Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:57 PM GMT

PDB ID	:	4W2F
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors	:	Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochek, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on	:	2014-09-12
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	NOT EXECUTED
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5967	10397	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			
11	CK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
13	CM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2871	Total	C	N	O	P	0	0	0
			61844	27523	11572	19878	2871			
25	DA	2800	Total	C	N	O	P	0	0	0
			60314	26840	11284	19390	2800			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
26	DB	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1429	916	256	253	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O	0	0	0
			873	550	174	149			
38	DS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
45	DZ	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CR	1	Total	Mg	0	0
			1	1		
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	906	Total	Mg	0	0
			906	906		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	AB	2	Total	Mg	0	0
			2	2		
56	DF	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CV	1	Total Mg 1 1	0	0
56	B8	3	Total Mg 3 3	0	0
56	BE	12	Total Mg 12 12	0	0
56	AW	4	Total Mg 4 4	0	0
56	DU	4	Total Mg 4 4	0	0
56	B1	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	AN	1	Total Mg 1 1	0	0
56	BP	6	Total Mg 6 6	0	0
56	AX	13	Total Mg 13 13	0	0
56	DR	1	Total Mg 1 1	0	0
56	BI	1	Total Mg 1 1	0	0
56	CA	201	Total Mg 201 201	0	0
56	B5	4	Total Mg 4 4	0	0
56	BB	30	Total Mg 30 30	0	0
56	BT	2	Total Mg 2 2	0	0
56	D8	2	Total Mg 2 2	0	0
56	AE	2	Total Mg 2 2	0	0
56	DB	21	Total Mg 21 21	0	0
56	CF	2	Total Mg 2 2	0	0
56	DT	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B9	1	Total Mg 1 1	0	0
56	BF	15	Total Mg 15 15	0	0
56	BX	6	Total Mg 6 6	0	0
56	B2	2	Total Mg 2 2	0	0
56	AA	233	Total Mg 233 233	0	0
56	BQ	7	Total Mg 7 7	0	0
56	CQ	2	Total Mg 2 2	0	0
56	D0	1	Total Mg 1 1	0	0
56	AR	1	Total Mg 1 1	0	0
56	DV	2	Total Mg 2 2	0	0
56	B6	2	Total Mg 2 2	0	0
56	AM	1	Total Mg 1 1	0	0
56	BU	10	Total Mg 10 10	0	0
56	AD	1	Total Mg 1 1	0	0
56	BN	4	Total Mg 4 4	0	0
56	CT	1	Total Mg 1 1	0	0
56	CG	1	Total Mg 1 1	0	0
56	BG	6	Total Mg 6 6	0	0
56	BY	3	Total Mg 3 3	0	0
56	DE	7	Total Mg 7 7	0	0
56	B3	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CJ	2	Total Mg 2 2	0	0
56	BR	3	Total Mg 3 3	0	0
56	CP	1	Total Mg 1 1	0	0
56	DA	673	Total Mg 673 673	0	0
56	DP	1	Total Mg 1 1	0	0
56	DW	3	Total Mg 3 3	0	0
56	D5	2	Total Mg 2 2	0	0
56	B7	3	Total Mg 3 3	0	0
56	AL	1	Total Mg 1 1	0	0
56	BV	5	Total Mg 5 5	0	0
56	DO	1	Total Mg 1 1	0	0
56	BO	5	Total Mg 5 5	0	0
56	CX	6	Total Mg 6 6	0	0
56	D1	1	Total Mg 1 1	0	0
56	DX	1	Total Mg 1 1	0	0
56	AH	1	Total Mg 1 1	0	0
56	BZ	3	Total Mg 3 3	0	0
56	DZ	1	Total Mg 1 1	0	0
56	BS	3	Total Mg 3 3	0	0
56	CW	4	Total Mg 4 4	0	0
56	DG	1	Total Mg 1 1	0	0

