

PDBID	molecule name
1ein	Lipase
3uu5	Proton-gated ion channel
3p4w	Proton-gated ion channel
3p50	Proton-gated ion channel
3uu6	Proton-gated ion channel
3uu8	Proton-gated ion channel
3uub	Proton-gated ion channel
4dos	Nuclear receptor subfamily 5 group A member 2
3h1j	MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I
1lpa	Colipase
4hfc	Proton-gated ion channel
5mvm	Proton-gated ion channel
5ejz	Cellulose synthase catalytic subunit [UDP-forming]
5j0z	Proton-gated ion channel
5mzr	Proton-gated ion channel
5mvm	Proton-gated ion channel
5mur	Proton-gated ion channel
5mzt	Proton-gated ion channel
4hfe	Proton-gated ion channel
4hfi	Proton-gated ion channel
4ila	Proton-gated ion channel
4ilb	Proton-gated ion channel
4hfh	Proton-gated ion channel
4hfb	Proton-gated ion channel
4ilc	Proton-gated ion channel
4qh5	Proton-gated ion channel
4p02	Cellulose synthase catalytic subunit [UDP-forming]
4p00	Cellulose synthase catalytic subunit [UDP-forming]
4hfd	Proton-gated ion channel
5eiy	Cellulose synthase catalytic subunit [UDP-forming]
4zzc	Proton-gated ion channel
4il9	Proton-gated ion channel
6yj4	NADH-ubiquinone oxidoreductase chain 3
3rw0	Ion_trans domain-containing protein
4zxh	Carrier domain-containing protein
5klv	Cytochrome b-c1 complex subunit 1, mitochondrial
5okd	Cytochrome b-c1 complex subunit 1, mitochondrial

Table 1: PDBIDs and molecules names used in the analysis of PC

PDBID	molecule name
5vb2	Ion_trans domain-containing protein
4ms2	Ion_trans domain-containing protein
5vb8	Ion_trans domain-containing protein
6mwa	Ion_trans domain-containing protein
6mwg	Ion_trans domain-containing protein
6mwd	Ion_trans domain-containing protein
6mvv	Ion_trans domain-containing protein
6haw	Cytochrome b-c1 complex subunit 1, mitochondrial
6mwb	Ion_trans domain-containing protein
6mvw	Ion_trans domain-containing protein
6c1k	Ion_trans domain-containing protein
5yua	Ion_trans domain-containing protein
6c1p	Ion_trans domain-containing protein
6c1e	Ion_trans domain-containing protein
6c1m	Ion_trans domain-containing protein
6p6x	Ion_trans domain-containing protein
6p6y	Ion_trans domain-containing protein
6ubs	Glycine receptor subunit alphaZ1
6mvy	Ion_trans domain-containing protein
6xvf	Cytochrome b-c1 complex subunit 1, mitochondrial
2h26	T-cell surface glycoprotein CD1b
3b7q	CRAL-TRIO domain-containing protein YKL091C
3b7z	CRAL-TRIO domain-containing protein YKL091C
6z5r	Light-harvesting complex 1 alpha chain
6z5s	Light harvesting complex 1 Protein W
6c15	T-cell surface glycoprotein CD1c
1dmh	Catechol 1,2-dioxygenase
1dlm	Catechol 1,2-dioxygenase
1dlt	Catechol 1,2-dioxygenase
1dlq	Catechol 1,2-dioxygenase
3n9t	INTRADIOL_DIOXYGENAS domain-containing protein
5kym	1-acyl-sn-glycerol-3-phosphate acyltransferase
2hh1	Reaction center protein L chain
2hg9	Reaction center protein L chain
5mzq	Proton-gated ion channel
6qpc	Anoctamin-6
6qp6	Anoctamin-6
5irz	Transient receptor potential cation channel subfamily V member 1
5irx	Transient receptor potential cation channel subfamily V member 1

