



STRUCTURAL
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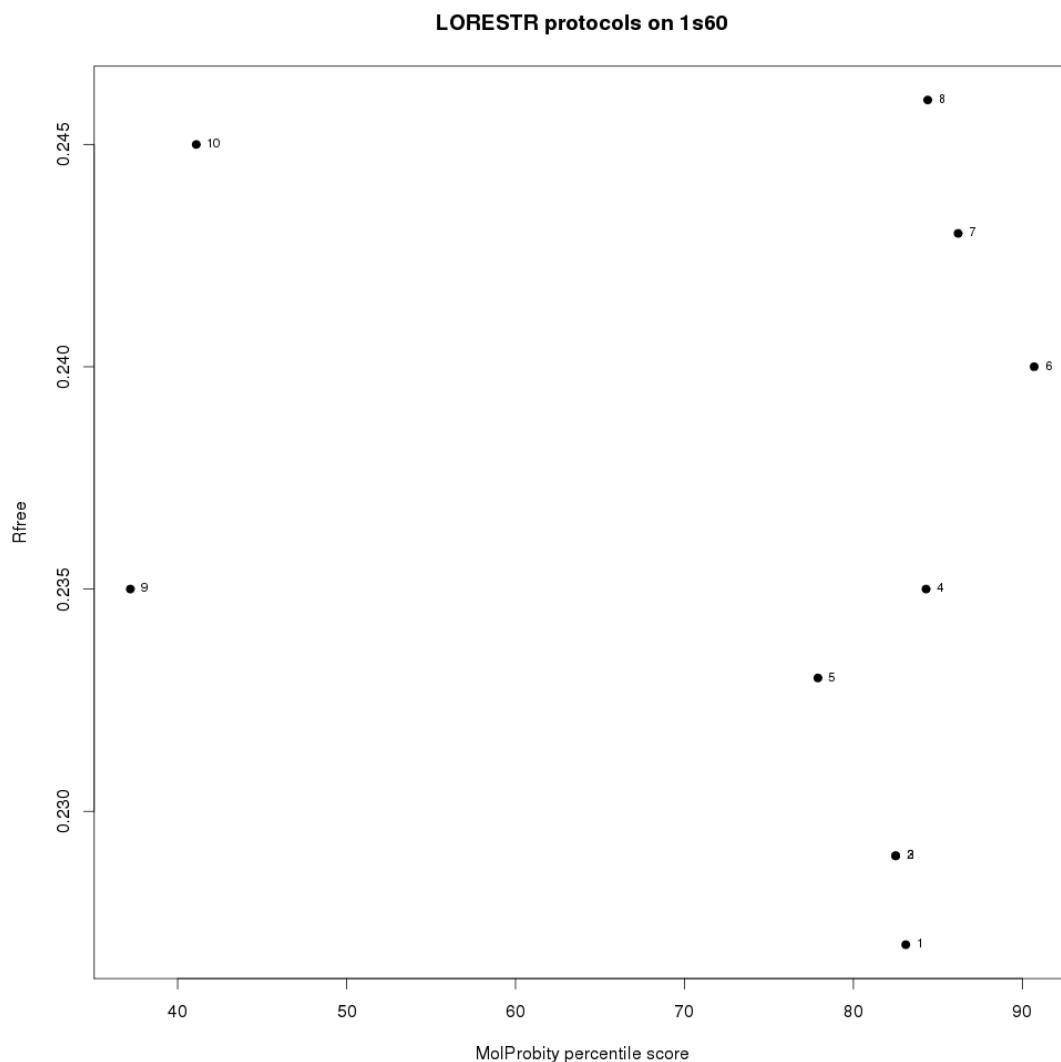
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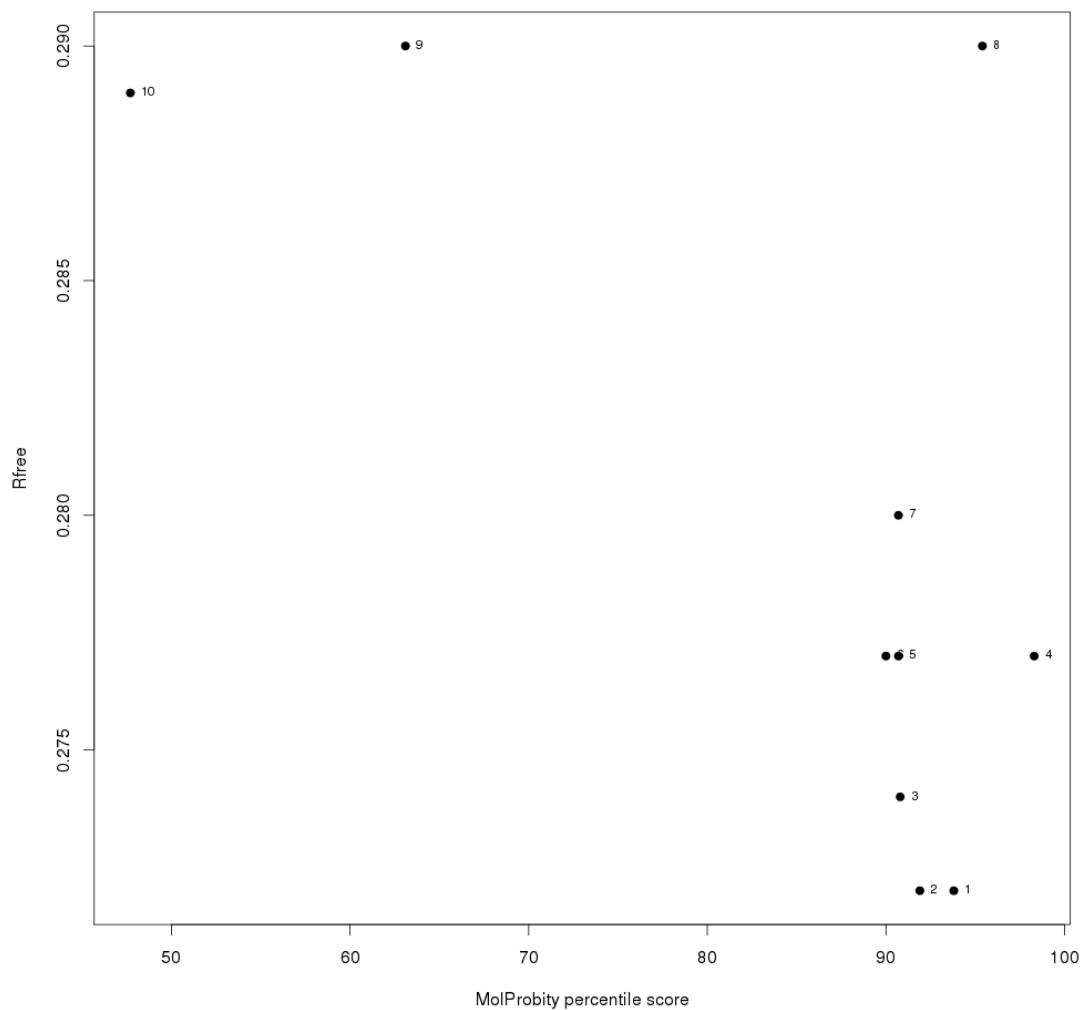
Supporting information for article:

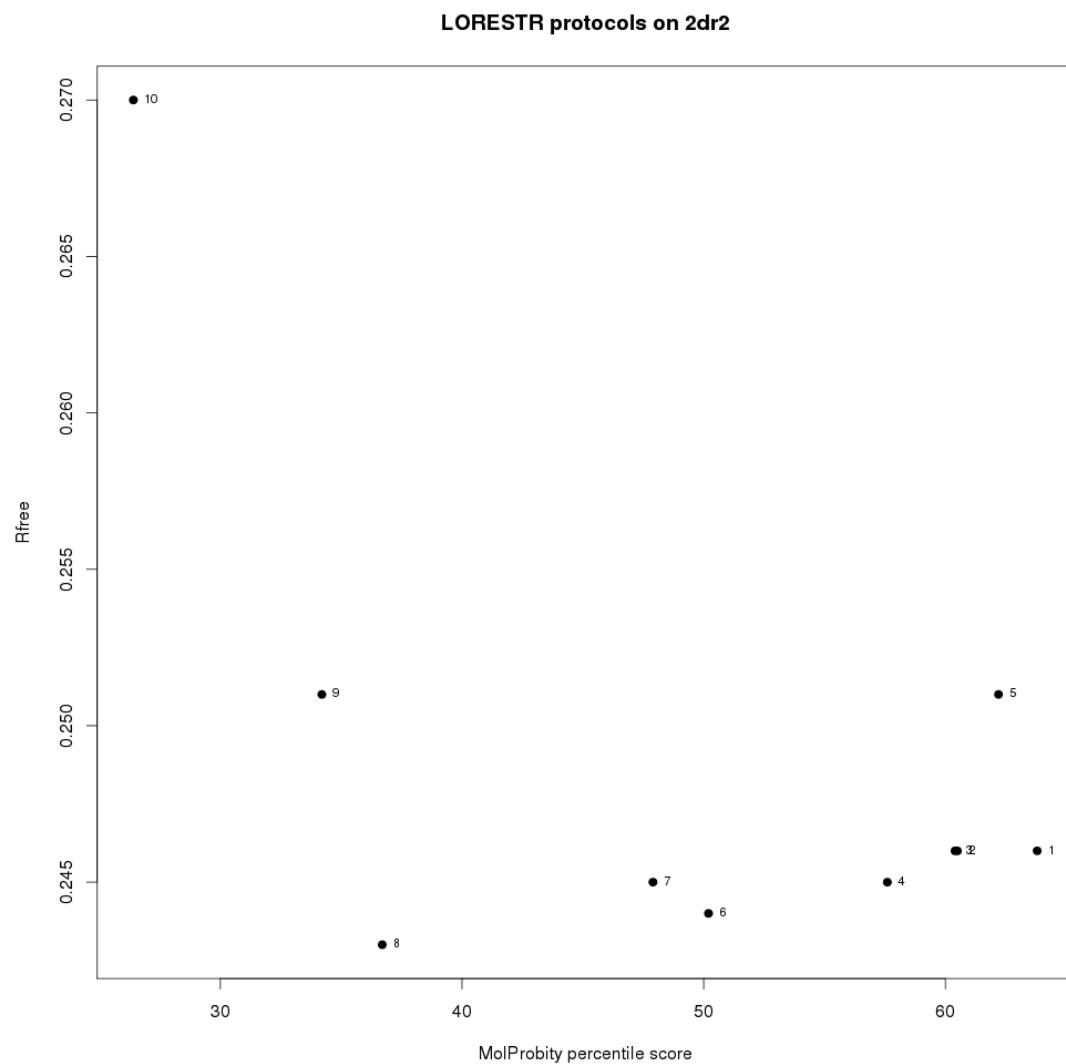
Automated refinement of macromolecular structures at low resolution using prior information

Oleg Kovalevskiy, Robert A. Nicholls and Garib N. Murshudov

Figure S1 Supporting information Scatterplots show performance of the LORESTR Q-score ranking on several random test cases; the numeric observation labels indicate the Q-score rank for a particular protocol that resulted in the corresponding R_{free} value and MolProbity percentile score.