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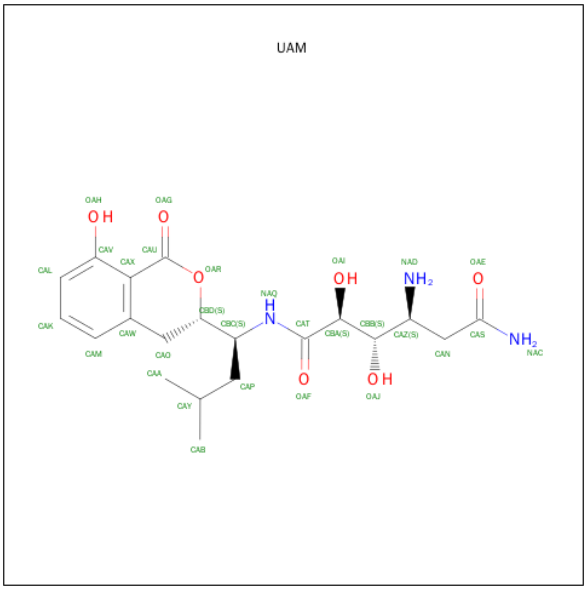
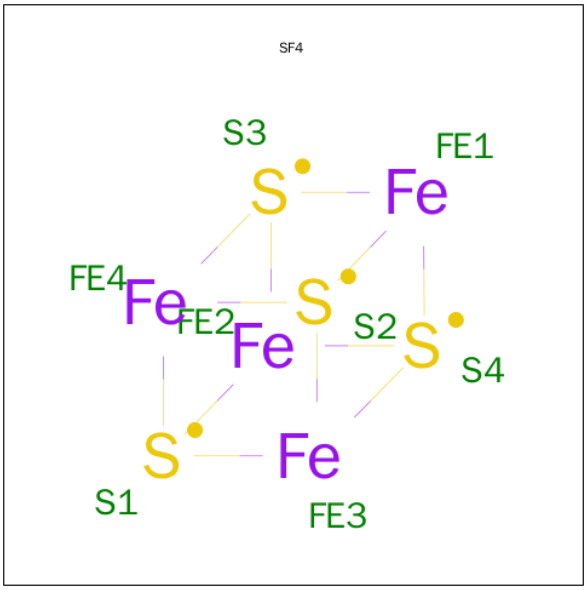
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CD	2	Total Mg 2 2	0	0
56	BD	13	Total Mg 13 13	0	0
56	AT	1	Total Mg 1 1	0	0
56	CL	2	Total Mg 2 2	0	0
56	B0	7	Total Mg 7 7	0	0
56	CE	1	Total Mg 1 1	0	0
56	BW	5	Total Mg 5 5	0	0
56	AY	2	Total Mg 2 2	0	0
56	DD	6	Total Mg 6 6	0	0
56	CK	1	Total Mg 1 1	0	0
56	AF	1	Total Mg 1 1	0	0
56	BH	1	Total Mg 1 1	0	0