Table 2: PDBIDs and molecules names used in the analysis of PC

PDBID	molecule name
4i9j	1-phosphatidylinositol phosphodiesterase
5ej1	Cellulose synthase catalytic subunit [UDP-forming]
6s7o	Dolichyl-diphosphooligosaccharide-protein glycosyltransferase subunit STT3A
6c26	Dolichyl-diphosphooligosaccharide-protein glycosyltransferase subunit STT3
6s7t	Dolichyl-diphosphooligosaccharide-protein glycosyltransferase subunit STT3B
1lsh	Vitellogenin
6uz8	Short transient receptor potential channel 6
4tso	DELTA-actitoxin-Afr1a
4tsp	DELTA-actitoxin-Afr1a
4tsq	DELTA-actitoxin-Afr1a
6iej	Cytosolic phospholipase A2
2a1l	Phosphatidylinositol transfer protein beta isoform
1t27	Phosphatidylinositol transfer protein alpha isoform
4f2a	Cholesteryl ester transfer protein
4nab	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
4uu1	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5d3i	Toll-like receptor 2
5uph	Lysosome membrane protein 2
5ylu	Potassium-transporting ATPase alpha chain 1
2obd	Cholesteryl ester transfer protein
5xa7	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5xab	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5xaa	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
6yu4	Sodium-dependent transporter
6vyk	Mechanosensitive channel MscS
6rld	Small-conductance mechanosensitive channel
6jxi	Potassium-transporting ATPase alpha chain 1
6jxh	Potassium-transporting ATPase alpha chain 1
6jxj	Potassium-transporting ATPase alpha chain 1
5xa8	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5xa9	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5ncq	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5ylv	Potassium-transporting ATPase alpha chain 1
7d91	Sodium/potassium-transporting ATPase subunit alpha-1
7k4b	Transient receptor potential cation channel subfamily V member 6
7ddl	Sodium/potassium-transporting ATPase subunit alpha-1
7bt2	Sarcoplasmic/endoplasmic reticulum calcium ATPase 2
7ddh	Sodium/potassium-transporting ATPase subunit alpha-1
7ddj	Sodium/potassium-transporting ATPase subunit alpha-1
7ddk	Sodium/potassium-transporting ATPase subunit alpha-1
7k4a	Transient receptor potential cation channel subfamily V member 6
7ado	ER membrane protein complex subunit 1
7d94	Sodium/potassium-transporting ATPase subunit alpha-1
6pw5	Ion.trans domain-containing protein

Table 3: PDBIDs and molecules names used in the analysis of PC

PDBID	molecule name
3cxh	Cytochrome b-c1 complex subunit 1, mitochondrial
3cx5	Cytochrome b-c1 complex subunit 1, mitochondrial
5klv	Cytochrome b-c1 complex subunit 1, mitochondrial
4rpe	Linoleate 9/13-lipoxygenase
6ymx	Cytochrome c oxidase subunit 1
6giq	Cytochrome b-c1 complex subunit 1, mitochondrial
6nhg	Cytochrome b-c1 complex subunit 1, mitochondrial
3ar5	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3ar4	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
2dqs	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
2agv	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3jtc	Endothelial protein C receptor
3nan	Calcium-transporting ATPase
3w5c	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3nam	Calcium-transporting ATPase
3w5b	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3zuy	Transporter
3zux	Transporter
3w5a	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
2eau	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3ar3	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3ar7	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3ar6	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
1l8j	Endothelial protein C receptor
1lqv	Endothelial protein C receptor
4cz8	Na ⁺ /H ⁺ Exchanger domain-containing protein
4ycn	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
5jmn	Multidrug efflux pump subunit AcrB
4j2t	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
3w5d	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
4v3e	IT4VAR07 CIDRA
4v3d	HB3VAR03 CIDRA DOMAIN
5a1s	Citrate-sodium symporter
4ycm	Sarcoplasmic/endoplasmic reticulum calcium ATPase 1
4n31	Signal peptidase I
2vwa	Early transcribed membrane protein 13
3pg7	Neurofibromin
5td3	Catechol 1,2-dioxygenase
5vxt	Catechol 1,2-dioxygenase
6wlw	V-type proton ATPase 21 kDa proteolipid subunit
6wbn	Pannexin-1
6wbg	Pannexin-1
6wbf	Pannexin-1
6wbm	Pannexin-1