LORESTR protocols on 2zo2



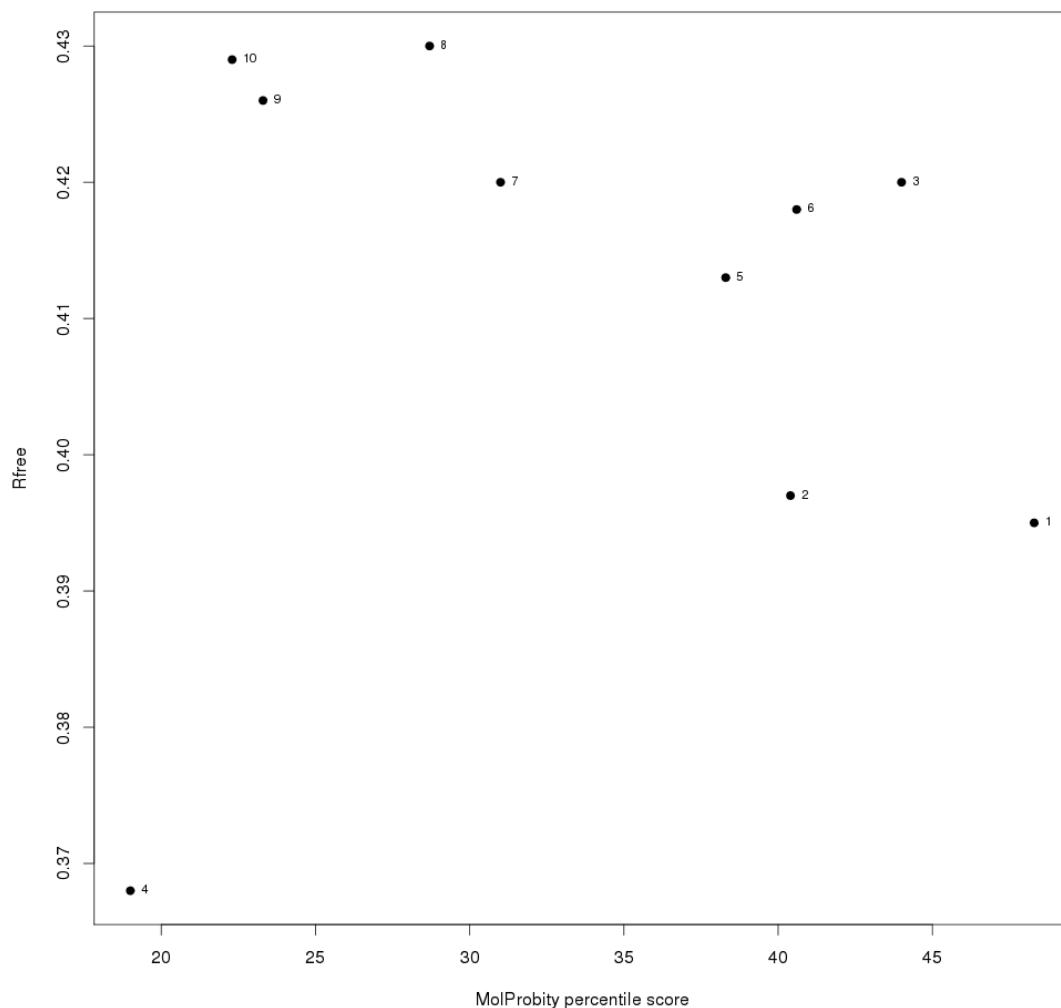
LORESTR protocols on 3l1g

Table S1 Details of the test sets

Subset 1: more than two homologues, used for refinement with multiple homologues

Subset 2: have homologues with 75%-90% sequence identity

Subset 3: cases where multiple homologues performed better or equal to a single homologue

Subset 4: cases where multiple homologues performed worse than a single homologue

PDB code	Reported resolution	Resolution of the data	Subset 1	Subset 2	Subset 3	Subset 4	Number of homologues	High-resolution homologues (PDB code, resolution, sequence identity, RMSD)
2rgr	3.0	3.0	X				3	3l4j (2.5 Å, 99.7%, 2.79 Å), 1bjt (2.5 Å, 100.0%, 15.90 Å), 1bgw (2.7 Å, 100.0%, 15.20 Å),
2is2	3.0	3.0	X		X		3	3lfu (1.8 Å, 99.8%, 14.50 Å), 2is6 (2.2 Å, 100.0%, 3.01 Å), 2is1 (2.9 Å, 100.0%, 1.22 Å),
1ob5	3.1	3.0	X				7	2c78 (1.4 Å, 98.0%, 4.41 Å), 2c77 (1.6 Å, 97.8%, 4.01 Å), 1exm (1.7 Å, 97.5%, 2.34 Å), 1ha3 (2.0 Å, 97.4%, 1.35 Å), 1b23 (2.6 Å, 100.0%, 2.58 Å), 1ttt (2.7 Å, 100.0%, 2.54 Å), 1tui (2.7 Å, 100.0%, 11.10 Å),
2c9m	3.0	3.0	X			X	11	3ar7 (2.1 Å, 100.0%, 15.40 Å), 3n5k (2.2 Å, 100.0%, 15.50 Å), 1wpg (2.3 Å, 100.0%, 15.30 Å), 2agv (2.4 Å, 100.0%, 15.40 Å), 2zbf (2.4 Å, 100.0%, 14.30 Å), 2zbd (2.4 Å, 100.0%, 13.90 Å), 1su4 (2.4 Å, 100.0%, 4.61 Å), 3fpb (2.5 Å, 100.0%, 15.40 Å), 3b9b (2.6 Å, 100.0%, 14.10 Å), 1vfp (2.9 Å, 100.0%, 14.00 Å), 2eat (2.9 Å, 100.0%, 15.50 Å),
3b9r	3.0	3.0	X			X	11	3ar7 (2.1 Å, 100.0%, 4.41 Å), 3n5k (2.2 Å, 100.0%, 1.43 Å), 1wpg (2.3 Å, 100.0%, 1.46 Å), 2agv (2.4 Å, 100.0%, 4.46 Å), 2zbf (2.4 Å, 100.0%, 2.60 Å), 2zbd (2.4 Å, 100.0%, 11.60 Å), 1su4 (2.4 Å, 100.0%, 13.40 Å), 3fpb (2.5 Å, 100.0%, 1.55 Å), 3b9b (2.6 Å, 100.0%, 3.81 Å), 1vfp (2.9 Å, 100.0%, 11.80 Å), 2eat (2.9 Å, 100.0%, 4.39 Å),

2pkg	3.3	3.3	X				4	1b3u (2.3 Å, 100.0%, 6.24 Å), 2ie4 (2.6 Å, 100.0%, 5.59 Å), 3fga (2.7 Å, 99.8%, 2.83 Å), 3dw8 (2.9 Å, 100.0%, 2.05 Å),
3s4u	3.3	3.3	X		X		3	3p7i (1.7 Å, 99.7%, 7.71 Å), 3quj (2.2 Å, 97.6%, 7.99 Å), 3qk6 (2.4 Å, 97.7%, 7.90 Å),
1lwt	3.2	3.2	X				3	1dfa (2.0 Å, 98.0%, 3.80 Å), 1jva (2.1 Å, 97.5%, 1.31 Å), 1ef0 (2.1 Å, 97.8%, 2.44 Å),
1lws	3.5	3.5	X				3	1dfa (2.0 Å, 98.0%, 3.80 Å), 1jva (2.1 Å, 97.5%, 1.30 Å), 1ef0 (2.1 Å, 97.8%, 2.77 Å),
1u88	3.5	3.5	X			X	6	1dug (1.8 Å, 99.5%, 0.69 Å), 3crt (1.9 Å, 99.0%, 0.76 Å), 1m9a (2.1 Å, 99.5%, 0.67 Å), 4ecb (2.2 Å, 99.5%, 1.47 Å), 1gta (2.4 Å, 99.5%, 0.68 Å), 1b8x (2.7 Å, 99.5%, 0.83 Å),
3ks2	3.3	3.3	X				2	3gz1 (2.1 Å, 100.0%, 7.46 Å), 3gyz (2.1 Å, 100.0%, 5.61 Å),
1a7b	3.1	3.1	X			X	2	1cdc (2.0 Å, 100.0%, 7.32 Å), 1a64 (2.0 Å, 100.0%, 0.76 Å),
2dut	3.0	3.0	X				3	2h4p (1.7 Å, 100.0%, 6.97 Å), 2h4q (2.1 Å, 97.6%, 4.49 Å), 2h4r (2.7 Å, 100.0%, 1.17 Å),
1l5t	3.0	3.0	X				6	1h45 (1.9 Å, 98.7%, 6.26 Å), 1h44 (2.0 Å, 99.4%, 6.01 Å), 1dsn (2.0 Å, 99.0%, 6.77 Å), 1hse (2.2 Å, 99.1%, 6.07 Å), 1vfe (2.3 Å, 99.4%, 6.31 Å), 1vfd (2.5 Å, 99.4%, 6.30 Å),
1jkt	3.5	3.5	X	X		X	13	3bhy (1.2 Å, 82.1%, 1.26 Å), 2w4j (1.3 Å, 100.0%, 1.44 Å), 2a2a (1.5 Å, 77.9%, 1.72 Å), 3bqr (1.8 Å, 81.7%, 6.39 Å), 2xuu (1.8 Å, 99.6%, 1.55 Å), 2yab (1.9 Å, 78.2%, 1.60 Å), 2w4k (1.9 Å, 100.0%, 1.56 Å), 2j90 (2.0 Å, 81.1%, 6.08 Å), 2xz (2.0 Å, 100.0%, 1.68 Å), 2x0g (2.2 Å, 100.0%, 1.52 Å), 1wvw (2.4 Å, 100.0%, 1.49 Å), 2y4p (2.6 Å, 100.0%, 5.49 Å), 1zws (2.9 Å, 77.9%, 1.65 Å),
2atq	3.2	3.2	X		X		5	3qex (1.7 Å, 99.6%, 6.21 Å), 3l8b (2.1 Å, 100.0%, 3.27 Å), 1ih7 (2.2 Å, 99.8%, 2.73 Å),