- Molecule 57 is Amicoumacin A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C N O 30 20 3 7	0	0
57	CA	1	Total C N O 30 20 3 7	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AD	1	Total Fe S 8 4 4	0	0
58	CD	1	Total Fe S 8 4 4	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	B5	1	Total Zn 1 1	0	0
59	B4	1	Total Zn 1 1	0	0
59	CN	1	Total Zn 1 1	0	0
59	BY	1	Total Zn 1 1	0	0
59	B9	1	Total Zn 1 1	0	0
59	DY	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	D5	1	Total Zn 1 1	0	0
59	D4	1	Total Zn 1 1	0	0
59	AN	1	Total Zn 1 1	0	0
59	D6	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0
59	B6	1	Total Zn 1 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AX	1	Total K 1 1	0	0
60	CX	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	264	Total O 264 264	0	0
61	AB	1	Total O 1 1	0	0
61	AE	2	Total O 2 2	0	0
61	AJ	1	Total O 1 1	0	0
61	AL	4	Total O 4 4	0	0
61	AM	1	Total O 1 1	0	0
61	AQ	1	Total O 1 1	0	0
61	AV	4	Total O 4 4	0	0
61	AW	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AX	11	Total O 11 11	0	0
61	AY	1	Total O 1 1	0	0
61	BA	1486	Total O 1486 1486	0	0
61	BB	43	Total O 43 43	0	0
61	BD	19	Total O 19 19	0	0
61	BE	20	Total O 20 20	0	0
61	BF	14	Total O 14 14	0	0
61	BG	5	Total O 5 5	0	0
61	BH	1	Total O 1 1	0	0
61	BI	2	Total O 2 2	0	0
61	BN	2	Total O 2 2	0	0
61	BO	7	Total O 7 7	0	0
61	BP	19	Total O 19 19	0	0
61	BQ	5	Total O 5 5	0	0
61	BR	5	Total O 5 5	0	0
61	BS	5	Total O 5 5	0	0
61	BT	5	Total O 5 5	0	0
61	BU	8	Total O 8 8	0	0
61	BV	6	Total O 6 6	0	0
61	BW	1	Total O 1 1	0	0
61	BX	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BY	3	Total O 3 3	0	0
61	BZ	1	Total O 1 1	0	0
61	B0	8	Total O 8 8	0	0
61	B1	3	Total O 3 3	0	0
61	B2	4	Total O 4 4	0	0
61	B3	3	Total O 3 3	0	0
61	B4	1	Total O 1 1	0	0
61	B5	4	Total O 4 4	0	0
61	B6	1	Total O 1 1	0	0
61	B7	4	Total O 4 4	0	0
61	B8	8	Total O 8 8	0	0
61	CA	204	Total O 204 204	0	0
61	CD	1	Total O 1 1	0	0
61	CG	1	Total O 1 1	0	0
61	CI	1	Total O 1 1	0	0
61	CJ	4	Total O 4 4	0	0
61	CL	4	Total O 4 4	0	0
61	CO	1	Total O 1 1	0	0
61	CP	1	Total O 1 1	0	0
61	CR	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	CW	2	Total O 2 2	0	0
61	CX	6	Total O 6 6	0	0
61	DA	1039	Total O 1039 1039	0	0
61	DB	10	Total O 10 10	0	0
61	DD	17	Total O 17 17	0	0
61	DE	8	Total O 8 8	0	0
61	DF	6	Total O 6 6	0	0
61	DI	2	Total O 2 2	0	0
61	DN	1	Total O 1 1	0	0
61	DO	3	Total O 3 3	0	0
61	DP	12	Total O 12 12	0	0
61	DQ	1	Total O 1 1	0	0
61	DR	3	Total O 3 3	0	0
61	DT	3	Total O 3 3	0	0
61	DU	1	Total O 1 1	0	0
61	DV	1	Total O 1 1	0	0
61	DW	2	Total O 2 2	0	0
61	DX	2	Total O 2 2	0	0
61	DY	1	Total O 1 1	0	0
61	DZ	2	Total O 2 2	0	0
61	D0	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	D1	4	Total O 4 4	0	0
61	D2	1	Total O 1 1	0	0
61	D3	1	Total O 1 1	0	0
61	D5	2	Total O 2 2	0	0
61	D7	5	Total O 5 5	0	0
61	D8	5	Total O 5 5	0	0
61	D9	1	Total O 1 1	0	0

MolProbity and EDS were not executed - this setion will therefore be empty.

3 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40	Depositor
% Data completeness (in resolution range)	99.7 (256.12-2.40)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298643	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

MolProbity was not executed - this section will therefore be empty.

4.2 Too-close contacts

MolProbity was not executed - this section will therefore be empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity was not executed - this section will therefore be empty.

4.3.2 Protein sidechains

MolProbity was not executed - this section will therefore be empty.

4.3.3 RNA

MolProbity was not executed - this section will therefore be empty.

4.4 Non-standard residues in protein, DNA, RNA chains

validation-pack and Mogul were not executed - this section will therefore be empty.

4.5 Carbohydrates

validation-pack and Mogul were not executed - this section will therefore be empty.

4.6 Ligand geometry

validation-pack and Mogul were not executed - this section will therefore be empty.

4.7 Other polymers

validation-pack and Mogul were not executed - this section will therefore be empty.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

5.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

5.4 Ligands

EDS was not executed - this section will therefore be empty.

5.5 Other polymers

EDS was not executed - this section will therefore be empty.