



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:07 AM UTC

PDB ID : 8UVR / pdb_00008uvr
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with spectinomycin, mRNA, deacylated A- and E-site tRNA^{phe}, and deacylated P-site tRNA^{met} at 2.60Å resolution
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Deposited on : 2023-11-03
Resolution : 2.60 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	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.60 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

There are 61 unique types of molecules in this entry. The entry contains 300591 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			2136	1349	423	361	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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			1117	719	207	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
			873	550	174	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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O		0	0	0
			199	122	48	29				
52	2u	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 53 is a RNA chain called MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Deacylated tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1116	Total	Mg	0	0
			1116	1116		
56	1B	39	Total	Mg	0	0
			39	39		
56	1D	15	Total	Mg	0	0
			15	15		
56	1E	14	Total	Mg	0	0
			14	14		
56	1F	15	Total	Mg	0	0
			15	15		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1I	1	Total 1	Mg 1	0	0
56	1N	5	Total 5	Mg 5	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	4	Total 4	Mg 4	0	0
56	1Q	8	Total 8	Mg 8	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	13	Total 13	Mg 13	0	0
56	1V	9	Total 9	Mg 9	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	5	Total 5	Mg 5	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	10	10	Total 10	Mg 10	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	5	Total 5	Mg 5	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	10	Total 10	Mg 10	0	0
56	16	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	4	Total 4	Mg 4	0	0
56	18	8	Total 8	Mg 8	0	0
56	19	2	Total 2	Mg 2	0	0
56	1a	214	Total 214	Mg 214	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	9	Total 9	Mg 9	0	0
56	1x	13	Total 13	Mg 13	0	0
56	1y	2	Total 2	Mg 2	0	0
56	2A	880	Total 880	Mg 880	0	0
56	2B	19	Total 19	Mg 19	0	0
56	2D	8	Total 8	Mg 8	0	0
56	2E	10	Total 10	Mg 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2F	8	Total 8	Mg 8	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2S	1	Total 1	Mg 1	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	4	Total 4	Mg 4	0	0
56	21	2	Total 2	Mg 2	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	6	Total 6	Mg 6	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	4	Total 4	Mg 4	0	0
56	29	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2a	235	Total 235	Mg 235	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	3	Total 3	Mg 3	0	0
56	2f	3	Total 3	Mg 3	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2l	6	Total 6	Mg 6	0	0
56	2q	4	Total 4	Mg 4	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	3	Total 3	Mg 3	0	0
56	2w	9	Total 9	Mg 9	0	0
56	2x	7	Total 7	Mg 7	0	0
56	2y	7	Total 7	Mg 7	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1	Total 1	K 1	0	0
57	2A	1	Total 1	K 1	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

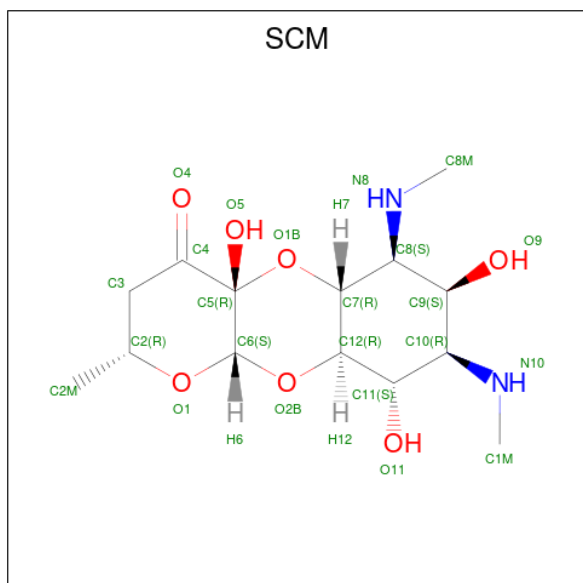
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total 1	Zn 1	0	0
58	14	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$).



