



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 05:04 AM UTC

PDB ID : 4V5Q / pdb_00004v5q
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a near- cognate codon on the 70S ribosome
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
Resolution : 3.10 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

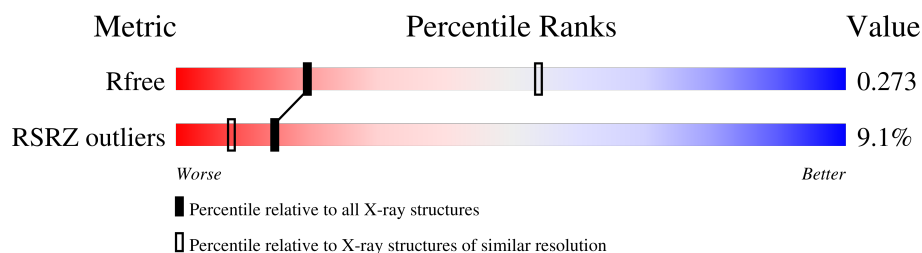
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307194 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
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	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
			1612	1016	314	281	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	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
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	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	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	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	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	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	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	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	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
12	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			
13	CM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	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
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	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	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	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	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
19	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	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	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			
23	CX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
27	D1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
29	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			
30	D4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	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	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
37	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
38	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
39	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
41	DF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
42	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
43	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	391	130	130			
44	DJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			
45	DK	140	Total	C	N	O	0	0	0
			700	420	140	140			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
46	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
50	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O		0	0	0
			770	486	154	130				
51	DS	98	Total	C	N	O		0	0	0
			770	486	154	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
52	DT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
54	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			
56	DX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
57	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

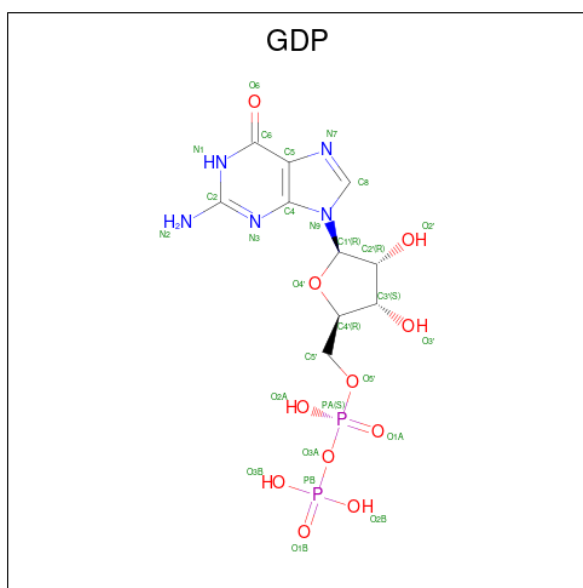
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			
58	DZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

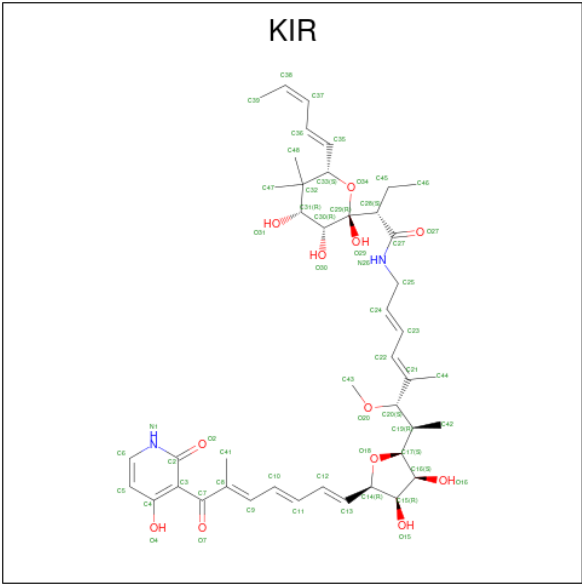
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 61 is KIRROMYCIN (CCD ID: KIR) (formula: C₄₃H₆₀N₂O₁₂).



3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 98.7 (50.00-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.238 , 0.275 0.237 , 0.273	Depositor DCC
R_{free} test set	69565 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	307194	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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](#)

