



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 10:35 PM BST

PDB ID : 5FDV
Title : Crystal structure of the Pyrrhocoricin antimicrobial peptide bound to the
Thermus thermophilus 70S ribosome
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian,
M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-12-16
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

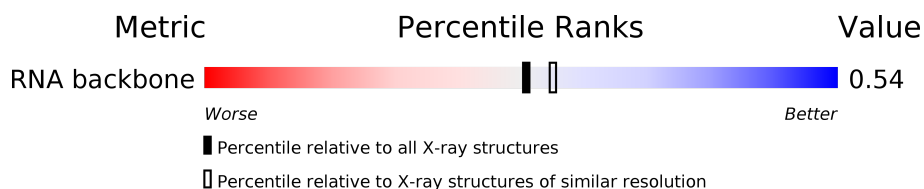
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
RNA backbone	3102	1227 (3.10-2.50)

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 293583 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61862	27535	11569	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61751	27486	11547	19852	2866			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			
33	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
34	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
35	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
36	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
37	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
38	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
39	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
40	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
41	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			
43	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
44	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
45	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
46	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
47	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
48	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
49	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
50	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
51	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
52	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 53 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
53	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 54 is a protein called Pyrrhocoricin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	16	Total	C	N	O	0	0	0
			120	79	20	21			
54	2y	16	Total	C	N	O	0	0	0
			120	79	20	21			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2E	4	Total	Mg	0	0
			4	4		
55	17	2	Total	Mg	0	0
			2	2		
55	2d	3	Total	Mg	0	0
			3	3		
55	1N	4	Total	Mg	0	0
			4	4		
55	20	5	Total	Mg	0	0
			5	5		
55	18	3	Total	Mg	0	0
			3	3		
55	1o	1	Total	Mg	0	0
			1	1		
55	2W	1	Total	Mg	0	0
			1	1		
55	1Y	1	Total	Mg	0	0
			1	1		
55	13	1	Total	Mg	0	0
			1	1		
55	1f	1	Total	Mg	0	0
			1	1		
55	2h	2	Total	Mg	0	0
			2	2		
55	1P	2	Total	Mg	0	0
			2	2		
55	2B	18	Total	Mg	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2a	197	Total 197	Mg 197	0	0
55	1k	1	Total 1	Mg 1	0	0
55	1E	5	Total 5	Mg 5	0	0
55	1b	1	Total 1	Mg 1	0	0
55	2l	2	Total 2	Mg 2	0	0
55	2F	9	Total 9	Mg 9	0	0
55	28	2	Total 2	Mg 2	0	0
55	2e	2	Total 2	Mg 2	0	0
55	1W	2	Total 2	Mg 2	0	0
55	1A	945	Total 945	Mg 945	0	0
55	1t	1	Total 1	Mg 1	0	0
55	2P	2	Total 2	Mg 2	0	0
55	1X	1	Total 1	Mg 1	0	0
55	1y	1	Total 1	Mg 1	0	0
55	25	3	Total 3	Mg 3	0	0
55	2b	1	Total 1	Mg 1	0	0
55	1D	14	Total 14	Mg 14	0	0
55	2N	1	Total 1	Mg 1	0	0
55	1e	1	Total 1	Mg 1	0	0
55	2G	3	Total 3	Mg 3	0	0
55	2f	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1V	1	Total 1	Mg 1	0	0
55	2X	3	Total 3	Mg 3	0	0
55	1a	226	Total 226	Mg 226	0	0
55	2Q	5	Total 5	Mg 5	0	0
55	15	4	Total 4	Mg 4	0	0
55	1R	3	Total 3	Mg 3	0	0
55	2U	2	Total 2	Mg 2	0	0
55	1G	3	Total 3	Mg 3	0	0
55	11	3	Total 3	Mg 3	0	0
55	1d	5	Total 5	Mg 5	0	0
55	2n	1	Total 1	Mg 1	0	0
55	1H	2	Total 2	Mg 2	0	0
55	21	2	Total 2	Mg 2	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2R	2	Total 2	Mg 2	0	0
55	2D	10	Total 10	Mg 10	0	0
55	2q	1	Total 1	Mg 1	0	0
55	1U	3	Total 3	Mg 3	0	0
55	27	2	Total 2	Mg 2	0	0
55	19	2	Total 2	Mg 2	0	0
55	1l	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2V	3	Total 3	Mg 3	0	0
55	1F	12	Total 12	Mg 12	0	0
55	2H	1	Total 1	Mg 1	0	0
55	10	7	Total 7	Mg 7	0	0
55	1g	1	Total 1	Mg 1	0	0
55	2o	1	Total 1	Mg 1	0	0
55	1Q	4	Total 4	Mg 4	0	0
55	2A	837	Total 837	Mg 837	0	0
55	1h	2	Total 2	Mg 2	0	0
55	1B	26	Total 26	Mg 26	0	0
55	2S	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

