

Supporting Information (SI)

Biophysical and computational analysis of interaction 2D MoS₂ nanosheets with human haemoglobin coupled with NIR activated photothermal therapy

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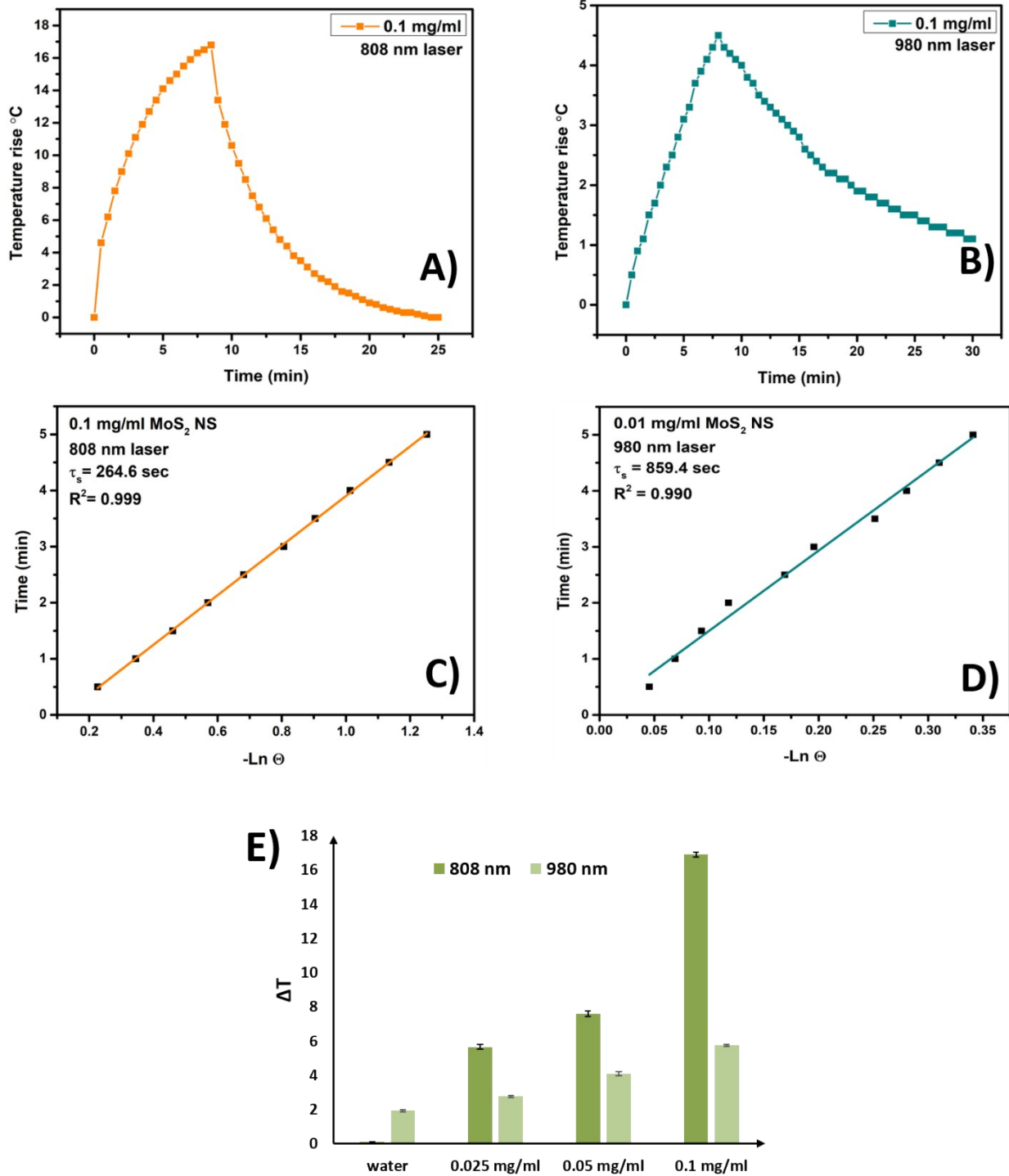


Figure S1 A, B) Photothermal conversion efficiency of MoS₂ NS using 808 nm (1.2 W) and 980 nm (0.2 W) laser. **C, D)** Calculation of heat dissipation constant using negative logarithm plot of $-\ln \Theta$ vs Time (min). **E)** Plot of MoS₂ Concentration (mg/ml) and water vs change in temperature (°C) using 808 nm (1.2 W) and 980 nm laser (0.2 W).