								2dtu (2.4 Å, 99.9%, 3.13 Å), 1clq (2.7 Å, 99.8%, 2.32 Å),
3vqk	4.5	4.5	X				4	3aab (1.9 Å, 98.1%, 4.28 Å), 3vql (1.9 Å, 100.0%, 1.69 Å), 3aac (2.4 Å, 98.1%, 7.16 Å), 3vqm (2.5 Å, 100.0%, 1.64 Å),
3dpn	3.3	3.2	X			X	3	3dor (2.2 Å, 97.1%, 6.04 Å), 3dpm (2.4 Å, 96.7%, 6.42 Å), 3dja (2.9 Å, 95.8%, 6.40 Å),
3e3j	6.7	6.7	X			X	4	1msw (2.1 Å, 99.9%, 16.00 Å), 1qln (2.4 Å, 99.9%, 6.34 Å), 1aro (2.8 Å, 99.6%, 6.16 Å), 1h38 (2.9 Å, 99.9%, 16.60 Å),
2waf	3.3	3.3	X			X	2	2wad (2.2 Å, 91.1%, 6.22 Å), 2wae (2.3 Å, 90.9%, 6.21 Å),
2hzv	3.1	3.1	X				2	2hza (2.1 Å, 100.0%, 5.64 Å), 1q5v (2.3 Å, 98.2%, 4.70 Å),
3lco	3.4	3.4	X			X	3	2i1m (1.8 Å, 95.8%, 1.52 Å), 3lcd (2.5 Å, 99.3%, 3.65 Å), 2ogv (2.7 Å, 98.6%, 1.81 Å),
3idq	3.7	3.7	X			X	4	2woj (2.0 Å, 100.0%, 2.62 Å), 3zs9 (2.1 Å, 100.0%, 2.54 Å), 3h84 (2.3 Å, 100.0%, 2.43 Å), 3a36 (2.8 Å, 99.6%, 2.37 Å),
1gub	3.1	3.0	X		X		2	1gud (1.7 Å, 100.0%, 1.05 Å), 1rpj (1.8 Å, 100.0%, 3.95 Å),
1t38	3.2	3.2	X	X			3	3l00 (1.7 Å, 86.8%, 1.12 Å), 1qnt (1.9 Å, 99.3%, 0.76 Å), 3kzy (1.9 Å, 86.8%, 1.11 Å),
3l8j	3.0	3.0	X		X		2	3ajm (2.3 Å, 100.0%, 3.77 Å), 3l8i (2.5 Å, 100.0%, 1.74 Å),
1w8b	3.0	2.8	X				6	2bz6 (1.6 Å, 100.0%, 0.98 Å), 2c4f (1.7 Å, 100.0%, 1.02 Å), 2flb (1.9 Å, 100.0%, 1.25 Å), 1jbu (2.0 Å, 100.0%, 3.94 Å), 1fak (2.1 Å, 100.0%, 1.13 Å), 1qfk (2.8 Å, 100.0%, 1.19 Å),
3p39	3.1	3.1	X	X		X	14	3rv (1.8 Å, 92.4%, 0.78 Å), 2rhk (1.9 Å, 87.4%, 1.63 Å), 3o9r (2.0 Å, 92.4%, 0.73 Å), 3m5r (2.0 Å, 82.6%, 2.30 Å), 2gx9 (2.1 Å, 85.4%, 1.68 Å), 3ee9 (2.1 Å, 85.2%, 2.36 Å), 3o9t (2.2 Å, 82.8%, 1.72 Å), 3kwg (2.2 Å, 86.1%, 2.39 Å), 3l4q (2.3 Å, 90.0%, 3.18 Å),