Table 4: PDBIDs and molecules names used in the analysis of PC

PDBID	name
6z16	Multisubunit Na ⁺ /H ⁺ antiporter, A subunit
6ymy	Cytochrome c oxidase subunit 1
6wm2	V-type proton ATPase subunit E 1
1p84	Ubiquinol-cytochrome C reductase complex core protein I
3szd	Probable porin
3m9i	Lens fiber major intrinsic protein
5ejz	Cellulose synthase catalytic subunit [UDP-forming]
4p02	Cellulose synthase catalytic subunit [UDP-forming]
4pd4	Cytochrome b-c1 complex subunit 1, mitochondrial
4p00	Cellulose synthase catalytic subunit [UDP-forming]
4qn9	N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D
5ej1	Cellulose synthase catalytic subunit [UDP-forming]
6zk9	NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial
6zkb	Mitochondrial complex I, 49 kDa subunit
1m57	Cytochrome c oxidase subunit 1
1n69	Saposin-B
1m56	Cytochrome c oxidase subunit 1
5weh	Cytochrome c oxidase subunit 1
6zqv	Genome polyprotein
2x72	Rhodopsin
2qgu	Probable signal peptide protein
3wmm	Photosynthetic reaction center cytochrome c subunit
1yp0	Steroidogenic factor 1
1zdt	Steroidogenic factor 1
1kb9	Cytochrome b-c1 complex subunit 1, mitochondrial
1eys	PHOTOSYNTHETIC REACTION CENTER
5y5s	Photosynthetic reaction center cytochrome c subunit
5w7l	Bac_transf domain-containing protein
6t15	Cytochrome b-c1 complex subunit 1, mitochondrial
5z39	PH domain-containing protein
6hu9	Cytochrome b-c1 complex subunit 1, mitochondrial
5irz	Transient receptor potential cation channel subfamily V member 1
5irx	Transient receptor potential cation channel subfamily V member 1
6cud	Short transient receptor potential channel 3
6o72	Transient receptor potential cation channel subfamily M member 8
6o6r	Transient receptor potential cation channel subfamily M member 8
2e2x	Neurofibromin
3peg	Neurofibromin
3p7z	Neurofibromin

Table 5: PDBIDs and molecules names used in the analysis of PC

PDBID	name
6rd5	ASA-10: Polytomella F-ATP synthase associated subunit 10
6xiw	Sodium leak channel non-selective protein
6lum	Succinate dehydrogenase subunit C
6tyi	Biopolymer transport protein ExbB
5jwy	Phosphatidylglycerophosphatase B
6uza	Short transient receptor potential channel 6
3l9r	Ig-like domain-containing protein
6or2	Membrane protein, MmpL family protein
6w2y	Gamma-aminobutyric acid type B receptor subunit 1
2ein	Cytochrome c oxidase subunit 1
2eil	Cytochrome c oxidase subunit 1
2eij	Cytochrome c oxidase subunit 1
3ag3	Cytochrome c oxidase subunit 1
3abm	Cytochrome c oxidase subunit 1
2y69	Cytochrome c oxidase subunit 1
2eik	Cytochrome c oxidase subunit 1
2dyr	Cytochrome c oxidase subunit 1
2r40	Ecdysone receptor
1r20	NR LBD domain-containing protein
3ae5	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ixp	NR LBD domain-containing protein
3vr8	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3vr9	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
1zoy	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
1g2n	NR LBD domain-containing protein
1nek	Succinate dehydrogenase flavoprotein subunit
1r1k	Ecdysone receptor
3ae8	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae9	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3aeb	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae2	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae4	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae3	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3abv	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae6	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3aea	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3ae1	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3aef	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
1nen	Succinate dehydrogenase flavoprotein subunit
4ytm	Succinate dehydrogenase flavoprotein
3vra	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial
3vrb	Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Table 6: PDBIDs and molecules names used in the analysis of PC

