

Serine and Cysteine π -Interactions in Nature: A Comparison of the Frequency and Stability of Contacts Involving Oxygen and Sulphur

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Table S1: PDB IDs for the crystal structures searched, as well as the type(s) of interactions identified and the residues involved.

PDB ID	YEAR	Res.	Cys/Ser		Nucleotide/Amino Acid			Type	Closet		Energy			Energy-Cationic		
			Res ID	Chain	Res #	Res ID	Chain		Res #	Contact Distance	Max	Min	Range	Max	Min	Range
2WBS	2011	1.70	Ser	a	415	His	a	416	both	4.185	-1.8	-7.7	-9.8	10.3	-20.2	30.5
2XHI	2011	1.6	Ser	a	115	His	a	111	both	3.859	1.5	-11.5	-4.1	-1.7	-27.6	25.9
3HP6	2011	1.81	Ser	d	785	Phe	d	781	both	3.683	2	-8.3	-10.3			
3HP6	2011	1.81	Ser	a	742	Phe	a	743	both	3.478	1.2	-15.5	-16.7			
3HP6	2011	1.81	Ser	a	785	Phe	a	781	both	3.457	2.8	-12.1	-14.9			
3HT3	2011	1.70	Ser	d	785	Phe	d	781	both	3.568	2.1	-9.5	-11.6			
3HT3	2011	1.70	Ser	a	785	Phe	a	781	both	3.482	2.6	-11.8	-14.4			
3NCI	2011	1.79	Cys	a	845	Phe	a	803	both	3.915	-2.5	-12.9	-10.4			
3NCI	2011	1.79	Ser	a	565	dG	t	4	both	3.395	-5.2	-10.6	-5.4			
3NCI	2011	1.79	Ser	a	281	Tyr	a	277	CH	3.430	-6.8	-18.8	-12			
3NDK	2011	2.0	Cys	a	845	Phe	a	803	both	3.953	-3.4	-13.8	-10.4			
3NDK	2011	2.0	Ser	a	565	dG	t	4	both	3.529	-3.6	-11.6	-8			
3NDK	2011	2.0	Ser	a	783	His	a	804	both	3.456	0	-19	-20.3	5.2	-33.4	38.6
3NDK	2011	2.0	Ser	a	281	Tyr	a	277	CH	3.398	-6.9	-19.2	-12.3			
3OGU	2011	1.85	Cys	a	239	Phe	a	223	CH	3.559	-12.1	-15.5	-3.4			
3OSG	2011	2.00	Cys	a	86	Phe	a	78	both	4.053	-0.4	-7.1	-6.7			
3PNC	2011	2.0	Cys	a	477	Phe	a	456	CH	3.505	-10.3	-15.2	-4.9			
3PNC	2011	2.0	Cys	a	300	Tyr	a	296	both	3.761	-3.8	-9.5	-5.4			
3PNC	2011	2.0	Ser	a	439	His	a	434	both	3.704	10	-3.8	-15.2	25.4	-8	33.4
3PO4	2011	1.80	Ser	a	644	Trp	a	645	both	3.611	3.9	-8.4	-12.3			
3PV8	2011	1.52	Ser	a	785	Phe	a	781	both	3.610	2.1	-10.6	-12.7			
3PV8	2011	1.52	Ser	d	785	Phe	d	781	both	3.816	2	-9.1	-11.1			
3PX0	2011	1.73	Ser	a	785	Phe	a	781	both	3.544	1.9	-10.4	-12.3			
3PX0	2011	1.73	Ser	d	785	Phe	d	781	both	3.828	2.3	-9.5	-11.8			
3QEP	2011	1.80	Cys	a	845	Phe	a	803	both	3.850	-3	-14	-11			
3QEP	2011	1.80	Ser	a	783	His	a	804	both	3.415	0	-17.8	-19.2	5.7	-31.8	37.5
3QEP	2011	1.80	Ser	a	281	Tyr	a	277	CH	3.557	-6.6	-17.8	-11.2			
3QER	2012	1.96	Cys	a	845	Phe	a	803	both	3.953	-3.2	-13.6	-10.4			
3QER	2012	1.96	Ser	a	119	His	a	131	both	3.154	-6.1	-18.2	-22.1	17.6	-38.2	55.8
3QER	2012	1.96	Ser	a	783	His	a	804	both	3.428	-0.5	-18.3	-20.2	6.6	-31.8	38.4
3QER	2012	1.96	Ser	a	281	Tyr	a	277	CH	3.508	-5.9	-17.9	-12			
3QNN	2012	1.92	Cys	a	845	Phe	a	803	both	3.885	-3	-13.7	-10.7			
3QNN	2012	1.92	Ser	a	119	His	a	131	both	3.125	-3	-17.7	-21	18	-39.6	57.6
3QNN	2012	1.92	Ser	a	783	His	a	804	both	3.334	-0.2	-19	-20	5.3	-34.1	39.4
3RJG	2012	2.00	Cys	a	239	Phe	a	223	CH	3.527	-11.1	-14.9	-3.8			
3RR7	2012	1.95	Ser	a	699	Phe	a	700	both	3.777	1.5	-12.7	-14.2			
3RZG	2012	1.62	Ser	a	125	Phe	a	124	both	4.596	1.7	-6.5	-8.2			
3S9H	2011	1.95	Cys	a	845	Phe	a	803	both	3.866	-2.5	-13.3	-10.8			
3S9H	2011	1.95	Ser	a	281	Tyr	a	277	CH	3.444	-7.4	-18.4	-11			
3SM4	2011	1.88	Cys	b	66	Phe	b	219	both	3.548	-4	-10.9	-6.9			
3SM4	2011	1.88	Cys	a	66	Phe	a	219	both	3.580	-3.2	-12.2	-9			
3SM4	2011	1.88	Cys	c	66	Phe	c	219	both	3.493	-1.9	-7.5	-5.6			
3SM4	2011	1.88	Ser	a	96	Phe	a	92	both	3.689	0.6	-14.9	-15.5			