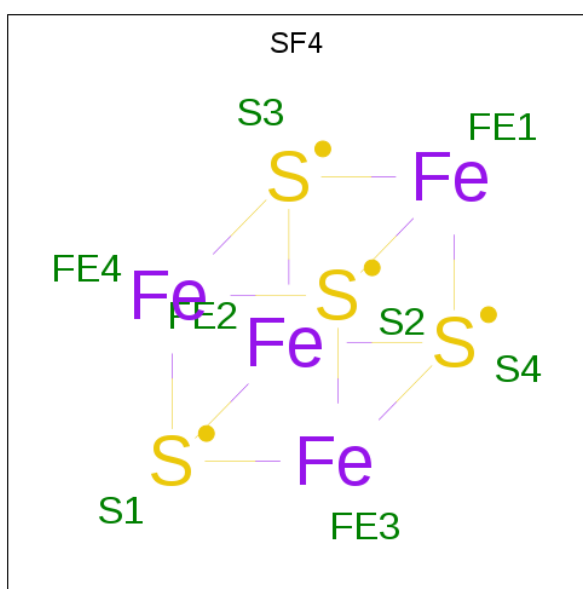
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Zn 1	0	0
56	14	1	Total 1	Zn 1	0	0
56	1n	1	Total 1	Zn 1	0	0
56	15	1	Total 1	Zn 1	0	0
56	29	1	Total 1	Zn 1	0	0
56	19	1	Total 1	Zn 1	0	0
56	26	1	Total 1	Zn 1	0	0
56	25	1	Total 1	Zn 1	0	0

