PDBe PDBePISA (Protein Interfaces, Surfaces and Assemblies)

http://pdbe.org/pisa/

This tutorial introduces the PDBePISA (PISA for short) service, which is a web-based interactive tool offered by the PDBe to investigate stability of formation of macromolecular complexes (protein, DNA/RNA and ligand). In addtion to a detailed analysis of surfaces, interfaces and assemblies for all entries in the Protein Data Bank (PDB), the service also allows upload and analysis of one's own PDB or mmCIF format coordinate files.

Background

The stability of a macromolecular complex in a biological system is essentially governed by the following physicochemical properties:

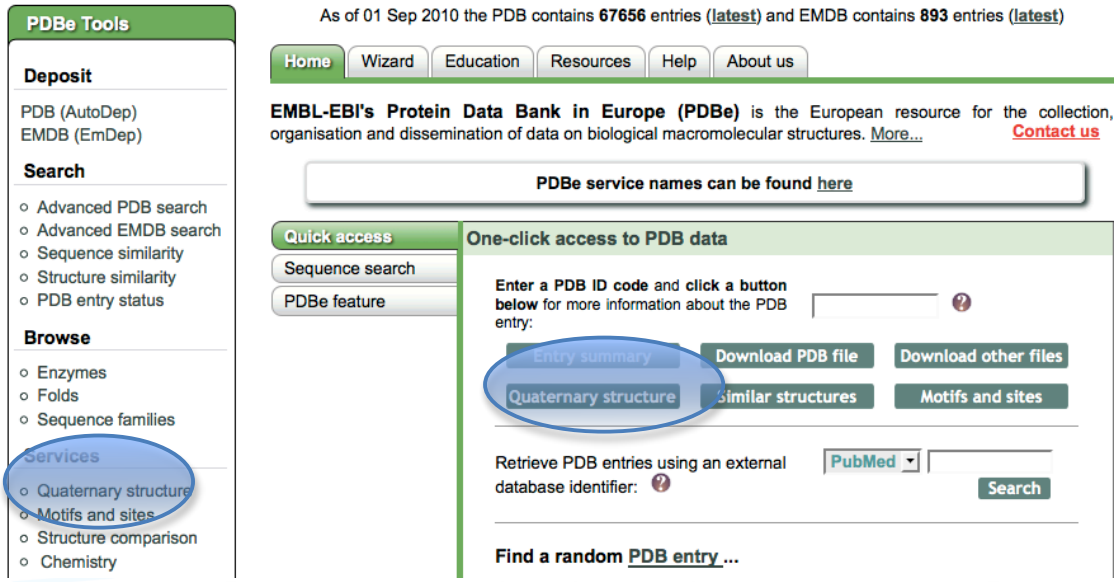
1) free energy of formation.
2) solvation energy gain.
3) interface area.
4) hydrogen bonds.
5) saltbridges across the interface.
6) hydrophobic specificity.

These interactions are also likely prevalent in crystal systems where protein molecules interact with one another in the crystallization solution and arrange themselves in orderly lattices to form crystals. Therefore, given that some crystallization conditions may mimic actual biological interactions in solution, the analysis of crystal interfaces and the prediction of higher order structures may actually reflect those present in a biological system. The PISA service uses all the criteria listed above in order to analyse a given structure and make a prediction of the possible stable complex. However, it is important to emphasize that PISA results are predictions and any conclusions drawn from the same must

be in light of other biological and experimental proof. The results from PISA may be used for validation of independent biochemical data if the structure of the protein under study is available.

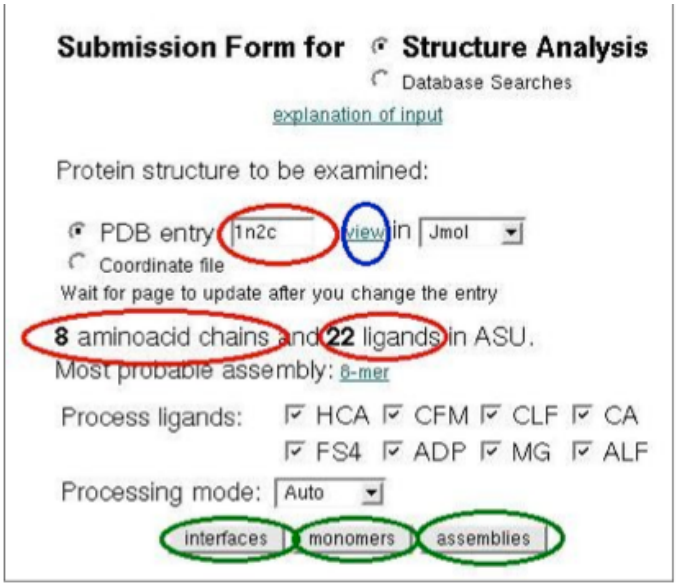
Tutorial

PISA may be accessed from multiple locations on the PDBe pages. You can access the service from the PDBe Home Page (http://pdbe.org/) as shown below.



You may also access PISA for a particular entry from the Summary Pages of a particular entry. Click on the link on the left hand sidebar to go to PISA. On the new page that comes up, choose “Start PDBePISA”.

This will open up a submission form. Type in the PDB Idcode 1N2C in the box provided.

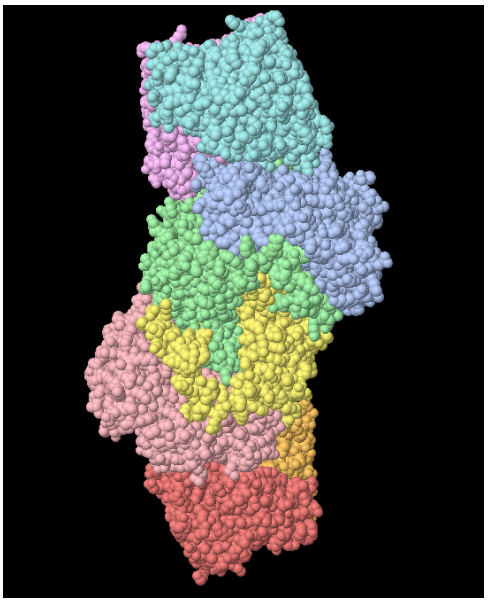


As soon as the file gets uploaded to the server, it will give you preliminary information regarding the PDB entry (number of proteins chains and bound ligands). The entry 1n2c has 8 protein chains and 22 ligands.

The most probable assembly is stated as an 8-mer.
[To know more about this PDB entry (e.g. Name of the protein, origin etc.), then go to the summary pages for this entry http://www.pdbe.org/1n2c/).

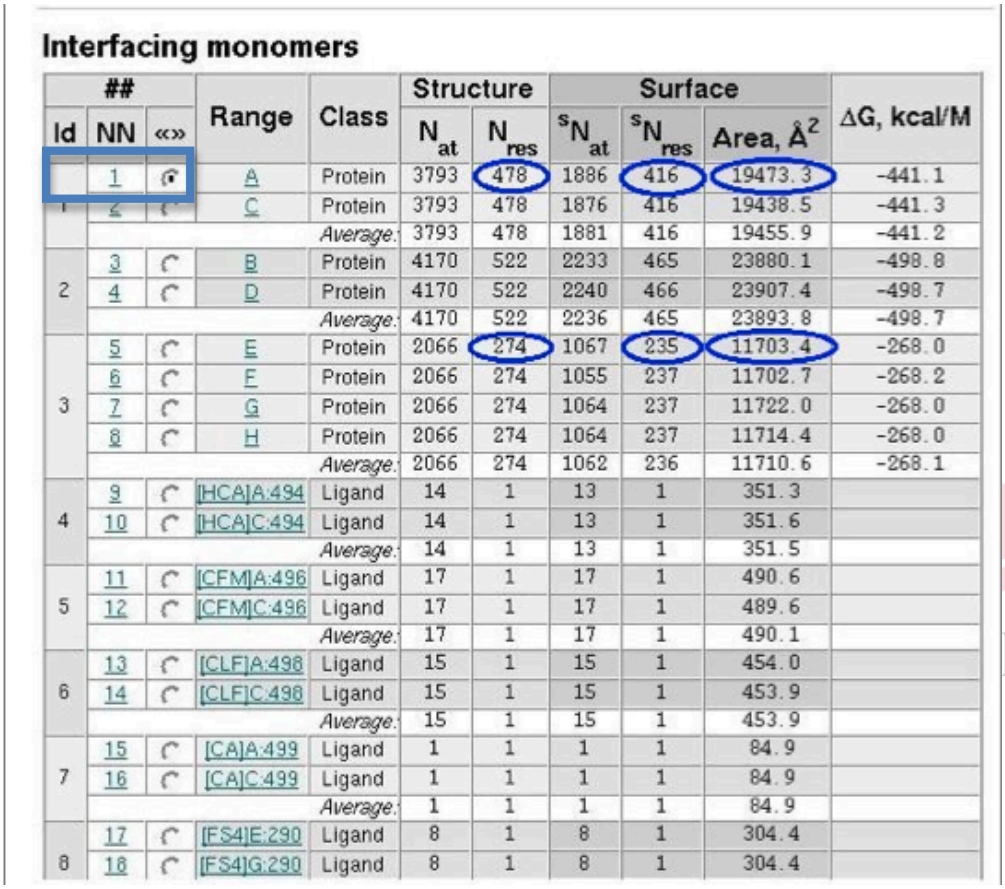
The atlas page for this entry gives us information that it is a nitrogenase complex structure stabilized by ADP- tetrafluoroaluminate. There are three different proteins NIFD (Chains A and B), NIFK (Chains C and D) and NIFH1 (Chains E, F, G, H).]