PDB ID	YEAR	Res.	Cys/Ser			Nucleotide/Amino Acid			Type	Closet		Energy			Energy-cationic		
			Res ID	Chain	Res #	Res ID	Chain	Res #		Contact Distance	Max	Min	Range	Max	Min	Range	
3SM4	2011	1.88	Ser	c	96	Phe	c	92	both	3.669	-0.2	-15.2	-15				
3SM4	2011	1.88	Ser	b	96	Phe	b	92	both	3.695	0.6	-15.1	-15.7				
3SQ0	2011	2.00	Cys	a	845	Phe	a	803	both	3.664	-2.5	-12.6	-10.1				
3SQ0	2011	2.00	Ser	a	281	Tyr	a	277	CH	3.948	-5.8	-16.8	-11				
3SV4	2012	1.99	Ser	a	699	Phe	a	700	both	3.663	0.4	-10.3	-10.7				
3TAN	2011	1.53	Ser	a	785	Phe	a	781	both	3.456	1.3	-9.5	-10.8				
3THV	2011	1.61	Ser	a	785	Phe	a	781	both	3.557	1.5	-9.4	-10.9				
3TI0	2011	1.62	Ser	a	785	Phe	a	781	both	3.510	2	-11.3	-13.3				
3UBY	2012	2.00	Cys	a	167	Tyr	a	159	CH	4.026	-8.9	-12.8	-7.9				
3UIQ	2012	1.88	Cys	a	845	Phe	a	803	both	3.868	34.1	23.6	-10.5				
3UIQ	2012	1.88	Ser	a	565	dA	t	4	both	3.331	-7.5	-13.3	-5.8				
3UIQ	2012	1.88	Ser	a	783	His	a	804	both	3.517	-0.6	-17.4	-19.5	6.3	-31.1	37.4	
3UIQ	2012	1.88	Ser	a	119	His	a	131	both	3.187	-4.4	-16.9	-21	16.9	-38.1	55	
3VAJ	2013	1.90	Ser	a	281	PHE	a	282	both	3.441	2.6	-9.9	-12.5				
3ZVM	2011	2.00	Cys	a	446	Phe	a	494	CH	4.292	-10.1	-12.8	-2.7				
4B21	2013	1.45	Cys	a	31	Trp	a	200	both	3.752	-4.1	-16.4	-12.3				
4B21	2013	1.45	Cys	a	31	Tyr	a	7	both	3.767	-3.6	-14.1	-10.6				
4B22	2013	1.90	Cys	a	31	Tyr	a	7	both	3.708	-3.6	-13.9	-10.3				
4B23	2013	2.00	Cys	a	31	Tyr	a	200	both	3.656	-4	-16.3	-12.3				
4B23	2013	2.00	Cys	a	31	Tyr	a	7	both	3.779	-3.6	-13.9	-10.3				
4B9S	2013	1.73	Ser	a	785	Phe	a	781	both	3.538	2.4	-10.7	-13.1				
4B9V	2013	2.00	Ser	a	785	Phe	a	781	lp	3.392	1.5	-9.6	-11.1				
4DIH	2012	1.80	Cys	h	122	Tyr	h	208	CH	4.604	-5.8	-9.2	-4.8				
4DIH	2012	1.80	Ser	l	14i	Tyr	l	14j	both	4.195	1.6	-4.8	-7.4				
4DL4	2012	2.00	Cys	a	72	Phe	a	57	both	3.817	-2.1	-13.4	-11.3				
4DOC	2012	1.95	Cys	a	239	Phe	a	223	CH	3.604	-11	-14.9	-3.9				
4DQI	2012	1.69	Ser	d	785	Phe	d	781	both	3.760	1.5	-8	-9.5				
4DQI	2012	1.69	Ser	a	785	Phe	a	781	both	3.774	2	-11.3	-13.3				
4DS4	2012	1.68	Ser	a	785	Phe	a	781	both	3.719	2.2	-12.3	-14.5				
4DS4	2012	1.68	Ser	d	785	Phe	d	781	both	3.725	2	-9.7	-11.7				
4DTJ	2012	1.90	Cys	a	845	Phe	a	803	both	3.870	-2.7	-13.5	-10.8				
4DTJ	2012	1.90	Ser	a	783	His	a	804	both	3.514	0	-17.5	-19.2	5.7	-31.3	37	
4DTJ	2012	1.90	Ser	a	281	Tyr	a	277	CH	3.520	-6.3	-17.8	-11.5				
4E0D	2012	1.58	Ser	a	785	Phe	a	781	both	3.754	2.1	-10.3	-12.4				
4E9F	2012	1.79	Ser	a	544	Tyr	a	540	lp	3.729	2.1	-8.4	-6.9				
4ECQ	2012	1.50	Cys	a	72	Phe	a	57	both	3.743	-3.6	-15.3	-11.7				
4ED0	2012	1.65	Cys	a	72	Phe	a	57	both	3.821	-3.4	-15.2	-11.8				
4EJY	2013	2.00	Cys	B	225	Phe	B	121	CH	3.938	-7.2	-14	-6.8				
4F1H	2012	1.66	Cys	a	322	Phe	a	324	CH	3.573	-11.1	-13.1	-2				
4F1H	2012	1.66	Ser	b	225	Phe	b	224	both	2.939	3.1	-13	-16.1				
4F5N	2012	1.80	Cys	a	239	Phe	a	223	CH	3.500	-11.5	-15.1	-3.6				
4FF2	2013	2.00	Ser	b	280	Phe	b	281	both	3.731	2.6	-9.7	-12.3				
4FJ7	2013	1.90	Cys	a	845	Phe	a	803	both	3.948	-1.6	-11.8	-10.2				
4FJ7	2013	1.90	Ser	a	119	His	a	131	both	3.206	-6.1	-17.6	-21	17.2	-37	54.2	
4FJ7	2013	1.90	Ser	a	783	His	a	804	both	3.477	0.2	-17.9	-19.3	5.3	-31.9	37.2	