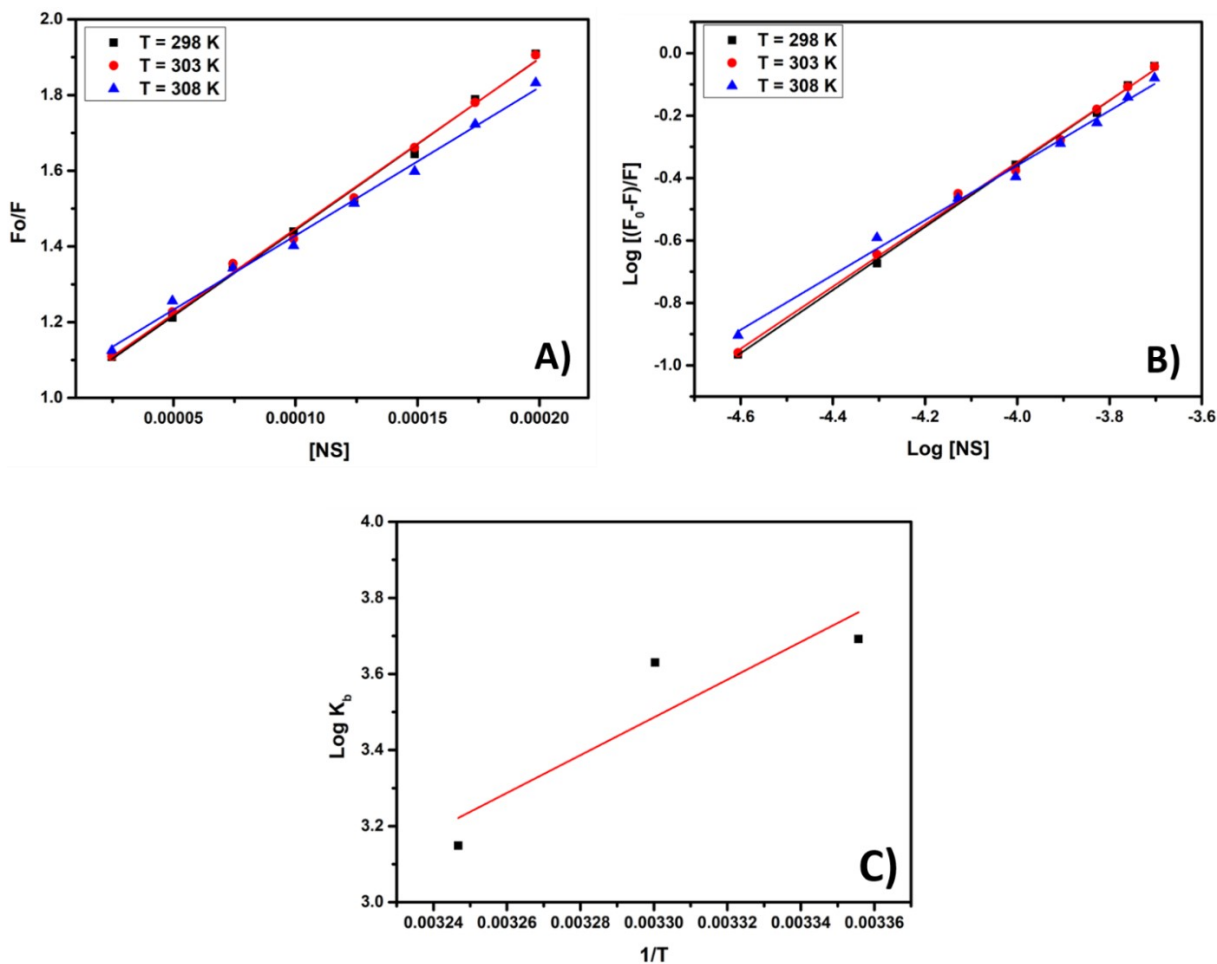


Figure S2 A) Stern Volmer Plot of 2.5 μM solution of Hb against the concentration of MoS₂ NS at 298, 303 and 308 K. B) Modified Stern Volmer plot of NS-Hb interaction for calculating binding constant. C) $\text{Log } K_b$ vs $1/T$ (Van't Hoff Plot) for calculating thermodynamic parameters.

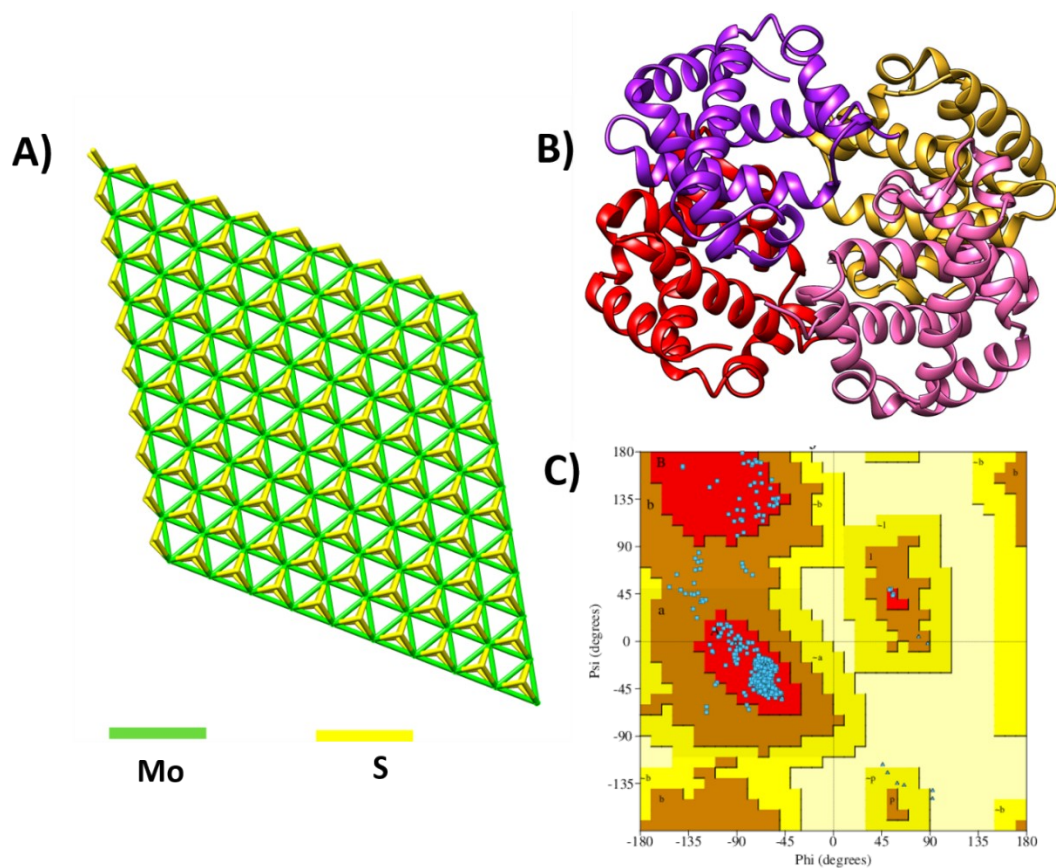


Figure S3 A) 2D structure of MoS₂ NS. B) 3D structure of haemoglobin. C) Ramachandran plot for 3D structure of haemoglobin.