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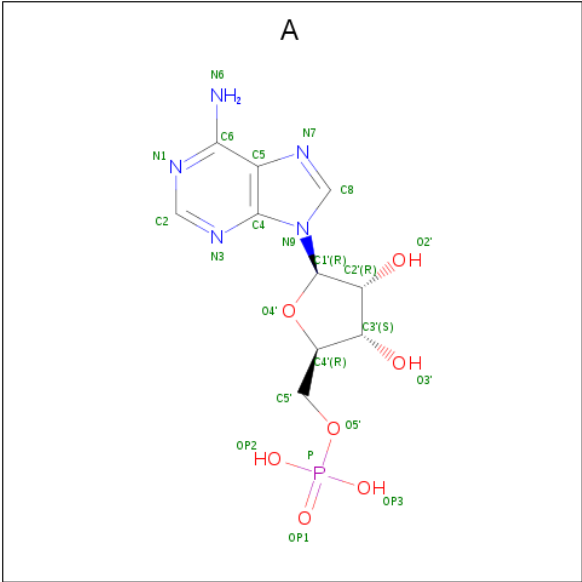
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	24	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1d	1	Total	Fe	S	0	0
			8	4	4		
57	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total P 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	43	Total O 43 43	0	0
59	1D	16	Total O 16 16	0	0
59	1E	17	Total O 17 17	0	0
59	1F	9	Total O 9 9	0	0
59	1G	2	Total O 2 2	0	0
59	1H	3	Total O 3 3	0	0
59	1N	8	Total O 8 8	0	0
59	1P	13	Total O 13 13	0	0
59	1Q	7	Total O 7 7	0	0
59	1R	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1T	5	Total 5	O 5	0	0
59	1U	5	Total 5	O 5	0	0
59	1V	3	Total 3	O 3	0	0
59	1W	2	Total 2	O 2	0	0
59	1X	4	Total 4	O 4	0	0
59	1Y	4	Total 4	O 4	0	0
59	10	5	Total 5	O 5	0	0
59	11	3	Total 3	O 3	0	0
59	13	1	Total 1	O 1	0	0
59	15	2	Total 2	O 2	0	0
59	16	2	Total 2	O 2	0	0
59	17	2	Total 2	O 2	0	0
59	18	9	Total 9	O 9	0	0
59	19	2	Total 2	O 2	0	0
59	1a	395	Total 395	O 395	0	0
59	1d	10	Total 10	O 10	0	0
59	1e	2	Total 2	O 2	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1m	2	Total 2	O 2	0	0
59	1n	1	Total 1	O 1	0	0
59	1p	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1t	1	Total 1	O 1	0	0
59	1y	2	Total 2	O 2	0	0
59	2A	1667	Total 1667	O 1667	0	0
59	2B	35	Total 35	O 35	0	0
59	2D	14	Total 14	O 14	0	0
59	2E	16	Total 16	O 16	0	0
59	2F	11	Total 11	O 11	0	0
59	2G	2	Total 2	O 2	0	0
59	2H	2	Total 2	O 2	0	0
59	2N	2	Total 2	O 2	0	0
59	2P	11	Total 11	O 11	0	0
59	2Q	4	Total 4	O 4	0	0
59	2R	4	Total 4	O 4	0	0
59	2T	2	Total 2	O 2	0	0
59	2U	2	Total 2	O 2	0	0
59	2V	2	Total 2	O 2	0	0
59	2W	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2X	5	Total 5	O 5	0	0
59	2Y	3	Total 3	O 3	0	0
59	20	7	Total 7	O 7	0	0
59	21	2	Total 2	O 2	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	26	2	Total 2	O 2	0	0
59	27	1	Total 1	O 1	0	0
59	28	6	Total 6	O 6	0	0
59	2a	387	Total 387	O 387	0	0
59	2c	1	Total 1	O 1	0	0
59	2d	6	Total 6	O 6	0	0
59	2e	4	Total 4	O 4	0	0
59	2f	1	Total 1	O 1	0	0
59	2h	1	Total 1	O 1	0	0
59	2j	1	Total 1	O 1	0	0
59	2l	3	Total 3	O 3	0	0
59	2m	2	Total 2	O 2	0	0
59	2o	1	Total 1	O 1	0	0
59	2t	1	Total 1	O 1	0	0
59	2y	1	Total 1	O 1	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.94Å 450.10Å 622.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (49.81-2.80)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.240	Depositor
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.044	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	293583	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, OMG, OMU, MA6, G7M, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, 4OC, M2G, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	1.57	577/69022 (0.8%)	2.06	3825/107739 (3.6%)
1	2A	1.21	119/68893 (0.2%)	1.72	1783/107533 (1.7%)
2	1B	1.15	4/2879 (0.1%)	1.89	110/4490 (2.4%)
2	2B	1.02	1/2874 (0.0%)	1.58	50/4482 (1.1%)
3	1D	0.93	0/2181	1.00	4/2940 (0.1%)
3	2D	0.78	0/2186	0.87	1/2944 (0.0%)
4	1E	0.99	0/1592	1.02	3/2149 (0.1%)
4	2E	0.79	0/1592	0.91	2/2149 (0.1%)
5	1F	0.95	0/1619	0.96	4/2193 (0.2%)
5	2F	0.73	0/1615	0.85	0/2188
6	1G	0.70	0/1451	0.86	0/1961
6	2G	0.78	1/1449 (0.1%)	0.86	0/1957
7	1H	0.80	0/1356	0.89	0/1834
7	2H	0.77	0/1350	0.85	0/1826
8	1I	0.77	2/1109 (0.2%)	0.92	2/1512 (0.1%)
8	2I	0.67	0/1091	0.87	2/1490 (0.1%)
9	1N	0.93	1/1148 (0.1%)	0.97	3/1547 (0.2%)
9	2N	0.64	0/1144	0.83	0/1543
10	1O	1.02	0/943	1.00	2/1269 (0.2%)
10	2O	0.81	0/943	0.86	1/1269 (0.1%)
11	1P	0.89	0/1152	0.96	2/1533 (0.1%)
11	2P	0.68	0/1152	0.83	0/1533
12	1Q	0.94	0/1143	0.94	0/1527
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.94	0/982	1.08	7/1312 (0.5%)
13	2R	0.70	0/982	0.90	1/1312 (0.1%)
14	1S	0.79	1/887 (0.1%)	0.98	2/1180 (0.2%)
14	2S	0.68	0/880	0.85	0/1172
15	1T	0.88	1/1105 (0.1%)	1.06	4/1477 (0.3%)
15	2T	0.73	0/1097	0.91	2/1468 (0.1%)
16	1U	1.08	2/977 (0.2%)	1.05	7/1301 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.73	0/977	0.83	0/1301
17	1V	0.94	0/786	0.98	2/1053 (0.2%)
17	2V	0.67	0/782	0.84	0/1049
18	1W	1.04	0/897	1.02	4/1205 (0.3%)
18	2W	0.83	0/897	0.84	1/1205 (0.1%)
19	1X	0.95	0/764	0.96	1/1025 (0.1%)
19	2X	0.76	0/764	0.86	2/1025 (0.2%)
20	1Y	0.86	0/823	0.96	1/1099 (0.1%)
20	2Y	0.79	0/823	0.92	0/1100
21	1Z	0.73	0/1620	0.83	1/2200 (0.0%)
21	2Z	0.70	0/1590	0.84	1/2162 (0.0%)
22	10	0.88	0/616	0.94	0/821
22	20	0.68	0/616	0.86	0/821
23	11	1.01	1/761 (0.1%)	0.96	1/1013 (0.1%)
23	21	0.79	0/766	0.92	2/1018 (0.2%)
24	12	0.87	0/590	0.94	0/781
24	22	0.77	0/594	0.81	0/785
25	13	0.92	0/474	0.94	0/635
25	23	0.62	0/469	0.80	1/630 (0.2%)
26	14	0.89	0/559	0.89	0/754
26	24	1.06	0/549	0.97	0/741
27	15	1.08	3/473 (0.6%)	1.07	6/639 (0.9%)
27	25	0.83	0/469	0.97	2/635 (0.3%)
28	16	0.98	2/460 (0.4%)	1.04	1/613 (0.2%)
28	26	0.68	0/456	0.80	0/608
29	17	1.08	0/426	1.08	1/561 (0.2%)
29	27	0.81	0/426	0.88	0/561
30	18	0.96	1/525 (0.2%)	0.95	2/691 (0.3%)
30	28	0.72	0/525	0.79	0/691
31	19	0.96	1/310 (0.3%)	1.09	2/407 (0.5%)
31	29	0.70	0/310	0.79	0/407
32	1a	1.14	55/35795 (0.2%)	1.70	881/55864 (1.6%)
32	2a	1.10	48/35890 (0.1%)	1.65	737/56012 (1.3%)
33	1x	0.66	0/776	0.79	0/1048
33	2x	0.72	0/761	0.79	0/1030
34	1b	0.77	0/1876	0.93	3/2533 (0.1%)
34	2b	0.78	0/1860	0.89	0/2518
35	1c	0.72	0/1582	0.80	0/2137
35	2c	0.81	0/1566	0.81	0/2119
36	1d	0.71	0/1695	0.84	0/2274
36	2d	0.70	0/1698	0.85	0/2277
37	1e	0.66	0/1149	0.88	0/1548
37	2e	0.68	0/1149	0.87	0/1548