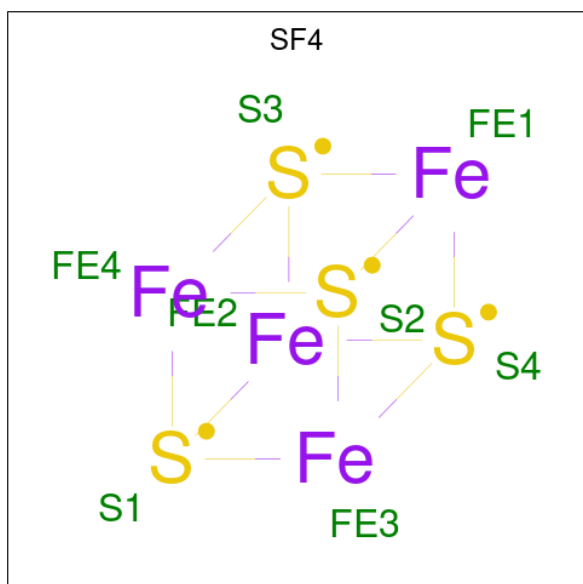
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1a	1	Total	C	N	O	0	0
			23	14	2	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	2a	1	Total	C	N	O	0	0
			23	14	2	7		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2167	Total	O	0	0
			2167	2167		
61	1B	69	Total	O	0	0
			69	69		
61	1D	27	Total	O	0	0
			27	27		
61	1E	25	Total	O	0	0
			25	25		
61	1F	21	Total	O	0	0
			21	21		
61	1G	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	2	Total	O	0	0
			2	2		
61	1I	1	Total	O	0	0
			1	1		
61	1N	5	Total	O	0	0
			5	5		
61	1O	5	Total	O	0	0
			5	5		
61	1P	24	Total	O	0	0
			24	24		
61	1Q	11	Total	O	0	0
			11	11		
61	1R	11	Total	O	0	0
			11	11		
61	1S	5	Total	O	0	0
			5	5		
61	1T	9	Total	O	0	0
			9	9		
61	1U	15	Total	O	0	0
			15	15		
61	1V	10	Total	O	0	0
			10	10		
61	1W	8	Total	O	0	0
			8	8		
61	1X	5	Total	O	0	0
			5	5		
61	1Y	3	Total	O	0	0
			3	3		
61	1Z	2	Total	O	0	0
			2	2		
61	10	18	Total	O	0	0
			18	18		
61	11	8	Total	O	0	0
			8	8		
61	12	3	Total	O	0	0
			3	3		
61	13	4	Total	O	0	0
			4	4		
61	14	1	Total	O	0	0
			1	1		
61	15	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	3	Total 3	O 3	0	0
61	17	8	Total 8	O 8	0	0
61	18	11	Total 11	O 11	0	0
61	1a	426	Total 426	O 426	0	0
61	1b	1	Total 1	O 1	0	0
61	1c	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1i	2	Total 2	O 2	0	0
61	1j	2	Total 2	O 2	0	0
61	1l	8	Total 8	O 8	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	2	Total 2	O 2	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1t	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	14	Total 14	O 14	0	0
61	1x	15	Total 15	O 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1y	1	Total 1	O 1	0	0
61	2A	1243	Total 1243	O 1243	0	0
61	2B	23	Total 23	O 23	0	0
61	2D	25	Total 25	O 25	0	0
61	2E	11	Total 11	O 11	0	0
61	2F	12	Total 12	O 12	0	0
61	2I	2	Total 2	O 2	0	0
61	2N	2	Total 2	O 2	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	10	Total 10	O 10	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	1	Total 1	O 1	0	0
61	2V	2	Total 2	O 2	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	2	Total 2	O 2	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	3	Total 3	O 3	0	0
61	21	11	Total 11	O 11	0	0
61	23	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	25	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	311	Total 311	O 311	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2g	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	5	Total 5	O 5	0	0
61	2p	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	3	Total 3	O 3	0	0
61	2x	3	Total 3	O 3	0	0
61	2y	14	Total 14	O 14	0	0

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	209.07Å 447.77Å 621.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.24 – 2.60	Depositor
% Data completeness (in resolution range)	98.8 (255.24-2.60)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.265	Depositor
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.181	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	300591	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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](#)