You may click on the View button (shown above) in blue to view the loaded PDB entry.



There are three buttons highlighted in green at the bottom of the submission page – **interfaces**, **monomers** and **assemblies**. Each of them provide structural information related to the protein of interest (energy of association, solvation energy, buried surface area, H-bonds and saltbridges etc.).

Monomers: Let us first start with the different monomers present in the PDB entry.
If you click on the monomers button, you get the following information about the corresponding PDB entry.



Interfacing monomers

##			Range	Class	Structure		Surface			ΔG, kcal/M
Id	NN	«»			N_{at}	N_{res}	$^{s}N_{at}$	$^{s}N_{res}$	Area, Å^2	
	1	◉	A	Protein	3793	478	1886	416	19473.3	-441.1
	2	○	C	Protein	3793	478	1876	416	19438.5	-441.3
				Average:	3793	478	1881	416	19455.9	-441.2
2	3	○	B	Protein	4170	522	2233	465	23880.1	-498.8
	4	○	D	Protein	4170	522	2240	466	23907.4	-498.7
				Average:	4170	522	2236	465	23893.8	-498.7
3	5	○	E	Protein	2066	274	1067	235	11703.4	-268.0
	6	○	F	Protein	2066	274	1055	237	11702.7	-268.2
	7	○	G	Protein	2066	274	1064	237	11722.0	-268.0
	8	○	H	Protein	2066	274	1064	237	11714.4	-268.0
				Average:	2066	274	1062	236	11710.6	-268.1
4	9	○	[HCA]A:494	Ligand	14	1	13	1	351.3	
	10	○	[HCA]C:494	Ligand	14	1	13	1	351.6	
				Average:	14	1	13	1	351.5	
5	11	○	[CFM]A:496	Ligand	17	1	17	1	490.6	
	12	○	[CFM]C:496	Ligand	17	1	17	1	489.6	
				Average:	17	1	17	1	490.1	
6	13	○	[CLF]A:498	Ligand	15	1	15	1	454.0	
	14	○	[CLF]C:498	Ligand	15	1	15	1	453.9	
				Average:	15	1	15	1	453.9	
7	15	○	[CA]A:499	Ligand	1	1	1	1	84.9	
	16	○	[CA]C:499	Ligand	1	1	1	1	84.9	
				Average:	1	1	1	1	84.9	
8	17	○	[FS4]E:290	Ligand	8	1	8	1	304.4	
	18	○	[FS4]G:290	Ligand	8	1	8	1	304.4	

For chain A, which represents the Molybdenum-iron protein, there are total 478 amino acids in the protein chain and 416 of them are surface exposed residues. The solvent accessible area for this protein 19473.3 $Å_2$ and the solvation energy for folding (ΔG) is -441.1 Kcal/M.

Similarly for chain E, there are a total 274 amino acids and of 235 of these are present on the surface of the protein. The solvent accessible surface area 11703.4$Å_2$ and energy of solvation (ΔG) for this structure is -268 kcal/M.

You may also view the individual protein chains in a 3-D graphical viewer by click on the letter (A, B, C, D, E, F, G, H) corresponding to the protein chain.

Identifying amino acid residues involved in interaction:
Click on the link that is represented as a number on the results page (highlighted

rectangle above). In our example it is **1** for chain **A** and **5** for chain **E**.
Click on link 1 for chain A. This will take you to the following page, where you get residue-by-residue solvent accessibility information.

Solvent accessibility (¤ interface engaged in PQS[1])

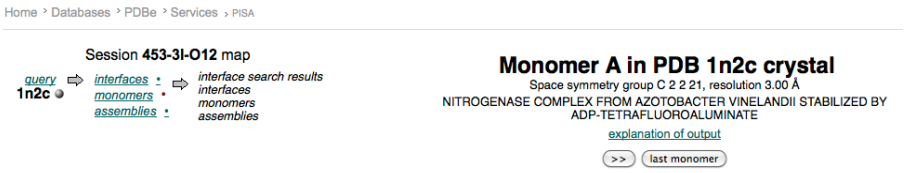
Inaccessible residues Solvent-accessible residues Interfacing residues

##	Monomer A	ASA, Å^2	Buried surface in interface						
			2¤	7¤	10¤	15¤	17¤	24¤	26¤
1	A:MET 4	82.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	A:SER 5	42.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	A:ARG 6	68.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	A:GLU 7	111.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	A:GLU 8	94.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	A:VAL 9	3.52	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	A:GLU 10	80.74	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	A:SER 11	55.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	A:LEU 12	9.52	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	A:ILE 13	5.36	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	A:GLN 14	81.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	A:GLU 15	94.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	A:VAL 16	5.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	A:LEU 17	2.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	A:GLU 18	133.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	A:VAL 19	86.65	47.95	0.00	0.00	0.00	0.00	0.00	0.00
17	A:TYR 20	15.29	6.45	0.00	0.00	0.00	0.00	0.00	0.00
18	A:PRO 21	95.12	68.33	0.00	0.00	0.00	0.00	0.00	0.00
19	A:GLU 22	113.74	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	A:LYS 23	165.23	41.89	0.00	0.00	0.00	0.00	0.00	0.00
21	A:ALA 24	11.01	10.86	0.00	0.00	0.00	0.00	0.00	0.00
22	A:ARG 25	73.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	A:LYS 26	121.28	0.00	0.00	0.00	0.00	0.00	0.00	0.00

All the residues are colour-coded depending on their solvent accessibility. The solvent exposed residues are grey, the interface residues are blue and the buried residues are black.

The Interfaces:

Let us now click at the interface button for this PDB entry 1n2c from the top of the page.



The results page will give us detailed information regarding the interface between two protein chains present in the complex structure.