							3p31 (2.5 Å, 99.2%, 1.81 Å), 3o9s (2.5 Å, 90.9%, 1.81 Å), 3o9q (2.5 Å, 91.7%, 0.86 Å), 3ee8 (2.6 Å, 85.2%, 2.42 Å), 3p38 (2.8 Å, 100.0%, 0.32 Å),
3o9u	3.2	3.2	X	X		14	3rvc (1.8 Å, 99.1%, 0.72 Å), 2rhk (1.9 Å, 89.7%, 1.70 Å), 3o9r (2.0 Å, 99.1%, 0.82 Å), 3m5r (2.0 Å, 87.1%, 1.81 Å), 2gx9 (2.1 Å, 95.7%, 0.72 Å), 3ee9 (2.1 Å, 89.7%, 1.73 Å), 3o9t (2.2 Å, 100.0%, 1.52 Å), 3kwg (2.2 Å, 88.8%, 1.78 Å), 3l4q (2.3 Å, 100.0%, 1.89 Å), 3p31 (2.5 Å, 92.2%, 1.85 Å), 3o9s (2.5 Å, 100.0%, 1.37 Å), 3o9q (2.5 Å, 99.1%, 0.69 Å), 3ee8 (2.6 Å, 89.7%, 1.88 Å), 3p38 (2.8 Å, 91.4%, 0.92 Å),
1ob2	3.4	3.4	X		X	10	1efc (2.0 Å, 100.0%, 11.20 Å), 2hcj (2.1 Å, 99.4%, 11.00 Å), 3u6b (2.1 Å, 99.7%, 10.80 Å), 2bvn (2.3 Å, 100.0%, 3.41 Å), 1d8t (2.4 Å, 99.7%, 11.20 Å), 3u6k (2.5 Å, 99.7%, 11.60 Å), 1efu (2.5 Å, 100.0%, 11.80 Å), 1dg1 (2.5 Å, 100.0%, 11.10 Å), 3u2q (2.7 Å, 99.7%, 11.80 Å), 2hdn (2.8 Å, 99.7%, 11.20 Å),
2fx3	3.4	3.4	X			10	1efc (2.0 Å, 99.7%, 1.21 Å), 2hcj (2.1 Å, 99.7%, 1.30 Å), 3u6b (2.1 Å, 100.0%, 1.30 Å), 2bvn (2.3 Å, 99.7%, 11.80 Å), 1d8t (2.4 Å, 100.0%, 1.25 Å), 3u6k (2.5 Å, 100.0%, 1.25 Å), 1efu (2.5 Å, 99.7%, 2.68 Å), 1dg1 (2.5 Å, 99.7%, 1.46 Å), 3u2q (2.7 Å, 100.0%, 1.09 Å), 2hdn (2.8 Å, 100.0%, 1.38 Å),
2cxf	3.1	3.1				1	2dwk (2.0 Å, 100.0%, 3.36 Å),
2cxl	3.2	3.2				1	2dwk (2.0 Å, 100.0%, 2.91 Å),
1juj	3.0	3.0	X			12	3gh0 (1.6 Å, 99.6%, 3.02 Å), 4e5o (1.7 Å, 93.4%, 2.85 Å), 4eb4 (1.7 Å, 93.4%, 0.52 Å), 1hvy (1.9 Å, 99.3%, 0.58 Å), 3ihi (1.9 Å, 93.2%, 0.71 Å), 1hzw (2.0 Å, 98.9%, 1.01 Å), 3n5e (2.3 Å, 98.5%, 2.41 Å), 2rd8 (2.5 Å,

							99.3%, 1.27 Å), 2tsr (2.6 Å, 92.9%, 0.78 Å), 3h9k (2.6 Å, 99.3%, 1.10 Å), 2rda (2.7 Å, 99.3%, 1.45 Å), 3gg5 (2.8 Å, 99.6%, 1.05 Å),
1fvf	3.2	3.2	X			2	1epu (2.4 Å, 96.5%, 3.05 Å), 1fvh (2.8 Å, 100.0%, 2.32 Å),
1rfq	3.0	3.0	X	X	49	2fxu (1.4 Å, 99.7%, 0.97 Å), 1wua (1.4 Å, 99.7%, 0.88 Å), 2v52 (1.4 Å, 100.0%, 1.20 Å), 1qz5 (1.4 Å, 99.7%, 1.31 Å), 3mn5 (1.5 Å, 99.1%, 1.88 Å), 2pbd (1.5 Å, 99.7%, 1.34 Å), 1j6z (1.5 Å, 99.7%, 1.53 Å), 3cip (1.6 Å, 91.4%, 1.08 Å), 2asm (1.6 Å, 100.0%, 0.99 Å), 1d4x (1.8 Å, 93.9%, 1.11 Å), 3sjh (1.8 Å, 100.0%, 0.84 Å), 2pav (1.8 Å, 99.7%, 1.14 Å), 2hf3 (1.8 Å, 93.3%, 1.12 Å), 2a40 (1.8 Å, 99.7%, 1.19 Å), 2a42 (1.9 Å, 99.7%, 1.09 Å), 2hmp (1.9 Å, 99.7%, 1.34 Å), 2gkj (1.9 Å, 99.7%, 1.23 Å), 1yag (1.9 Å, 87.3%, 1.08 Å), 1t44 (2.0 Å, 100.0%, 1.22 Å), 2gwk (2.0 Å, 99.7%, 1.12 Å), 3mn7 (2.0 Å, 93.3%, 1.07 Å), 3mn6 (2.0 Å, 93.3%, 1.12 Å), 3m6g (2.0 Å, 100.0%, 0.95 Å), 1esv (2.0 Å, 99.7%, 1.06 Å), 1c0g (2.0 Å, 90.9%, 1.04 Å), 3u8x (2.0 Å, 100.0%, 1.02 Å), 1yxq (2.0 Å, 99.7%, 0.94 Å), 3u9z (2.1 Å, 100.0%, 1.38 Å), 1kxp (2.1 Å, 100.0%, 0.90 Å), 1mdu (2.2 Å, 99.7%, 1.18 Å), 3ub5 (2.2 Å, 94.2%, 1.60 Å), 3chv (2.3 Å, 91.4%, 1.07 Å), 1rdw (2.3 Å, 100.0%, 0.99 Å), 2vyp (2.4 Å, 100.0%, 1.11 Å), 2v51 (2.4 Å, 100.0%, 1.00 Å), 1ma9 (2.4 Å, 99.7%, 1.03 Å), 4efh (2.5 Å, 92.8%, 1.08 Å), 2a5x (2.5 Å, 100.0%, 0.85 Å), 3el2 (2.5 Å, 93.3%, 1.05 Å), 2q97 (2.5 Å, 99.7%, 1.04 Å), 2q36 (2.5 Å, 100.0%, 0.93 Å), 2d1k (2.5 Å, 99.7%, 1.21 Å), 3daw (2.5 Å, 100.0%, 1.63 Å), 1p8z (2.6 Å, 100.0%, 0.94 Å), 2oan (2.6 Å, 94.1%, 1.06 Å),	

