

## Supplemental Material

**Supplementary Table 1. List of L-peptide bond containing ligands.** This list of 514 three-letter PDB ligand names defines non-standard peptides that may be covalently bound in a peptide chain or may be bound ligands. Presence of any of these names implied exclusion from our analysis.

0A0	0A1	0A2	0A5	0A8	0A9	0AA	0AB	0AC	0AF	0AG	0AH
0AK	0AY	0AZ	0CS	0NC	175	1LU	1PA	1TQ	1TY	200	23F
2AS	2FM	2LU	2ML	2MR	2MT	2TY	2VA	3AH	3MD	4DP	4F3
4FB	4FW	4HT	4PH	5CS	5HP	6CL	6CW	AA3	AA4	AAR	ABA
ACB	ACL	AEI	AFA	AGM	AHB	AHO	AHP	AIB	AKL	ALC	ALG
ALM	ALN	ALO	ALS	ALY	APH	API	APK	AR4	ARM	ASA	ASB
ASI	ASK	ASL	ASQ	AYA	AYG	AZK	AZY	B1F	B2A	B2F	B2I
B2V	B3A	B3D	B3E	B3K	B3S	B3X	B3Y	BAL	BBC	BCS	BCX
BFD	BHD	BIF	BLE	BLY	BMT	BNN	BOR	BPE	BSE	BTA	BTC
BUC	BUG	C12	C1X	C3Y	C5C	C6C	C99	CAB	CAF	CAS	CCL
CCS	CEA	CFY	CGA	CGU	CH6	CH7	CHG	CHP	CIR	CL0	CLB
CLD	CLE	CLG	CLH	CLV	CME	CMH	CML	CMT	CR0	CR2	CR5
CR7	CR8	CRF	CRK	CRO	CRQ	CRU	CRW	CRX	CS0	CS1	CS3
CS4	CSA	CSB	CSD	CSE	CSI	CSO	CSP	CSR	CSS	CSU	CSW
CSX	CSY	CSZ	CTH	CWR	CXM	CY0	CY1	CY3	CY4	CYA	CYD
CYF	CYG	CYM	CYQ	CYR	CZ2	CZZ	D11	DAB	DAH	DAL	DAR
DAS	DBS	DBU	DBY	DBZ	DCY	DDE	DGL	DGN	DHA	DHI	DHN
DIL	DIR	DIV	DLE	DLS	DLY	DM0	DMH	DMK	DNE	DNG	DNL
DNM	DNP	DNS	DOH	DON	DPH	DPL	DPN	DPP	DPQ	DPR	DSE
DSG	DSN	DSP	DTH	DTR	DTY	DVA	DYG	EFC	FCL	FGL	FGP
FLA	FLE	FME	FOE	FPA	FT6	FTR	FTY	GAU	GGL	GHG	GHP
GLH	GLQ	GLZ	GMA	GPL	GSC	GSU	GT9	GYC	GYS	H5M	HAC
HAR	HBN	HIA	HIC	HIP	HIQ	HLU	HMF	HMR	HPC	HPE	HPQ
HRG	HRP	HSE	HSL	HSO	HTI	HTR	HV5	HY3	HYP	I58	IAM
IAS	IGL	IIC	IIL	ILG	ILX	IML	IOY	IT1	IYR	IYT	K1R
KCX	KGC	KOR	KST	KYN	LA2	LAA	LAL	LCK	LCX	LDH	LED
LEF	LLP	LLY	LME	LNT	LPD	LPG	LPS	LTR	LVG	LYM	LYN
LYR	LYX	LYZ	M0H	M3L	MAA	MAI	MBQ	MC1	MCL	MCS	MDO
MEA	MEG	MEN	MEQ	MEU	MFC	MGG	MGN	MGY	MHL	MHO	MHS
MIS	MLE	MLL	MLY	MLZ	MME	MNL	MNV	MPQ	MSE	MSL	MSO
MVA	N10	N7P	NAL	NAM	NBQ	NC1	NCB	NDF	NEM	NEP	NFA
NHL	NIY	NLE	NLN	NLO	NLP	NLQ	NMC	NMM	NNH	NPH	NRQ
NTY	NVA	NYG	NZH	OAS	OCS	OCY	OHI	OHS	OMT	OPR	ORN
ORQ	OSE	OTY	OXX	P1L	P2Y	PAQ	PAS	PAT	PAU	PBB	PBF
PCA	PCC	PCS	PEC	PF5	PFF	PG1	PG9	PGY	PHA	PHD	PHI
PHL	PHM	PLE	PM3	POM	PPH	PPN	PR3	PRR	PRS	PSA	PSH
PTH	PTM	PTR	PVH	PYA	PYX	QLG	R1A	R1B	R1F	R7A	RC7
RCY	SAC	SAH	SAR	SBD	SBL	SCH	SCS	SCY	SDP	SEB	SEC
SEG	SEL	SEP	SET	SHC	SHP	SHR	SIB	SLZ	SMC	SME	SMF
SNC	SOC	SOY	STY	SUI	SVA	T11	TAV	TBG	TBM	TFQ	THC
TIH	TMB	TMD	TNB	TNR	TOX	TPL	TPO	TPQ	TQQ	TRG	TRN
TRO	TRQ	TRW	TRX	TTQ	TTS	TYB	TYI	TYN	TYO	TYQ	TYS
TYT	TYY	UMA	UNK	VAD	X9Q	XX1	XXY	XYG	YCM		

**Supplementary Table 2. List of frequently encountered buffer molecules.** The following table specifies 67 three-letter PDB names of ligands, which are found in crystallization buffers, and which in general do not have biological significance.

These names define ligands with letter 'B' in the *class* column of the main table.

PO4	SO4	GOL	EDO	BME	MPD	PEG	ACY	TRS	FMT	MES	CIT
PG4	DMS	IMD	EPE	IPA	PGE	MRD	1PE	FLC	TLA	EOH	P6G
BEN	DTT	BEZ	NHE	MLA	DOD	3PG	HTO	2PE	1PG	PGO	HEZ
PE4	MOH	15P	P33	TBU	13P	ACN	12P	PG6	PGR	7PE	NH3
ETX	P4C	PG5	PE8	PG0	PE5	PDO	P22	PE3	CE1	3PO	TME
9PE	8PE	PE9	PE7	PE6	PE2	PE1					