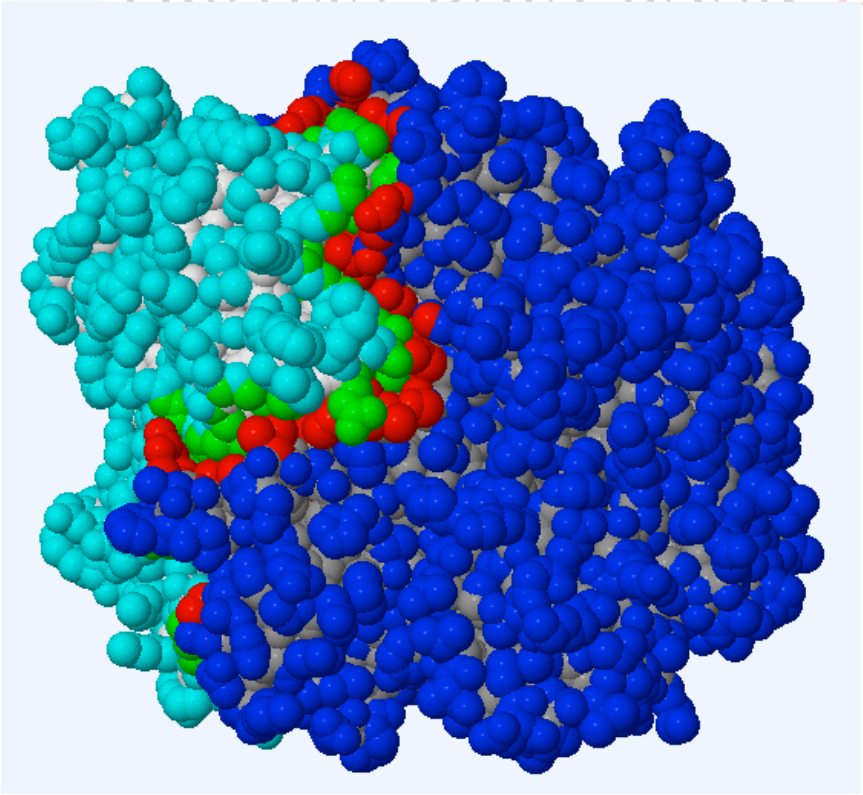
Found interfaces

##			Structure 1			×		Interface area, Å^2	$\Delta^i G$ kcal/M	$\Delta^i G$ P-value	N_{HB}	N_{SB}	N_{DS}	CSS
Id	NN	«»	Range	$^iN_{at}$	$^iN_{res}$		Range							
1	1	◉	D	469	119	◊	C	4367.5	-54.3	0.011	56	18	0	0.551
	2	○	B	474	120	◊	A	4360.2	-54.4	0.010	55	17	0	0.551
								4363.9	-54.3	0.011	56	18	0	0.551
2	3	○	D	322	77	◊	B	2872.0	-21.6	0.430	46	32	0	0.724
3	4	○	H	251	66	◊	G	2335.1	-12.4	0.400	31	15	0	0.302
	5	○	F	248	66	◊	E	2321.0	-12.4	0.398	31	14	0	0.302
								2328.0	-12.4	0.399	31	15	0	0.302
4	6	○	B	140	37	◊	C	1288.3	-15.5	0.177	17	6	0	0.306
	7	○	D	137	36	◊	A	1283.3	-15.3	0.181	16	7	0	0.306
								1285.8	-15.4	0.179	17	7	0	0.306
5	8	○	G	69	19	◊	D	554.0	1.5	0.724	5	3	0	0.004
	9	○	E	71	19	◊	B	549.2	1.4	0.703	5	4	0	0.004
								551.6	1.4	0.713	5	4	0	0.004
6	10	○	F	61	19	◊	A	514.0	-1.5	0.599	4	3	0	0.027
	11	○	H	60	19	◊	C	506.8	-1.8	0.576	4	5	0	0.027
								510.4	-1.7	0.588	4	4	0	0.027
7	12	○	F	52	16	◊	B	417.6	-7.8	0.088	4	2	0	0.030
	13	○	H	51	17	◊	D	405.0	-7.5	0.095	5	1	0	0.030
								411.3	-7.6	0.091	5	2	0	0.030
8	14	○	G	49	15	◊	C	392.9	-6.7	0.112	4	2	0	0.056
	15	○	E	48	15	◊	A	390.0	-6.7	0.109	4	2	0	0.056

In the above example, between chains C and D there are 18 saltbridges and 56 H-bonding interactions.

If you click on the link highlighted in red, you can visualize the interface region between the protein chains.

The interface region is highlighted in red and green as shown below.



Information regarding the specific residues involved in complex formation may be found by choosing the link under column name **NN** (highlighted in green).

Found interfaces

##			Structure 1			×		Interface area, Å^2	$\Delta^i G$ kcal/M	$\Delta^i G$ P-value	N_{HB}	N_{SB}	N_{DS}	CSS
Id	NN	«»	Range	$^iN_{at}$	$^iN_{res}$		Range							
	1		D	469	119		C	4367.5	-54.3	0.011	56	18	0	0.551

Hydrogen bonds

##	Structure 1	Dist. [Å]	Structure 2
1	D:ASN 137[ND2]	2.90	C:PRO 54[O]
2	D:TYR 142[OH]	2.81	C:LEU 56[O]
3	D:TYR 142[OH]	3.81	C:MET 57[O]
4	D:ARG 100[NH1]	3.90	C:THR 58[O]
5	D:GLN 93[NE2]	3.24	C:GLY 61[O]
6	D:TYR 447[OH]	3.30	C:GLN 90[O]
7	D:CYS 70[SG]	2.79	C:TYR 91[OH]
8	D:CYS 70[N]	3.21	C:TYR 91[OH]
9	D:LYS 34[NZ]	3.73	C:ILE 101[O]
10	D:ARG 453[NH2]	3.46	C:THR 104[O]
11	D:ASN 65[N]	2.83	C:ASN 113[O]
12	D:THR 63[N]	2.99	C:THR 115[O]
13	D:LYS 68[NZ]	3.02	C:ASP 117[OD1]
14	D:LYS 68[NZ]	2.90	C:ASP 117[OD2]
15	D:HIS 396[NE2]	3.80	C:ASP 117[OD2]
16	D:LEU 62[N]	2.95	C:GLU 137[OE1]
17	D:ALA 61[N]	3.23	C:GLU 137[OE1]
18	D:ALA 61[N]	3.10	C:GLU 137[OE2]
19	D:GLU 60[N]	2.93	C:GLU 137[OE2]
20	D:TYR 52[OH]	3.02	C:LEU 141[O]
21	D:SER 92[OG]	3.18	C:CYS 154[SG]
22	D:GLU 120[N]	3.04	C:PHE 186[O]
23	D:GLN 93[NE2]	2.79	C:VAL 189[O]
24	D:LYS 27[NZ]	2.90	C:GLU 261[OE1]
25	D:LYS 27[NZ]	2.98	C:GLU 261[OE2]
26	D:SER 2[N]	3.85	C:TYR 331[OH]
27	D:GLN 3[N]	3.14	C:GLU 334[OE1]
28	D:SER 2[OG]	3.17	C:GLU 334[OE2]
29	D:ARG 100[NH2]	3.70	C:LYS 426[O]
30	D:ASP 266[N]	3.70	C:LYS 433[O]
31	D:GLN 268[N]	3.03	C:LYS 433[O]
32	D:GLN 3[NE2]	3.33	C:ASP 454[O]

Salt bridges

##	Structure 1	Dist. [Å]	Structure 2
1	D:LYS 68[NZ]	3.02	C:ASP 117[OD1]
2	D:LYS 68[NZ]	2.90	C:ASP 117[OD2]
3	D:HIS 396[NE2]	3.80	C:ASP 117[OD2]
4	D:LYS 27[NZ]	2.90	C:GLU 261[OE1]
5	D:LYS 27[NZ]	2.98	C:GLU 261[OE2]
6	D:SER 2[N]	3.41	C:ASP 454[OD1]
7	D:SER 2[N]	3.36	C:ASP 454[OD2]
8	D:GLU 32[OE1]	2.90	C:LYS 76[NZ]
9	D:GLU 32[OE2]	3.01	C:LYS 76[NZ]
10	D:GLU 33[OE1]	3.16	C:ARG 210[NH2]
11	D:GLU 33[OE1]	3.53	C:LYS 146[NZ]
12	D:GLU 33[OE2]	2.99	C:ARG 210[NH1]
13	D:GLU 33[OE2]	3.20	C:ARG 210[NH2]
14	D:GLU 109[OE1]	2.71	C:LYS 433[NZ]
15	D:GLU 109[OE2]	3.37	C:LYS 433[NZ]
16	D:ASP 121[OD1]	3.49	C:LYS 51[NZ]
17	D:ASP 133[OD1]	3.93	C:LYS 23[NZ]
18	D:ASP 133[OD2]	3.01	C:LYS 23[NZ]

Disulfide bonds

##	Structure 1	Dist. [Å]	Structure 2
No disulfide bonds found			

Covalent bonds

##	Structure 1	Dist. [Å]	Structure 2
No covalent bonds found			

This page also provides information regarding the importance of the interface in complex formation.

