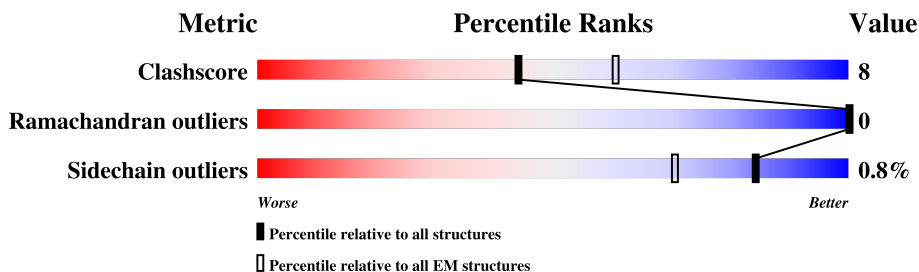
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.34 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	H	1582	 63% 11% 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7456 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-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	1173	7456	4723	1354	1359	20	0	0

V1573	SER
F1574	PHE
A1575	VAL
	ARG
	ALA
	ASP
	LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	499095	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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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	H	0.44	1/7590 (0.0%)	0.60	1/10453 (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	H	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	382	GLU	C-N	-5.13	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	387	LEU	CB-CG-CD1	-6.61	99.76	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	1339	TRP	Peptide
1	H	223	ASN	Peptide
1	H	229	THR	Peptide
1	H	589	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	7456	0	5845	100	0
All	All	7456	0	5845	100	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 (100) 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:H:1059:LEU:N	1:H:1064:TYR:HH	1.59	0.99
1:H:398:LYS:NZ	1:H:614:LEU:O	2.14	0.81
1:H:781:ASN:N	1:H:1206:GLU:OE2	2.15	0.72
1:H:369:GLN:HE22	1:H:370:ARG:NH1	1.91	0.69
1:H:1249:GLU:O	1:H:1253:GLU:HB2	1.94	0.67
1:H:741:SER:HB2	1:H:1218:ARG:HH12	1.61	0.66
1:H:482:SER:HB3	1:H:598:ARG:HH12	1.62	0.65
1:H:251:ALA:HB1	1:H:252:LYS:HD3	1.79	0.64
1:H:1346:GLN:HA	1:H:1368:LEU:HA	1.82	0.62
1:H:685:PHE:HA	1:H:697:SER:HA	1.82	0.62
1:H:306:ARG:NH2	1:H:437:ASN:OD1	2.34	0.61
1:H:684:GLY:HA2	1:H:735:GLY:HA3	1.84	0.59
1:H:236:PHE:O	1:H:239:THR:HB	2.03	0.59
1:H:741:SER:HB2	1:H:1218:ARG:NH1	2.17	0.59
1:H:832:GLY:HA2	1:H:836:GLN:H	1.68	0.59
1:H:452:LEU:HG	1:H:460:ALA:HB1	1.85	0.58
1:H:702:ARG:HG2	1:H:704:PRO:HD3	1.85	0.58
1:H:1550:MET:HA	1:H:1561:ASP:H	1.68	0.57
1:H:1501:SER:H	1:H:1531:ARG:NH1	2.02	0.56
1:H:1112:PHE:O	1:H:1116:THR:N	2.39	0.56
1:H:1245:ASN:OD1	1:H:1300:ARG:NH2	2.38	0.56
1:H:1350:LEU:HA	1:H:1401:GLY:HA3	1.88	0.55
1:H:400:MET:C	1:H:1215:ARG:HH12	2.09	0.55
1:H:1004:TYR:O	1:H:1008:ALA:N	2.36	0.54
1:H:392:GLN:HA	1:H:395:ILE:HD12	1.90	0.54
1:H:770:VAL:HG21	1:H:1218:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:686:PHE:N	1:H:696:LEU:O	2.41	0.54
1:H:851:VAL:H	1:H:884:VAL:HA	1.73	0.53
1:H:869:MET:O	1:H:893:TYR:OH	2.25	0.53
1:H:1153:ALA:HB1	1:H:1287:TYR:HB3	1.91	0.53
1:H:367:LEU:O	1:H:371:THR:OG1	2.23	0.53
1:H:288:TRP:HE1	1:H:607:VAL:HG11	1.73	0.52
1:H:1201:VAL:HA	1:H:1204:PHE:HD2	1.75	0.51
1:H:369:GLN:HE22	1:H:370:ARG:HH11	1.57	0.51
1:H:587:VAL:O	1:H:590:LEU:N	2.43	0.51
1:H:598:ARG:HH11	1:H:602:LYS:NZ	2.08	0.51
1:H:422:ALA:O	1:H:426:ASN:ND2	2.43	0.51
1:H:1454:ALA:O	1:H:1458:ALA:N	2.44	0.51
1:H:781:ASN:HA	1:H:824:GLY:HA3	1.92	0.51
1:H:320:ILE:HD11	1:H:1289:LEU:HD12	1.92	0.51
1:H:542:ILE:HA	1:H:545:PHE:HB3	1.93	0.50
1:H:456:LEU:HB2	1:H:460:ALA:HB2	1.92	0.50