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

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	$\# Z > 2$
24	4SU	CY	8	24	18,21,22	2.12	3 (16%)	25,30,33	1.85	4 (16%)
24	PSU	CY	55	24	18,21,22	1.14	2 (11%)	21,30,33	1.88	4 (19%)
24	OMC	CY	32	24	19,22,23	0.69	0	25,31,34	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	7MG	AY	46	24	23,26,27	2.61	3 (13%)	27,39,42	1.70	3 (11%)
24	5MU	AY	54	24	19,22,23	0.25	0	27,32,35	0.40	0
24	MIA	CY	37	24	28,31,32	1.29	2 (7%)	38,44,47	0.86	1 (2%)
24	H2U	AY	16	24	18,21,22	0.83	0	19,30,33	1.57	3 (15%)
24	OMC	AY	32	24	19,22,23	0.64	0	25,31,34	0.43	0
24	7MG	CY	46	24	23,26,27	2.54	3 (13%)	27,39,42	1.72	3 (11%)
24	H2U	CY	16	24	18,21,22	0.92	0	19,30,33	1.60	3 (15%)
24	H2U	AY	20	24	18,21,22	0.89	1 (5%)	19,30,33	1.75	4 (21%)
24	H2U	AY	17	24	18,21,22	0.80	0	19,30,33	1.60	4 (21%)
24	MIA	AY	37	24	28,31,32	1.12	2 (7%)	38,44,47	1.19	1 (2%)
24	5MU	CY	54	24	19,22,23	0.27	0	27,32,35	0.42	0
24	H2U	CY	17	24	18,21,22	0.90	0	19,30,33	1.66	4 (21%)
24	H2U	CY	20	24	18,21,22	0.88	0	19,30,33	1.80	5 (26%)
24	PSU	AY	55	24	18,21,22	1.02	2 (11%)	21,30,33	1.94	5 (23%)
24	4SU	AY	8	24	18,21,22	2.00	3 (16%)	25,30,33	1.83	5 (20%)

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
24	4SU	CY	8	24	-	0/7/25/26	0/2/2/2
24	PSU	CY	55	24	-	2/7/25/26	0/2/2/2
24	OMC	CY	32	24	-	0/9/27/28	0/2/2/2
24	7MG	AY	46	24	-	4/7/37/38	0/3/3/3
24	5MU	AY	54	24	-	2/7/25/26	0/2/2/2
24	MIA	CY	37	24	-	1/15/33/34	0/3/3/3
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2
24	7MG	CY	46	24	-	4/7/37/38	0/3/3/3
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	H2U	AY	20	24	-	4/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	MIA	AY	37	24	-	1/15/33/34	0/3/3/3
24	5MU	CY	54	24	-	2/7/25/26	0/2/2/2
24	H2U	CY	17	24	-	5/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	CY	20	24	-	4/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/7/25/26	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-11.70	1.38	1.45
24	CY	46	7MG	C8-N9	-11.42	1.38	1.45
24	CY	8	4SU	C4-N3	5.92	1.43	1.37
24	CY	37	MIA	C2-S10	5.49	1.80	1.75
24	AY	8	4SU	C4-N3	5.42	1.43	1.37

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	46	7MG	N9-C8-N7	7.00	113.28	103.37
24	AY	46	7MG	N9-C8-N7	6.90	113.14	103.37
24	AY	37	MIA	C11-S10-C2	6.39	107.05	102.25
24	AY	55	PSU	N1-C2-N3	4.94	120.38	115.17
24	CY	55	PSU	N1-C2-N3	4.64	120.06	115.17

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C2
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C1'-N1-C6
24	AY	37	MIA	N6-C12-C13-C14
24	AY	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	KIR	AZ	502	-	56,59,59	3.78	23 (41%)	60,84,84	1.79	11 (18%)
61	KIR	CZ	502	-	56,59,59	3.85	23 (41%)	60,84,84	1.78	12 (20%)
60	GDP	AZ	501	-	29,30,30	0.96	2 (6%)	45,47,47	1.73	9 (20%)
60	GDP	CZ	501	-	29,30,30	0.95	1 (3%)	45,47,47	1.74	10 (22%)

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	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	AZ	501	-	-	2/16/32/32	0/3/3/3
60	GDP	CZ	501	-	-	2/16/32/32	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-15.26	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.53	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.44	1.18	1.42
61	AZ	502	KIR	O30-C30	-12.24	1.18	1.42
61	AZ	502	KIR	O34-C33	-8.66	1.30	1.44

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C2-N3-C4	5.33	121.48	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C2-N3-C4	5.13	121.14	112.30
61	CZ	502	KIR	C6-N1-C2	-4.95	121.61	124.54
61	AZ	502	KIR	C6-N1-C2	-4.73	121.74	124.54
61	AZ	502	KIR	O29-C29-O34	-4.64	102.49	110.15

There are no chirality outliers.