This interface scored

0.548

in complexation significance score (CSS).

CSS ranges from 0 to 1 as interface relevance to complexation increases.

Achieved CSS implies that the interface plays an essential role in complexation

In addition to the saltbridge and H-bonding interactions between the residues, the results page also provides information about Buried and accessible surface areas and solvation energies of the interfacing residues.

Interfacing residues (not a contact table)

Display level: Residues

Inaccessible residues
Solvent-accessible residues

HSDC Residues making Hydrogen/Disulphide bond, Salt bridge or Covalent link
Interfacing residues

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

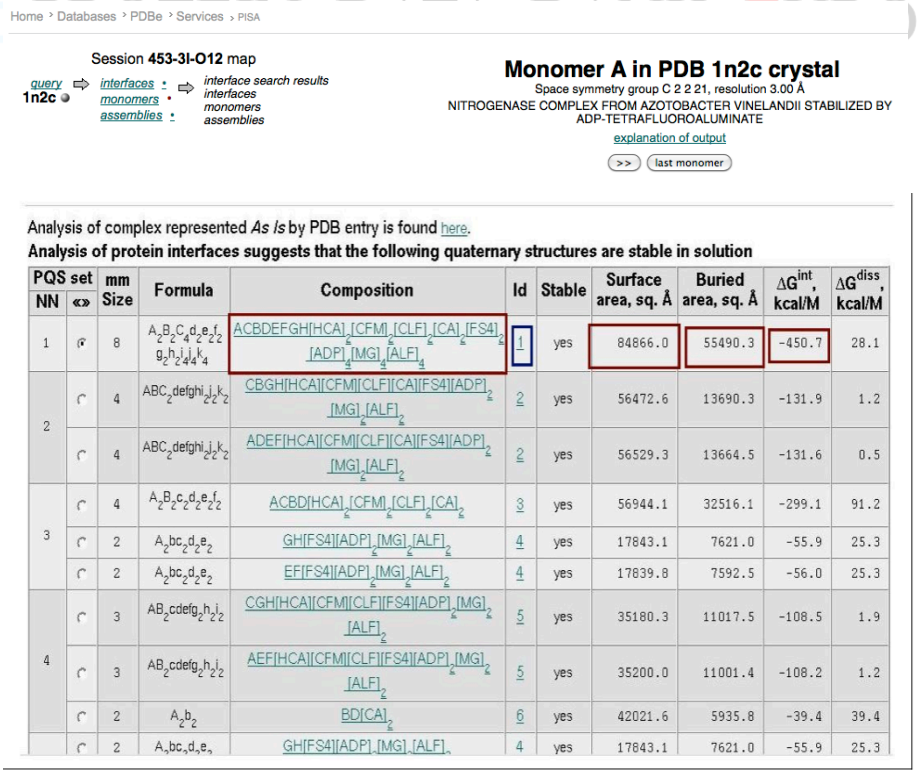
##	Structure 1	HSDC	ASA	BSA	Δ^iG
1	D:SER 2	HS	109.18	72.80 |||||||	-0.13
2	D:GLN 3	H	79.30	71.64 ||||||||||	0.21
3	D:GLN 4		93.12	0.00	0.00
4	D:VAL 5		129.40	89.67 |||||||	1.21
5	D:ASP 6		107.81	10.57		0.14
6	D:LYS 7		154.14	0.00	-0.00
7	D:ILE 8	H	123.53	101.65 |||||||||	1.34
8	D:LYS 9		54.02	0.74		-0.01
9	D:ALA 10		69.36	45.43 |||||||	0.69
10	D:SER 11		72.64	52.55 |||||||	0.17
11	D:TYR 12		170.20	0.00	0.00
12	D:PRO 13		53.69	0.00	-0.00
13	D:LEU 14		21.83	21.83 ||||||||||	0.35
14	D:PHE 15		93.51	71.76 |||||||	1.15
15	D:LEU 16		94.22	0.00	0.00
16	D:ASP 17		38.02	0.00	-0.00
17	D:GLN 18		118.45	0.00	-0.00
18	D:ASP 19		92.27	28.19 ||||	-0.29
19	D:TYR 20	H	53.43	53.43 ||||||||||	-0.01
20	D:LYS 21		102.43	0.00	0.00
21	D:ASP 22		60.06	0.00	-0.00

##	Structure 2	HSDC	ASA	BSA	Δ^iG
1	C:MET 4		83.01	0.00	-0.00
2	C:SER 5		43.58	0.00	-0.00
3	C:ARG 6		68.40	0.00	0.00
4	C:GLU 7		110.97	0.00	0.00
5	C:GLU 8		93.82	0.00	0.00
6	C:VAL 9		4.03	0.00	-0.00
7	C:GLU 10		80.52	0.00	-0.00
8	C:SER 11		56.14	0.00	-0.00
9	C:LEU 12		9.86	0.00	-0.00
10	C:ILE 13		5.52	0.00	0.00
11	C:GLN 14		82.44	0.00	0.00
12	C:GLU 15		93.93	0.00	0.00
13	C:VAL 16		4.83	0.00	-0.00
14	C:LEU 17		2.01	0.00	-0.00
15	C:GLU 18		132.87	0.00	-0.00
16	C:VAL 19		86.80	49.08 ||||||	0.39
17	C:TYR 20		16.11	7.22 |||||	0.11
18	C:PRO 21		96.13	68.58 |||||||	1.10
19	C:GLU 22		113.78	0.00	-0.00
20	C:LYS 23	HS	165.26	43.89 |||	-0.50
21	C:ALA 24		11.15	11.00 ||||||||||	0.17
22	C:ARG 25		73.29	0.00	-0.00

All the residues in this table are colour coded depending on their solvent accessibility (grey-surface exposed, black – buried, light blue – interfacing residues). The color red represents residues that are involved in **H**ydrogen/**D**isulphide bond, **S**alt bridge or **C**ovalent interactions.

Assemblies:

In order to get the quaternary structure information for 1N2C click on the "assemblies" button from the top of the page.



PQS set NN	«»	mm Size	Formula	Composition	Id	Stable	Surface area, sq. Å	Buried area, sq. Å	ΔG^{int}, kcal/M	ΔG^{diss}, kcal/M
1	◉	8	$A_2B_2C_4d_2e_2f_2g_2h_2i_4j_4k_4$	ACBDEFGH[HCA]$_2$[CFM]$_2$[CLF]$_2$[CA]$_2$[FS4]$_2$[ADP]$_4$[MG]$_4$[ALF]$_4$	1	yes	84866.0	55490.3	-450.7	28.1
2	○	4	$ABC_2defghi_2j_2k_2$	CBGH[HCA][CFM][CLF][CA][FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	2	yes	56472.6	13690.3	-131.9	1.2
	○	4	$ABC_2defghi_2j_2k_2$	ADEF[HCA][CFM][CLF][CA][FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	2	yes	56529.3	13664.5	-131.6	0.5
3	○	4	$A_2B_2c_2d_2e_2f_2$	ACBD[HCA]$_2$[CFM]$_2$[CLF]$_2$[CA]$_2$	3	yes	56944.1	32516.1	-299.1	91.2
	○	2	$A_2bc_2d_2e_2$	GH[FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	4	yes	17843.1	7621.0	-55.9	25.3
	○	2	$A_2bc_2d_2e_2$	EF[FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	4	yes	17839.8	7592.5	-56.0	25.3
4	○	3	$AB_2cdefg_2h_2i_2$	CGH[HCA][CFM][CLF][FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	5	yes	35180.3	11017.5	-108.5	1.9
	○	3	$AB_2cdefg_2h_2i_2$	AEF[HCA][CFM][CLF][FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	5	yes	35200.0	11001.4	-108.2	1.2
	○	2	A_2b_2	BD[CA]$_2$	6	yes	42021.6	5935.8	-39.4	39.4
	○	2	$A_2bc_2d_2e_2$	GH[FS4][ADP]$_2$[MG]$_2$[ALF]$_2$	4	yes	17843.1	7621.0	-55.9	25.3

For this entry the proposed quaternary structure by **PISA** is a hetero-octamer that is

already present as a stable assembly in the PDB file. In the **assemblies** result page **PISA** also gives information about the buried and accessible surface area, and free energy of solvation gained upon the formation of the entire complex structures.