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1f	0.72	0/827	0.81	0/1120
38	2f	0.70	0/829	0.84	0/1123
39	1g	0.71	1/1254 (0.1%)	0.77	0/1683
39	2g	0.73	0/1248	0.76	0/1676
40	1h	0.67	0/1118	0.83	0/1506
40	2h	0.61	0/1108	0.83	0/1494
41	1i	0.77	0/1005	0.82	0/1351
41	2i	0.84	0/985	0.88	0/1329
42	1j	0.79	0/732	0.84	0/993
42	2j	0.81	0/723	0.76	0/984
43	1k	0.73	0/849	0.85	0/1150
43	2k	0.67	0/848	0.86	1/1149 (0.1%)
44	1l	0.69	0/937	0.83	0/1260
44	2l	0.68	0/937	0.95	3/1260 (0.2%)
45	1m	0.68	0/924	0.83	0/1242
45	2m	0.76	0/905	0.82	0/1217
46	1n	0.74	0/501	0.93	2/664 (0.3%)
46	2n	0.75	0/501	0.82	1/664 (0.2%)
47	1o	0.72	0/739	0.86	0/985
47	2o	0.65	0/739	0.79	0/985
48	1p	0.69	0/697	0.85	0/939
48	2p	0.70	0/693	0.90	0/935
49	1q	0.73	0/836	0.86	0/1117
49	2q	0.67	0/836	0.85	1/1117 (0.1%)
50	1r	0.70	0/560	0.87	1/746 (0.1%)
50	2r	0.70	0/560	0.81	0/746
51	1s	0.73	0/663	0.81	0/895
51	2s	0.81	0/660	0.79	1/893 (0.1%)
52	1t	0.68	0/734	0.86	0/969
52	2t	0.64	0/736	0.85	0/976
53	1u	0.69	0/203	0.83	0/266
53	2u	0.73	0/203	0.87	0/266
54	1y	0.83	0/125	0.82	0/173
54	2y	0.69	0/125	0.74	0/173
All	All	1.17	821/310171 (0.3%)	1.62	7479/463547 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
30	18	0	1
44	2l	0	1
All	All	0	4