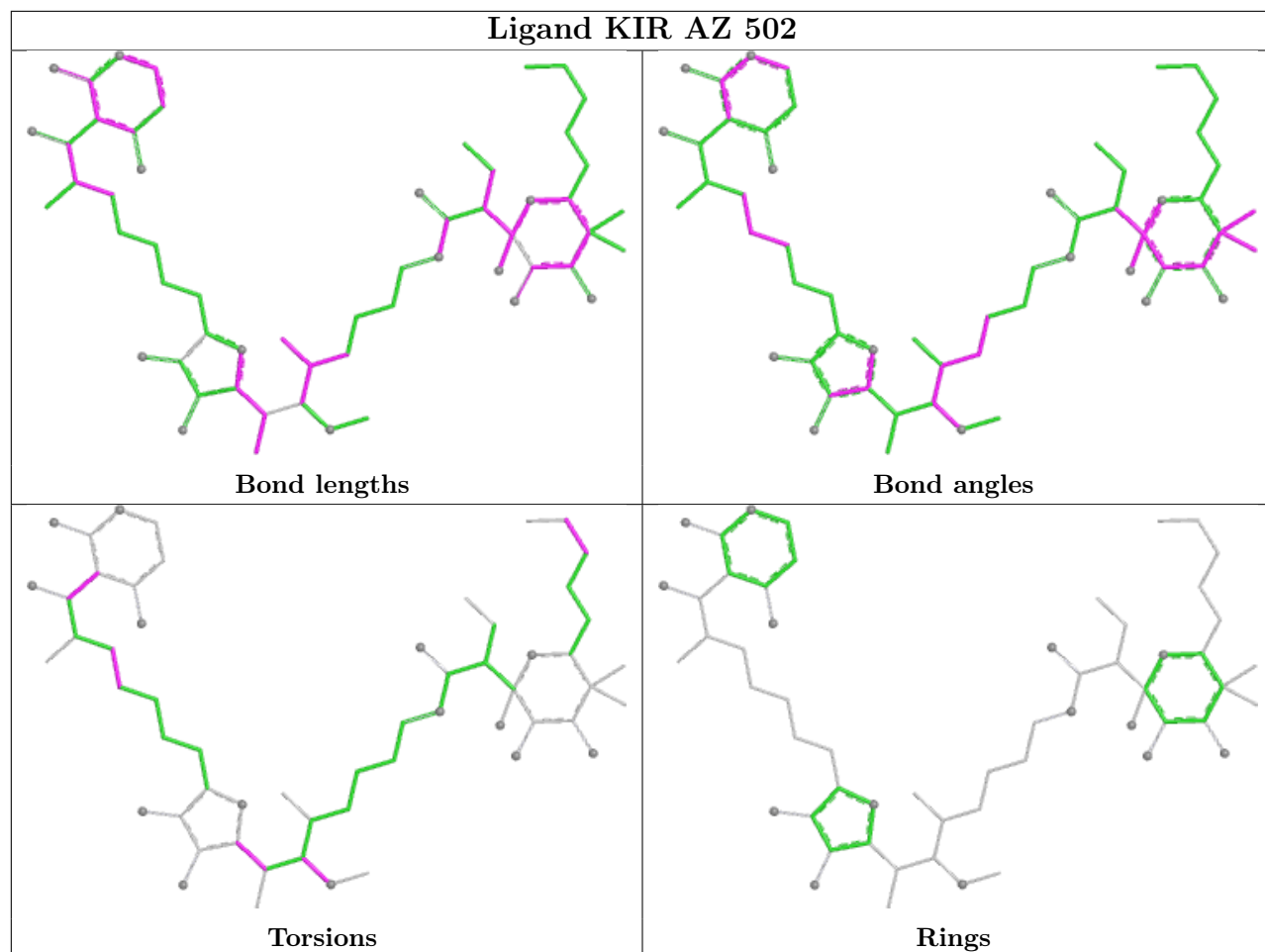
5 of 20 torsion outliers are listed below:

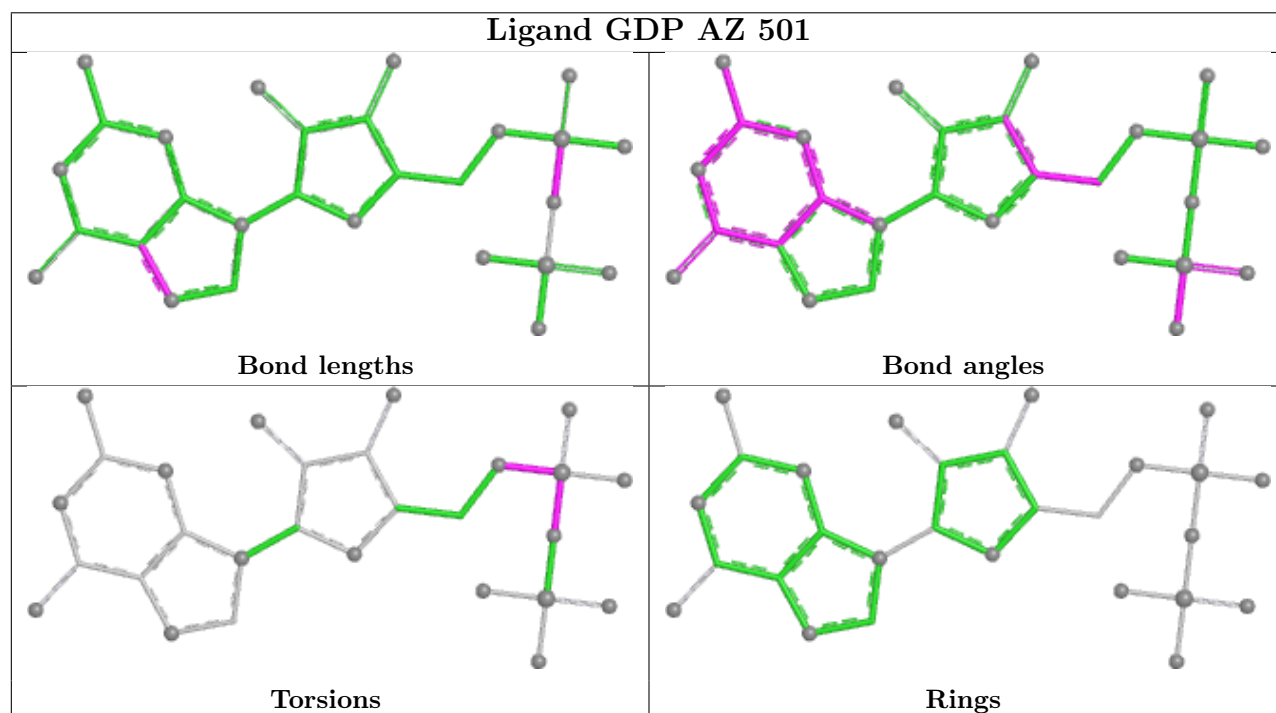
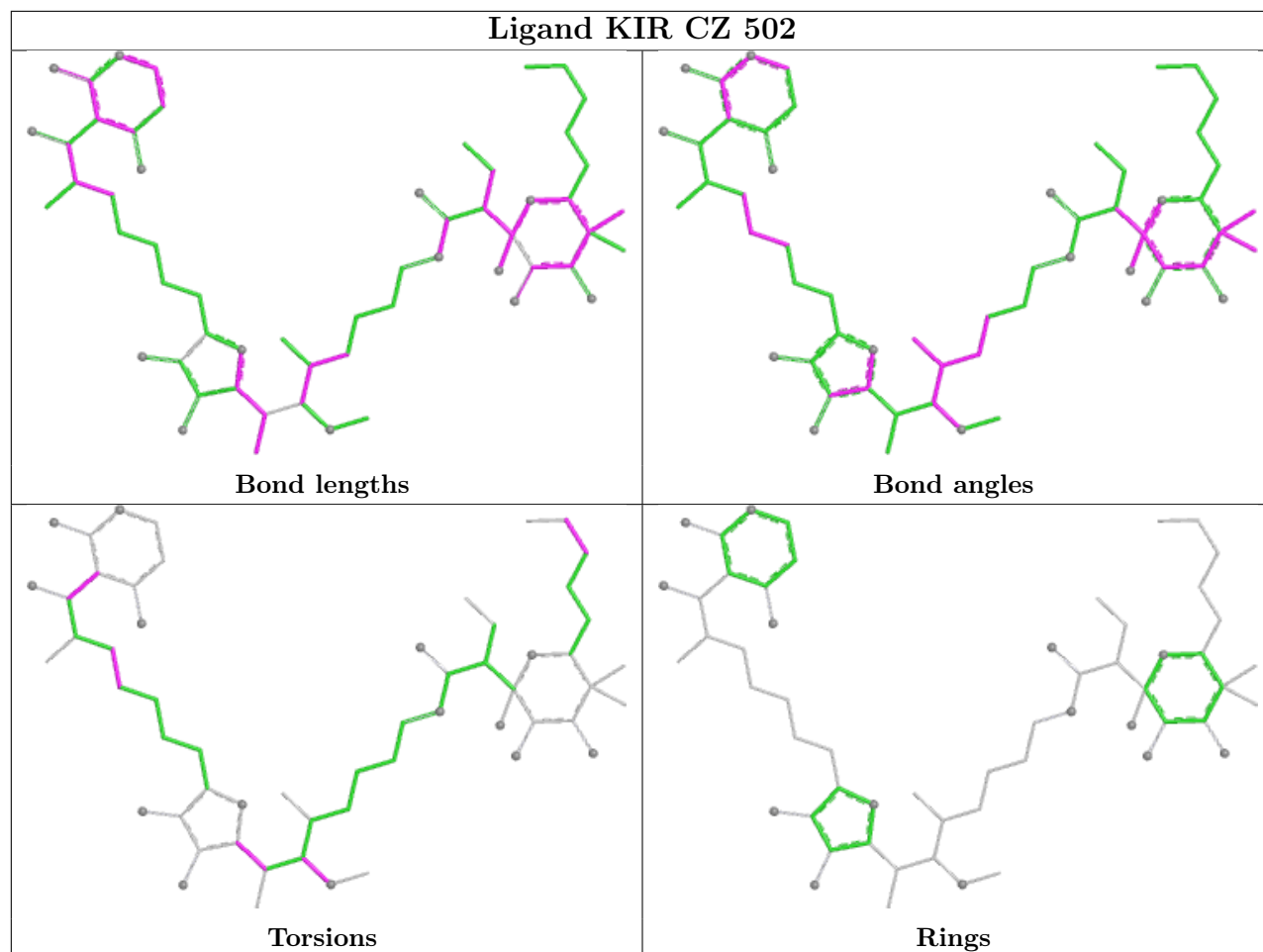
Mol	Chain	Res	Type	Atoms
60	AZ	501	GDP	C5'-O5'-PA-O1A
60	CZ	501	GDP	C5'-O5'-PA-O1A
61	AZ	502	KIR	C4-C3-C7-C8
61	AZ	502	KIR	O18-C17-C19-C42
61	CZ	502	KIR	C4-C3-C7-C8

