GAIA evaluates the quality of a given protein structure or a structural model based on different criteria. The statistics used by Gaia for comparison are generated from high resolution crystal structures. The observed and expected scores for different criteria used by Gaia to score the given structure are summarized in the table below. Values in cells with a red background indicate parameters that need immediate attention in order to refine the structure further.

This report is generated by Gaia, developed by the Dokholyan group.
Please cite : Kota, P., Ding, F., Ramachandran, S. and Dokholyan N.V. Bioinformatics (2011)

Table 1: Summary of scores for the input structure

Criterion		Observed	Target
Steric clashes		0.02	0.02
Hydrogen bonds	%Unsatisfied in shell	13.80	9.56
	%Unsatisfied in core	1.30	1.45
Solvent accessible surface area		190.55	221.64
Void volume		0.50	0.097

Steric clashes

Clash summary	
Number of residues	102
Number of contacts	1353
Number of clashes	35
Clash score	0.02

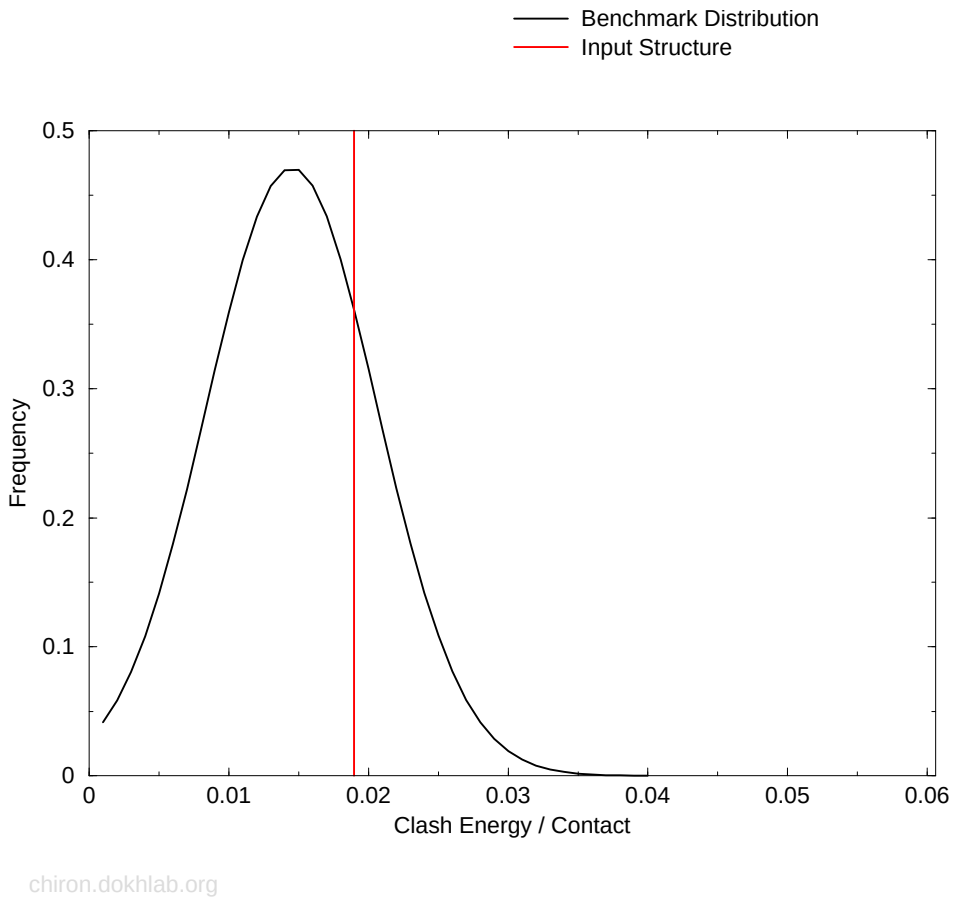

Figure 1: Comparison of clash-score with the distribution of clash-scores of high resolution crystal structures

