Session Map (id=736-O8-C44)
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Interfaces in PDB 7dn3

STRUCTURE OF HUMAN RNA POLYMERASE III ELONGATION COMPLEX

Interfaces

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## NN	«»	Structure 1 Range	N_{at}	N_{res}	Surface Å^2	×	Structure 2 Range	N_{at}	N_{res}	Surface Å^2	interface area, Å^2	Δ^iG kcal/mol	Δ^iG P-value	N_{HB}	N_{SB}	N_{DS}	CSS
1	◉	A	844	228	64526	◊	B	833	204	48874	8233.8	-101.8	0.004	93	20	0	0.000
2	○	O	274	75	24978	◊	Q	218	49	10471	2354.8	-22.6	0.561	10	2	0	0.000
3	○	M	239	51	12223	◊	N	191	48	7103	2066.6	-28.7	0.384	27	4	0	0.000
4	○	C	204	51	18867	◊	K	196	47	7175	2038.3	-34.4	0.011	15	8	0	0.000
5	○	G	206	53	10648	◊	D	187	49	8929	1963.5	-28.1	0.219	15	3	0	0.000
6	○	A	211	56	64526	◊	F	196	51	5471	1891.1	-26.4	0.214	12	2	0	0.000
7	○	P	177	49	10590	◊	O	210	60	24978	1844.7	-17.6	0.649	12	5	0	0.000
8	○	A	193	57	64526	◊	O	212	51	24978	1809.1	-7.8	0.684	14	2	0	0.000
9	○	B	200	57	48874	◊	C	186	52	18867	1798.9	-6.4	0.700	29	10	0	0.000
10	○	A	172	44	64526	◊	H	188	50	6921	1796.3	-18.2	0.096	21	9	0	0.000
11	○	A	191	60	64526	◊	E	178	46	11589	1717.2	-10.5	0.444	17	9	0	0.000
12	○	B	179	55	48874	◊	J	139	31	4505	1461.4	-18.2	0.382	15	1	0	0.000
13	○	A	153	40	64526	◊	I	122	35	5222	1333.1	-18.3	0.310	11	0	0	0.000
14	○	A	126	29	64526	◊	G	163	44	10648	1327.7	-11.3	0.564	10	0	0	0.000
15	○	B	140	44	48874	◊	L	110	27	4427	1159.0	-9.6	0.441	13	5	0	0.000
16	○	C	107	31	18867	◊	J	86	25	4505	944.4	-7.3	0.588	8	5	0	0.000
17	○	A	94	23	64526	◊	K	102	28	7175	919.4	-3.5	0.712	15	4	0	0.000
18	○	B	89	29	48874	◊	M	87	23	12223	826.9	1.4	0.878	8	1	0	0.000
19	○	X	82	16	3839	◊	Y	77	16	5505	733.3	-9.5	0.734	26	0	0	0.000
20	○	A	81	25	64526	◊	Y	72	8	5505	680.5	-4.8	0.707	9	0	0	0.000
21	○	B	70	22	48874	◊	N	71	23	7103	655.3	-9.6	0.363	3	0	0	0.000
22	○	C	80	20	18867	◊	L	56	11	4427	627.7	-1.2	0.666	14	8	0	0.000
23	○	P	59	16	10590	◊	Q	51	14	10471	513.8	-8.3	0.597	3	1	0	0.000
24	○	A	49	18	64526	◊	C	54	11	18867	455.6	-4.1	0.400	4	0	0	0.000
25	○	I	52	13	5222	◊	M	53	19	12223	434.1	-3.9	0.612	1	0	0	0.000

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interface # 1 in PDB 7dn3

STRUCTURE OF HUMAN RNA POLYMERASE III ELONGATION COMPLEX

interface #1/61 XML << < > >>

Interface Summary

XML

	Structure 1		Structure 2	
Selection range	A		B	
class	Protein		Protein	
symmetry operation	x,y,z		x,y,z	
symmetry ID	1_555		0_555	
Number of atoms				
interface	844	8.3%	833	10.1%
surface	5853	57.7%	4584	55.5%
total	10152	100.0%	8254	100.0%
Number of residues				
interface	228	17.6%	204	19.5%
surface	1215	94.0%	971	93.0%
total	1293	100.0%	1044	100.0%
Solvent-accessible area, Å				
interface	8078.7	12.5%	8388.9	17.2%
total	64526.4	100.0%	48874.1	100.0%
Solvation energy, kcal/mol				
isolated structure	-1164.7	100.0%	-971.6	100.0%
gain on complex formation	-47.7	4.1%	-54.1	5.6%
average gain	-25.5	2.2%	-28.1	2.9%
P-value	0.009		0.001	