The worst 5 of 821 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2026	G	N7-C5	-11.28	1.32	1.39
1	1A	2040	G	P-OP2	-11.24	1.29	1.49
1	1A	354	A	N9-C4	-10.67	1.31	1.37
1	1A	1814	A	N3-C4	-10.29	1.28	1.34
1	2A	1046	A	N9-C4	9.81	1.43	1.37

The worst 5 of 7479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-33.37	70.65	110.70
32	1a	1520	G	O5'-P-OP1	-31.38	73.04	110.70
32	1a	1520	G	O5'-P-OP2	26.23	142.18	110.70
32	1a	1520	G	OP1-P-OP2	-24.67	82.60	119.60
32	2a	1208	C	OP1-P-OP2	-24.65	82.62	119.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	18	13	ARG	Peptide
19	1X	93	GLU	Peptide
19	2X	93	GLU	Peptide
44	2l	86	ARG	Peptide

4.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	396 (13%)	0
1	2A	2856/2915 (97%)	414 (14%)	0
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	5 (4%)	0
32	1a	1494/1521 (98%)	319 (21%)	0
32	2a	1498/1521 (98%)	305 (20%)	0
All	All	8948/9112 (98%)	1444 (16%)	0

5 of 1444 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G
1	1A	70	A

There are no RNA pucker outliers to report.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2435 ligands modelled in this entry, 1 is modelled with single atom and 2432 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.56

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.