84 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$
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	27,32,35	1.83	7 (25%)
54	4SU	2w	8	54	18,21,22	1.82	6 (33%)	25,30,33	1.99	4 (16%)
1	5MC	1A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	967	32	19,22,23	1.79	3 (15%)	26,32,35	1.16	3 (11%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	4 (19%)
55	4SU	2x	8	55	18,21,22	2.14	5 (27%)	25,30,33	1.38	3 (12%)
1	2MA	2A	2503	1,56	22,25,26	1.45	5 (22%)	32,37,40	2.30	9 (28%)
54	MIA	2y	37	54	21,24,32	1.60	3 (14%)	30,35,47	2.10	8 (26%)
55	5MC	1x	32	55	19,22,23	1.62	3 (15%)	26,32,35	1.22	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.21	3 (11%)
54	MIA	1y	37	54	21,24,32	1.62	4 (19%)	30,35,47	2.04	7 (23%)
54	MIA	2w	37	54	24,27,32	2.08	5 (20%)	32,39,47	2.51	11 (34%)
1	5MU	1A	1915	1	19,22,23	1.37	5 (26%)	27,32,35	2.29	8 (29%)
32	M2G	1a	966	32	24,27,28	1.34	4 (16%)	33,40,43	1.89	7 (21%)
32	2MG	1a	1207	32,56	23,26,27	1.22	3 (13%)	33,38,41	2.29	8 (24%)
54	G7M	2y	46	54	23,26,27	1.58	4 (17%)	34,39,42	1.79	4 (11%)
32	5MC	2a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.23	3 (11%)
43	0TD	2l	92	43	8,9,10	4.52	1 (12%)	6,11,13	1.32	1 (16%)
55	5MU	1x	54	55,56	19,22,23	1.40	5 (26%)	27,32,35	1.95	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	3 (11%)
32	G7M	2a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.75	5 (14%)
54	5MU	1y	54	54	19,22,23	1.50	6 (31%)	27,32,35	2.04	6 (22%)
1	5MC	2A	1942	1	19,22,23	1.72	3 (15%)	26,32,35	1.19	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	1.94	10 (30%)
54	4SU	1y	8	54	18,21,22	1.79	5 (27%)	25,30,33	1.66	5 (20%)
1	5MU	2A	1939	1,56	19,22,23	1.48	6 (31%)	27,32,35	2.20	8 (29%)
43	0TD	1l	92	43	8,9,10	4.63	1 (12%)	6,11,13	8.17	2 (33%)
54	5MU	1w	54	54	19,22,23	1.42	5 (26%)	27,32,35	1.68	5 (18%)
32	5MC	2a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	3 (11%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.03	3 (14%)
1	5MC	1A	1962	1,56	19,22,23	1.73	3 (15%)	26,32,35	1.25	3 (11%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.83	6 (18%)
1	OMU	1A	2552	1,56	19,22,23	1.21	3 (15%)	25,31,34	1.81	5 (20%)
32	5MC	1a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.32	5 (19%)
54	PSU	1y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.93	4 (19%)
54	5MU	2y	54	54	19,22,23	1.50	5 (26%)	27,32,35	1.82	8 (29%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	2.10	4 (19%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.91	4 (19%)
32	4OC	2a	1402	32,56	20,23,24	0.78	0	25,32,35	0.96	1 (4%)