Table 2: List of clashes

$Atom_i$	Res_i	$Atom_j$	Res_j	d_{acc}	d_{obs}	ΔG_{VDWR}
CB	6	SG	11	3.950	3.029	0.854
SG	6	CB	11	3.950	2.991	0.915
CA	7	SG	28	4.255	3.260	0.421
O	7	NE2	26	3.200	2.410	2.032
O	7	CD2	26	3.598	3.055	0.503
CB	7	SG	28	3.950	2.953	0.976
SG	7	CB	28	3.950	3.020	0.868
O	9	CD2	26	3.598	3.093	0.376
CA	11	OE1	15	3.965	3.230	0.411
CA	20	O	44	3.965	3.242	0.387
CA	20	SG	40	4.255	3.281	0.400
CB	20	SG	40	3.950	3.086	0.765
SG	20	CA	40	4.255	3.309	0.372
SG	20	CB	40	3.950	2.949	0.981
CB	21	O	43	3.660	2.906	1.347
CG	34	OE2	85	3.660	3.077	0.902
OE2	34	OE2	85	3.200	2.586	1.109
O	36	CB	40	3.660	3.204	0.372
CA	44	O	98	3.660	3.007	1.015
O	47	CA	95	3.660	3.174	0.467
CA	52	O	102	3.660	3.015	0.988
O	52	CG	56	3.660	3.231	0.301
CB	57	SG	62	3.950	2.886	1.083
SG	57	CB	62	3.950	3.042	0.833
CB	58	SG	79	3.950	2.997	0.905
SG	58	CB	79	3.950	3.029	0.855
CA	62	OE1	66	3.965	3.038	0.809
CB	62	OE1	66	3.660	3.087	0.753
CA	63	ND2	75	3.965	3.201	0.576
CB	63	ND2	75	3.660	3.254	0.301
O	65	CB	68	3.660	3.230	0.303
CA	71	SG	91	4.255	3.325	0.355
CB	71	SG	91	3.950	3.030	0.854
SG	71	CB	91	3.950	3.037	0.842
O	87	CB	91	3.660	3.191	0.413

End of Table 2

Hydrogen bonds

Table 3: List of hydrogen bonds

$Atom_i$	$ResName_i$	Res_i	$Atom_j$	$ResName_j$	Res_j	$Type$
N	GLY	1	OE1	GLU	4	BS/SB
N	GLU	4	O	GLY	1	BB
N	GLN	5	O	GLY	1	BB
NE2	GLN	5	O	ILE	10	BS/SB
N	CYS	6	O	ILE	2	BB
N	CYS	7	O	VAL	3	BB
N	THR	8	O	GLU	4	BB
N	SER	9	O	GLN	5	BB
N	CYS	11	O	GLN	25	BB
N	SER	12	OE1	GLN	15	BS/SB
N	GLN	15	O	SER	12	BB
N	LEU	16	O	SER	12	BB
N	GLU	17	O	LEU	13	BB
N	ASN	18	O	GLN	15	BB
N	TYR	19	O	LEU	16	BB
N	CYS	20	O	GLU	17	BB
N	ASN	21	O	GLY	44	BB
N	GLN	25	O	CYS	11	BB
N	LEU	27	O	CYS	6	BB
N	HIS	31	O	CYS	28	BB
N	LEU	32	O	CYS	28	BB
N	VAL	33	O	GLY	29	BB
N	GLU	34	O	SER	30	BB
N	ALA	35	O	HIS	31	BB
N	LEU	36	O	LEU	32	BB
N	TYR	37	O	VAL	33	BB
N	LEU	38	O	GLU	34	BB
N	VAL	39	O	ALA	35	BB
N	CYS	40	O	LEU	36	BB
N	GLY	41	O	TYR	37	BB
N	ARG	43	O	CYS	40	BB
NE	ARG	43	O	ASN	21	BS/SB
NH1	ARG	43	O	ASN	21	BS/SB
N	GLY	44	O	CYS	40	BB
N	PHE	45	O	TYR	98	BB
N	PHE	46	O	TYR	19	BB
N	TYR	47	O	PHE	96	BB

