



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2023 – 12:30 AM EDT

PDB ID : 6OF6
Title : Crystal structure of tRNA^{Ala}(GGC) bound to cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-03-28
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
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) : 2.35.1

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 3.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 298675 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	Total 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1500	Total 32249	C 14354	N 5984	O 10412	P 1499	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	XB	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	XC	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	Total 1674	C 1050	N 333	O 284	S 7	0	0	0
4	XD	208	Total 1674	C 1050	N 333	O 284	S 7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	XI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	XJ	99	801	504	157	139	1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	QK	119	885	549	168	165	3	0	0	0
11	XK	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	QL	125	975	614	196	164	1	0	0	0
12	XL	125	975	614	196	164	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	121	964	597	199	166	2	0	0	0
13	XM	121	964	597	199	166	2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	QO	88	734	459	147	126	2	0	0	0
15	XO	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-site tRNA^{Ala}(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1627	725	296	530	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			416	186	85	126	19			
24	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 25 is a RNA chain called A-site tRNA^{Ala}(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
27	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
28	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
29	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
30	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
32	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
33	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
34	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
36	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
37	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 38 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
38	YD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
39	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 40 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
40	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 41 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	YH	170	1307	829	245	232	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	RI	146	1136	726	201	208	1	0	0	0
43	YI	146	1136	726	201	208	1	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	RN	138	1104	712	206	182	4	0	0	0
44	YN	138	1104	712	206	182	4	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	RO	122	933	588	171	170	4	0	0	0
45	YO	122	933	588	171	170	4	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	RP	150	1145	712	232	198	3	0	0	0
46	YP	150	1145	712	232	198	3	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	RQ	141	1122	715	212	188	7	0	0	0
47	YQ	141	1122	715	212	188	7	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
48	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 49 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
49	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
50	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 51 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
51	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 52 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
52	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 53 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
53	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 54 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
54	YX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 55 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
55	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 56 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
56	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	124	Total	Mg	0	0
			124	124		
57	QD	1	Total	Mg	0	0
			1	1		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QK	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QL	1	Total Mg 1 1	0	0
57	QM	1	Total Mg 1 1	0	0
57	QV	6	Total Mg 6 6	0	0
57	QX	1	Total Mg 1 1	0	0
57	R0	1	Total Mg 1 1	0	0
57	R1	1	Total Mg 1 1	0	0
57	R5	1	Total Mg 1 1	0	0
57	R8	1	Total Mg 1 1	0	0
57	R9	1	Total Mg 1 1	0	0
57	RA	378	Total Mg 378 378	0	0
57	RB	4	Total Mg 4 4	0	0
57	RD	2	Total Mg 2 2	0	0
57	RE	8	Total Mg 8 8	0	0
57	RF	2	Total Mg 2 2	0	0
57	RG	1	Total Mg 1 1	0	0
57	RI	1	Total Mg 1 1	0	0
57	RP	3	Total Mg 3 3	0	0
57	RR	2	Total Mg 2 2	0	0
57	RT	2	Total Mg 2 2	0	0
57	XA	123	Total Mg 123 123	0	0
57	XB	2	Total Mg 2 2	0	0