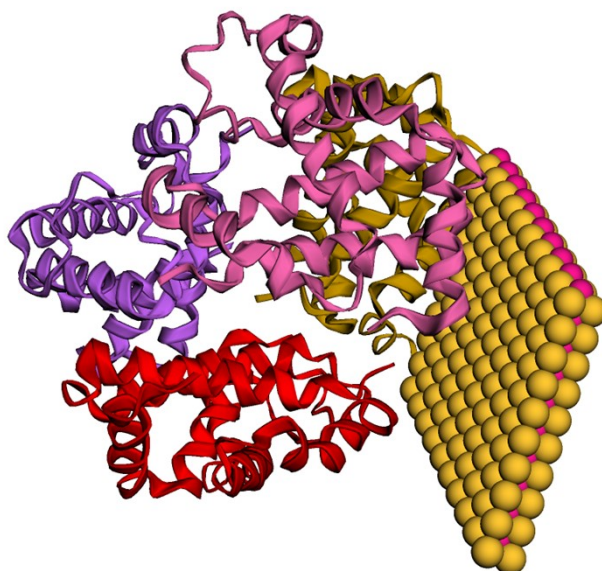


Figure S4 Surface view interaction of MoS₂ NS with human haemoglobin via molecular docking analysis.

Table S1: Binding constants for interaction of Hb with MoS₂ NS at 298 K, 303 K and 308 K.

Binding Constants	Temperature (K)		
	298 K	303 K	308 K
Stern Volmer Constant K_{sv} (M^{-1})(10^3)	4.537	4.497	3.918
Quenching Constant K_q ($M^{-1} s^{-1}$) (10^{11})	4.537	4.497	3.918
Binding Constant K_b (M^{-1})	4897.78	4265.79	1380.38
Number of binding sites n	1.011	0.995	0.999

Table S2: Thermodynamic parameters of interaction of Hb with MoS₂ NS.

	ΔG (kJ/mol)	ΔH (kJ/mol)	$T\Delta S$ (kJ/mol)
MoS ₂ NS	-9.3211	-41.2562	-31.9351

Table S3: Percentage content of secondary structure of protein for Hb only and Hb with MoS₂ NS

Secondary structures	Details of secondary structures	Percentage content of secondary structure			
		Hb	Hb+ MoS ₂ NS (0.00304 mg/ml)	Hb+ MoS ₂ NS (0.00608 mg/ml)	Hb+ MoS ₂ NS (0.01216 mg/ml)
Helix	Helix 1 (Regular)	21.0	19.7	18.9	17.3
	Helix 2 (Distorted)	11.4	11.3	10.6	10.6
Antiparallel	Anti 1 (Left-twisted)	0.0	0.0	0.0	0.0
	Anti 2 (Relaxed)	0.0	0.0	1.8	0.4
	Anti 3 (Right twisted)	13.0	12.7	12.8	13.9
Parallel		7.4	8.1	9.4	7.6
Turns		17.4	17.2	16.1	17.9
Others		29.7	31.0	30.4	32.3

Table S4: The detailed molecular interactions were evaluated using PDBsum

List of protein-ligand interactions

Hydrogen bonds

<----- A T O M 1 ----->						<----- A T O M 2 ----->					
Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	2152	OD1	ASP 94	B	<--	5297	S1	LIG 0	Z		3.01
2.	2152	OD1	ASP 94	B	<--	5343	S29	LIG 0	Z		3.19
3.	2847	OE2	GLU 23	C	<--	5314	S9	LIG 0	Z		1.93

4.	2847	OE2	GLU	23	C	<--	5315	S10	LIG	0	Z	2.18
5.	2847	OE2	GLU	23	C	<--	5323	S18	LIG	0	Z	2.93
6.	2847	OE2	GLU	23	C	<--	5324	S19	LIG	0	Z	3.10
7.	2881	OE1	GLU	27	C	<--	5323	S18	LIG	0	Z	2.06
8.	2902	O	GLU	30	C	<--	5319	S14	LIG	0	Z	3.14
9.	2906	OE1	GLU	30	C	<--	5312	S7	LIG	0	Z	3.15
10.	2906	OE1	GLU	30	C	<--	5321	S16	LIG	0	Z	2.47
11.	2906	OE1	GLU	30	C	<--	5478	S83	LIG	0	Z	2.52
12.	2907	OE2	GLU	30	C	<--	5469	S74	LIG	0	Z	1.88
13.	2907	OE2	GLU	30	C	<--	5478	S83	LIG	0	Z	2.55
14.	3009	NZ	LYS	40	C	-->	5316	S11	LIG	0	Z	2.85
15.	3009	NZ	LYS	40	C	-->	5317	S12	LIG	0	Z	1.93
16.	3092	O	LEU	48	C	<--	5310	S5	LIG	0	Z	1.85
17.	3092	O	LEU	48	C	<--	5460	S65	LIG	0	Z	3.11
18.	3106	N	HIS	50	C	-->	5460	S65	LIG	0	Z	2.96
19.	3112	ND1	HIS	50	C	-->	5469	S74	LIG	0	Z	2.82
20.	3672	NE2	HIS	112	C	-->	5323	S18	LIG	0	Z	2.15

Non-bonded contacts

<----- A T O M 1 ----->

<----- A T O M 2 ----->

	Atom	Atom	Res	Res		Atom	Atom	Res	Res			
	no.	name	name	no.	Chain	no.	name	name	no.	Chain	Distance	
1.	2151	CG	ASP	94	B	5343	S29	LIG	0	Z	3.64	
2.	2152	OD1	ASP	94	B	5297	S1	LIG	0	Z	3.01	