View: structure 1 | interface | structure 2

Download: structure 1 | interface | structure 2

This interface scored

0.000

in Complex Formation Significance Score (CSS).
CSS ranges from 0 to 1 as interface relevance to complex formation increases.

Achieved CSS implies that the interface does not play any role in complex formation and seems to be a result of crystal packing only

Hydrogen bonds

XML

##	Structure 1	Dist. [Å]	Structure 2
1	A:ARG 855[NH2]	2.39	B:PRO 481[O]
2	A:ARG 816[NH1]	3.56	B:GLU 638[O]

Salt bridges

XML

##	Structure 1	Dist. [Å]	Structure 2
1	A:ARG 484[NE]	3.67	B:GLU 892[OE2]
2	A:LYS 877[NZ]	3.07	B:GLU1049[OE1]

No disulfide bonds found
No covalent bonds found

Interfacing residues (not a contact table)

XML Display level: Interface atoms

Inaccessible residues
Solvent-accessible residues
HSDC Residues making **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent link
Interfacing residues

ASA Accessible Surface Area, Å² **BSA** Buried Surface Area, Å² **ΔᴵG** Solvation energy effect, kcal/mol |||| Buried area percentage, one bar per 10%

##	Structure 1	HSDC	ASA	BSA	ΔᴵG
1	A:GLU 4		220.28	0.00	0.00
2	A:GLN 5		178.81	0.00	0.00
3	A:PHE 6		163.91	0.00	0.00
4	A:ARG 7		184.07	0.00	0.00
5	A:GLU 8		113.51	0.00	0.00
6	A:THR 9		80.56	0.00	0.00
7	A:ASP 10		132.27	0.00	0.00
8	A:VAL 11		98.53	36.66 ||||	0.34
	[C]				
	[O]				
	[CG1]				
	[CG2]				
9	A:ALA 12		95.84	63.60 |||||||	0.62
	[N]				
	[CA]				
	[C]				
	[O]				
	[CB]				
10	A:LYS 13		170.11	111.92 |||||||	0.82
	[N]	H			
	[CA]				
	[C]				
	[O]				
	[CB]				
	[CG]				
	[CD]				
	[CE]				

##	Structure 2	HSDC	ASA	BSA	ΔᴵG
1	B:VAL 23		109.30	0.00	0.00
2	B:GLU 24		152.70	0.00	0.00
3	B:GLU 25		47.38	0.00	0.00
4	B:LYS 26		25.97	0.00	0.00
5	B:TRP 27		48.76	0.00	0.00
6	B:ARG 28		102.99	0.00	0.00
7	B:LEU 29		0.16	0.00	0.00
8	B:LEU 30		0.00	0.00	0.00
9	B:PRO 31		33.40	0.00	0.00
10	B:ALA 32		7.12	0.00	0.00
11	B:PHE 33		0.17	0.00	0.00
12	B:LEU 34		20.74	0.00	0.00
13	B:LYS 35		163.24	0.00	0.00
14	B:VAL 36		60.18	0.00	0.00
15	B:LYS 37		40.99	0.00	0.00
16	B:GLY 38		0.00	0.00	0.00
17	B:LEU 39		15.04	0.00	0.00
18	B:VAL 40		6.72	0.00	0.00
19	B:LYS 41		71.36	0.00	0.00
20	B:GLN 42		0.65	0.00	0.00
21	B:HIS 43		1.05	0.00	0.00
22	B:ILE 44		20.41	0.00	0.00
23	B:ASP 45		45.33	0.00	0.00
24	B:SER 46		6.14	0.00	0.00
25	B:PHE 47		0.00	0.00	0.00
26	B:ASN 48		34.06	0.00	0.00
27	B:TYR 49		56.66	0.00	0.00