

CRYST1	7.057	7.035	16.961	90.02	90.03	119.59	P 1	0	
ATOM	1 S	UNK A	1	3.613	2.023	10.833	1.00	0.00	S
ATOM	2 O	UNK A	1	3.597	2.016	12.322	1.00	0.00	O
ATOM	3 O	UNK A	1	4.965	1.249	8.041	1.00	0.00	O
ATOM	4 H	UNK A	1	5.722	0.807	7.579	1.00	0.00	H
ATOM	5 O	UNK A	1	3.649	3.602	8.124	1.00	0.00	O
ATOM	6 H	UNK A	1	3.640	4.336	7.465	1.00	0.00	H
ATOM	7 O	UNK A	1	2.328	1.279	7.895	1.00	0.00	O
ATOM	8 H	UNK A	1	1.514	0.840	7.533	1.00	0.00	H
ATOM	9 Al	UNK A	1	-1.666	3.016	8.499	1.00	0.00	Al
ATOM	10 O	UNK A	1	-1.139	3.385	6.680	1.00	0.00	O
ATOM	11 Al	UNK A	1	3.653	-0.004	8.481	1.00	0.00	Al
ATOM	12 O	UNK A	1	0.105	5.486	6.645	1.00	0.00	O
ATOM	13 Al	UNK A	1	1.864	3.085	8.506	1.00	0.00	Al
ATOM	14 O	UNK A	1	1.328	3.363	6.648	1.00	0.00	O
ATOM	15 O	UNK A	1	2.392	2.730	10.330	1.00	0.00	O
ATOM	16 O	UNK A	1	3.603	0.611	10.324	1.00	0.00	O
ATOM	17 O	UNK A	1	4.858	2.715	10.358	1.00	0.00	O
ATOM	18 S	UNK A	1	0.092	4.062	6.159	1.00	0.00	S
ATOM	19 O	UNK A	1	0.072	4.039	4.673	1.00	0.00	O
ATOM	20 O	UNK A	1	1.467	4.856	8.902	1.00	0.00	O
ATOM	21 H	UNK A	1	2.165	5.249	9.478	1.00	0.00	H
ATOM	22 O	UNK A	1	0.110	2.506	8.918	1.00	0.00	O
ATOM	23 H	UNK A	1	0.100	1.670	9.450	1.00	0.00	H
ATOM	24 O	UNK A	1	-1.165	4.828	9.105	1.00	0.00	O
ATOM	25 H	UNK A	1	-1.987	5.277	9.433	1.00	0.00	H
ATOM	26 S	UNK A	1	3.582	6.094	5.187	1.00	0.00	S
ATOM	27 O	UNK A	1	-3.448	6.107	6.667	1.00	0.00	O
ATOM	28 O	UNK A	1	-2.106	5.287	2.405	1.00	0.00	O
ATOM	29 H	UNK A	1	-1.359	4.852	1.921	1.00	0.00	H
ATOM	30 O	UNK A	1	0.035	1.439	2.225	1.00	0.00	O
ATOM	31 H	UNK A	1	0.017	2.374	1.894	1.00	0.00	H
ATOM	32 O	UNK A	1	2.247	5.270	2.453	1.00	0.00	O
ATOM	33 H	UNK A	1	1.603	4.907	1.797	1.00	0.00	H
ATOM	34 Al	UNK A	1	1.811	0.931	2.845	1.00	0.00	Al
ATOM	35 O	UNK A	1	2.325	1.291	1.003	1.00	0.00	O
ATOM	36 Al	UNK A	1	3.613	4.043	2.852	1.00	0.00	Al
ATOM	37 O	UNK A	1	3.550	3.408	1.023	1.00	0.00	O
ATOM	38 Al	UNK A	1	5.294	0.946	2.813	1.00	0.00	Al
ATOM	39 O	UNK A	1	4.773	1.271	0.979	1.00	0.00	O
ATOM	40 O	UNK A	1	5.813	0.693	4.693	1.00	0.00	O
ATOM	41 O	UNK A	1	3.587	4.685	4.689	1.00	0.00	O
ATOM	42 O	UNK A	1	1.198	0.706	4.657	1.00	0.00	O
ATOM	43 S	UNK A	1	3.550	2.003	0.503	1.00	0.00	S
ATOM	44 O	UNK A	1	3.536	2.016	15.977	1.00	0.00	O
ATOM	45 O	UNK A	1	4.940	2.752	3.253	1.00	0.00	O
ATOM	46 H	UNK A	1	-1.432	3.144	3.849	1.00	0.00	H
ATOM	47 O	UNK A	1	3.552	0.426	3.287	1.00	0.00	O
ATOM	48 H	UNK A	1	0.091	5.671	3.757	1.00	0.00	H
ATOM	49 O	UNK A	1	2.282	2.717	3.440	1.00	0.00	O
ATOM	50 H	UNK A	1	1.502	3.206	3.821	1.00	0.00	H
ATOM	51 Al	UNK A	1	-1.729	5.126	14.110	1.00	0.00	Al
ATOM	52 O	UNK A	1	-1.217	4.858	15.990	1.00	0.00	O

