Acta Crystallographica Section D

Volume 70 (2014)

Supporting information for article:

Structural and biophysical analysis of interactions between cod and human uracil-DNA N-glycosylase (UNG) and UNG inhibitor (Ugi)

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Table S1 Protein-protein interface data of hUNG-Ugi and cUNG-Ugi from PISA and WHAT IF calculations.

Protein-Ugi		Interface area (Å^2)	Hydrogen bonds (<3.5Å)	Electrostatic interactions (<6Å)
hUNG-Ugi		1093	12	3
cUNG-Ugi	A+B	1035	14	4
	C+D	1053	12	3
	E+F	1050	14	4
	G+H	1061	14	3
	I+J	1033	13	4
	K+L	1045	12	3
	M+N	1025	13	2
	O+P	1041	10	2
cUNG-Ugi	Average	1043	12.8	3.1

Table S2 Hydrogen bonds and electrostatic interactions in the cUNG-Ugi complex (eight complexes in one asymmetric unit) and hUNG-Ugi. Hydrogen bonds (<3.5 Å) were analyzed with PISA, and the WHAT IF Web Interface was used to identify electrostatic interactions with interatomic distance of <6 Å.

Hydrogen bond distances (Å)

cUNG-Ugi chains									Interacting atoms		cUNG average		hUNG
	AB	CD	EF	GH	IJ	KL	MN	OP	Ugi	UNG	Dist	Stdev	Dist
	2.91	2.86	2.78	3.07			3.30		Gln19 O	Gln152 $N\varepsilon_2$	2.98	0.21	3.05
	3.02	2.94	2.85	2.95	2.69	2.74	2.81	2.74	Glu20 $O\varepsilon_1$	Ser169 N	2.84	0.12	2.98
	2.72	2.47	2.56	2.64	2.75	2.51	2.64	2.61	Glu20 $O\varepsilon_2$	Ser169 $O\gamma$	2.61	0.10	3.06
	3.09	2.66	3.09	3.04	3.20	3.01	3.14	2.97	Ser 21 $O\gamma$	His148 $N\varepsilon_2$	3.03	0.16	2.79
	2.82	2.66	2.64	2.75	2.57	2.74	2.85	2.59	Leu23 N	Gln144 $O\varepsilon_1$	2.70	0.10	2.97
	3.04	2.80	2.73	3.11	3.09	3.09	2.96	3.06	Leu23 O	Gln144 $N\varepsilon_2$	2.99	0.14	2.94
	2.96	2.65	2.38	3.05	2.97	2.88	2.74	2.85	Glu28 $O\varepsilon_2$	Ser247 N	2.81	0.22	3.08
			2.76						Glu28 $O\varepsilon_2$	Ser247 $O\gamma$	2.76		
			3.27						Glu31 O	Arg276 $N\eta_1$	3.27		
					2.34	2.97			Glu31 $O\varepsilon_1$	Arg276 $N\eta_2$	2.66	0.45	2.98
	3.38		3.46	3.38	3.42	3.45	3.35		Met56 $S\delta$	Leu272 N	3.41	0.04	
	2.96	3.29	2.76	3.04	2.63	2.76	2.84	2.83	Asp61 $O\delta_1$	Asn215 $N\delta_2$	2.89	0.21	3.04
	3.24							3.10	Asp61 $O\delta_2$	Asn215 $N\delta_2$	3.17	0.10	
	2.70	2.82	2.68	3.02	2.67	2.98	2.79	3.10	Asp61 $O\delta_2$	Lys218 $N\zeta$	2.85	0.17	2.64
	3.47			2.43					Ala62 O	Lys218 $N\zeta$	2.95	0.74	
	2.83	3.46	2.76	3.38	3.27		3.24		Tyr65 $O\eta$	Ala214 N	3.16	0.29	
		2.55		2.76	2.68	2.77	2.71	2.50	Tyr65 $O\eta$	Ala214 O	2.66	0.11	2.84
	2.82	2.80	2.57	2.67	2.78	2.58	2.76	3.04	Gln73 $N\varepsilon_2$	Pro271 O	2.75	0.15	2.80
Aver.	3.00	2.83	2.81	2.95	2.85	2.87	2.93	2.85			2.92	0.07	2.93

Electrostatic interaction distances (Å)

cUNG-Ugi chains									Interacting atoms		cUNG average		hUNG
	AB	CD	EF	GH	IJ	KL	MN	OP	Ugi	cUNG	Dist	Stdev	Dist
	5.53	5.52	5.46	5.53	5.42	5.35	5.58	5.54	Glu20 $O\varepsilon_2$	His268 $N\delta_1$	5.49	0.08	5.93
			5.22						Glu28 $O\varepsilon_2$	His250 $N\delta_1$	5.22		
					2.34				Glu31 $O\varepsilon_1$	Arg276 $N\eta_1$	2.34		
	4.36								Glu31 $O\varepsilon_1$	Arg276 $N\eta_2$	4.36		2.98
				4.41		2.97			Glu31 $O\varepsilon_2$	Arg276 $N\eta_2$	3.69	1.02	
		5.65							Asp40 $O\delta_2$	Lys251 $N\zeta$	5.65		
	5.95		5.95		5.85				Asp40 $O\delta_2$	Lys218 $N\zeta$	5.92	0.06	
	2.70	2.82	2.68	3.02	2.67	2.98	2.79	3.10	Asp61 $O\delta_2$	Lys218 $N\zeta$	2.85	0.17	2.64
Aver.	4.64	4.66	4.83	4.32	4.07	3.77	4.19	4.32			4.44	0.33	3.85

Table S3 Calculated accessible surface area (ASA) with Surface Racer 5.0 for cUNG (chain E) and hUNG (chain E) from the UNG-UGI complexes.

Protein	cUNG	hUNG	Difference
Chain	E	E	(cUNG – hUNG)
PDB	4LYL	1UGH	
TOTAL ASA	10376	10497	-122
Polar ASA	4838	4831	7
Non-polar ASA	5537	5666	-129
Polar back bone ASA	1241	1294	-53
Non-polar back bone	690	807	-117
Polar side chain ASA	3597	3537	61
Non-polar side chain ASA	4847	4859	-12
+charge ASA	1574	1548	26
-charge ASA	849	690	159