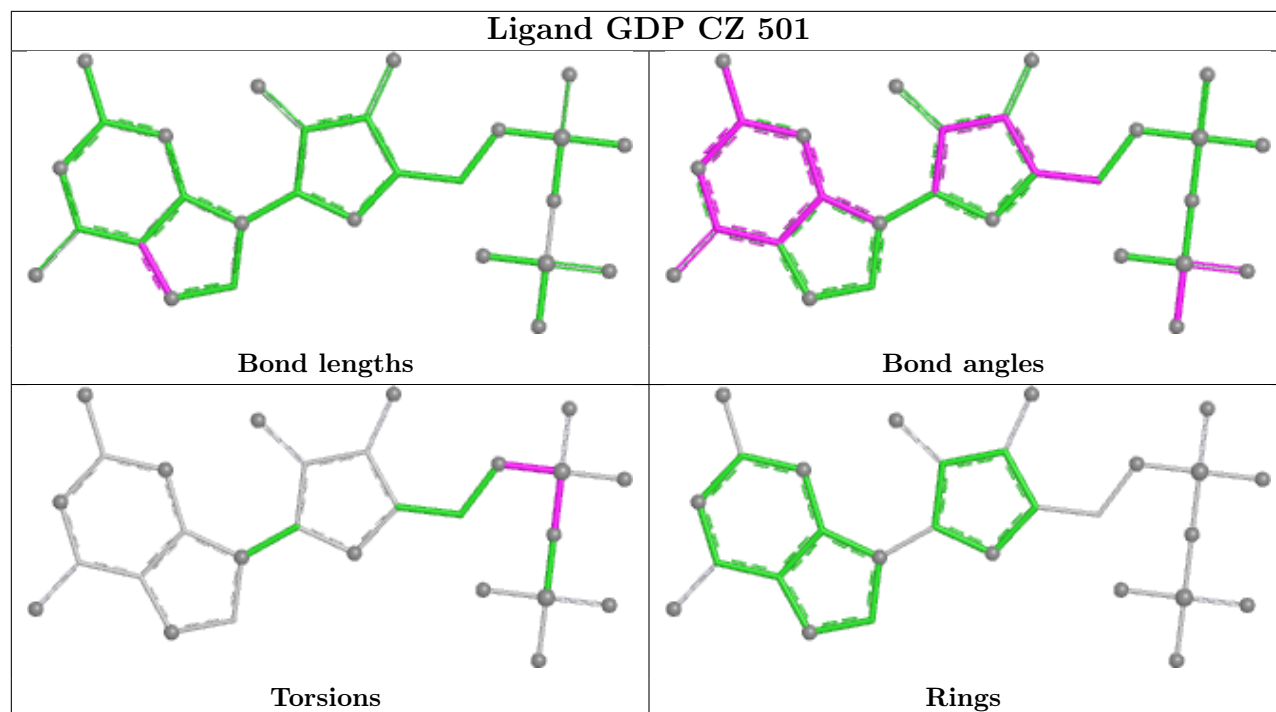
There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.12	76 (5%) 33 18	22, 58, 151, 200	0
1	CA	1504/1522 (98%)	0.36	61 (4%) 41 23	39, 79, 157, 200	0
2	AB	234/256 (91%)	0.38	11 (4%) 36 19	33, 66, 135, 154	0
2	CB	234/256 (91%)	0.45	9 (3%) 44 25	50, 89, 142, 150	0
3	AC	206/239 (86%)	-0.08	3 (1%) 72 52	25, 49, 78, 88	0
3	CC	206/239 (86%)	0.30	5 (2%) 59 38	53, 80, 106, 113	0
4	AD	208/209 (99%)	0.99	28 (13%) 7 4	59, 88, 122, 126	0
4	CD	208/209 (99%)	1.01	30 (14%) 6 3	79, 105, 125, 135	0
5	AE	150/162 (92%)	-0.23	0 100 100	30, 45, 71, 97	0
5	CE	150/162 (92%)	-0.02	0 100 100	48, 63, 85, 102	0
6	AF	101/101 (100%)	0.22	0 100 100	48, 74, 94, 105	0
6	CF	101/101 (100%)	0.52	2 (1%) 65 44	79, 98, 111, 119	0
7	AG	155/156 (99%)	0.25	5 (3%) 50 30	39, 65, 96, 117	0
7	CG	155/156 (99%)	0.51	5 (3%) 50 30	71, 95, 115, 127	0
8	AH	138/138 (100%)	-0.13	1 (0%) 84 68	32, 49, 69, 74	0
8	CH	138/138 (100%)	0.06	1 (0%) 84 68	46, 64, 80, 87	0
9	AI	127/128 (99%)	0.54	10 (7%) 18 10	32, 68, 111, 124	0
9	CI	127/128 (99%)	0.91	15 (11%) 9 5	66, 106, 132, 139	0
10	AJ	98/105 (93%)	0.72	6 (6%) 27 15	33, 70, 112, 125	0
10	CJ	98/105 (93%)	1.15	17 (17%) 4 2	66, 109, 144, 148	0
11	AK	119/129 (92%)	0.04	2 (1%) 69 48	32, 50, 92, 118	0
11	CK	119/129 (92%)	0.48	5 (4%) 40 22	52, 76, 100, 120	0
12	AL	124/132 (93%)	0.13	0 100 100	33, 61, 85, 124	0
12	CL	124/132 (93%)	0.30	1 (0%) 82 65	47, 72, 99, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.63	9 (7%)	21	11	43, 72, 103, 131	0
13	CM	124/126 (98%)	0.79	15 (12%)	8	5	76, 99, 122, 142	0
14	AN	60/61 (98%)	0.32	3 (5%)	34	18	30, 53, 78, 84	0
14	CN	60/61 (98%)	0.95	5 (8%)	17	9	65, 83, 102, 105	0
15	AO	88/89 (98%)	-0.04	0	100	100	36, 54, 82, 88	0
15	CO	88/89 (98%)	0.15	2 (2%)	61	39	44, 68, 90, 98	0
16	AP	83/88 (94%)	0.56	2 (2%)	59	38	61, 74, 98, 133	0
16	CP	83/88 (94%)	0.63	1 (1%)	76	58	74, 90, 110, 132	0
17	AQ	99/105 (94%)	0.04	1 (1%)	79	61	40, 60, 79, 89	0
17	CQ	99/105 (94%)	0.30	2 (2%)	65	44	53, 71, 91, 102	0
18	AR	70/88 (79%)	-0.03	0	100	100	39, 60, 90, 99	0
18	CR	70/88 (79%)	0.34	0	100	100	56, 81, 108, 118	0
19	AS	78/93 (83%)	0.71	8 (10%)	12	6	52, 73, 117, 127	0
19	CS	78/93 (83%)	0.98	10 (12%)	7	4	81, 97, 126, 132	0
20	AT	99/106 (93%)	0.68	9 (9%)	15	8	55, 80, 126, 130	0