Click on the Id shown above in blue to see details of the predicted assembly.
Click on the Composition section for set 1 to graphically view the assembly formed.

Assembly Summary

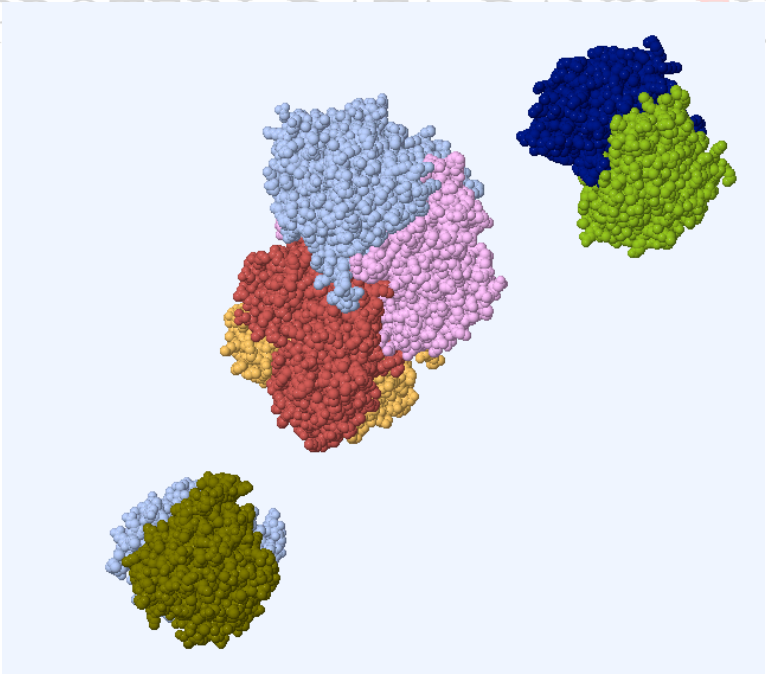
Multimeric state	8	**Surface area, Å^2**	84849.0	**ΔG^{int}, kcal/mol**	-452.5	**TΔS^{diss}, kcal/mol**	30.4
Copies in unit cell	8	**Buried area, Å^2**	55491.5	**ΔG^{diss}, kcal/mol**	28.1	**Symmetry number**	2
Formula	$A_2B_2C_4a_2b_2c_2d_2e_4f_4g_4h_2$					**Biomolecule (R350)**	1
Composition	ACBDEFGH[HCA]$_2$[CFM]$_2$[CA]$_2$[CLF]$_2$[MG]$_4$[ALF]$_4$[ADP]$_4$[SF4]$_2$						
Dissociation pattern	ACBD[HCA]$_2$[CFM]$_2$[CA]$_2$[CLF]$_2$ + EF[MG]$_2$[ALF]$_2$[ADP]$_2$[SF4] + GH[MG]$_2$[ALF]$_2$[ADP]$_2$[SF4]						

view assembly | view dissociated | in Jmol | download assembly | remark 350

Engaged interfaces

Id	##		Interfacing structures	N_{occ}	Diss.	Sym.ID	Buried area, Å^2	Δ^iG, kcal/mol	N_{HB}	N_{SB}	N_{DS}	CSS
1	1	◉	D + C	1		1_555	4367.5 (8%)	-54.3 (12%)	56 (14%)	18 (15%)	0	0.548
	2	○	B + A	1		1_555	4360.1 (8%)	-54.4 (12%)	55 (13%)	17 (14%)	0	0.548
						Average:	4363.8 (8%)	-54.3 (12%)	56 (14%)	18 (15%)	0	0.548
2	3	○	D + B	1		1_555	2872.0 (5%)	-21.6 (5%)	46 (11%)	24 (20%)	0	0.719
3	4	○	H + G	1		1_555	2335.1 (4%)	-12.4 (3%)	31 (8%)	15 (12%)	0	0.302
	5	○	F + E	1		1_555	2321.0 (4%)	-12.4 (3%)	31 (8%)	14 (11%)	0	0.302
						Average:	2328.0 (4%)	-12.4 (3%)	31 (8%)	15 (12%)	0	0.302

The "View Dissociated" button will graphically show how the assembly is put together. In the case of this entry the program suggests that chains A,B,C,D form the core of the assembly and then chains E,F,G and H bind on either side of this core protein to form a stable assembly.

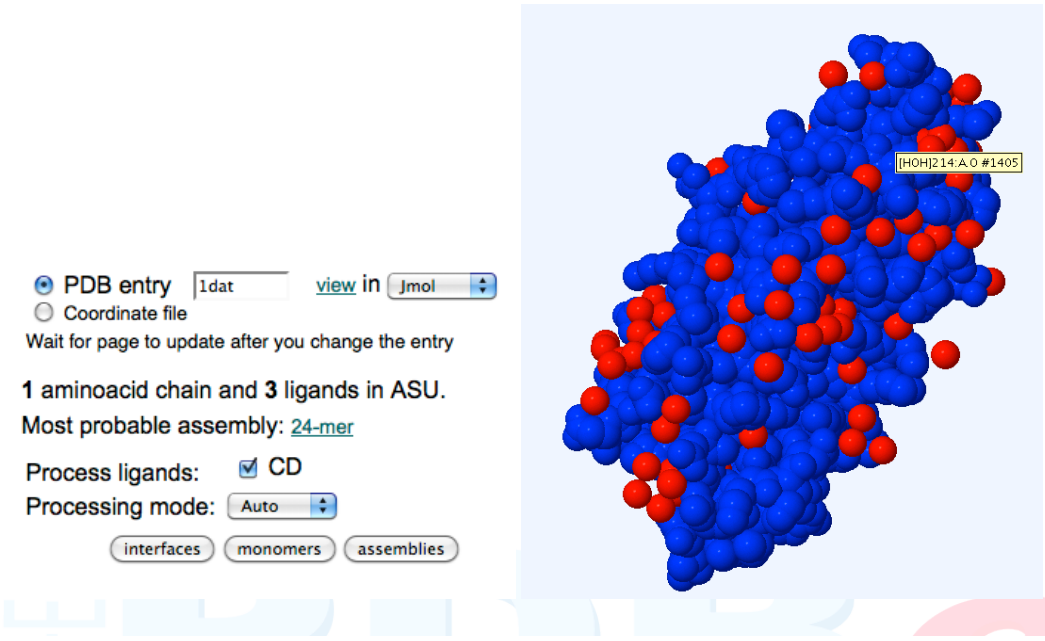


Therefore, using PISA you can get valuable information about the type of complexes that can be formed based on chemical stability and crystal contacts. The residue-by-residue information provided by PISA can be used to identify the

amino acids that are crucial to the formation of stable complexes which can be biologically relevant.

Some other interesting assemblies to look at:

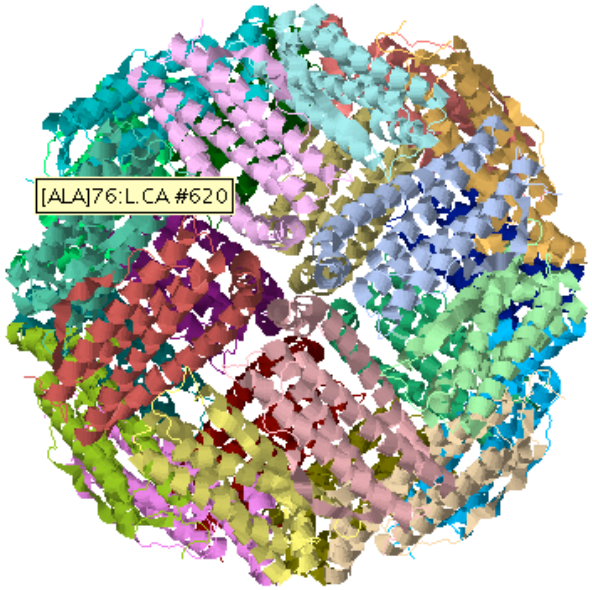
1DAT: Single chain in the deposited entry, but stable complex is a 24-mer.