54	MIA	1w	37	54	28,31,32	2.40	7 (25%)	38,44,47	2.73	12 (31%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.93	1 (4%)
54	PSU	1w	32	54,56	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
1	5MU	2A	1915	1,56	19,22,23	1.44	6 (31%)	27,32,35	2.22	6 (22%)
32	PSU	1a	516	32	18,21,22	1.40	3 (16%)	21,30,33	1.93	4 (19%)
1	OMG	1A	2251	1,55,56	23,26,27	1.23	3 (13%)	32,38,41	1.99	6 (18%)
32	UR3	1a	1498	32	19,22,23	0.95	0	26,32,35	1.79	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.33	3 (16%)	21,30,33	2.09	3 (14%)
32	G7M	1a	527	32,56	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	1.93	4 (19%)
32	2MG	2a	1207	32,56	23,26,27	1.26	4 (17%)	33,38,41	2.14	7 (21%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.91	4 (19%)
55	4SU	1x	8	55	18,21,22	2.26	5 (27%)	25,30,33	1.68	5 (20%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	21,30,33	2.12	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.11	1 (5%)	26,32,35	1.82	4 (15%)
55	5MU	2x	54	55	19,22,23	1.44	6 (31%)	27,32,35	1.88	5 (18%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	5MU	1A	1939	1,56	19,22,23	1.41	4 (21%)	27,32,35	2.10	6 (22%)
1	OMG	2A	2251	1,55,56	23,26,27	1.23	3 (13%)	32,38,41	2.06	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.44	0	33,38,41	2.05	10 (30%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.00	5 (23%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.25	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
54	4SU	1w	8	54	18,21,22	1.89	5 (27%)	25,30,33	1.86	4 (16%)
54	G7M	1w	46	54	23,26,27	1.57	4 (17%)	34,39,42	1.60	4 (11%)
1	5MC	2A	1962	1,56	19,22,23	1.57	3 (15%)	26,32,35	1.08	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	1.03	1 (4%)
54	PSU	2y	55	54	18,21,22	1.35	3 (16%)	21,30,33	1.91	4 (19%)
55	PSU	2x	55	55	18,21,22	1.41	2 (11%)	21,30,33	1.91	5 (23%)
54	4SU	2y	8	54	18,21,22	1.73	4 (22%)	25,30,33	2.78	5 (20%)
1	2MA	1A	2503	1,56	22,25,26	1.38	4 (18%)	32,37,40	2.40	9 (28%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.04	9 (27%)
1	PSU	1A	2605	1,56	18,21,22	1.35	2 (11%)	21,30,33	2.14	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	1.00	0
54	PSU	2y	39	54	18,21,22	1.49	2 (11%)	21,30,33	1.63	4 (19%)
54	PSU	2y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	4 (19%)
1	OMU	2A	2552	1,56	19,22,23	1.19	3 (15%)	25,31,34	1.78	5 (20%)
32	5MC	2a	967	32	19,22,23	1.72	3 (15%)	26,32,35	1.10	2 (7%)
54	G7M	1y	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.82	4 (11%)
54	PSU	1y	39	54	18,21,22	1.44	2 (11%)	21,30,33	1.86	5 (23%)
54	G7M	2w	46	54	23,26,27	1.49	3 (13%)	34,39,42	1.79	5 (14%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)