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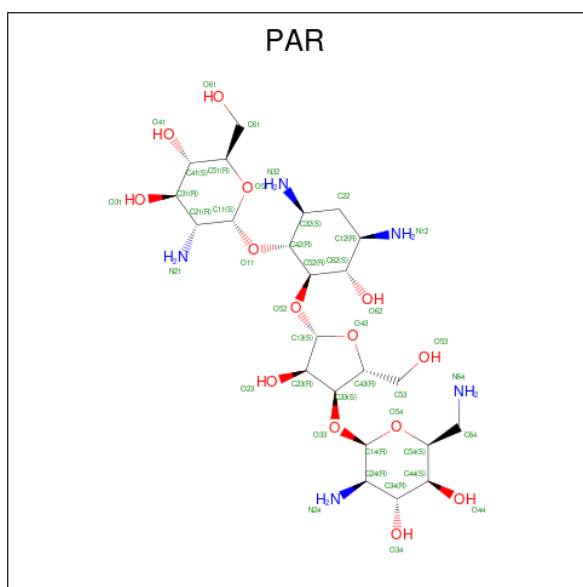
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	XD	1	Total Mg 1 1	0	0
57	XF	1	Total Mg 1 1	0	0
57	XJ	1	Total Mg 1 1	0	0
57	XK	1	Total Mg 1 1	0	0
57	XL	2	Total Mg 2 2	0	0
57	XM	1	Total Mg 1 1	0	0
57	XV	7	Total Mg 7 7	0	0
57	XX	1	Total Mg 1 1	0	0
57	Y0	3	Total Mg 3 3	0	0
57	Y2	3	Total Mg 3 3	0	0
57	Y3	1	Total Mg 1 1	0	0
57	Y4	2	Total Mg 2 2	0	0
57	Y5	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	Y8	3	Total Mg 3 3	0	0
57	YA	457	Total Mg 457 457	0	0
57	YB	8	Total Mg 8 8	0	0
57	YD	4	Total Mg 4 4	0	0
57	YE	6	Total Mg 6 6	0	0
57	YF	5	Total Mg 5 5	0	0
57	YG	2	Total Mg 2 2	0	0

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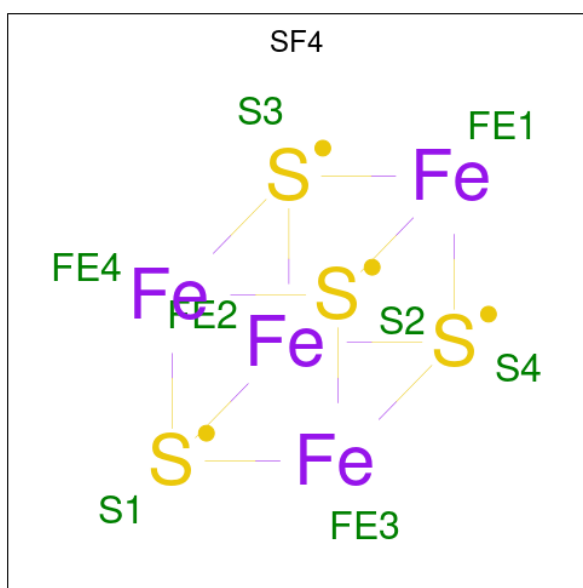
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YH	5	Total 5	Mg 5	0	0
57	YI	1	Total 1	Mg 1	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	7	Total 7	Mg 7	0	0
57	YQ	4	Total 4	Mg 4	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YT	2	Total 2	Mg 2	0	0
57	YU	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YW	1	Total 1	Mg 1	0	0
57	YX	2	Total 2	Mg 2	0	0
57	YY	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
58	QA	1	42	23	5	14	0	0
58	XA	1	42	23	5	14	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

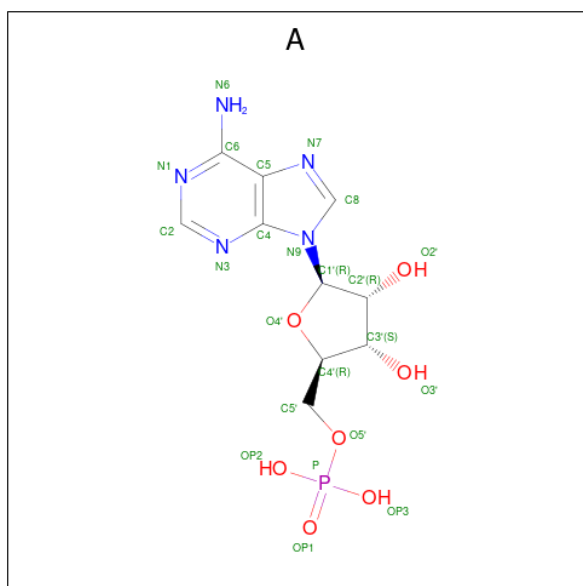


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe S		
59	QD	1	8	4 4	0	0
59	XD	1	8	4 4	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	QN	1	Total	Zn	0	0
			1	1		
60	XN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	QY	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	QA	1	Total	O	0	0
			1	1		
62	QX	1	Total	O	0	0
			1	1		