Analysis of complex represented *As Is* by PDB entry is found here.

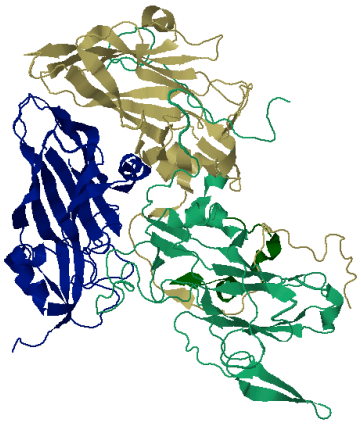
Analysis of protein interfaces suggests that the following quaternary structures are stable in solution

PQS set NN	PQS set «»	mm Size	Formula	Composition	Id	Biomol R350	Stable	Surface area, sq. Å	Buried area, sq. Å	ΔG^{int}, kcal/mol	ΔG^{diss}, kcal/mol
	⊙	24	A_{24}	A_{24}	1	1	yes	137880	93980	-263.8	254.5



2WS9: 4 chains in the PDB file. Actual assembly 240-mer.

Viruses are special in the PDB in that not all the chains that are present in the so-called crystallographic asymmetric unit are deposited. Instead, only the minimum number of chains that can uniquely describe a icosahedral repeat unit are deposited in the PDB. Symmetry operations are then used to generate the full viral capsid.



Protein structure to be examined:

PDB entry 2ws9 view in Jmol

Coordinate file

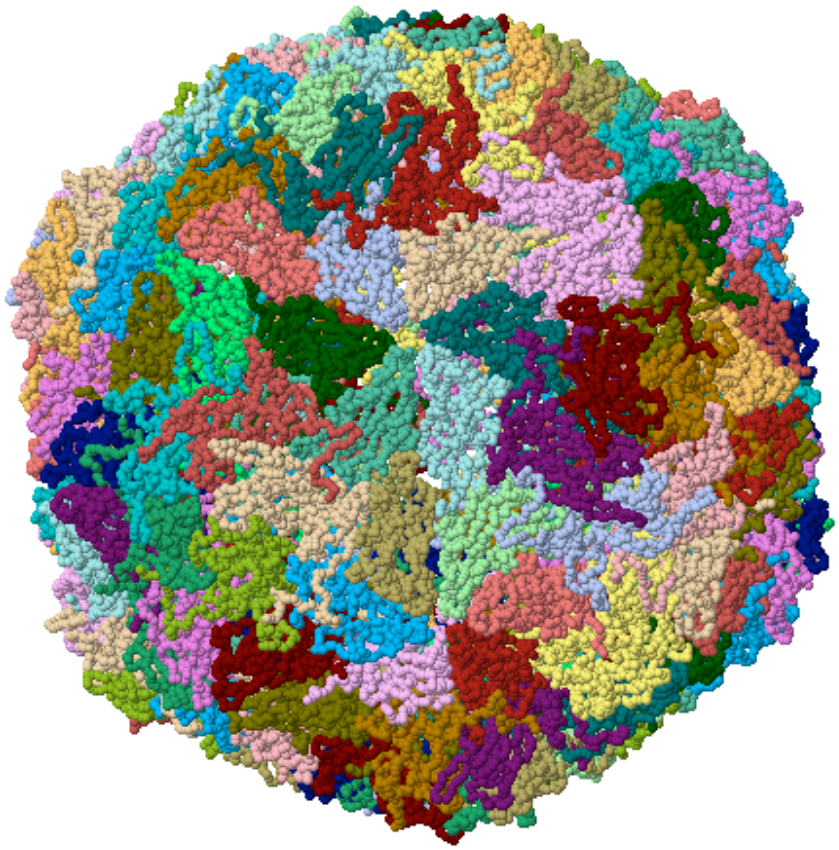
Wait for page to update after you change the entry