PDBID	name
4g33	Linoleate 9/13-lipoxygenase
5ir4	Lipoxygenase LoxA
5lc8	Linoleate 9/13-lipoxygenase
5ir5	Lipoxygenase LoxA
4g32	Linoleate 9/13-lipoxygenase
6a9j	Autophagy-related protein 2
6adq	Cytochrome aa3 subunit 2
7bh1	Potassium-transporting ATPase potassium-binding subunit
7bgy	Potassium-transporting ATPase potassium-binding subunit
7lc3	Potassium-transporting ATPase potassium-binding subunit
7bh2	Potassium-transporting ATPase potassium-binding subunit
5jxd	Tumor necrosis factor alpha-induced protein 8
5h5a	Mitochondrial distribution and morphology protein 12
6pqo	Transient receptor potential cation channel subfamily A member 1
6ppp	Transient receptor potential cation channel subfamily A member 1
6x16	Glutamate transporter homologue GltPh
6vyi	Diacylglycerol O-acyltransferase 1
6w98	F5/8 type C domain-containing protein
6uz3	Sodium channel protein type 5 subunit alpha, Green fluorescent protein
6uw4	Transient receptor potential cation channel subfamily V member 3
6x15	Glutamate transporter homologue GltPh
6agf	Sodium channel protein type 4 subunit alpha
6br8	Protein A6 homolog
6br9	Protein A6 homolog
6vz1	Diacylglycerol O-acyltransferase 1
6uwf	Glutamate transporter homolog
6uz0	Sodium channel protein type 5 subunit alpha, Green fluorescent protein
6ppq	Transient receptor potential cation channel subfamily A member 1
7k18	Green fluorescent protein
7kv8	Envelope protein E
7cu3	Sodium leak channel non-selective protein
2qjk	Cytochrome b
2qjy	Cytochrome b
2fyn	Cytochrome b
3ayg	COX1 domain-containing protein
2qjp	Cytochrome b
3ayf	COX1 domain-containing protein
5kkz	Cytochrome b
5kli	Cytochrome b
6qq6	Nitric oxide reductase subunit B
1pp9	Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Table 7: PDBIDs and molecules names used in the analysis of PC

PDBID	name
3h1l	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
3tgu	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
3h1k	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
3l70	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
3l75	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
3l71	Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i
2bcc	Cytochrome b-c1 complex subunit 1, mitochondrial

Table 8: PDBIDs and molecules names used in the analysis of PC

PDBID	molecule name
3mtx	Lymphocyte antigen 86
4c7r	Glycine betaine transporter BetP
4doj	Glycine betaine transporter BetP
5azb	Phosphatidylglycerol-prolipoprotein diacylglyceryl transferase
4opc	Digeranylgeranyllycerophospholipid reductase
4phz	unknown peptide
5azc	Phosphatidylglycerol-prolipoprotein diacylglyceryl transferase
6z5r	Light-harvesting complex 1 alpha chain
6z5s	Light harvesting complex 1 Protein W
6tyi	Biopolymer transport protein ExbB
6tjv	NAD(P)H-quinone oxidoreductase subunit 1
2hhk	Reaction center protein L chain
2cyd	V-type sodium ATPase subunit K
2bhw	Chlorophyll a-b binding protein AB80, chloroplastic
1rwt	Chlorophyll a-b binding protein, chloroplastic
2axt	Photosystem II protein D1 1
2bl2	V-type sodium ATPase subunit K
3jcu	Photosystem II protein D1
5t85	Antibody 10E8 FAB HEAVY CHAIN
2ein	Cytochrome c oxidase subunit 1
2eil	Cytochrome c oxidase subunit 1
2eij	Cytochrome c oxidase subunit 1
2irv	Rhomboid protease GlpG
3ag3	Cytochrome c oxidase subunit 1
3abm	Cytochrome c oxidase subunit 1
2y69	Cytochrome c oxidase subunit 1
2eik	Cytochrome c oxidase subunit 1
2dyr	Cytochrome c oxidase subunit 1
3oz2	Digeranylgeranyllycerophospholipid reductase
4i7z	Cytochrome b6
5wki	T-cell surface glycoprotein CD1b
5wl1	T-cell surface glycoprotein CD1b
2r9r	Voltage-gated potassium channel subunit beta-2
3wmm	Photosynthetic reaction center cytochrome c subunit
4jta	Voltage-gated potassium channel subunit beta-2
4jtc	Voltage-gated potassium channel subunit beta-2
4jtd	Voltage-gated potassium channel subunit beta-2
3lnm	Voltage-gated potassium channel subunit beta-2