1:H:1142:CYS:SG	1:H:1301:ASN:ND2	2.84	0.50
1:H:1110:MET:HA	1:H:1113:PHE:HD2	1.76	0.50
1:H:1552:LEU:HB3	1:H:1557:ILE:HA	1.94	0.49
1:H:1037:TRP:HE1	1:H:1061:GLN:HB2	1.78	0.49
1:H:1501:SER:OG	1:H:1531:ARG:NH1	2.46	0.48
1:H:222:VAL:HB	1:H:227:LYS:HZ3	1.76	0.48
1:H:684:GLY:O	1:H:698:ASN:N	2.46	0.48
1:H:1192:LEU:O	1:H:1196:THR:OG1	2.21	0.48
1:H:686:PHE:HA	1:H:732:LYS:HA	1.95	0.48
1:H:387:LEU:HD11	1:H:432:PHE:HD2	1.78	0.48
1:H:1404:ILE:HA	1:H:1409:ASP:HA	1.95	0.48
1:H:442:PRO:HA	1:H:445:ILE:HD12	1.96	0.48
1:H:875:GLU:O	1:H:879:ASP:N	2.47	0.47
1:H:1059:LEU:N	1:H:1064:TYR:OH	2.36	0.47
1:H:550:ILE:HA	1:H:553:ALA:HB3	1.96	0.47
1:H:802:VAL:O	1:H:806:CYS:N	2.46	0.47
1:H:1160:VAL:HG12	1:H:1161:THR:HG23	1.96	0.47
1:H:1270:ASN:O	1:H:1277:SER:OG	2.32	0.46
1:H:1352:VAL:HA	1:H:1398:MET:HA	1.96	0.46
1:H:1247:TRP:NE1	1:H:1251:CYS:SG	2.86	0.46
1:H:396:TYR:HA	1:H:399:ILE:HD12	1.98	0.46
1:H:1434:GLY:O	1:H:1475:ILE:N	2.48	0.46
1:H:1552:LEU:HA	1:H:1558:LEU:H	1.79	0.46
1:H:267:CYS:HA	1:H:270:PHE:HD2	1.81	0.46
1:H:1182:PHE:CE2	1:H:1248:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:466:VAL:O	1:H:470:LEU:HB2	2.16	0.45
1:H:1155:THR:O	1:H:1158:SER:OG	2.32	0.45
1:H:1233:SER:HA	1:H:1236:ILE:HG22	1.99	0.45
1:H:419:ASN:HA	1:H:422:ALA:HB3	1.98	0.45
1:H:1164:PHE:HZ	1:H:1259:VAL:HG13	1.82	0.44
1:H:711:ILE:H	1:H:887:VAL:HA	1.82	0.44
1:H:685:PHE:O	1:H:733:VAL:N	2.40	0.44
1:H:1435:THR:HA	1:H:1474:ILE:HA	1.98	0.43
1:H:1231:THR:O	1:H:1235:ASN:ND2	2.51	0.43
1:H:1024:HIS:HE1	1:H:1145:ARG:HA	1.83	0.43
1:H:370:ARG:HB3	1:H:1253:GLU:HG2	2.00	0.43
1:H:1182:PHE:CG	1:H:1248:LEU:HD13	2.54	0.43
1:H:347:SER:O	1:H:351:PHE:N	2.50	0.42
1:H:445:ILE:HG12	1:H:590:LEU:HD21	2.02	0.42
1:H:1240:PHE:HD1	1:H:1240:PHE:HA	1.71	0.42
1:H:1562:LYS:HA	1:H:1563:PRO:HA	1.86	0.42
1:H:1569:GLN:O	1:H:1573:VAL:N	2.52	0.42
1:H:419:ASN:O	1:H:423:ILE:N	2.38	0.42
1:H:1283:LEU:HA	1:H:1286:THR:HG22	2.01	0.42
1:H:888:THR:OG1	1:H:889:HIS:N	2.53	0.42
1:H:367:LEU:HA	1:H:367:LEU:HD23	1.87	0.41
1:H:396:TYR:OH	1:H:1223:PHE:HB3	2.20	0.41
1:H:797:GLN:O	1:H:801:MET:N	2.49	0.41
1:H:253:LEU:HA	1:H:253:LEU:HD23	1.90	0.41
1:H:377:TYR:O	1:H:381:ILE:HG12	2.20	0.41
1:H:226:SER:O	1:H:230:TYR:N	2.43	0.41
1:H:832:GLY:HA3	1:H:859:ALA:HB1	2.01	0.41
1:H:1281:VAL:O	1:H:1284:GLY:N	2.54	0.41
1:H:1523:VAL:O	1:H:1528:PHE:N	2.44	0.41
1:H:1156:VAL:HG21	1:H:1287:TYR:HE2	1.86	0.40
1:H:1223:PHE:HD1	1:H:1223:PHE:HA	1.66	0.40
1:H:1165:LEU:HA	1:H:1168:LEU:HB3	2.02	0.40
1:H:739:TRP:HB2	1:H:741:SER:H	1.86	0.40

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	H	1159/1582 (73%)	1047 (90%)	112 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	H	474/1373 (34%)	470 (99%)	4 (1%)	83	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	252	LYS
1	H	354	ASN
1	H	377	TYR
1	H	1296	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	354	ASN
1	H	369	GLN
1	H	427	GLN
1	H	491	HIS

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Mol	Chain	Res	Type
1	H	1235	ASN
1	H	1296	ASN
1	H	1301	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.