Total **120** aminoacid chains in ASU

including **116** NCS-mates. **119** NCS-mates ignored

Most probable assembly: 240-mer

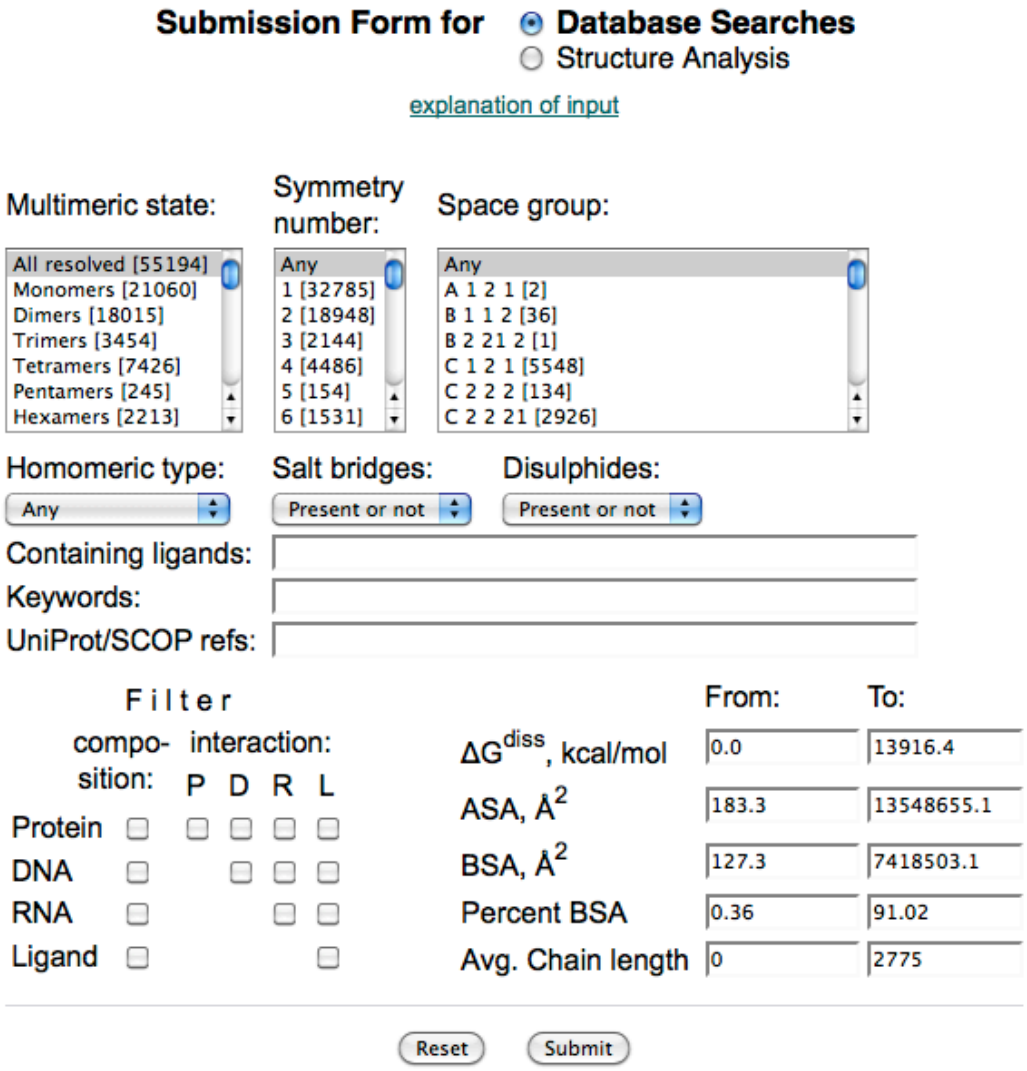
interfaces monomers assemblies



PISA Database Searches

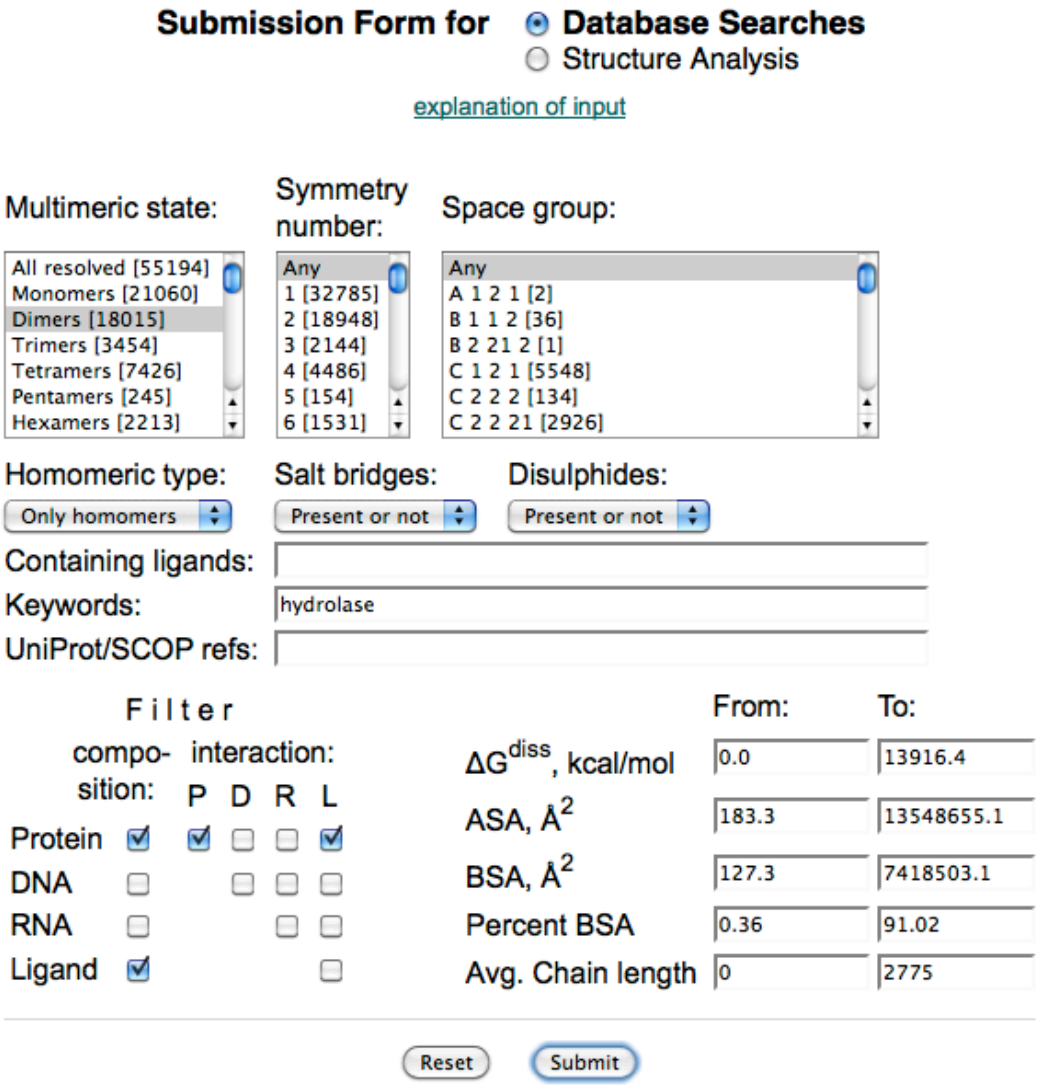
PISA maintains a database of all entries in the PDB and can be used to rapidly search for entries that match a particular criterion. These could be

1) Oligomeric State
2) Symmetry/Space Group
3) Number of Salt bridges and/or Disulphide Bonds
4) UniProt/SCOP references
5) Composition etc.

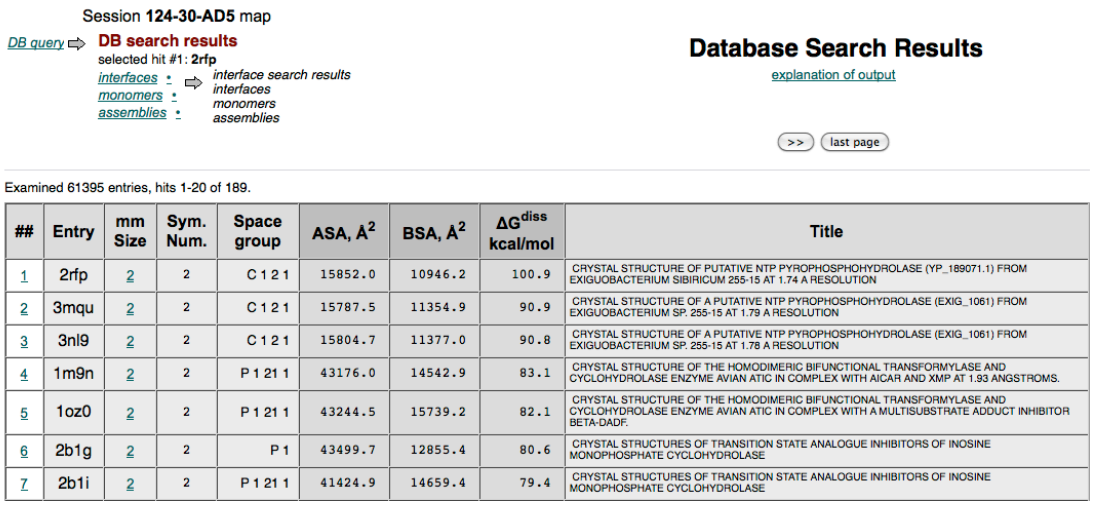


In order to see the Database Search form, choose the Database Search radio button instead of the Structure Analysis button from the PISA submission form page.

In order to do a search for all entries in the PDB that are of enzyme class "hydrolase" and contain protein and ligand molecules, where the protein interacts with the ligand and protein, and the predicted PISA assembly is homodimeric, the submission form could look as shown below.



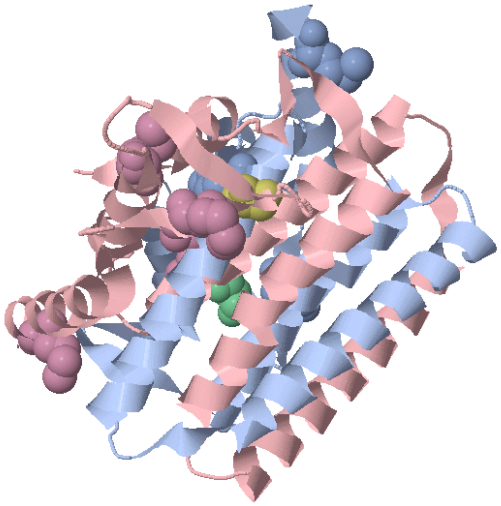
Click on the Submit button to see the results.



Choose 2rfp shown for further analysis. Click on the first column to see details of the interfaces. Click on the mm Size column to view this graphically as shown below.

Examined 61395 entries, hits 1-20 of 189.

##	Entry	mm Size	Sym. Num.	Space group	ASA, Å^2	BSA, Å^2	ΔG^{diss} kcal/mol	Title
1	2rfp	2	2	C 1 2 1	15852.0	10946.2	100.9	CRYSTAL STRUCTURE OF PUTATIVE NTP PYROPHOSPHOHYDROLASE (YP_189071.1) FROM EXIGUOBACTERIUM SIBIRICUM 255-15 AT 1.74 A RESOLUTION
2	3mqu	2	2	C 1 2 1	15787.5	11354.9	90.9	CRYSTAL STRUCTURE OF A PUTATIVE NTP PYROPHOSPHOHYDROLASE (EXIG_1061) FROM EXIGUOBACTERIUM SP. 255-15 AT 1.79 A RESOLUTION
3	3nl9	2	2	C 1 2 1	15804.7	11377.0	90.8	CRYSTAL STRUCTURE OF A PUTATIVE NTP PYROPHOSPHOHYDROLASE (EXIG_1061) FROM EXIGUOBACTERIUM SP. 255-15 AT 1.78 A RESOLUTION
4	1m9n	2	2	P 1 21 1	43176.0	14542.9	83.1	CRYSTAL STRUCTURE OF THE HOMODIMERIC BIFUNCTIONAL TRANSFORMYLASE AND CYCLOHYDROLASE ENZYME AVIAN ATIC IN COMPLEX WITH AICAR AND XMP AT 1.93 ANGSTROMS.