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

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	211.26Å 452.33Å 626.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20	Depositor
% Data completeness (in resolution range)	91.2 (44.53-3.20)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.232	Depositor
Wilson B-factor (Å ²)	73.8	Xtrriage
Anisotropy	0.170	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	298675	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1222 ligands modelled in this entry, 1217 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	A	QY	101	-	18,24,25	0.65	0	18,35,38	0.86	1 (5%)
58	PAR	QA	1711	-	45,45,45	0.54	0	64,67,67	0.95	2 (3%)
59	SF4	QD	501	4	0,12,12	-	-	-	-	-
58	PAR	XA	1717	-	45,45,45	0.53	0	64,67,67	0.86	1 (1%)
59	SF4	XD	501	4	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	A	QY	101	-	-	0/3/25/26	0/3/3/3
58	PAR	QA	1711	-	-	3/18/94/94	0/4/4/4
59	SF4	QD	501	4	-	-	0/6/5/5
58	PAR	XA	1717	-	-	2/18/94/94	0/4/4/4
59	SF4	XD	501	4	-	-	0/6/5/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	QA	1711	PAR	C13-O52-C52	-2.82	110.99	117.96
58	XA	1717	PAR	C13-O52-C52	-2.71	111.26	117.96
58	QA	1711	PAR	O52-C13-C23	2.56	113.28	107.96
61	QY	101	A	C5-C6-N6	2.03	123.43	120.35

There are no chirality outliers.

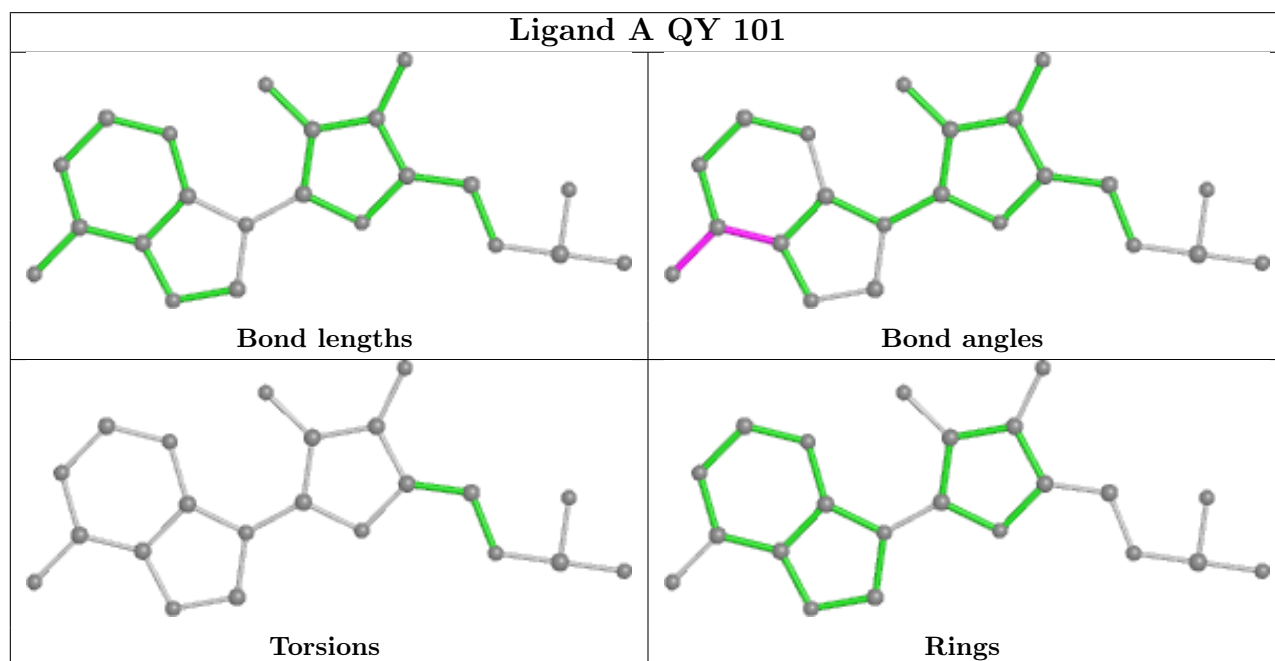
All (5) torsion outliers are listed below:

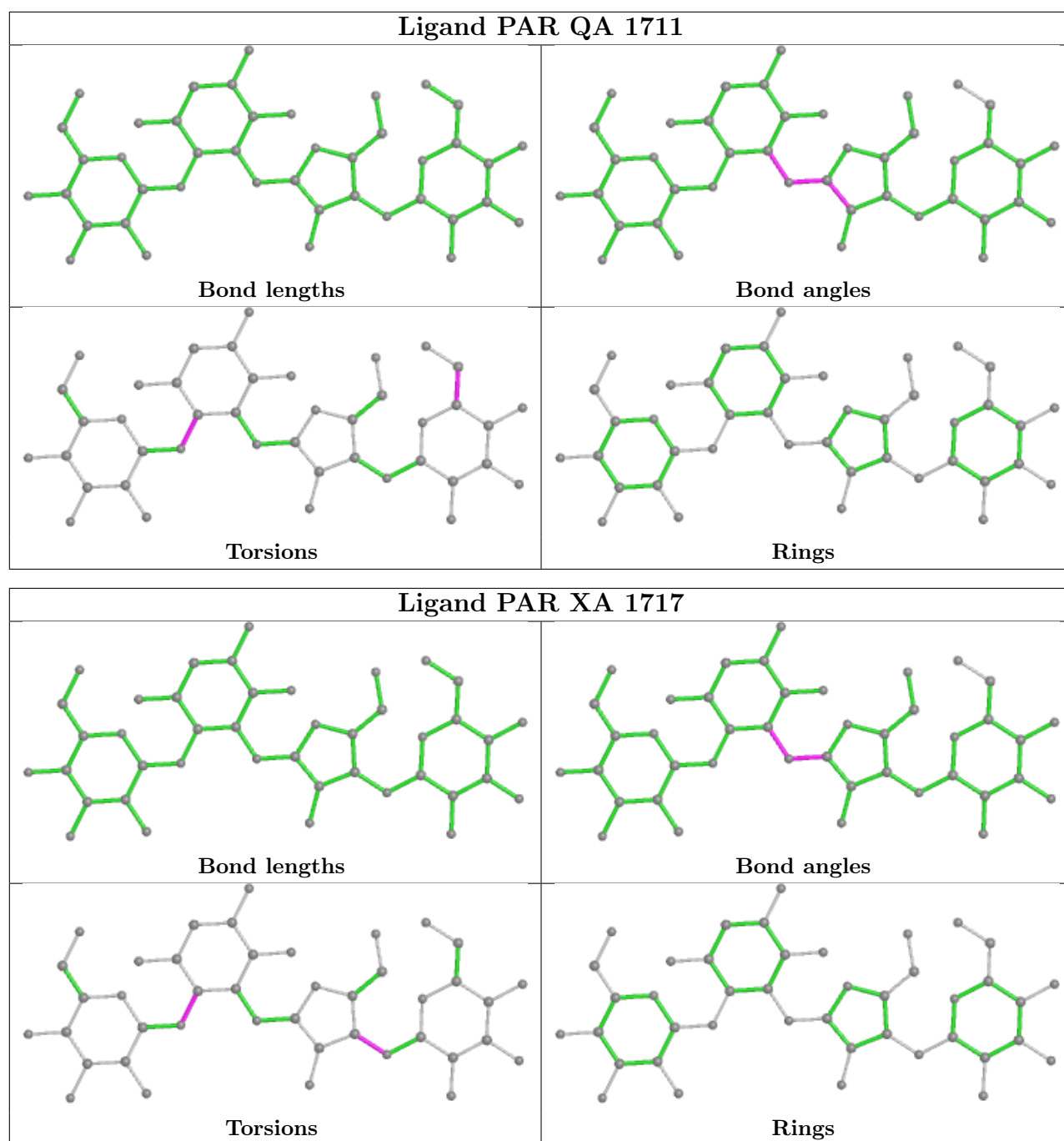
Mol	Chain	Res	Type	Atoms
58	QA	1711	PAR	O54-C54-C64-N64
58	XA	1717	PAR	C23-C33-O33-C14
58	QA	1711	PAR	C52-C42-O11-C11
58	XA	1717	PAR	C52-C42-O11-C11
58	QA	1711	PAR	C44-C54-C64-N64

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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.