BB - Backbone-backbone ; SS - Sidechain-sidechain ; BS/SB - Backbone-sidechain

Continued on next page

Table 3 – continued from previous page

$Atom_i$	$ResName_i$	Res_i	$Atom_j$	$ResName_j$	Res_j	$Type$
N	LYS	50	OE2	GLU	4	BS/SB
N	GLY	52	OE2	GLU	55	BS/SB
N	GLU	55	O	GLY	52	BB
N	GLN	56	O	GLY	52	BB
NE2	GLN	56	OH	TYR	70	SS
N	CYS	57	O	ILE	53	BB
N	CYS	58	O	VAL	54	BB
N	THR	59	O	VAL	54	BB
N	SER	60	O	GLU	55	BB
N	ILE	61	OG	SER	60	BS/SB
N	CYS	62	O	GLN	76	BB
N	SER	63	OE1	GLN	66	BS/SB
N	GLN	66	O	SER	63	BB
NE2	GLN	66	OE1	GLN	56	SS
N	LEU	67	O	SER	63	BB
N	GLU	68	O	LEU	64	BB
N	ASN	69	O	GLN	66	BB
N	TYR	70	O	LEU	67	BB
N	CYS	71	O	GLU	68	BB
N	ASN	72	O	GLY	95	BB
ND2	ASN	72	O	ARG	94	BS/SB
N	GLN	76	O	CYS	62	BB
ND1	HIS	77	O	CYS	58	BS/SB
N	LEU	78	O	CYS	57	BB
N	HIS	82	O	CYS	79	BB
N	LEU	83	O	CYS	79	BB
N	VAL	84	O	GLY	80	BB
N	GLU	85	O	SER	81	BB
N	ALA	86	O	HIS	82	BB
N	LEU	87	O	LEU	83	BB
N	TYR	88	O	VAL	84	BB
N	LEU	89	O	GLU	85	BB
N	VAL	90	O	ALA	86	BB
N	CYS	91	O	LEU	87	BB
N	GLY	92	O	TYR	88	BB
N	ARG	94	O	CYS	91	BB
NE	ARG	94	O	ASN	72	BS/SB
NH1	ARG	94	O	ASN	72	BS/SB
N	GLY	95	O	GLY	92	BB
N	PHE	96	O	TYR	47	BB
N	PHE	97	O	TYR	70	BB
N	TYR	98	O	PHE	45	BB
N	ALA	102	O	THR	99	BB

BB - Backbone-backbone ; SS - Sidechain-sidechain ; BS/SB - Backbone-sidechain

End of Table 3

Unsatisfied hydrogen bond partners in the shell

Shell hydrogen bond summary	
# Unsatisfied partners	40
% Unsatisfied partners	13.80

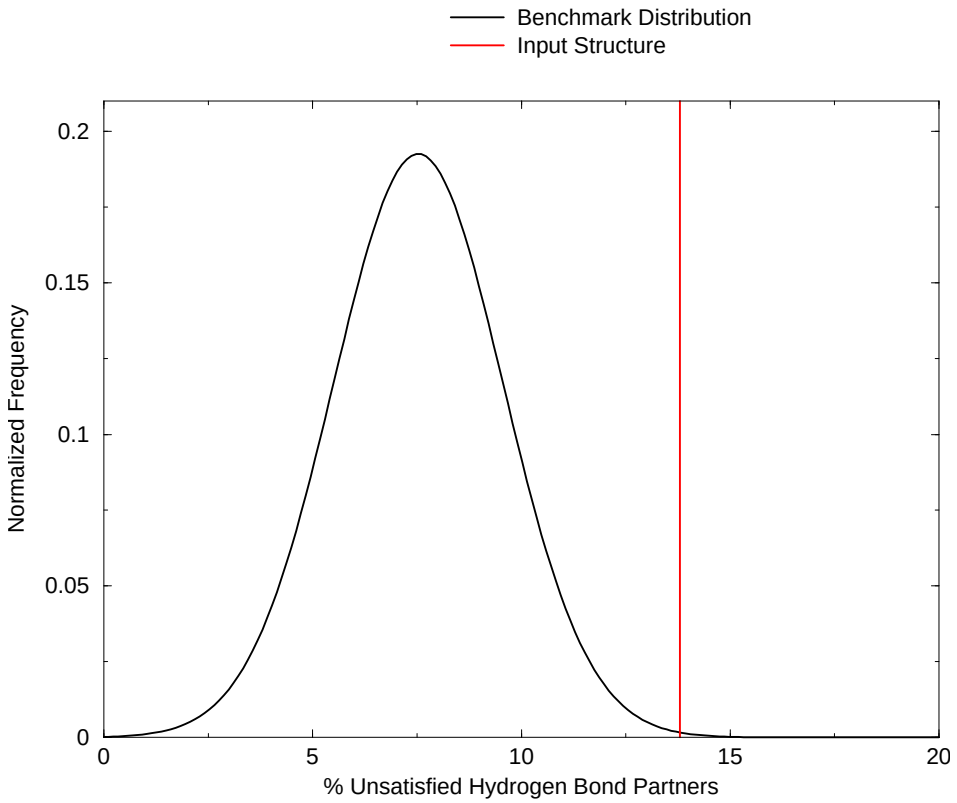

Figure 2: Comparison of %unsatisfied hydrogen bonds in the shell with the distribution from high resolution crystal structures