PDB ID	YEAR	Res.	Cys/Ser			Nucleotide/Amino Acid			Type	Closet		Energy			Energy-cationic		
			Res ID	Chain	Res #	Res ID	Chain	Res #		Contact Distance	Max	Min	Range	Max	Min	Range	
4FJ7	2013	1.90	Ser	a	281	Tyr	a	277	CH	3.529	-7	-18.1	-11.1				
4FJ9	2013	1.97	Cys	a	845	Phe	a	803	both	3.950	-3.8	-14.4	-10.6				
4FJ9	2013	1.97	Ser	a	119	His	a	131	both	3.265	-1.7	-18.5	-20.1	17.2	-37	54.2	
4FJ9	2013	1.97	Ser	a	783	His	a	804	both	3.575	0.4	-17	-18.7	5.7	-30.7	36.4	
4FJ9	2013	1.97	Ser	a	281	Tyr	a	277	CH	3.506	-6.8	-17.8	-11				
4FJJ	2013	1.99	Cys	a	845	Phe	a	803	both	3.944	-3.9	-14.8	-10.9				
4FJJ	2013	1.99	Ser	a	783	His	a	804	both	3.458	1.2	-17.5	-19.7	5.5	-32.4	37.9	
4FJJ	2013	1.99	Ser	a	119	His	a	131	both	3.359	-5.7	-17.2	-19.3	14.6	-33.5	48.1	
4FJJ	2013	1.99	Ser	a	281	Tyr	a	277	CH	3.425	-6.5	-18	-11.5				
4FJK	2013	2.00	Cys	a	845	Phe	a	803	both	3.931	-3.5	-14.1	-10.6				
4FJK	2013	2.00	Ser	a	783	His	a	804	both	3.320	-0.3	-18.6	-19.5	5.6	-33.5	39.1	
4FJK	2013	2.00	Ser	a	119	His	a	131	both	3.319	-6.1	-16.3	-19.2	16.3	-34.2	50.5	
4FJK	2013	2.00	Ser	a	281	Tyr	a	277	CH	3.579	-7.3	-16.7	-9.4				
4FK2	2013	1.98	Cys	a	845	Phe	a	803	both	3.783	-2.8	-14.1	-11.3				
4FK2	2013	1.98	Ser	a	783	His	a	804	both	3.426	0.3	-17.7	-19	5.5	-31.6	37.1	
4FPV	2012	1.73	Cys	a	239	dT	c	1	both	3.850	1.1	-9.8	-10.9				
4FPV	2012	1.73	Cys	b	322	Phe	b	324	CH	3.611	-10.4	-13.6	-3.2				
4FPV	2012	1.73	Cys	a	322	Phe	a	324	CH	3.649	-11.3	-14.1	-2.8				
4FPV	2012	1.73	Ser	b	225	Phe	b	224	both	3.074	1.5	-15.4	-16.9				
4G92	2012	1.80	Ser	c	77	His	c	80	both	4.323	-2.5	-10.8	-8.6	12.7	-12.9	25.6	
4GLX	2012	1.90	Cys	a	112	Phe	a	269	CH	4.440	-3	-4.3	-1.3				
4GLX	2012	1.90	Ser	a	254	Phe	a	223	CH	4.812	-6.1	-7.8	-1.7				
4HSB	2013	1.9	Cys	a	191	TRP	a	21	both	3.397	1.8	-12.5	-14.3				
4HSB	2013	1.9	Cys	a	31	TRP	a	200	both	3.713	-3.1	-15.7	-12.6				
4HSB	2013	1.9	Cys	a	31	Tyr	a	7	both	3.659	-3.1	-13.8	-10.8				
4IBU	2013	1.7	Cys	b	182	His	b	178	lp	2.956	6.5	-10.3	-8.3	-18.2	-24.5	6.3	
4IBU	2013	1.7	Cys	d	182	His	d	178	lp	3.422	-2.4	-15.1	-6.3	-22.1	-28.6	6.5	
4IBU	2013	1.7	Cys	c	182	His	c	178	lp	3.638	-1.9	-12.1	-8.3	-22.5	-27.3	4.8	
4IBU	2013	1.7	Ser	b	106	Tyr	b	107	both	3.552	0.8	-11.3	-9.9				
4IBU	2013	1.7	Cys	b	229	Trp	b	146	CH	3.830	-15.7	-23.8	-8.1				
4IBU	2013	1.7	Ser	d	106	Tyr	d	107	both	3.306	0.8	-13.4	-11.4				
4J9L	2013	1.9	Cys	a	72	Phe	a	57	both	3.763	-3.3	-14.2	-10.9				
4J9L	2013	1.9	Ser	a	288	His	a	289	lp	3.588	1	-11.9	-3	-8.3	-23.9	15.6	
4JRP	2013	2.0	Cys	a	51	Phe	a	84	CH	3.739	-8.3	-14.1	-5.8				
4JRP	2013	2.0	Ser	b	127	Trp	b	126	CH	4.246	-8.7	-13.9	-5.2				
4JWM	2013	2.0	Cys	a	239	Phe	a	223	CH	3.612	-10.9	-14.6	-3.7				
4K98	2013	1.9	Cys	a	419	His	a	422	both	3.674	-2.3	-17	-6.2	0.0	-28.7	28.7	
4K98	2013	1.9	Cys	a	459	Phe	a	455	both	3.496	-1.4	-10.1	-8.7				
4KLD	2013	1.9	Cys	a	239	Phe	a	223	CH	3.724	-10.7	-14.2	-3.5				
4L5R	2013	1.9	Ser	c	238	Phe	c	221	both	4.130	-1.5	-9.8	-8.3				
2XZF	2011	1.80															
3OQG	2011	1.8															
3OR3	2011	2.0															
3Q8P	2011	2.0															
3QZ7	2011	2.0															

