wwPDB EM Validation Summary Report

Mar 15, 2025 – 09:07 pm GMT

PDB ID	:	8QJU
EMDB ID	:	EMD-18449
Title	:	Structure of the human 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2 (PLCG2) protein
Authors	:	Faille, A.; Warren, A.J.
Deposited on	:	2023-09-13
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

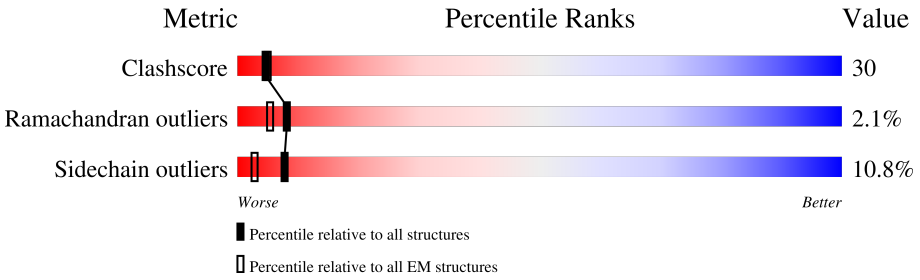
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1265	41% 37% 5% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8578 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 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2.

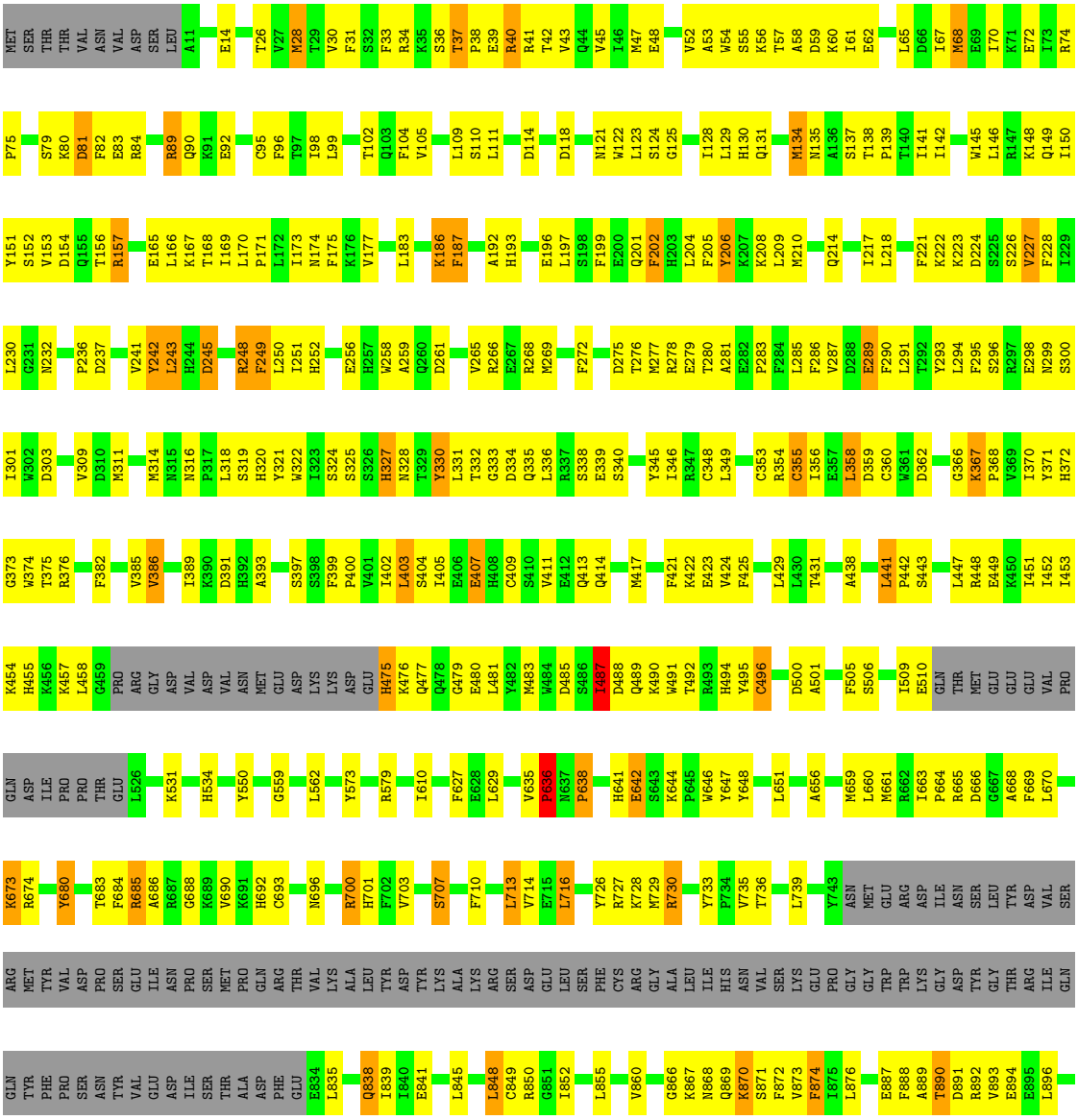
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1045	8578	5470	1470	1595	43	0	0