Table 4: List of unsatisfied partners in the shell

Atom	*ResName*	*Res*
N	ILE	2
N	VAL	3
N	ILE	10
SG	CYS	11
N	LEU	13
N	TYR	14
SG	CYS	20
ND2	ASN	21
N	VAL	23
O	VAL	23
N	ASN	24
N	HIS	26
NE2	HIS	26
O	LEU	27
N	CYS	28
SG	CYS	40
O	GLY	41
N	GLU	42
O	GLU	42
O	PHE	46
N	THR	48
N	ALA	51
N	VAL	54
O	GLN	56
O	SER	60
N	LEU	64
N	TYR	65
SG	CYS	71
N	VAL	74
O	VAL	74
N	ASN	75
N	HIS	77
O	LEU	78
N	CYS	79
SG	CYS	91
N	GLU	93
O	PHE	97
N	THR	99
N	LYS	101
O	ALA	102

End of Table 4

Unsatisfied hydrogen bond partners in the core

Core hydrogen bond summary	
# Unsatisfied partners	4
% Unsatisfied partners	1.30

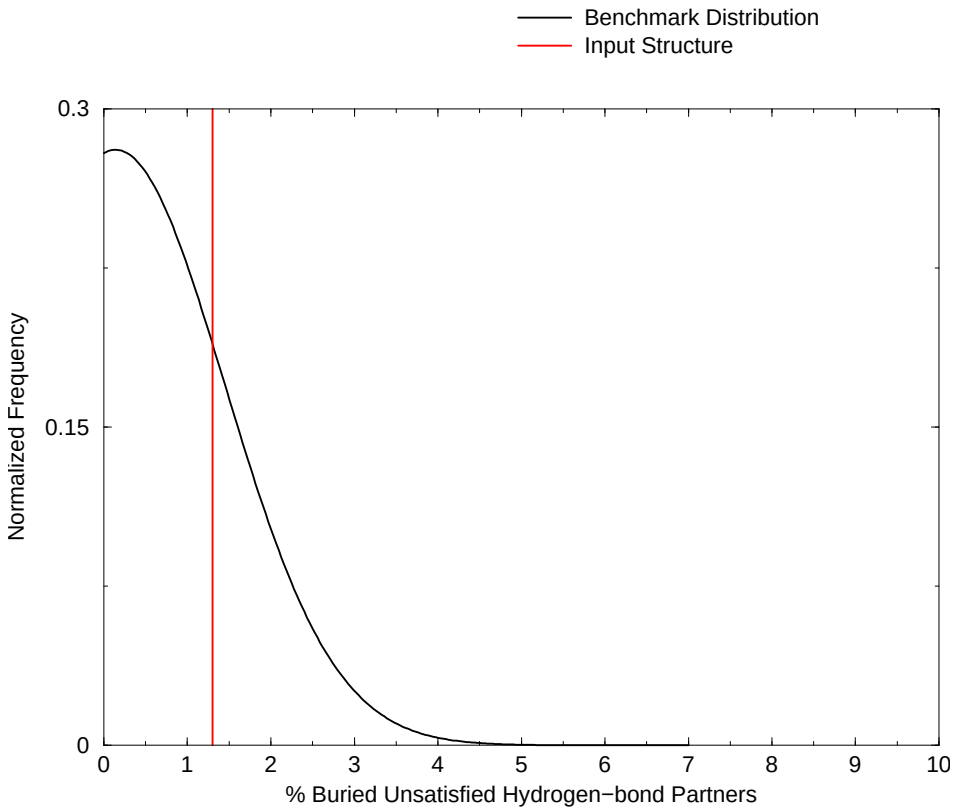

Figure 3: Comparison of %unsatisfied hydrogen bonds in the core with the distribution from high resolution crystal structures

Table 5: List of unsatisfied partners in the core

Atom	*ResName*	*Res*
SG	CYS	6
N	ILE	53
SG	CYS	57
SG	CYS	62
		End of Table 5

Solvent excluded surface area (SASA)