PDB ID	YEAR	Res.	Cys/Ser			Nucleotide/Amino Acid			Type	Closet Contact Distance	Energy			Energy-cationic		
			Res ID	Chain	Res #	Res ID	Chain	Res #			Max	Min	Range	Max	Min	Range
3RAX	2011	1.89														
3RH4	2011	1.92														
3RTV	2012	1.90														
3S57	2012	1.60														
3SAR	2012	1.95														
3SPD	2011	1.91														
3T3F	2012	1.90														
3TED	2011	2.00														
3U6C	2012	1.80														
3U7F	2011	1.80														
3V6T	2012	1.85														
3V9W	2012	1.70														
3VK8	2012	2.00														
3VKE	2012	1.77														
3VOK	2012	2.00														
3VXV	2013	2.00														
3ZDA	2013	1.50														
3ZDB	2013	1.47														
3ZDC	2013	1.53														
3ZDD	2013	1.50														
4A75	2012	1.75														
4AIK	2012	1.85														
4BWJ	2013	1.55														
4C8L	2013	1.70														
4C8M	2013	1.57														
4C8N	2013	1.88														
4C8O	2013	1.75														
4DF8	2012	2.00														
4EA4	2012	2.00														
4ELU	2012	1.80														
4F4W	2013	1.90														
4FBT	2013	2.00														
4FF3	2013	2.00														
4G4O	2013	2.0														
4GZ1	2012	1.50														
4HC9	2012	1.60														
4IX7	2013	1.6														
4K1G	2013	1.9														
4LB5	2013	2.0														
4LJR	2013	1.8														
4M9V	2013	1.0														
4MDE	2013	1.8														
4NDH	2013	1.9														