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
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	0/7/25/26	0/3/3/3
54	MIA	2y	37	54	-	2/7/25/34	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/7/25/34	0/3/3/3
54	MIA	2w	37	54	-	4/11/29/34	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	2MG	1a	1207	32,56	-	2/9/27/28	0/3/3/3
54	G7M	2y	46	54	-	0/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	4/7/12/14	-
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	4SU	1y	8	54	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	0/9/29/30	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,56	-	0/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	2/7/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/9/27/28	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	1/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.76	1.69	1.82
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
54	1w	37	MIA	C2-S10	-7.73	1.69	1.75
54	1w	37	MIA	C13-C14	6.92	1.53	1.32
54	2w	37	MIA	C2-S10	-6.78	1.70	1.75

The worst 5 of 401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	19.78	137.91	102.36
54	1w	37	MIA	C12-C13-C14	-8.91	111.02	127.01
1	1A	2503	2MA	C5-C4-N3	-8.39	118.34	127.18
54	2y	8	4SU	C4-N3-C2	-8.28	119.38	127.31
54	2w	37	MIA	C5-C4-N3	-8.11	118.63	127.18

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	G7M	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 [i](#)

Of 2844 ligands modelled in this entry, 2840 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
59	SCM	2a	3236	-	23,25,25	0.81	1 (4%)	27,39,39	1.60	4 (14%)
60	SF4	1d	501	35	0,12,12	-	-	-		
60	SF4	2d	303	35	0,12,12	-	-	-		
59	SCM	1a	1815	-	23,25,25	0.74	0	27,39,39	1.64	4 (14%)

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
59	SCM	2a	3236	-	-	1/4/57/57	0/3/3/3
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5
59	SCM	1a	1815	-	-	0/4/57/57	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2a	3236	SCM	O5-C5	2.44	1.43	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2a	3236	SCM	C8M-N8-C8	5.39	121.19	114.23
59	1a	1815	SCM	C1M-N10-C10	4.92	120.57	114.23
59	1a	1815	SCM	C8M-N8-C8	4.27	119.74	114.23
59	2a	3236	SCM	C1M-N10-C10	3.64	118.93	114.23
59	2a	3236	SCM	O1-C2-C3	3.55	113.56	108.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

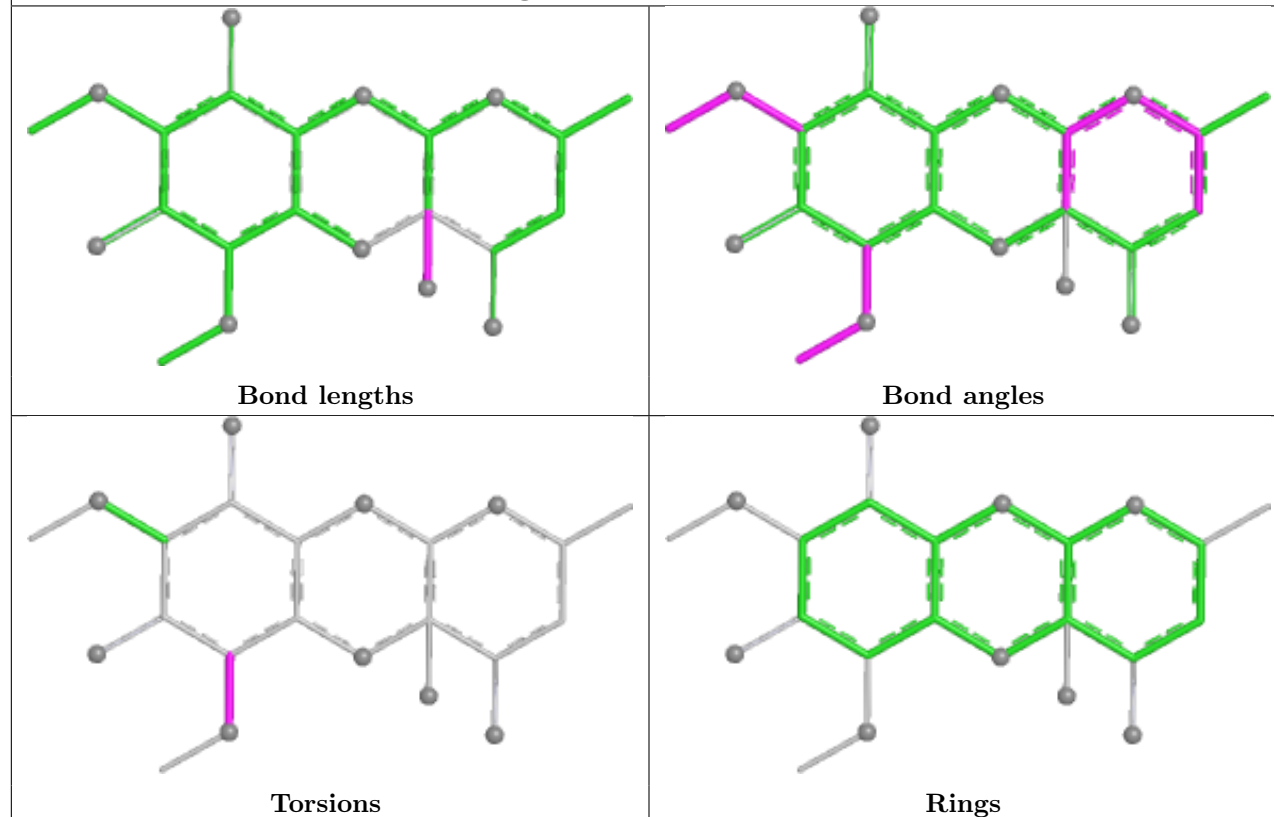
Mol	Chain	Res	Type	Atoms
59	2a	3236	SCM	C9-C8-N8-C8M

There are no ring outliers.

