

Dataset S2. PDB cluster codes

Cluster Number	PDB	Residues
1	2ww8	Glu54-Chain A, Glu103-Chain A, Lys731-Chain A
	6o6y	Lys231-Chain A, Glu250-Chain A, Glu422-Chain A
	5gw9	Lys24-Chain A, Asp28-Chain A, Asp110-Chain A
	3oyv	Lys116-Chain A, Glu137-Chain A, Asp147-Chain A
	5xwi	Glu279-Chain A, Lys330-Chain A, Asp334-Chain A
	5k4b	Lys248-Chain A, Glu350-Chain A, Glu359-Chain B
	4q8k	Glu188-Chain A, Glu221-Chain A, Lys349-Chain A
	5ziq	Lys129-Chain B, Glu186-Chain B, Glu190-Chain B
	4xxl	Glu72-Chain A, Lys108-Chain A, Asp112-Chain A
	6os7	Lys183-Chain A, Glu200-Chain A, Glu357-Chain B
	3drf	Asp504-Chain A, Lys525-Chain A, Asp529-Chain A
	3l1n	Lys30-Chain A, Asp34-Chain A, Asp49-Chain A
	3k6o	Asp119-Chain A, Lys193-Chain B, Asp195-Chain B
	6sa9	Asp55-Chain A, Lys31-Chain B, Asp35-Chain B
	5dl8	Lys300-Chain B, Glu303-Chain B, Glu343-Chain B
	3pty	Lys747-Chain A, Asp754-Chain A, Asp1051-Chain A
2pd2	Glu33-Chain B, Glu94-Chain B, Lys98-Chain B	
2	2o16	Asp134-Chain A, Lys63-Chain B, Asp134-Chain B
	2zod	Asp136-Chain A, Lys140-Chain A, Asp136-Chain B
	3cra	Lys119-Chain A, Glu122-Chain A, Asp61-Chain B
	6lce	Asp129-Chain A, Lys134-Chain A, Glu151-Chain A
	3cay	Glu7-Chain C, Glu18-Chain J, Lys22-Chain J
	5xwi	Glu58-Chain A, Lys234-Chain A, Glu309-Chain A
	5x93	Glu299-Chain A, Lys303-Chain A, Glu1021-Chain A
	3m6z	Asp31-Chain A, Glu123-Chain A, Lys282-Chain A
	3lp5	Lys73-Chain A, Asp77-Chain A, Glu153-Chain A
	4u9v	Lys97-Chain B, Glu100-Chain B, Glu139-Chain B
	2xu3	Lys17-Chain A, Glu50-Chain A, Glu86-Chain A
	3ot2	Glu28-Chain A, Lys123-Chain A, Asp159-Chain B
	5dwa	Glu173-Chain A, Asp223-Chain A, Lys224-Chain A
	3m6z	Asp31-Chain B, Glu123-Chain B, Lys282-Chain B
3hr0	Asp538-Chain A, Lys541-Chain A, Glu662-Chain A	
3	3lrk	Asp35-Chain A, Asp72-Chain A, Lys147-Chain A
	5coz	Glu306-Chain A, Lys309-Chain A, Asp368-Chain A
	2ygk	Glu77-Chain A, Lys304-Chain A, Asp308-Chain A
	4whn	Glu9-Chain C, Glu13-Chain C, Lys49-Chain C
	3sd7	Asp11-Chain A, Lys144-Chain A, Asp172-Chain A
	4yn8	Asp8-Chain A, Asp50-Chain A, Lys99-Chain A
	4i90	Glu207-Chain A, Asp210-Chain A, Lys214-Chain A

	6kqs	Asp100-Chain A, Lys453-Chain A, Glu497-Chain A
	4ri2	Lys34-Chain A, Glu37-Chain A, Asp98-Chain A
4	4zr8	Glu92-Chain B, Glu95-Chain B, Lys98-Chain B
	5fc2	Glu1773-Chain B, Lys1776-Chain B, Glu1777-Chain B
	4hye	Glu141-Chain A, Glu143-Chain B, Lys180-Chain B
	3e6c	Lys62-Chain C, Asp64-Chain C, Glu72-Chain C
	1c3c	Lys387-Chain A, Glu391-Chain A, Glu395-Chain A
	4qdc	Lys166-Chain A, Glu298-Chain A, Glu302-Chain A
	3mgg	Lys224-Chain A, Glu235-Chain A, Glu239-Chain A
5	3nua	Glu91-Chain A, Lys178-Chain A, Glu180-Chain A
	3sdb	Asp372-Chain A, Asp482-Chain A, Lys510-Chain A
	4q6j	Glu36-Chain A, Glu122-Chain A, Lys173-Chain A
	5gt5	Lys271-Chain A, Asp272-Chain A, Asp296-Chain A
	4wep	Asp92-Chain A, Asp95-Chain A, Lys107-Chain A
	3q1n	Lys216-Chain A, Asp231-Chain A, Glu291-Chain A
6	2zfn	Lys105-Chain A, Glu109-Chain A, Glu232-Chain A
	4z39	Glu21-Chain A, Lys28-Chain A, Asp116-Chain B
	3i42	Glu25-Chain A, Asp69-Chain A, Lys120-Chain A
	5ytq	Lys69-Chain A, Glu72-Chain A, Glu39-Chain B
	2qvg	Glu14-Chain A, Asp66-Chain A, Lys118-Chain A
	5x5j	Glu19-Chain A, Asp63-Chain A, Lys112-Chain A
7	4hzi	Glu236-Chain A, Glu240-Chain A, Lys261-Chain A
	4i6k	Glu132-Chain A, Asp157-Chain A, Lys188-Chain A
	5jaz	Lys205-Chain A, Asp231-Chain A, Glu318-Chain A
	5i6r	Lys6-Chain A, Glu12-Chain A, Glu16-Chain A
	2xxp	Lys172-Chain A, Glu195-Chain A, Asp454-Chain A
	3o3o	Asp82-Chain A, Lys347-Chain A, Glu329-Chain B
8	2yk4	Glu159-Chain A, Lys161-Chain A, Asp209-Chain A
	6w40	Glu3-Chain A, Asp73-Chain B, Lys75-Chain B
	2rc3	Lys24-Chain A, Glu32-Chain A, Asp146-Chain A
	6dyf	Glu18-Chain A, Glu92-Chain A, Lys95-Chain A
	3mvp	Lys151-Chain A, Asp179-Chain A, Glu187-Chain B
	5cdv	Glu246-Chain A, Asp329-Chain A, Lys346-Chain A