Cartesian Coordinates of MP2/6-31G(d) optimized monomers.

Cytosine

N	-1.1543457	0.0000000	-1.0189133
C	-0.0139117	0.0000000	-1.7560353
H	-0.1272167	0.0000000	-2.8360553
C	1.1916173	0.0000000	-1.1291663
H	2.1199753	0.0000000	-1.6876203
C	1.1537363	0.0000000	0.3086437
N	2.3257473	0.0000000	0.9946257
H	2.2819673	0.0000000	2.0040787
H	3.2218923	0.0000000	0.5346417
N	0.0467983	0.0000000	1.0285047
C	-1.1807517	0.0000000	0.4004987
O	-2.2682307	0.0000000	0.9686247
H	-2.0680117	0.0000000	-1.4593653

Thymine

N	0.07951237	0.00000000	-1.66480782
C	-1.15138563	0.00000000	-1.04033782
H	-2.00858163	0.00000000	-1.70774182
C	-1.28017063	0.00000000	0.30790218
C	-2.59536563	0.00000000	1.02178618
H	-3.42614263	0.00000000	0.31108918
H	-2.68216463	0.87905500	1.66644018
H	-2.68216463	-0.87905500	1.66644018
C	-0.06560763	0.00000000	1.12248918
O	-0.04194263	0.00000000	2.35240018
N	1.12688237	0.00000000	0.38354318
H	1.98718637	0.00000000	0.92599118
C	1.29131437	0.00000000	-0.99306382
O	2.37852137	0.00000000	-1.55705982
H	0.15166237	0.00000000	-2.67527082

Guanine

N	-2.18566412	0.00000000	0.70037686
C	-1.84512912	0.00000000	2.03313286
H	-2.59376312	0.00000000	2.81476986
N	-0.53659812	0.00000000	2.22998686
C	-0.01248812	0.00000000	0.95511886
C	1.36268288	0.00000000	0.52803386
O	2.40747388	0.00000000	1.16851486
N	1.40931288	0.00000000	-0.90234814
H	2.35902288	0.00000000	-1.26567514
C	0.33848788	0.00000000	-1.76442214
N	0.62098288	0.00000000	-3.09840914
H	1.55983788	0.00000000	-3.46173614
H	-0.15748712	0.00000000	-3.73937014
N	-0.91566012	0.00000000	-1.37320414
C	-1.01560712	0.00000000	-0.01289614
H	-3.11577712	0.00000000	0.29853386