MSA summary	
Total MSA	4869.93
Rescaled MSA	119.47

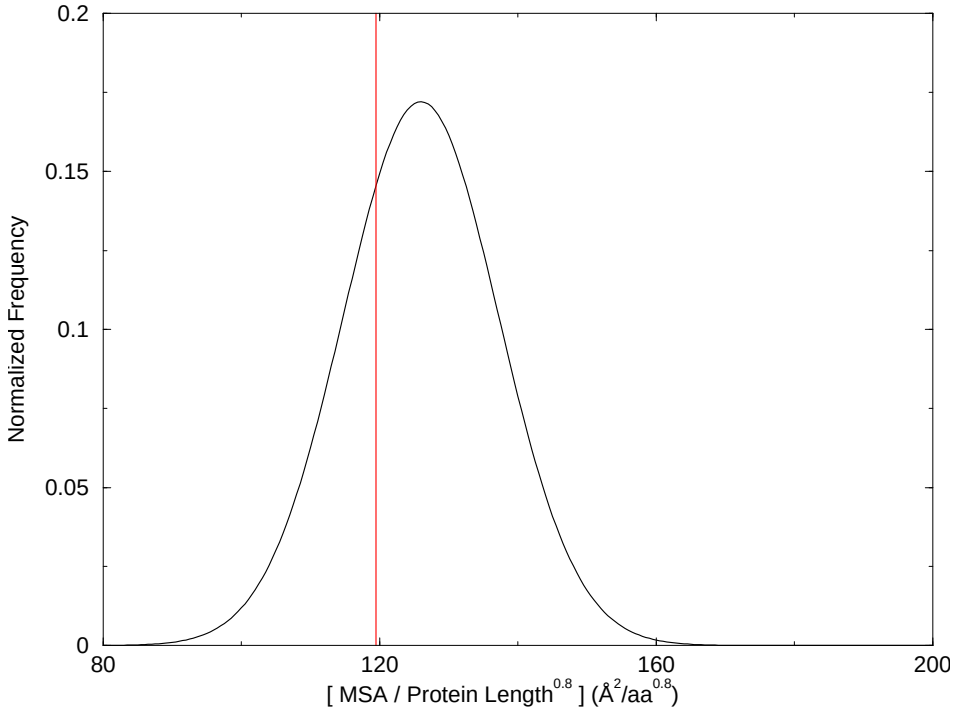

Figure 4: Comparison of rescaled solvent excluded surface area with the distribution from high resolution crystal structures

Void volume

The total void volume of the input structure is **51.08** $\mathring{A}^3$. In order to eliminate bias due to length of the protein, we normalize the void volume by the chain length. The rescaled volume of the input structure is **0.50** $\mathring{A}^3$. The red line in the plot above represents the rescaled void volume of the input structure in context of the distribution generated from high resolution crystal structures.

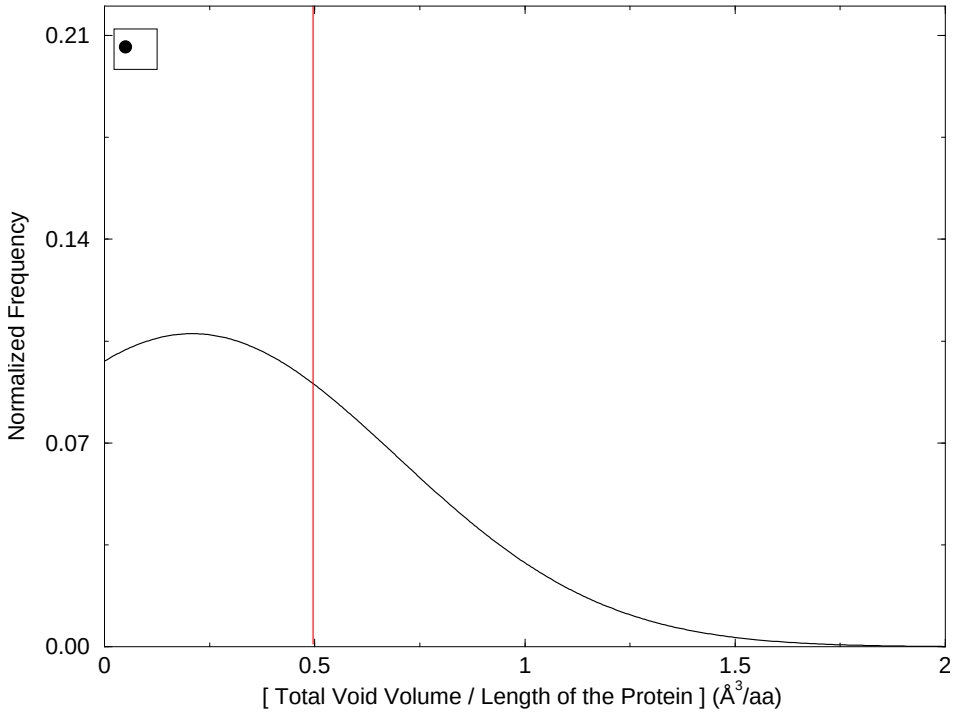

Figure 5: Comparison of rescaled void volume with the distribution from high resolution crystal structures

Table 6: List of voids

$Void$	$Volume(\mathring{A}^{\mathbf{3}})$
1	0.000
2	0.000
	End of Table 6