20	CT	99/106 (93%)	0.59	7 (7%)	22	12	74, 90, 120, 122	0
21	AU	24/27 (88%)	0.48	2 (8%)	17	9	41, 55, 79, 99	0
21	CU	24/27 (88%)	1.45	5 (20%)	2	1	74, 92, 105, 113	0
22	AV	76/76 (100%)	0.18	5 (6%)	24	13	35, 72, 107, 124	0
22	AW	76/76 (100%)	2.01	31 (40%)	0	0	64, 140, 185, 199	0
22	CV	76/76 (100%)	0.75	8 (10%)	11	6	51, 86, 120, 137	0
22	CW	76/76 (100%)	1.98	32 (42%)	0	0	94, 170, 191, 200	0
23	AX	17/27 (62%)	1.13	8 (47%)	0	0	31, 91, 142, 143	0
23	CX	17/27 (62%)	3.55	15 (88%)	0	0	69, 122, 155, 157	0
24	AY	68/77 (88%)	1.03	8 (11%)	9	5	57, 140, 177, 197	0
24	CY	68/77 (88%)	1.15	9 (13%)	7	4	73, 142, 175, 198	0
25	AZ	385/405 (95%)	1.33	76 (19%)	3	1	87, 124, 151, 169	0
25	CZ	385/405 (95%)	2.11	194 (50%)	0	0	111, 133, 156, 170	0
26	B0	84/85 (98%)	0.47	4 (4%)	35	19	58, 73, 107, 122	0
26	D0	84/85 (98%)	0.99	7 (8%)	17	9	69, 86, 113, 123	0
27	B1	93/98 (94%)	0.74	13 (13%)	6	4	45, 69, 129, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.65	6 (6%) 25 13	59, 86, 133, 139	0
28	B2	71/72 (98%)	2.22	32 (45%) 0 0	130, 143, 155, 158	0
28	D2	71/72 (98%)	0.92	9 (12%) 8 4	100, 122, 136, 143	0
29	B3	59/60 (98%)	0.42	1 (1%) 69 48	65, 81, 106, 122	0
29	D3	59/60 (98%)	0.52	2 (3%) 48 28	60, 93, 106, 126	0
30	B4	44/71 (61%)	2.24	21 (47%) 0 0	111, 140, 167, 173	0
30	D4	44/71 (61%)	2.08	17 (38%) 1 0	136, 163, 184, 186	0
31	B5	59/60 (98%)	1.10	9 (15%) 5 3	62, 87, 148, 163	0
31	D5	59/60 (98%)	1.26	7 (11%) 9 5	63, 92, 145, 154	0
32	B6	50/54 (92%)	1.82	17 (34%) 1 0	57, 84, 103, 110	0
32	D6	50/54 (92%)	1.63	14 (28%) 1 1	73, 97, 116, 122	0
33	B7	48/49 (97%)	0.61	3 (6%) 26 14	51, 64, 101, 121	0
33	D7	48/49 (97%)	0.79	4 (8%) 17 9	64, 73, 104, 125	0
34	B8	63/65 (96%)	1.10	11 (17%) 4 2	56, 73, 91, 115	0
34	D8	63/65 (96%)	1.33	18 (28%) 1 1	72, 85, 101, 120	0
35	B9	37/37 (100%)	1.43	8 (21%) 2 1	73, 85, 103, 104	0
35	D9	37/37 (100%)	2.37	17 (45%) 0 0	67, 96, 107, 120	0
36	BA	2901/2915 (99%)	0.51	200 (6%) 23 12	26, 77, 181, 200	0
36	DA	2901/2915 (99%)	0.67	240 (8%) 17 9	37, 87, 180, 200	0
37	BB	119/122 (97%)	0.52	4 (3%) 48 28	59, 85, 112, 132	0
37	DB	119/122 (97%)	0.70	4 (3%) 48 28	69, 101, 126, 132	0
38	BC	228/229 (99%)	0.51	22 (9%) 13 7	50, 79, 160, 173	0
38	DC	228/229 (99%)	0.61	15 (6%) 24 13	68, 102, 170, 180	0