Adenine

N	-2.145943	0.141083	0.000000
C	-1.901685	1.491125	0.000000
H	-2.706825	2.215287	0.000000
N	-0.610998	1.795581	0.000000
C	0.004874	0.559615	0.000000
C	1.364021	0.184843	0.000000
N	2.357787	1.102692	0.000000
H	3.316882	0.788506	0.000000
H	2.139972	2.087842	0.000000
N	1.677448	-1.121094	0.000000
C	0.667637	-2.020724	0.000000
H	0.979653	-3.062975	0.000000
N	-0.653903	-1.805562	0.000000
C	-0.920157	-0.488588	0.000000
H	-3.047377	-0.321672	0.000000

His⁺

C	0.215178	1.172663	0.000000
N	1.122098	0.127966	0.000000
C	-1.025605	0.607946	0.000000
H	2.132363	0.223587	0.000000
C	0.473409	-1.040153	0.000000
N	-0.833261	-0.762500	0.000000
H	-2.008616	1.052698	0.000000
H	0.920684	-2.023006	0.000000
H	-1.569004	-1.461408	0.000000
H	0.525071	2.206147	0.000000

His

C	1.1377116	0.3293768	0.0000000
N	0.0177486	1.1278098	0.0000000
C	0.6535356	-0.9600682	0.0000000
H	0.0072346	2.1397748	0.0000000
C	-1.0743074	0.3069578	0.0000000
N	-0.7235474	-0.9705632	0.0000000
H	1.2205446	-1.8810042	0.0000000
H	-2.0873264	0.6867338	0.0000000
H	2.1374496	0.7378438	0.0000000

Phe

C	-1.209663000	-0.698399000	0.000000000
C	-1.209663000	0.698399000	0.000000000
C	0.000000000	1.396798000	0.000000000
C	1.209663000	0.698399000	0.000000000
C	1.209663000	-0.698399000	0.000000000
C	0.000000000	-1.396798000	0.000000000
H	2.151407000	1.242116000	0.000000000
H	0.000000000	2.484231000	0.000000000
H	-2.151408000	1.242116000	0.000000000
H	-2.151408000	-1.242116000	0.000000000
H	0.000000000	-2.484231000	0.000000000
H	2.151407000	-1.242116000	0.000000000

Trp

C	-1.6361404	-1.1368351	0.0000000
C	-2.3823514	0.0185269	0.0000000
C	-0.2598594	-0.7474761	0.0000000
H	-3.4560784	0.1568389	0.0000000
N	-1.5357974	1.1078809	0.0000000
C	-0.2284364	0.6749959	0.0000000
C	0.9604676	-1.4502321	0.0000000
H	-1.8312804	2.0748479	0.0000000
C	0.9680946	1.4037829	0.0000000
C	2.1485316	-0.7333971	0.0000000
H	0.9698186	-2.5386311	0.0000000
H	0.9728736	2.4921269	0.0000000
C	2.1528086	0.6793459	0.0000000
H	3.0971616	-1.2649741	0.0000000
H	3.1023076	1.2094869	0.0000000
H	-2.0310124	-2.1445671	0.0000000

Tyr

C	-0.8019391	-0.4419713	0.0000000
C	-0.7734581	0.9556997	0.0000000
C	0.4518949	1.6177797	0.0000000
C	1.6501029	0.8971467	0.0000000
C	1.6117509	-0.4970653	0.0000000
C	0.3888809	-1.1723533	0.0000000
H	2.5359099	-1.0701493	0.0000000
H	2.6034389	1.4183027	0.0000000
H	0.4706249	2.7049567	0.0000000
H	-1.7153311	1.4970317	0.0000000
H	0.3646009	-2.2614373	0.0000000
O	-2.0417591	-1.0372913	0.0000000
H	-1.9178861	-2.0028823	0.0000000

Cys

S	0.66100000	-0.08700000	0.00000000
H	0.89800000	1.23300000	0.00000000
C	-1.15100000	0.01900000	0.00000000
H	-1.52400000	-1.00600000	-0.00100000
H	-1.52500000	0.52200000	0.89300000
H	-1.52500000	0.52300000	-0.89200000

Ser

O	0.75100000	0.12300000	0.00000000
H	1.13200000	-0.77000000	0.00000000
C	-0.66600000	-0.02000000	0.00000000
H	-1.07500000	0.99100000	0.00000000
H	-1.03200000	-0.54300000	-0.89200000
H	-1.03200000	-0.54300000	0.89200000