Table 9: PDBIDs and molecule names of PG lipids

PDBID	name
6tos	Orexin receptor type 1
6to7	Orexin receptor type 1
6tot	Orexin receptor type 1
6tp6	Orexin receptor type 1
6tod	Orexin receptor type 1
6cju	Cyclic nucleotide-binding domain-containing protein
6cjt	Cyclic nucleotide-binding domain-containing protein
6bw5	UDP-N-acetylglucosamine–dolichyl-phosphate N-acetylglucosaminophosphotransferase
6bw6	UDP-N-acetylglucosamine–dolichyl-phosphate N-acetylglucosaminophosphotransferase
6tp4	Orexin receptor type 1
6tq6	Orexin receptor type 1
6tq7	Orexin receptor type 1
6tq4	Orexin receptor type 1
6v35	Calcium-activated potassium channel subunit alpha-1
6tp3	Orexin receptor type 1
6tq9	Orexin receptor type 1
7cge	Lipid asymmetry maintenance ABC transporter permease subunit MlaE
1ymt	Steroidogenic factor 1
7kc4	Protein Wnt-8a
1yok	Nuclear receptor subfamily 5 group A member 2
4nh2	Ammonium transporter
4oni	Nuclear receptor subfamily 5 group A member 2
5eg1	Microcin-J25 export ATP-binding/permease protein McjD
3tx7	Catenin beta-1
6rck	Outer membrane protein C
6uxp	Bcl-2 homologous antagonist/killer
6hsy	Toluene tolerance protein Ttg2D

Table 10: PDBIDs and molecule names of PG lipids

PDBID	name
3kaa	Hepatitis A virus cellular receptor 2 homolog
3bib	T-cell immunoglobulin and mucin domain-containing protein 4
1dsy	Protein kinase C alpha type
6wlw	V-type proton ATPase 21 kDa proteolipid subunit
6wm2	V-type proton ATPase subunit E 1
6b8o	Triggering receptor expressed on myeloid cells 2
6snd	LN01 light chain
6roh	Probable phospholipid-transporting ATPase DRS2
3d9s	Aquaporin-5
5dye	Aquaporin-5
5c5x	Aquaporin-5
6u9w	P2X purinoceptor 7
6u9v	P2X purinoceptor 7
4b2z	Oxysterol-binding protein homolog 6
6lcp	Phospholipid-transporting ATPase
6lcr	Phospholipid-transporting ATPase
6i3y	PRELI domain-containing protein 1, mitochondrial
6vp0	Diacylglycerol O-acyltransferase 1
6tt7	ATP synthase subunit alpha
6sp2	Membrane protein TMS1d
7bsu	ATP11C
7bsv	ATP11C
6k7m	Phospholipid-transporting ATPase
2hj6	Reaction center protein L chain
4hyt	Sodium/potassium-transporting ATPase subunit alpha-1
4res	Sodium/potassium-transporting ATPase subunit alpha-1
6uxn	Bcl-2 homologous antagonist/killer
6nhh	Cytochrome b

Table 11: PDBIDs and molecule names of protein structures used in the analysis of PS headgroup structures.