								2q1n (2.7 Å, 100.0%, 0.99 Å), 3ue5 (2.8 Å, 100.0%, 1.10 Å), 1atn (2.8 Å, 99.7%, 1.31 Å), 3buz (2.8 Å, 100.0%, 1.01 Å),
3n6s	3.1	3.1	X		X		2	3mva (2.2 Å, 100.0%, 1.78 Å), 3n7q (2.4 Å, 100.0%, 3.05 Å),
3oz0	3.0	3.0	X			X	6	2awh (2.0 Å, 99.6%, 1.61 Å), 3gz9 (2.0 Å, 99.2%, 2.59 Å), 2b50 (2.0 Å, 99.6%, 2.34 Å), 3sp9 (2.3 Å, 100.0%, 2.82 Å), 2xyj (2.3 Å, 100.0%, 2.86 Å), 2q5g (2.7 Å, 100.0%, 1.74 Å),
3prj	3.1	3.1	X		X		7	2q3e (2.0 Å, 100.0%, 0.86 Å), 2qg4 (2.1 Å, 100.0%, 2.19 Å), 3tf5 (2.3 Å, 100.0%, 2.67 Å), 3khu (2.3 Å, 99.8%, 1.82 Å), 3itk (2.4 Å, 99.8%, 2.38 Å), 3ptz (2.5 Å, 100.0%, 0.31 Å), 3tdk (2.8 Å, 100.0%, 0.35 Å),
2qnc	3.1	3.1	X		X		3	1e7l (1.3 Å, 100.0%, 1.62 Å), 1en7 (2.4 Å, 99.4%, 2.23 Å), 1e7d (2.8 Å, 99.4%, 1.24 Å),
2qrn	3.4	3.2	X		X		8	1p5z (1.6 Å, 100.0%, 0.67 Å), 2no7 (1.7 Å, 98.7%, 0.78 Å), 2zi6 (1.8 Å, 99.1%, 1.22 Å), 2zia (1.8 Å, 98.6%, 0.71 Å), 3qeo (1.9 Å, 97.8%, 1.73 Å), 2zi7 (2.0 Å, 98.6%, 0.85 Å), 3mjr (2.1 Å, 98.7%, 1.56 Å), 3ipy (2.5 Å, 100.0%, 1.65 Å),
4dt0	3.6	3.6	X				2	2dm9 (1.9 Å, 100.0%, 2.87 Å), 2dma (2.0 Å, 96.6%, 2.95 Å),
1s60	3.0	3.0	X				2	2vbq (2.0 Å, 100.0%, 0.60 Å), 1s5k (2.4 Å, 100.0%, 2.50 Å),
2dpu	3.1	3.1	X			X	3	1bm9 (2.0 Å, 99.1%, 2.14 Å), 2efw (2.5 Å, 100.0%, 1.33 Å), 1f4k (2.5 Å, 100.0%, 0.74 Å),
3l1g	3.3	3.3	X			X	3	2y1y (2.0 Å, 98.7%, 1.49 Å), 2y1z (2.5 Å, 97.6%, 2.49 Å), 2wj7 (2.6 Å, 100.0%, 1.62 Å),
3id2	3.1	3.1	X			X	3	2zpm (1.0 Å, 91.9%, 1.17 Å), 3id4 (1.6 Å, 97.8%, 1.81 Å), 3id3 (2.0 Å, 98.9%, 2.18 Å),
2r8a	3.0	3.0	X			X	6	3pgu (1.7 Å, 99.2%, 0.82 Å), 3pgs (1.9 Å, 99.2%, 0.91 Å), 2r88 (2.6 Å, 98.6%, 0.59 Å),

								1t16 (2.6 Å, 99.2%, 0.71 Å), 1t1l (2.8 Å, 99.2%, 0.90 Å), 2r4p (2.9 Å, 99.2%, 0.69 Å),
2r4n	3.2	3.1	X		X	6		3pgu (1.7 Å, 99.2%, 1.94 Å), 3pgs (1.9 Å, 99.3%, 0.83 Å), 2r88 (2.6 Å, 98.9%, 0.97 Å), 1t16 (2.6 Å, 99.5%, 0.59 Å), 1t1l (2.8 Å, 99.5%, 0.93 Å), 2r4p (2.9 Å, 99.5%, 0.57 Å),
2c86	3.0	3.0	X			2		2gec (1.3 Å, 92.5%, 1.91 Å), 2bxx (1.9 Å, 100.0%, 1.19 Å),
3km2	3.1	3.1	X		X	4		3pu7 (1.8 Å, 100.0%, 0.36 Å), 3hog (1.9 Å, 100.0%, 2.28 Å), 3km1 (2.0 Å, 100.0%, 0.74 Å), 1srd (2.0 Å, 90.2%, 0.68 Å),
3hl9	3.4	3.4	X			2		3hld (2.0 Å, 98.5%, 2.06 Å), 3hlb (2.5 Å, 100.0%, 0.47 Å),
3cl9	3.3	3.3	X		X	4		3irm (2.1 Å, 99.4%, 1.71 Å), 3inv (2.4 Å, 99.4%, 1.81 Å), 2h2q (2.4 Å, 100.0%, 1.50 Å), 3kjs (2.5 Å, 100.0%, 0.95 Å),
1i0e	3.5	3.5	X	X		6		1qh4 (1.4 Å, 81.6%, 1.41 Å), 1u6r (1.6 Å, 96.2%, 1.38 Å), 3drb (2.0 Å, 80.3%, 1.45 Å), 1vrp (2.1 Å, 83.9%, 1.44 Å), 1g0w (2.3 Å, 80.8%, 1.45 Å), 2crk (2.4 Å, 96.4%, 0.75 Å),
4a5t	3.5	3.5				1		4dur (2.5 Å, 100.0%, 1.93 Å),
3auw	3.6	3.6	X		X	2		3agw (2.2 Å, 100.0%, 1.16 Å), 2e4f (2.3 Å, 100.0%, 1.31 Å),
2akq	3.0	3.0	X	X		8		1beb (1.8 Å, 99.4%, 0.57 Å), 3uev (1.9 Å, 98.7%, 1.45 Å), 1uz2 (1.9 Å, 99.4%, 1.88 Å), 3kza (2.0 Å, 84.4%, 0.91 Å), 1yup (2.1 Å, 94.9%, 0.65 Å), 3ph5 (2.4 Å, 98.7%, 0.58 Å), 2q39 (2.5 Å, 100.0%, 1.30 Å), 2r56 (2.8 Å, 98.7%, 1.27 Å),
2bx5	3.1	3.1				1		2z5y (2.2 Å, 99.8%, 1.22 Å),
2zgk	3.0	3.0	X	X	X	12		2zgr (1.9 Å, 99.4%, 0.94 Å), 2zgl (1.9 Å, 100.0%, 0.92 Å), 2zgm (1.9 Å, 100.0%, 0.90 Å), 1ww7 (1.9 Å, 88.6%, 1.59 Å), 2zgq (1.9 Å, 99.4%, 0.96 Å), 3afk (1.9 Å, 100.0%, 0.95 Å), 3m3c (2.0 Å, 100.0%, 0.93 Å), 3m3o (2.1 Å,