3.	2152	OD1	ASP	94	B	---	5343	S29	LIG	0	Z	3.19
4.	2153	OD2	ASP	94	B	---	5343	S29	LIG	0	Z	3.58
5.	2637	O	HIS	146	B	---	5316	S11	LIG	0	Z	3.63
6.	2639	CG	HIS	146	B	---	5494	S99	LIG	0	Z	3.46
7.	2640	ND1	HIS	146	B	---	5297	S1	LIG	0	Z	3.60
8.	2640	ND1	HIS	146	B	---	5325	Mo10	LIG	0	Z	3.83
9.	2640	ND1	HIS	146	B	---	5343	S29	LIG	0	Z	3.28
10.	2640	ND1	HIS	146	B	---	5494	S99	LIG	0	Z	2.08
11.	2640	ND1	HIS	146	B	---	5494	S99	LIG	0	Z	3.51
12.	2641	CD2	HIS	146	B	---	5297	S1	LIG	0	Z	3.87
13.	2641	CD2	HIS	146	B	---	5343	S29	LIG	0	Z	3.47
14.	2642	CE1	HIS	146	B	---	5297	S1	LIG	0	Z	2.61
15.	2642	CE1	HIS	146	B	---	5325	Mo10	LIG	0	Z	2.79
16.	2642	CE1	HIS	146	B	---	5343	S29	LIG	0	Z	2.10
17.	2642	CE1	HIS	146	B	---	5353	Mo20	LIG	0	Z	3.88
18.	2642	CE1	HIS	146	B	---	5494	S99	LIG	0	Z	1.97
19.	2642	CE1	HIS	146	B	---	5494	S99	LIG	0	Z	3.42
20.	2643	NE2	HIS	146	B	---	5297	S1	LIG	0	Z	2.79
21.	2643	NE2	HIS	146	B	---	5325	Mo10	LIG	0	Z	3.59
22.	2643	NE2	HIS	146	B	---	5343	S29	LIG	0	Z	2.24
23.	2643	NE2	HIS	146	B	---	5494	S99	LIG	0	Z	3.29
24.	2644	OXT	HIS	146	B	---	5494	S99	LIG	0	Z	3.79
25.	2822	ND1	HIS	20	C	---	5306	Mo9	LIG	0	Z	3.22
26.	2824	CE1	HIS	20	C	---	5306	Mo9	LIG	0	Z	3.17
27.	2841	C	GLU	23	C	---	5304	Mo7	LIG	0	Z	3.87
28.	2842	O	GLU	23	C	---	5303	Mo6	LIG	0	Z	3.80

29.	2842	O	GLU	23	C	---	5304	Mo7	LIG	0	Z	3.23
30.	2844	CG	GLU	23	C	---	5304	Mo7	LIG	0	Z	2.88
31.	2844	CG	GLU	23	C	---	5305	Mo8	LIG	0	Z	2.91
32.	2844	CG	GLU	23	C	---	5314	S9	LIG	0	Z	2.63
33.	2845	CD	GLU	23	C	---	5304	Mo7	LIG	0	Z	3.49
34.	2845	CD	GLU	23	C	---	5305	Mo8	LIG	0	Z	1.90
35.	2845	CD	GLU	23	C	---	5314	S9	LIG	0	Z	2.39
36.	2845	CD	GLU	23	C	---	5315	S10	LIG	0	Z	2.71
37.	2846	OE1	GLU	23	C	---	5305	Mo8	LIG	0	Z	2.80
38.	2846	OE1	GLU	23	C	---	5306	Mo9	LIG	0	Z	3.69
39.	2846	OE1	GLU	23	C	---	5314	S9	LIG	0	Z	3.41
40.	2846	OE1	GLU	23	C	---	5315	S10	LIG	0	Z	2.68
41.	2847	OE2	GLU	23	C	---	5304	Mo7	LIG	0	Z	3.13
42.	2847	OE2	GLU	23	C	---	5305	Mo8	LIG	0	Z	0.80
43.	2847	OE2	GLU	23	C	---	5306	Mo9	LIG	0	Z	3.44
44.	2847	OE2	GLU	23	C	---	5314	S9	LIG	0	Z	1.93
45.	2847	OE2	GLU	23	C	---	5315	S10	LIG	0	Z	2.18
46.	2847	OE2	GLU	23	C	---	5323	S18	LIG	0	Z	2.93
47.	2847	OE2	GLU	23	C	---	5324	S19	LIG	0	Z	3.10
48.	2847	OE2	GLU	23	C	---	5415	Mo82	LIG	0	Z	3.30
49.	2847	OE2	GLU	23	C	---	5424	Mo91	LIG	0	Z	3.45
50.	2847	OE2	GLU	23	C	---	5494	S99	LIG	0	Z	3.88
51.	2855	CD1	TYR	24	C	---	5305	Mo8	LIG	0	Z	3.63
52.	2857	CE1	TYR	24	C	---	5305	Mo8	LIG	0	Z	3.22
53.	2857	CE1	TYR	24	C	---	5306	Mo9	LIG	0	Z	3.79
54.	2857	CE1	TYR	24	C	---	5324	S19	LIG	0	Z	3.54