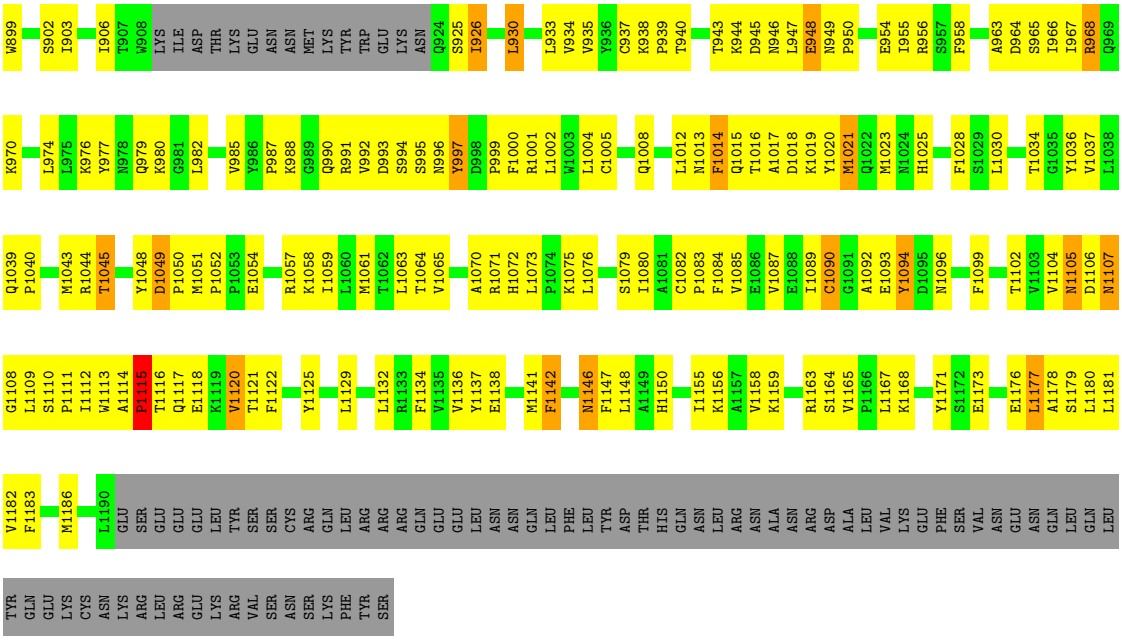
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2

Chain A:




W899 S902 I903 I906 T907 W908 LYS ILE ASP THR LYS GLU ASN ASN MET LYS TYR TRP GLU LYS ASN Q924 S925 I926 L930 L933 V934 V935 Y936 C937 K938 P939 T940 T943 K944 D945 N946 L947 E948 N949 P950 E954 I955 R956 S957 F958 A963 D964 S965 I966 I967 R968 Q969
K970 L974 L975 K976 Y977 N978 Q979 K980 G981 L982 V985 Y986 P987 K988 G989 Q990 R991 V992 D993 S994 S995 N996 Y997 D998 P999 F1000 R1001 L1002 W1003 L1004 C1005 Q1008 L1012 N1013 F1014 Q1015 T1016 A1017 D1018 K1019 Y1020 M1021 Q1022 M1023 N1024 H1025 F1028 S1029 L1030 T1034 G1035 Y1036 V1037 L1038
Q1039 P1040 M1043 R1044 T1045 Y1048 D1049 P1050 M1051 P1052 P1053 E1054 R1057 K1058 I1059 L1060 M1061 T1062 L1063 T1064 V1065 A1070 R1071 H1072 L1073 P1074 K1075 L1076 S1079 I1080 A1081 C1082 P1083 F1084 V1085 E1086 V1087 E1088 I1089 C1090 G1091 A1092 E1093 Y1094 D1095 N1096 F1099 T1102 V1103 V1104 N1105 D1106 N1107
G1108 L1109 S1110 P1111 I1112 W1113 A1114 P1115 T1116 Q1117 E1118 K1119 V1120 T1121 F1122 Y1125 L1129 L1132 R1133 F1134 V1135 V1136 Y1137 E1138 M1141 F1142 N1146 F1147 L1148 A1149 H1150 I1155 K1156 A1157 V1158 K1159 R1163 S1164 V1165 P1166 L1167 K1168 Y1171 S1172 E1173 E1176 L1177 A1178 S1179 L1180 L1181
V1182 F1183 M1186 L1190 GLU SER GLU GLU GLU LEU TYR SER SER CYS ARG GLN LEU ARG ARG ARG GLN GLU GLU LEU ASN ASN GLN LEU PHE LEU TYR ASP THR HIS GLN ASN LEU ARG ASN ALA ASN ARG ASP ALA LEU VAL LYS GLU PHE SER VAL ASN GLU ASN GLN LEU GLN LEU
TYR GLN GLU LYS CYS ASN LYS ARG LEU ARG GLU LYS ARG VAL SER ASN SER LYS PHE TYR SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130911	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/8779	0.65	0/11849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8578	0	8475	511	0
All	All	8578	0	8475	511	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 30.

The worst 5 of 511 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:138:THR:CG2	1:A:139:PRO:HD3	1.69	1.21
1:A:138:THR:HG22	1:A:139:PRO:HD3	1.31	1.11
1:A:138:THR:CG2	1:A:272:PHE:HE1	1.68	1.07
1:A:170:LEU:HD12	1:A:173:ILE:HD11	1.38	1.05
1:A:138:THR:CG2	1:A:272:PHE:CE1	2.41	1.02

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	1035/1265 (82%)	922 (89%)	91 (9%)	22 (2%)	5 32

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	227	VAL
1	A	327	HIS
1	A	355	CYS
1	A	948	GLU

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	950/1158 (82%)	847 (89%)	103 (11%)	5 24

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	659	MET
1	A	736	THR
1	A	1142	PHE
1	A	673	LYS

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Mol	Chain	Res	Type
1	A	707	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	868	ASN
1	A	1146	ASN
1	A	1031	ASN
1	A	413	GLN
1	A	856	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.