								99.4%, 0.90 Å), 3m3e (2.1 Å, 99.4%, 0.94 Å), 3m3q (2.2 Å, 100.0%, 0.93 Å), 1ww6 (2.2 Å, 88.6%, 0.69 Å), 2zgu (2.4 Å, 99.4%, 1.34 Å),
1xcp	3.2	3.2	X		X		8	2afh (2.1 Å, 99.7%, 0.98 Å), 1fp6 (2.1 Å, 99.7%, 1.16 Å), 1g20 (2.2 Å, 96.5%, 1.74 Å), 2nip (2.2 Å, 99.7%, 1.04 Å), 1g1m (2.2 Å, 99.7%, 1.03 Å), 2afk (2.3 Å, 99.6%, 1.73 Å), 1m34 (2.3 Å, 99.6%, 1.76 Å), 1rw4 (2.5 Å, 98.9%, 1.65 Å),
1kog	3.5	3.5	X				3	1evl (1.6 Å, 100.0%, 0.57 Å), 1fyf (1.6 Å, 100.0%, 0.56 Å), 1evk (2.0 Å, 100.0%, 1.65 Å),
1u6b	3.1	3.1	X			X	9	1nu4 (1.8 Å, 100.0%, 1.64 Å), 1urn (1.9 Å, 100.0%, 0.88 Å), 1m5o (2.2 Å, 100.0%, 0.65 Å), 3egz (2.2 Å, 96.7%, 0.69 Å), 1sj3 (2.2 Å, 100.0%, 1.23 Å), 3mxh (2.3 Å, 100.0%, 0.93 Å), 1oia (2.4 Å, 97.8%, 1.30 Å), 2nz4 (2.5 Å, 100.0%, 0.66 Å), 3cul (2.8 Å, 95.7%, 0.74 Å),
3iwn	3.2	3.2	X			X	9	1nu4 (1.8 Å, 100.0%, 1.44 Å), 1urn (1.9 Å, 100.0%, 0.64 Å), 1m5o (2.2 Å, 100.0%, 0.65 Å), 3egz (2.2 Å, 96.7%, 0.62 Å), 1sj3 (2.2 Å, 100.0%, 0.59 Å), 3mxh (2.3 Å, 100.0%, 0.90 Å), 1oia (2.4 Å, 97.7%, 1.10 Å), 2nz4 (2.5 Å, 100.0%, 0.57 Å), 3cul (2.8 Å, 96.7%, 0.68 Å),
3p49	3.5	3.5	X				9	1nu4 (1.8 Å, 100.0%, 1.85 Å), 1urn (1.9 Å, 100.0%, 0.88 Å), 1m5o (2.2 Å, 100.0%, 0.88 Å), 3egz (2.2 Å, 96.7%, 0.83 Å), 1sj3 (2.2 Å, 100.0%, 0.89 Å), 3mxh (2.3 Å, 100.0%, 0.76 Å), 1oia (2.4 Å, 97.7%, 1.23 Å), 2nz4 (2.5 Å, 100.0%, 0.87 Å), 3cul (2.8 Å, 95.7%, 0.91 Å),
2dr2	3.0	3.0	X				6	1r6u (2.0 Å, 96.8%, 0.99 Å), 1r6t (2.1 Å, 96.5%, 0.95 Å), 2qui (2.4 Å, 100.0%, 0.85 Å), 1o5t (2.5 Å, 100.0%, 1.34 Å), 2quk (2.8 Å, 100.0%, 1.18 Å), 2azx (2.8 Å, 96.8%, 0.82 Å),

1dcm	3.0	2.6	X			X	2	1dbw (1.6 Å, 100.0%, 1.35 Å), 1d5w (2.3 Å, 99.2%, 1.72 Å),
2zni	3.1	3.1	X		X		2	3dsq (2.1 Å, 100.0%, 1.50 Å), 2znj (2.5 Å, 100.0%, 1.59 Å),
3fbr	3.5	3.5	X		X		4	3dnu (1.5 Å, 97.8%, 1.13 Å), 3dnt (1.7 Å, 97.6%, 0.80 Å), 2wiu (2.4 Å, 99.8%, 1.55 Å), 3dnv (2.7 Å, 99.5%, 1.10 Å),
2zys	3.1	3.1	X		X		2	2zyr (1.8 Å, 100.0%, 0.63 Å), 2zyh (1.8 Å, 99.8%, 1.51 Å),
1gc4	3.3	3.3	X				4	1b5p (1.8 Å, 99.5%, 1.20 Å), 5bj3 (2.2 Å, 100.0%, 0.71 Å), 1gck (2.5 Å, 99.5%, 1.16 Å), 1bkg (2.6 Å, 99.0%, 0.58 Å),
1gc3	3.3	3.3	X		X		4	1b5p (1.8 Å, 99.5%, 1.02 Å), 5bj3 (2.2 Å, 100.0%, 0.62 Å), 1gck (2.5 Å, 99.5%, 1.01 Å), 1bkg (2.6 Å, 99.0%, 0.69 Å),
2zo2	3.1	3.1	X	X		X	11	3fde (1.4 Å, 100.0%, 1.44 Å), 2zkd (1.6 Å, 98.9%, 1.23 Å), 3bi7 (1.7 Å, 86.5%, 0.78 Å), 2zkg (1.8 Å, 98.9%, 0.62 Å), 2pb7 (1.9 Å, 87.0%, 1.05 Å), 2zo1 (2.0 Å, 100.0%, 1.26 Å), 3f8j (2.0 Å, 99.0%, 1.24 Å), 2zo0 (2.2 Å, 100.0%, 1.32 Å), 3clz (2.2 Å, 87.7%, 1.36 Å), 3f8i (2.3 Å, 100.0%, 1.19 Å), 2zkf (2.5 Å, 98.9%, 1.23 Å),
4dx0	3.4	3.4	X	X		X	6	2br9 (1.8 Å, 72.6%, 1.36 Å), 1o9d (2.3 Å, 87.2%, 1.02 Å), 3axy (2.4 Å, 89.5%, 1.34 Å), 3e6y (2.5 Å, 87.2%, 1.11 Å), 3m50 (2.6 Å, 89.0%, 0.56 Å), 2o98 (2.7 Å, 87.3%, 1.06 Å),
2x0n	3.2	3.2	X	X			4	3ids (1.8 Å, 90.2%, 1.37 Å), 1i32 (2.6 Å, 80.7%, 1.22 Å), 1a7k (2.8 Å, 80.7%, 1.23 Å), 1gyp (2.8 Å, 80.7%, 1.24 Å),
1fb5	3.5	3.5	X			X	2	1oth (1.9 Å, 98.1%, 1.36 Å), 1fvo (2.6 Å, 98.1%, 1.25 Å),
2xrg	3.2	3.2	X		X		2	3nkq (1.7 Å, 98.3%, 1.05 Å), 2xr9 (2.0 Å, 99.9%, 1.18 Å),