55.	2860	OH	TYR	24	C	---	5306	Mo9	LIG	0	Z	3.43
56.	2860	OH	TYR	24	C	---	5324	S19	LIG	0	Z	3.82
57.	2870	C	ALA	26	C	---	5302	Mo5	LIG	0	Z	3.62
58.	2870	C	ALA	26	C	---	5303	Mo6	LIG	0	Z	3.63
59.	2871	O	ALA	26	C	---	5302	Mo5	LIG	0	Z	2.94
60.	2874	N	GLU	27	C	---	5303	Mo6	LIG	0	Z	2.90
61.	2874	N	GLU	27	C	---	5321	S16	LIG	0	Z	3.79
62.	2875	CA	GLU	27	C	---	5302	Mo5	LIG	0	Z	3.61
63.	2875	CA	GLU	27	C	---	5303	Mo6	LIG	0	Z	2.58
64.	2875	CA	GLU	27	C	---	5321	S16	LIG	0	Z	2.70
65.	2875	CA	GLU	27	C	---	5322	S17	LIG	0	Z	3.33
66.	2876	C	GLU	27	C	---	5321	S16	LIG	0	Z	3.40
67.	2877	O	GLU	27	C	---	5321	S16	LIG	0	Z	3.23
68.	2878	CB	GLU	27	C	---	5303	Mo6	LIG	0	Z	2.61
69.	2878	CB	GLU	27	C	---	5304	Mo7	LIG	0	Z	3.43
70.	2878	CB	GLU	27	C	---	5321	S16	LIG	0	Z	3.18
71.	2878	CB	GLU	27	C	---	5322	S17	LIG	0	Z	2.20
72.	2879	CG	GLU	27	C	---	5303	Mo6	LIG	0	Z	3.36
73.	2879	CG	GLU	27	C	---	5321	S16	LIG	0	Z	3.11
74.	2879	CG	GLU	27	C	---	5322	S17	LIG	0	Z	1.98
75.	2880	CD	GLU	27	C	---	5304	Mo7	LIG	0	Z	3.76
76.	2880	CD	GLU	27	C	---	5322	S17	LIG	0	Z	2.22
77.	2880	CD	GLU	27	C	---	5323	S18	LIG	0	Z	3.23
78.	2880	CD	GLU	27	C	---	5494	S99	LIG	0	Z	3.88
79.	2881	OE1	GLU	27	C	---	5304	Mo7	LIG	0	Z	2.75
80.	2881	OE1	GLU	27	C	---	5322	S17	LIG	0	Z	2.05

81.	2881	OE1	GLU	27	C	---	5323	S18	LIG	0	Z	2.06
82.	2881	OE1	GLU	27	C	---	5494	S99	LIG	0	Z	3.53
83.	2882	OE2	GLU	27	C	---	5322	S17	LIG	0	Z	3.34
84.	2899	N	GLU	30	C	---	5301	Mo4	LIG	0	Z	3.55
85.	2899	N	GLU	30	C	---	5302	Mo5	LIG	0	Z	3.79
86.	2899	N	GLU	30	C	---	5320	S15	LIG	0	Z	3.17
87.	2900	CA	GLU	30	C	---	5301	Mo4	LIG	0	Z	2.75
88.	2900	CA	GLU	30	C	---	5302	Mo5	LIG	0	Z	3.55
89.	2900	CA	GLU	30	C	---	5319	S14	LIG	0	Z	3.06
90.	2900	CA	GLU	30	C	---	5320	S15	LIG	0	Z	2.05
91.	2901	C	GLU	30	C	---	5319	S14	LIG	0	Z	3.50
92.	2901	C	GLU	30	C	---	5320	S15	LIG	0	Z	2.76
93.	2902	O	GLU	30	C	---	5319	S14	LIG	0	Z	3.14
94.	2902	O	GLU	30	C	---	5320	S15	LIG	0	Z	3.40
95.	2903	CB	GLU	30	C	---	5301	Mo4	LIG	0	Z	2.41
96.	2903	CB	GLU	30	C	---	5302	Mo5	LIG	0	Z	2.29
97.	2903	CB	GLU	30	C	---	5311	S6	LIG	0	Z	3.34
98.	2903	CB	GLU	30	C	---	5319	S14	LIG	0	Z	3.36
99.	2903	CB	GLU	30	C	---	5320	S15	LIG	0	Z	0.71
100.	2903	CB	GLU	30	C	---	5321	S16	LIG	0	Z	3.18
101.	2903	CB	GLU	30	C	---	5388	Mo55	LIG	0	Z	3.05
102.	2903	CB	GLU	30	C	---	5494	S99	LIG	0	Z	3.84
103.	2903	CB	GLU	30	C	---	5494	S99	LIG	0	Z	3.77
104.	2904	CG	GLU	30	C	---	5301	Mo4	LIG	0	Z	2.65
105.	2904	CG	GLU	30	C	---	5302	Mo5	LIG	0	Z	3.16
106.	2904	CG	GLU	30	C	---	5311	S6	LIG	0	Z	3.40

107.	2904	CG	GLU	30	C	---	5319	S14	LIG	0	Z	2.83
108.	2904	CG	GLU	30	C	---	5320	S15	LIG	0	Z	0.89
109.	2904	CG	GLU	30	C	---	5321	S16	LIG	0	Z	3.73
110.	2904	CG	GLU	30	C	---	5379	Mo46	LIG	0	Z	3.41
111.	2904	CG	GLU	30	C	---	5388	Mo55	LIG	0	Z	2.10
112.	2904	CG	GLU	30	C	---	5494	S99	LIG	0	Z	2.32
113.	2904	CG	GLU	30	C	---	5494	S99	LIG	0	Z	2.89
114.	2905	CD	GLU	30	C	---	5301	Mo4	LIG	0	Z	3.13
115.	2905	CD	GLU	30	C	---	5302	Mo5	LIG	0	Z	2.88
116.	2905	CD	GLU	30	C	---	5311	S6	LIG	0	Z	2.68
117.	2905	CD	GLU	30	C	---	5319	S14	LIG	0	Z	3.87
118.	2905	CD	GLU	30	C	---	5320	S15	LIG	0	Z	1.82
119.	2905	CD	GLU	30	C	---	5321	S16	LIG	0	Z	3.47
120.	2905	CD	GLU	30	C	---	5379	Mo46	LIG	0	Z	3.49
121.	2905	CD	GLU	30	C	---	5388	Mo55	LIG	0	Z	0.73
122.	2905	CD	GLU	30	C	---	5389	Mo56	LIG	0	Z	3.63
123.	2905	CD	GLU	30	C	---	5397	Mo64	LIG	0	Z	3.04
124.	2905	CD	GLU	30	C	---	5398	Mo65	LIG	0	Z	3.42
125.	2905	CD	GLU	30	C	---	5469	S74	LIG	0	Z	3.10
126.	2905	CD	GLU	30	C	---	5478	S83	LIG	0	Z	2.86
127.	2905	CD	GLU	30	C	---	5494	S99	LIG	0	Z	2.40
128.	2905	CD	GLU	30	C	---	5494	S99	LIG	0	Z	2.06
129.	2906	OE1	GLU	30	C	---	5302	Mo5	LIG	0	Z	2.49
130.	2906	OE1	GLU	30	C	---	5311	S6	LIG	0	Z	3.02
131.	2906	OE1	GLU	30	C	---	5312	S7	LIG	0	Z	3.15
132.	2906	OE1	GLU	30	C	---	5320	S15	LIG	0	Z	2.31