ATOM	53	Al	UNK	A	1	0.066	2.098	14.158	1.00	0.00	Al
ATOM	54	O	UNK	A	1	0.019	2.726	15.985	1.00	0.00	O
ATOM	55	Al	UNK	A	1	1.837	5.109	14.121	1.00	0.00	Al
ATOM	56	O	UNK	A	1	1.226	4.856	15.945	1.00	0.00	O
ATOM	57	S	UNK	A	1	0.004	0.080	11.789	1.00	0.00	S
ATOM	58	O	UNK	A	1	0.006	0.075	10.309	1.00	0.00	O
ATOM	59	O	UNK	A	1	1.382	0.808	14.562	1.00	0.00	O
ATOM	60	H	UNK	A	1	2.113	1.224	15.088	1.00	0.00	H
ATOM	61	O	UNK	A	1	3.583	4.596	14.563	1.00	0.00	O
ATOM	62	H	UNK	A	1	3.580	3.763	15.095	1.00	0.00	H
ATOM	63	O	UNK	A	1	5.795	0.782	14.733	1.00	0.00	O
ATOM	64	H	UNK	A	1	5.007	1.251	15.122	1.00	0.00	H
ATOM	65	S	UNK	A	1	0.028	4.141	16.481	1.00	0.00	S
ATOM	66	O	UNK	A	1	0.053	4.145	1.000	1.00	0.00	O
ATOM	67	O	UNK	A	1	1.401	3.335	13.698	1.00	0.00	O
ATOM	68	H	UNK	A	1	2.119	2.906	13.170	1.00	0.00	H
ATOM	69	O	UNK	A	1	0.062	5.603	13.539	1.00	0.00	O
ATOM	70	H	UNK	A	1	3.525	0.402	13.143	1.00	0.00	H
ATOM	71	O	UNK	A	1	-1.301	3.326	13.711	1.00	0.00	O
ATOM	72	H	UNK	A	1	5.019	2.905	13.200	1.00	0.00	H
ATOM	73	O	UNK	A	1	2.360	5.520	12.309	1.00	0.00	O
ATOM	74	O	UNK	A	1	0.015	1.512	12.288	1.00	0.00	O
ATOM	75	O	UNK	A	1	-2.251	5.482	12.287	1.00	0.00	O
ATOM	76	H	UNK	A	1	-0.116	3.194	11.520	1.00	0.00	H
ATOM	77	H	UNK	A	1	-0.485	4.453	10.446	1.00	0.00	H
ATOM	78	H	UNK	A	1	-0.003	4.733	12.122	1.00	0.00	H
ATOM	79	O	UNK	A	1	0.059	4.144	11.287	1.00	0.00	O
ATOM	80	H	UNK	A	1	4.286	1.405	5.445	1.00	0.00	H
ATOM	81	H	UNK	A	1	3.015	1.701	6.497	1.00	0.00	H
ATOM	82	H	UNK	A	1	2.984	2.239	4.822	1.00	0.00	H
ATOM	83	O	UNK	A	1	3.540	2.025	5.667	1.00	0.00	O
ATOM	84	H	UNK	A	1	-0.493	0.383	16.124	1.00	0.00	H
ATOM	85	H	UNK	A	1	0.877	-0.342	16.738	1.00	0.00	H
ATOM	86	H	UNK	A	1	0.010	0.642	17.794	1.00	0.00	H
ATOM	87	O	UNK	A	1	-0.023	0.019	16.966	1.00	0.00	O
CONNECT	1	2	15	16	17						
CONNECT	2	68	70	72	1						
CONNECT	3	11	4								
CONNECT	4	3									
CONNECT	5	13	6								
CONNECT	6	5									
CONNECT	7	13	11	81	8						
CONNECT	8	7									
CONNECT	9	24	22	10							
CONNECT	10	18	9								
CONNECT	11	16	7	3							
CONNECT	12	18									
CONNECT	13	20	15	22	14	7	5				
CONNECT	14	18	81	13							
CONNECT	15	13	1								
CONNECT	16	11	1								
CONNECT	17	1									
CONNECT	18	19	14	12	10						
CONNECT	19	46	48	50	18						

CONNECT	20	21	13			
CONNECT	21	20				
CONNECT	22	23	13	9		
CONNECT	23	58	22			
CONNECT	24	25	77	9		
CONNECT	25	24				
CONNECT	26	41				
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CONNECT	28	29				
CONNECT	29	66	28			
CONNECT	30	31	34			
CONNECT	31	66	30			
CONNECT	32	33	36			
CONNECT	33	66	32			
CONNECT	34	42	47	49	35	30
CONNECT	35	43	34			
CONNECT	36	41	37	45	49	32
CONNECT	37	43	36			
CONNECT	38	40	39	45	47	
CONNECT	39	43	38			
CONNECT	40	80	38			
CONNECT	41	36	26			
CONNECT	42	82	34			
CONNECT	43	39	37	35		
CONNECT	44	62	64	60		
CONNECT	45	38	36			
CONNECT	46	19				
CONNECT	47	80	82	38	34	
CONNECT	48	19				
CONNECT	49	82	50	36	34	
CONNECT	50	49	19			
CONNECT	51	52	69	71	75	
CONNECT	52	65	51			
CONNECT	53	67	71	54	59	74
CONNECT	54	65	84	53		
CONNECT	55	56	61	67	69	73
CONNECT	56	65	55			
CONNECT	57	58	74			
CONNECT	58	57	23			
CONNECT	59	84	60	53		
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CONNECT	61	62	55			
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CONNECT	65	56	54	52		
CONNECT	66	33	31	29		
CONNECT	67	68	55	53		
CONNECT	68	67	2			
CONNECT	69	78	55	51		
CONNECT	70	2				
CONNECT	71	76	78	53	51	
CONNECT	72	2				
CONNECT	73	78	55			

CONNECT 74 76 57 53
CONNECT 75 78 51
CONNECT 76 79 74 71
CONNECT 77 79 24
CONNECT 78 79 75 73 71 69
CONNECT 79 78 77 76
CONNECT 80 83 47 40
CONNECT 81 83 14 7
CONNECT 82 83 49 47 42
CONNECT 83 82 81 80
CONNECT 84 87 59 54
CONNECT 85 87
CONNECT 86 87
CONNECT 87 86 85 84