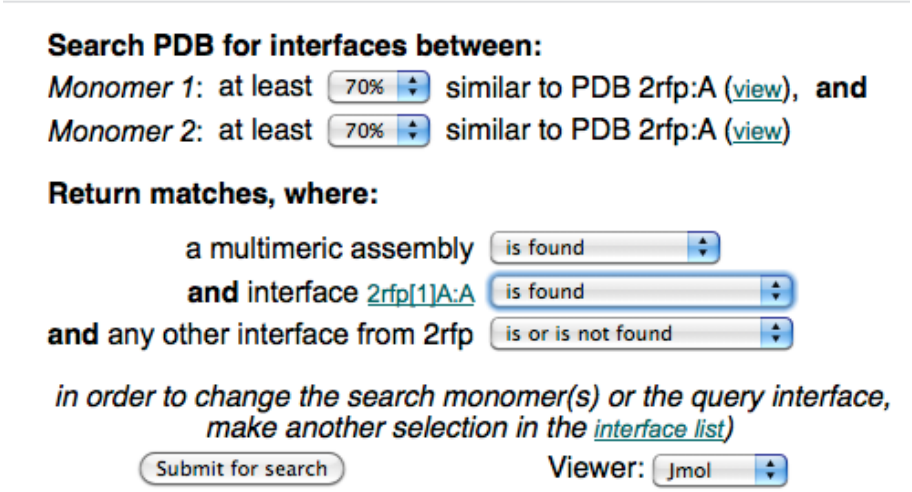
When you view the interface details, as shown below, you may also choose to search the entire PDB for other structures that have similar interfaces.

Found interfaces

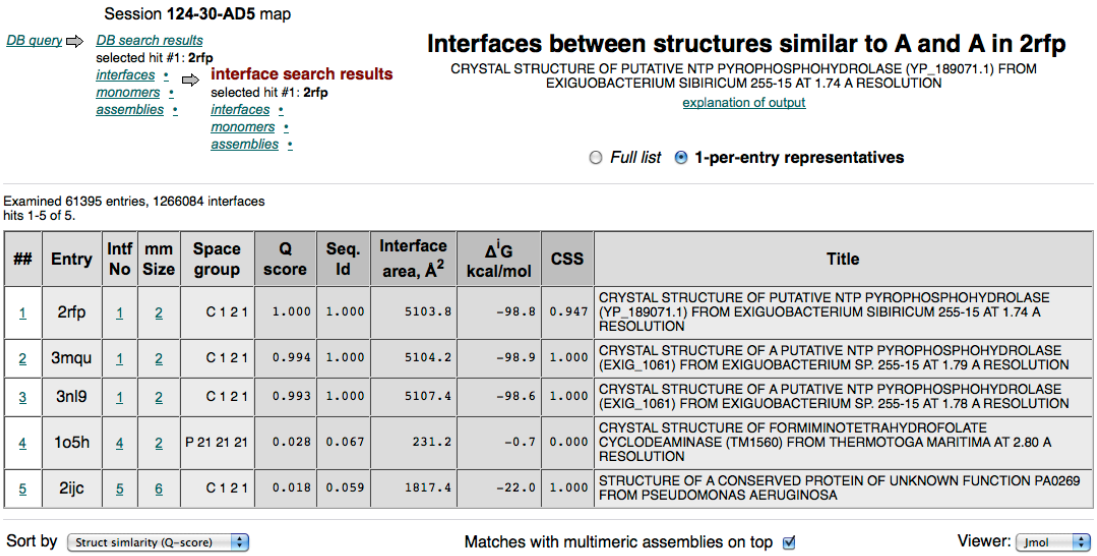
##		Structure 1			×	Structure 2					Interface area, Å^2	$\Delta^i G$ kcal/mol	$\Delta^i G$ P-value
NN	«»	Range	$^iN_{at}$	$^iN_{res}$		Range	Symmetry op-n	Sym.ID	$^iN_{at}$	$^iN_{res}$			
1	◉	A	512	106	◊	A	-x,y,-z+1	2_556	508	106	5103.8	-98.8	0.033
2	○	A	41	14	◊	A	-x,y,-z	2_555	41	14	393.7	-8.0	0.302
3	○	A	37	12	x	A	x-1/2,y+1/2,z	3_455	43	14	380.7	-2.4	0.702
4	○	A	15	5	◊	A	-x+1,y,-z+1	2_656	15	5	116.4	-0.1	0.797
5	○	A	13	4	x	A	-x+1/2,y-1/2,-z+1	4_546	10	4	109.2	0.5	0.841
6	○	[GOL]A:171	6	1	f	A	x,y,z	1_555	16	7	105.8	-0.1	0.735
7	○	[GOL]A:171	5	1	◊	A	-x,y,-z+1	2_556	10	4	78.8	-1.3	0.419
8	○	A	4	1	x	A	x,y,z-1	1_554	6	3	46.4	-0.4	0.558
9	○	A	6	2	x	A	-x-1/2,y-1/2,-z+1	4_446	2	1	36.3	-0.4	0.323
10	○	A	3	1	x	A	-x-1/2,y-1/2,-z	4_445	4	1	29.4	0.9	0.861
11	○	A	2	1	x	A	x-1/2,y-1/2,z	3_445	3	2	17.4	0.4	0.818
12	○	A	2	1	◊	A	-x-1,y,-z	2_455	2	1	13.3	-0.4	0.400

>> view selected interface
>> details of selected interface
>> download selected interface
>> search PDB for interfaces between structures similar to those making the selected interface

This is a memory intensive search. Choosing this option will bring up another submission form where certain parameters may be tweaked for the search.



Once the search has finished, you will be presented with a results section containing entries that have similar interface to the one submitted.



##	Entry	Intf No	mm Size	Space group	Q score	Seq. Id	Interface area, Å^2	Δ^iG kcal/mol	CSS	Title
1	2rfp	1	2	C 1 2 1	1.000	1.000	5103.8	-98.8	0.947	CRYSTAL STRUCTURE OF PUTATIVE NTP PYROPHOSPHOHYDROLASE (YP_189071.1) FROM EXIGUOBACTERIUM SIBIRICUM 255-15 AT 1.74 A RESOLUTION
2	3mqu	1	2	C 1 2 1	0.994	1.000	5104.2	-98.9	1.000	CRYSTAL STRUCTURE OF A PUTATIVE NTP PYROPHOSPHOHYDROLASE (EXIG_1061) FROM EXIGUOBACTERIUM SP. 255-15 AT 1.79 A RESOLUTION
3	3nl9	1	2	C 1 2 1	0.993	1.000	5107.4	-98.6	1.000	CRYSTAL STRUCTURE OF A PUTATIVE NTP PYROPHOSPHOHYDROLASE (EXIG_1061) FROM EXIGUOBACTERIUM SP. 255-15 AT 1.78 A RESOLUTION
4	1o5h	4	2	P 21 21 21	0.028	0.067	231.2	-0.7	0.000	CRYSTAL STRUCTURE OF FORMIMINOTETRAHYDROFOLATE CYCLODEAMINASE (TM1560) FROM THERMOTOGA MARITIMA AT 2.80 A RESOLUTION
5	2ijc	5	6	C 1 2 1	0.018	0.059	1817.4	-22.0	1.000	STRUCTURE OF A CONSERVED PROTEIN OF UNKNOWN FUNCTION PA0269 FROM PSEUDOMONAS AERUGINOSA

The results suggest that there are 4 entries that may have similar interfaces (the first is the same as the query). PDB entry 2JIC is a hexamer and interface 5 of this entry is a potential match to our query. However, the Q-score is very low (0.018). Q-scores range from 0 to 1 for unrelated to identical interfaces. The only entries with a high Q-score are that of the same protein. This suggests that this interface found in our query structure is unique to the PDB under the given search criteria. Changing the query parameters could produce different results.

This ends our tutorial on PDBePISA. We hope you found this useful and will be able to use this tool in your future research and analysis. There is extensive online help available for the program (all column header terms provide pop-up help in a separate window), and if you need to get in touch with the PDBe regarding any aspect of the programme, please email pdbehelp@ebi.ac.uk and we will try to assist you in any way possible.