133.	2906	OE1	GLU	30	C	---	5321	S16	LIG	0	Z	2.47
134.	2906	OE1	GLU	30	C	---	5388	Mo55	LIG	0	Z	1.64
135.	2906	OE1	GLU	30	C	---	5397	Mo64	LIG	0	Z	1.85
136.	2906	OE1	GLU	30	C	---	5398	Mo65	LIG	0	Z	3.18
137.	2906	OE1	GLU	30	C	---	5478	S83	LIG	0	Z	2.52
138.	2906	OE1	GLU	30	C	---	5494	S99	LIG	0	Z	3.46
139.	2906	OE1	GLU	30	C	---	5494	S99	LIG	0	Z	1.60
140.	2906	OE1	GLU	30	C	---	5494	S99	LIG	0	Z	3.68
141.	2907	OE2	GLU	30	C	---	5301	Mo4	LIG	0	Z	3.27
142.	2907	OE2	GLU	30	C	---	5302	Mo5	LIG	0	Z	3.69
143.	2907	OE2	GLU	30	C	---	5310	S5	LIG	0	Z	3.73
144.	2907	OE2	GLU	30	C	---	5311	S6	LIG	0	Z	2.58
145.	2907	OE2	GLU	30	C	---	5319	S14	LIG	0	Z	3.89
146.	2907	OE2	GLU	30	C	---	5320	S15	LIG	0	Z	2.81
147.	2907	OE2	GLU	30	C	---	5379	Mo46	LIG	0	Z	2.75
148.	2907	OE2	GLU	30	C	---	5388	Mo55	LIG	0	Z	0.58
149.	2907	OE2	GLU	30	C	---	5389	Mo56	LIG	0	Z	2.73
150.	2907	OE2	GLU	30	C	---	5397	Mo64	LIG	0	Z	3.67
151.	2907	OE2	GLU	30	C	---	5398	Mo65	LIG	0	Z	3.22
152.	2907	OE2	GLU	30	C	---	5469	S74	LIG	0	Z	1.88
153.	2907	OE2	GLU	30	C	---	5478	S83	LIG	0	Z	2.55
154.	2907	OE2	GLU	30	C	---	5479	S84	LIG	0	Z	3.69
155.	2907	OE2	GLU	30	C	---	5494	S99	LIG	0	Z	2.18
156.	2907	OE2	GLU	30	C	---	5494	S99	LIG	0	Z	2.78
157.	2907	OE2	GLU	30	C	---	5494	S99	LIG	0	Z	3.85
158.	2909	N	ARG	31	C	---	5320	S15	LIG	0	Z	3.44

159.	2939	CB	PHE	33	C	---	5300	Mo3	LIG	0	Z	3.76
160.	2939	CB	PHE	33	C	---	5318	S13	LIG	0	Z	3.17
161.	2939	CB	PHE	33	C	---	5319	S14	LIG	0	Z	3.52
162.	2940	CG	PHE	33	C	---	5300	Mo3	LIG	0	Z	3.86
163.	2942	CD2	PHE	33	C	---	5300	Mo3	LIG	0	Z	3.20
164.	2942	CD2	PHE	33	C	---	5319	S14	LIG	0	Z	3.73
165.	2952	CG	LEU	34	C	---	5319	S14	LIG	0	Z	3.78
166.	2952	CG	LEU	34	C	---	5494	S99	LIG	0	Z	3.24
167.	2952	CG	LEU	34	C	---	5494	S99	LIG	0	Z	3.28
168.	2953	CD1	LEU	34	C	---	5494	S99	LIG	0	Z	3.84
169.	2953	CD1	LEU	34	C	---	5494	S99	LIG	0	Z	2.72
170.	2953	CD1	LEU	34	C	---	5494	S99	LIG	0	Z	3.51
171.	2953	CD1	LEU	34	C	---	5494	S99	LIG	0	Z	3.89
172.	2954	CD2	LEU	34	C	---	5494	S99	LIG	0	Z	2.25
173.	2954	CD2	LEU	34	C	---	5494	S99	LIG	0	Z	3.78
174.	2954	CD2	LEU	34	C	---	5494	S99	LIG	0	Z	3.64
175.	2954	CD2	LEU	34	C	---	5494	S99	LIG	0	Z	3.51
176.	3006	CG	LYS	40	C	---	5317	S12	LIG	0	Z	3.49
177.	3007	CD	LYS	40	C	---	5298	Mo1	LIG	0	Z	3.55
178.	3007	CD	LYS	40	C	---	5299	Mo2	LIG	0	Z	3.26
179.	3007	CD	LYS	40	C	---	5317	S12	LIG	0	Z	2.05
180.	3007	CD	LYS	40	C	---	5318	S13	LIG	0	Z	3.52
181.	3008	CE	LYS	40	C	---	5298	Mo1	LIG	0	Z	3.70
182.	3008	CE	LYS	40	C	---	5316	S11	LIG	0	Z	3.23
183.	3008	CE	LYS	40	C	---	5317	S12	LIG	0	Z	2.32
184.	3009	NZ	LYS	40	C	---	5298	Mo1	LIG	0	Z	3.58