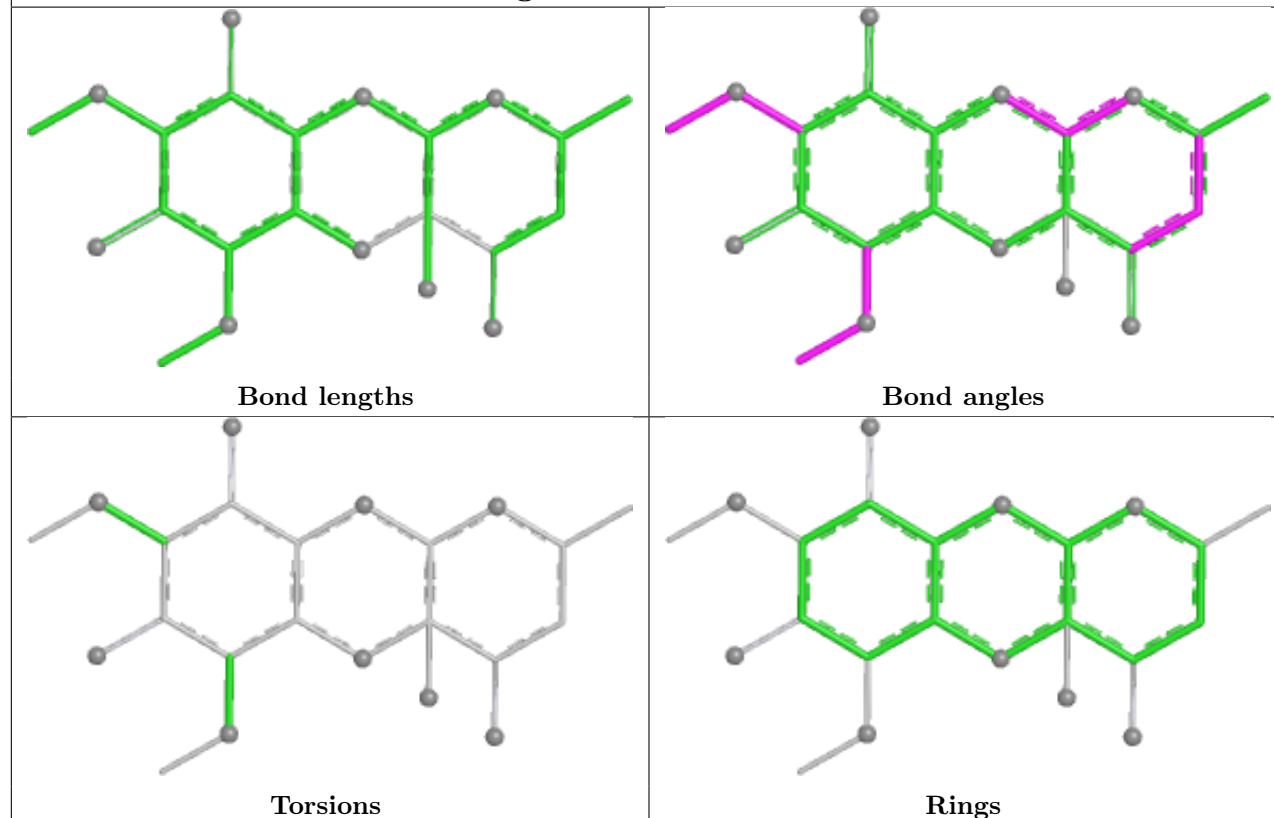
No monomer is involved in short contacts.

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.

Ligand SCM 2a 3236



Ligand SCM 1a 1815



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.