1de9	3.0	3.0	X			X	7	2o3h (1.9 Å, 99.3%, 0.65 Å), 1hd7 (1.9 Å, 99.6%, 0.57 Å), 3u8u (2.1 Å, 99.6%, 0.98 Å), 1bix (2.2 Å, 99.6%, 0.51 Å), 1e9n (2.2 Å, 99.6%, 0.73 Å), 1dew (2.6 Å, 100.0%, 0.66 Å), 2isi (2.8 Å, 99.6%, 0.85 Å),
3uvf	3.0	3.0	X	X		X	2	2qoj (2.4 Å, 84.6%, 1.03 Å), 3eh8 (2.7 Å, 85.4%, 0.75 Å),
2fpf	3.0	3.0	X		X		2	2fpe (1.8 Å, 96.7%, 0.56 Å), 2fpd (2.0 Å, 96.7%, 0.50 Å),
1u9o	3.3	3.3	X			X	2	3q0w (1.6 Å, 100.0%, 1.01 Å), 3q0v (1.9 Å, 100.0%, 0.83 Å),
1xqg	3.1	3.1					1	1wz9 (2.1 Å, 97.2%, 1.01 Å),
2xz0	3.0	3.0	X	X			3	2uw1 (1.9 Å, 82.0%, 0.64 Å), 1oq4 (2.4 Å, 100.0%, 0.89 Å), 1oq9 (2.4 Å, 100.0%, 0.74 Å),
1nph	3.0	3.0					1	2fh1 (1.6 Å, 94.2%, 0.90 Å),
2wrf	3.1	3.1	X				3	2wr1 (2.1 Å, 93.6%, 1.04 Å), 2wr7 (2.5 Å, 94.7%, 0.89 Å), 2wr4 (2.5 Å, 93.0%, 0.93 Å),
2nre	4.0	3.5					1	1dj0 (1.5 Å, 100.0%, 1.11 Å),
1uaz	3.4	3.4	X	X	X		3	2ei4 (2.1 Å, 85.0%, 0.70 Å), 2z55 (2.5 Å, 85.0%, 0.74 Å), 1vgo (2.5 Å, 86.1%, 0.72 Å),
3i78	3.0	3.0	X	X		X	5	3beu (1.1 Å, 98.7%, 0.75 Å), 1os8 (1.6 Å, 90.1%, 0.86 Å), 2fmj (1.6 Å, 92.3%, 0.85 Å), 1sgt (1.7 Å, 88.7%, 0.88 Å), 3i77 (2.1 Å, 96.1%, 0.90 Å),
2ahd	3.0	3.0	X				2	1s3l (2.4 Å, 100.0%, 0.85 Å), 1s3n (2.5 Å, 100.0%, 0.36 Å),
1jod	3.2	3.0	X		X		2	1f35 (2.3 Å, 100.0%, 0.77 Å), 1job (2.4 Å, 96.9%, 0.89 Å),
3i5s	3.0	3.0	X				2	3i5r (1.7 Å, 100.0%, 0.80 Å), 1pht (2.0 Å, 100.0%, 0.55 Å),
3fdf	3.2	3.2	X		X		2	3p9y (2.1 Å, 93.2%, 0.79 Å), 3omx (2.3 Å, 94.2%, 0.85 Å),
3fmv	3.3	3.3	X				2	3p9y (2.1 Å, 93.2%, 0.62 Å), 3omx (2.3 Å, 94.2%, 0.82 Å),

3n5u	3.2	3.2	X		X		6	3e7a (1.6 Å, 100.0%, 0.51 Å), 3egg (1.9 Å, 100.0%, 0.52 Å), 1jk7 (1.9 Å, 98.0%, 0.70 Å), 1it6 (2.0 Å, 98.0%, 0.53 Å), 2o8g (2.5 Å, 97.6%, 0.48 Å), 1s70 (2.7 Å, 92.9%, 0.60 Å),
2v9z	3.0	3.0	X				3	3g9x (0.9 Å, 96.9%, 0.66 Å), 3fbw (1.2 Å, 97.3%, 0.77 Å), 1bn7 (1.5 Å, 96.9%, 0.72 Å),
4ddf	3.1	3.1	X	X	X		3	3n79 (1.5 Å, 95.1%, 0.59 Å), 3pac (1.9 Å, 88.0%, 0.75 Å), 3vcd (2.4 Å, 100.0%, 0.41 Å),
3b1k	3.3	3.3	X			X	2	3b1j (2.2 Å, 100.0%, 0.67 Å), 3b20 (2.4 Å, 100.0%, 0.86 Å),
2ayg	3.1	3.1	X				2	1r8h (1.9 Å, 100.0%, 0.73 Å), 2aye (2.3 Å, 100.0%, 0.67 Å),
2ayb	3.2	3.2	X			X	2	1r8h (1.9 Å, 100.0%, 0.69 Å), 2aye (2.3 Å, 100.0%, 0.69 Å),
3red	3.0	3.0	X	X	X		2	1ju2 (1.5 Å, 86.7%, 0.50 Å), 3gdp (1.6 Å, 86.7%, 0.44 Å),
3g1k	3.1	3.1	X				9	3g91 (1.2 Å, 99.6%, 0.54 Å), 3g00 (1.7 Å, 99.6%, 0.55 Å), 3ga6 (1.9 Å, 99.6%, 0.55 Å), 3fzi (1.9 Å, 100.0%, 0.58 Å), 3g2d (2.3 Å, 99.6%, 0.53 Å), 3g2c (2.3 Å, 100.0%, 0.61 Å), 3g8v (2.4 Å, 99.6%, 0.55 Å), 3g0r (2.4 Å, 99.6%, 0.55 Å), 3g4t (2.6 Å, 100.0%, 0.53 Å),
1wac	3.0	2.9	X			X	2	1uvj (1.9 Å, 99.7%, 0.52 Å), 1hi8 (2.5 Å, 95.9%, 0.60 Å),
2g3k	3.0	3.0	X				2	2j9v (2.0 Å, 98.9%, 0.50 Å), 2j9u (2.0 Å, 98.9%, 0.40 Å),
4dfs	3.8	3.8	X		X		3	3azy (1.6 Å, 99.2%, 0.55 Å), 3azx (1.8 Å, 99.2%, 0.48 Å), 3azz (1.8 Å, 99.2%, 0.54 Å),
2bvg	3.2	3.2	X		X		2	2bvf (1.9 Å, 100.0%, 0.52 Å), 2bvh (2.9 Å, 100.0%, 0.48 Å),
2abm	3.2	3.2	X				2	2o9g (1.9 Å, 98.7%, 0.43 Å), 2o9d (2.3 Å, 98.7%, 0.42 Å),