185.	3009	NZ	LYS	40	C	---	5316	S11	LIG	0	Z	2.85
186.	3009	NZ	LYS	40	C	---	5317	S12	LIG	0	Z	1.93
187.	3009	NZ	LYS	40	C	---	5361	Mo28	LIG	0	Z	3.45
188.	3009	NZ	LYS	40	C	---	5494	S99	LIG	0	Z	2.68
189.	3009	NZ	LYS	40	C	---	5494	S99	LIG	0	Z	3.60
190.	3089	N	LEU	48	C	---	5309	S4	LIG	0	Z	3.56
191.	3090	CA	LEU	48	C	---	5299	Mo2	LIG	0	Z	3.72
192.	3090	CA	LEU	48	C	---	5300	Mo3	LIG	0	Z	3.68
193.	3090	CA	LEU	48	C	---	5309	S4	LIG	0	Z	2.51
194.	3091	C	LEU	48	C	---	5300	Mo3	LIG	0	Z	3.37
195.	3091	C	LEU	48	C	---	5309	S4	LIG	0	Z	1.92
196.	3091	C	LEU	48	C	---	5310	S5	LIG	0	Z	3.01
197.	3091	C	LEU	48	C	---	5460	S65	LIG	0	Z	3.81
198.	3092	O	LEU	48	C	---	5300	Mo3	LIG	0	Z	2.42
199.	3092	O	LEU	48	C	---	5309	S4	LIG	0	Z	1.72
200.	3092	O	LEU	48	C	---	5310	S5	LIG	0	Z	1.85
201.	3092	O	LEU	48	C	---	5370	Mo37	LIG	0	Z	3.48
202.	3092	O	LEU	48	C	---	5379	Mo46	LIG	0	Z	3.54
203.	3092	O	LEU	48	C	---	5460	S65	LIG	0	Z	3.11
204.	3093	CB	LEU	48	C	---	5299	Mo2	LIG	0	Z	2.39
205.	3093	CB	LEU	48	C	---	5300	Mo3	LIG	0	Z	3.15
206.	3093	CB	LEU	48	C	---	5308	S3	LIG	0	Z	3.31
207.	3093	CB	LEU	48	C	---	5309	S4	LIG	0	Z	2.22
208.	3094	CG	LEU	48	C	---	5299	Mo2	LIG	0	Z	3.09
209.	3094	CG	LEU	48	C	---	5309	S4	LIG	0	Z	3.71
210.	3095	CD1	LEU	48	C	---	5298	Mo1	LIG	0	Z	3.75

211.	3095	CD1	LEU	48	C	---	5299	Mo2	LIG	0	Z	2.63
212.	3095	CD1	LEU	48	C	---	5308	S3	LIG	0	Z	3.85
213.	3098	N	SER	49	C	---	5309	S4	LIG	0	Z	2.82
214.	3098	N	SER	49	C	---	5310	S5	LIG	0	Z	3.83
215.	3098	N	SER	49	C	---	5460	S65	LIG	0	Z	3.89
216.	3099	CA	SER	49	C	---	5309	S4	LIG	0	Z	3.46
217.	3099	CA	SER	49	C	---	5310	S5	LIG	0	Z	3.73
218.	3099	CA	SER	49	C	---	5460	S65	LIG	0	Z	3.12
219.	3100	C	SER	49	C	---	5310	S5	LIG	0	Z	3.06
220.	3100	C	SER	49	C	---	5460	S65	LIG	0	Z	3.35
221.	3100	C	SER	49	C	---	5469	S74	LIG	0	Z	3.71
222.	3101	O	SER	49	C	---	5310	S5	LIG	0	Z	3.11
223.	3106	N	HIS	50	C	---	5310	S5	LIG	0	Z	3.25
224.	3106	N	HIS	50	C	---	5379	Mo46	LIG	0	Z	3.86
225.	3106	N	HIS	50	C	---	5460	S65	LIG	0	Z	2.96
226.	3106	N	HIS	50	C	---	5469	S74	LIG	0	Z	2.65
227.	3107	CA	HIS	50	C	---	5310	S5	LIG	0	Z	3.57
228.	3107	CA	HIS	50	C	---	5311	S6	LIG	0	Z	3.45
229.	3107	CA	HIS	50	C	---	5469	S74	LIG	0	Z	2.19
230.	3107	CA	HIS	50	C	---	5478	S83	LIG	0	Z	3.76
231.	3108	C	HIS	50	C	---	5469	S74	LIG	0	Z	3.63
232.	3110	CB	HIS	50	C	---	5389	Mo56	LIG	0	Z	3.47
233.	3110	CB	HIS	50	C	---	5469	S74	LIG	0	Z	2.05
234.	3110	CB	HIS	50	C	---	5470	S75	LIG	0	Z	3.35
235.	3110	CB	HIS	50	C	---	5478	S83	LIG	0	Z	3.24
236.	3110	CB	HIS	50	C	---	5479	S84	LIG	0	Z	2.71