39	BD	275/276 (99%)	0.06	8 (2%) 53 32	30, 49, 83, 105	0
39	DD	275/276 (99%)	0.23	13 (4%) 36 19	42, 61, 91, 111	0
40	BE	204/206 (99%)	0.74	22 (10%) 11 6	50, 79, 128, 140	0
40	DE	204/206 (99%)	0.78	24 (11%) 9 5	47, 84, 133, 138	0
41	BF	207/210 (98%)	0.99	28 (13%) 7 4	53, 112, 162, 170	0
41	DF	207/210 (98%)	1.07	28 (13%) 7 4	62, 118, 161, 170	0
42	BG	181/182 (99%)	0.81	19 (10%) 11 6	63, 86, 117, 130	0
42	DG	181/182 (99%)	0.76	12 (6%) 24 13	89, 108, 136, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	1.17	28 (17%) 4 2	92, 134, 152, 156	0
43	DH	159/180 (88%)	1.18	24 (15%) 5 3	87, 129, 146, 154	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.66	7 (5%) 33 18	63, 89, 125, 134	0
46	DN	138/140 (98%)	0.56	6 (4%) 40 22	69, 90, 125, 133	0
47	BO	122/122 (100%)	0.04	1 (0%) 82 65	46, 63, 77, 85	0
47	DO	122/122 (100%)	0.18	1 (0%) 82 65	47, 67, 83, 89	0
48	BP	146/150 (97%)	1.54	38 (26%) 1 1	55, 103, 133, 150	0
48	DP	146/150 (97%)	1.42	36 (24%) 2 1	64, 115, 137, 153	0
49	BQ	141/141 (100%)	0.26	4 (2%) 55 34	46, 64, 86, 128	0
49	DQ	141/141 (100%)	0.37	6 (4%) 40 22	51, 66, 90, 126	0
50	BR	117/118 (99%)	0.68	7 (5%) 27 15	60, 85, 107, 126	0
50	DR	117/118 (99%)	0.80	7 (5%) 27 15	57, 90, 105, 123	0
51	BS	98/112 (87%)	1.13	19 (19%) 3 1	63, 90, 116, 126	0
51	DS	98/112 (87%)	1.38	21 (21%) 2 1	77, 102, 126, 128	0
52	BT	137/146 (93%)	0.62	6 (4%) 39 21	58, 84, 142, 167	0
52	DT	137/146 (93%)	0.73	11 (8%) 18 10	63, 90, 147, 169	0
53	BU	117/118 (99%)	0.63	6 (5%) 33 18	64, 79, 111, 128	0
53	DU	117/118 (99%)	0.70	9 (7%) 19 10	63, 86, 110, 124	0
54	BV	101/101 (100%)	1.01	10 (9%) 13 7	62, 116, 129, 136	0
54	DV	101/101 (100%)	0.97	12 (11%) 9 5	71, 115, 134, 136	0
55	BW	113/113 (100%)	0.54	6 (5%) 32 17	65, 90, 116, 141	0
55	DW	113/113 (100%)	0.67	8 (7%) 22 12	73, 93, 123, 145	0
56	BX	92/96 (95%)	1.07	12 (13%) 7 4	75, 95, 110, 118	0
56	DX	92/96 (95%)	0.93	8 (8%) 16 9	82, 100, 116, 120	0
57	BY	100/110 (90%)	1.50	29 (29%) 1 1	108, 134, 162, 168	0
57	DY	100/110 (90%)	1.61	34 (34%) 1 0	107, 136, 160, 169	0
58	BZ	183/206 (88%)	0.69	16 (8%) 16 9	56, 83, 120, 132	0
58	DZ	183/206 (88%)	0.71	12 (6%) 24 13	62, 88, 120, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21996/23370 (94%)	0.63	2003 (9%) 15 8	22, 84, 151, 200	0