237.	3111	CG	HIS	50	C	---	5388	Mo55	LIG	0	Z	3.68
238.	3111	CG	HIS	50	C	---	5389	Mo56	LIG	0	Z	3.84
239.	3111	CG	HIS	50	C	---	5398	Mo65	LIG	0	Z	3.41
240.	3111	CG	HIS	50	C	---	5469	S74	LIG	0	Z	2.77
241.	3111	CG	HIS	50	C	---	5478	S83	LIG	0	Z	2.14
242.	3111	CG	HIS	50	C	---	5479	S84	LIG	0	Z	2.40
243.	3111	CG	HIS	50	C	---	5488	S93	LIG	0	Z	3.59
244.	3112	ND1	HIS	50	C	---	5311	S6	LIG	0	Z	3.46
245.	3112	ND1	HIS	50	C	---	5312	S7	LIG	0	Z	3.85
246.	3112	ND1	HIS	50	C	---	5388	Mo55	LIG	0	Z	2.71
247.	3112	ND1	HIS	50	C	---	5389	Mo56	LIG	0	Z	3.68
248.	3112	ND1	HIS	50	C	---	5397	Mo64	LIG	0	Z	3.20
249.	3112	ND1	HIS	50	C	---	5398	Mo65	LIG	0	Z	2.49
250.	3112	ND1	HIS	50	C	---	5469	S74	LIG	0	Z	2.82
251.	3112	ND1	HIS	50	C	---	5478	S83	LIG	0	Z	0.80
252.	3112	ND1	HIS	50	C	---	5479	S84	LIG	0	Z	2.61
253.	3112	ND1	HIS	50	C	---	5487	S92	LIG	0	Z	3.70
254.	3112	ND1	HIS	50	C	---	5488	S93	LIG	0	Z	3.11
255.	3112	ND1	HIS	50	C	---	5494	S99	LIG	0	Z	3.65
256.	3113	CD2	HIS	50	C	---	5478	S83	LIG	0	Z	2.82
257.	3113	CD2	HIS	50	C	---	5479	S84	LIG	0	Z	3.02
258.	3113	CD2	HIS	50	C	---	5488	S93	LIG	0	Z	3.20
259.	3114	CE1	HIS	50	C	---	5312	S7	LIG	0	Z	3.58
260.	3114	CE1	HIS	50	C	---	5388	Mo55	LIG	0	Z	3.64
261.	3114	CE1	HIS	50	C	---	5397	Mo64	LIG	0	Z	2.80
262.	3114	CE1	HIS	50	C	---	5398	Mo65	LIG	0	Z	2.60

263.	3114	CE1	HIS	50	C	---	5407	Mo74	LIG	0	Z	3.40
264.	3114	CE1	HIS	50	C	---	5478	S83	LIG	0	Z	1.24
265.	3114	CE1	HIS	50	C	---	5479	S84	LIG	0	Z	3.26
266.	3114	CE1	HIS	50	C	---	5487	S92	LIG	0	Z	2.52
267.	3114	CE1	HIS	50	C	---	5488	S93	LIG	0	Z	2.29
268.	3114	CE1	HIS	50	C	---	5494	S99	LIG	0	Z	3.89
269.	3115	NE2	HIS	50	C	---	5398	Mo65	LIG	0	Z	3.52
270.	3115	NE2	HIS	50	C	---	5478	S83	LIG	0	Z	2.43
271.	3115	NE2	HIS	50	C	---	5479	S84	LIG	0	Z	3.48
272.	3115	NE2	HIS	50	C	---	5487	S92	LIG	0	Z	3.08
273.	3115	NE2	HIS	50	C	---	5488	S93	LIG	0	Z	2.34
274.	3118	N	GLY	51	C	---	5311	S6	LIG	0	Z	3.48
275.	3668	CG	HIS	112	C	---	5324	S19	LIG	0	Z	3.18
276.	3669	ND1	HIS	112	C	---	5305	Mo8	LIG	0	Z	3.68
277.	3669	ND1	HIS	112	C	---	5306	Mo9	LIG	0	Z	3.75
278.	3669	ND1	HIS	112	C	---	5323	S18	LIG	0	Z	3.62
279.	3669	ND1	HIS	112	C	---	5324	S19	LIG	0	Z	1.87
280.	3670	CD2	HIS	112	C	---	5323	S18	LIG	0	Z	3.50
281.	3670	CD2	HIS	112	C	---	5324	S19	LIG	0	Z	3.68
282.	3671	CE1	HIS	112	C	---	5305	Mo8	LIG	0	Z	2.86
283.	3671	CE1	HIS	112	C	---	5323	S18	LIG	0	Z	2.31
284.	3671	CE1	HIS	112	C	---	5324	S19	LIG	0	Z	1.69
285.	3671	CE1	HIS	112	C	---	5424	Mo91	LIG	0	Z	3.60
286.	3671	CE1	HIS	112	C	---	5494	S99	LIG	0	Z	3.18
287.	3672	NE2	HIS	112	C	---	5305	Mo8	LIG	0	Z	3.46
288.	3672	NE2	HIS	112	C	---	5323	S18	LIG	0	Z	2.15

289.	3672	NE2	HIS	112	C	---	5324	S19	LIG	0	Z	2.97
290.	5044	CB	LYS	120	D	---	5494	S99	LIG	0	Z	3.31
291.	5047	CE	LYS	120	D	---	5426	Mo93	LIG	0	Z	3.52
292.	5081	CG2	THR	123	D	---	5494	S99	LIG	0	Z	3.35
293.	5088	CB	PRO	124	D	---	5494	S99	LIG	0	Z	3.18
294.	5089	CG	PRO	124	D	---	5321	S16	LIG	0	Z	3.69
295.	5089	CG	PRO	124	D	---	5494	S99	LIG	0	Z	2.86
296.	5089	CG	PRO	124	D	---	5494	S99	LIG	0	Z	3.24
297.	5090	CD	PRO	124	D	---	5494	S99	LIG	0	Z	3.62
298.	5090	CD	PRO	124	D	---	5494	S99	LIG	0	Z	3.29
299.	5090	CD	PRO	124	D	---	5494	S99	LIG	0	Z	3.25
300.	5096	CG	PRO	125	D	---	5494	S99	LIG	0	Z	3.14
301.	5096	CG	PRO	125	D	---	5494	S99	LIG	0	Z	3.30
302.	5096	CG	PRO	125	D	---	5494	S99	LIG	0	Z	3.39
303.	5097	CD	PRO	125	D	---	5494	S99	LIG	0	Z	3.29
304.	5097	CD	PRO	125	D	---	5494	S99	LIG	0	Z	3.86
305.	5097	CD	PRO	125	D	---	5494	S99	LIG	0	Z	3.85

Number of hydrogen bonds: 20

Number of non-bonded contacts: 305