The worst 5 of 2003 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	D9	1	MET	12.3
31	D5	2	ALA	10.8
25	AZ	63	ILE	10.7
14	CN	2	ALA	10.0
14	AN	2	ALA	9.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	H2U	CY	16	20/21	0.26	0.18	194,198,199,199	0
24	H2U	CY	17	20/21	0.33	0.17	199,199,200,200	0
24	H2U	CY	20	20/21	0.41	0.18	188,191,192,192	0
24	PSU	CY	55	20/21	0.42	0.19	158,161,162,162	0
24	H2U	AY	16	20/21	0.49	0.20	196,198,199,200	0
24	PSU	AY	55	20/21	0.51	0.18	156,161,162,162	0
24	H2U	AY	17	20/21	0.52	0.17	199,199,200,200	0
24	H2U	AY	20	20/21	0.64	0.14	186,189,193,193	0
24	7MG	AY	46	24/25	0.78	0.15	145,150,151,151	0
24	5MU	CY	54	21/22	0.79	0.16	139,149,151,155	0
24	4SU	CY	8	20/21	0.79	0.19	143,145,147,148	0
24	7MG	CY	46	24/25	0.80	0.15	148,153,154,154	0
24	4SU	AY	8	20/21	0.81	0.20	142,144,146,146	0
24	5MU	AY	54	21/22	0.81	0.14	139,150,152,154	0
24	MIA	CY	37	29/30	0.83	0.16	80,87,95,99	0
24	MIA	AY	37	29/30	0.87	0.18	64,78,89,98	0
24	OMC	CY	32	21/22	0.87	0.11	108,114,121,121	0
24	OMC	AY	32	21/22	0.88	0.12	101,105,115,115	0

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
61	KIR	CZ	502	57/57	0.64	0.23	122,131,140,141	0
61	KIR	AZ	502	57/57	0.75	0.20	115,122,129,130	0
60	GDP	CZ	501	28/28	0.75	0.17	137,140,141,141	0
60	GDP	AZ	501	28/28	0.77	0.16	129,133,138,138	0
59	ZN	D4	101	1/1	0.92	0.08	196,196,196,196	0
59	ZN	D9	101	1/1	0.94	0.08	141,141,141,141	0
59	ZN	AN	101	1/1	0.98	0.05	48,48,48,48	0
59	ZN	B9	101	1/1	0.99	0.04	113,113,113,113	0
59	ZN	CD	301	1/1	0.99	0.17	79,79,79,79	0
59	ZN	AD	301	1/1	0.99	0.17	74,74,74,74	0
59	ZN	B4	101	1/1	0.99	0.04	112,112,112,112	0
59	ZN	CN	101	1/1	1.00	0.02	77,77,77,77	0

5.5 Other polymers

There are no such residues in this entry.