wwPDB EM Validation Summary Report (i)

May 13, 2024 – 11:38 pm BST

PDB ID	:	6RXU
EMDB ID	:	EMD-10052
Title	:	Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state B1
Authors	:	Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2019-06-10
Resolution	:	3.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

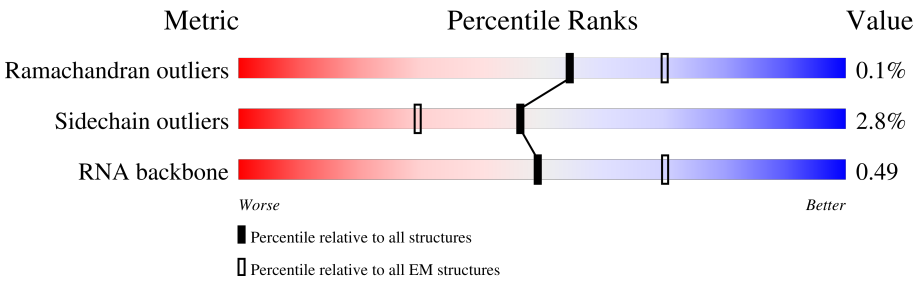
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	UA	904	92% • 7%
2	UB	907	56% 44%
3	UC	648	11% 89%
4	UD	884	87% 13%
5	UF	414	79% 20%
6	UG	558	84% • 14%
7	UJ	1802	60% • 40%
8	UK	270	80% 20%
9	UL	962	81% • 18%

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Mol	Chain	Length	Quality of chain
10	UM	912	79% 20%
11	UN	938	19% 81%
12	UO	557	89% 10%
13	UQ	960	81% 18%
14	UR	618	72% 28%
15	UU	1049	85% 14%
16	UX	193	98%
17	UZ	391	58% 40%
18	CA	313	77% 23%
18	CB	313	75% 24%
19	CC	523	74% 26%
20	CD	582	72% 28%
21	CE	127	94% 5%
21	CF	127	91% 6%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 211834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UA	839	6366	4101	1136	1105	24	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	512	4079	2576	781	711	11	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	772	6071	3851	1093	1103	24	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3717	2369	700	636	12	0	0

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UJ	1090	8416	5408	1452	1525	31	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UK	217	1687	1062	351	269	5	0	0

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	UL	785	6175	3940	1088	1130	17	0	0

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UM	729	5643	3590	995	1045	13	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UN	177	1401	892	263	239	7	0	0

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	UO	504	3819	2422	699	684	14	0	0

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	UQ	789	6008	3831	1037	1119	21	0	0

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UR	447	3491	2209	656	616	10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UU	902	6734	4336	1236	1136	26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	UX	190	1470	932	282	246	10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UZ	235	1819	1186	331	299	3	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CA	242	1778	1149	327	293	9	0	0
18	CB	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Nop56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CD	420	3150	2023	560	557	10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	CE	121	879	557	165	154	3	0	0
21	CF	120	864	550	161	150	3	0	0

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	CG	416	3245	2065	587	580	13	0	0

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	CH	389	2888	1827	526	525	10	0	0

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	CI	822	6486	4169	1213	1077	27	0	0

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	CJ	179	1434	918	283	226	7	0	0

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	CK	297	2329	1476	445	400	8	0	0

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	CL	231	1786	1114	339	327	6	0	0

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CM	445	3501	2195	672	619	15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CN	226	1762	1119	306	327	10	0	0
29	CO	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CP	233	1893	1209	340	335	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	CQ	175	1361	862	250	242	7	0	0

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CR	760	5989	3851	1024	1087	27	0	0
32	CS	760	5989	3851	1024	1087	27	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	CT	131	1035	656	197	178	4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Ca	225	1821	1160	341	315	5	0	0

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Cb	232	1851	1179	340	325	7	0	0

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Cc	192	1464	926	278	253	7	0	0

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Cd	226	1819	1138	363	313	5	0	0

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Ce	159	1279	810	237	232	0	0

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Cf	174	1398	872	283	242	1	0	0

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Cg	159	1242	801	255	184	2	0	0

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	Ch	66	546	355	101	90	0	0

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Ci	115	808	506	156	141	5	0	0

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Cj	126	943	613	177	151	2	0	0

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ck	140	1163	750	224	184	5	0	0

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Cm	126	985	632	184	164	5	0	0

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Cn	96	702	456	134	110	2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Co	92	741	474	139	126	2	0	0

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	Cp	61	455	284	97	74	0	0

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	CU	176	1337	822	265	244	6	0	0

- Molecule 50 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	C1	1575	33604	14992	6023	11014	1575	0	0

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	C2	230	4891	2182	856	1623	230	0	0

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	CW	382	2924	1857	530	524	13	0	0

- Molecule 53 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	UT	2033	16053	10338	2819	2828	68	0	0

- Molecule 54 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	UH	359	2809	1773	496	527	13	0	0

- Molecule 55 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	UE	125	972	608	183	175	6	0	0
55	UI	125	972	608	183	175	6	0	0

- Molecule 56 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	US	451	3672	2389	608	660	15	0	0

- Molecule 57 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Cl	80	633	400	115	117	1	0	0

- Molecule 58 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	CX	267	2130	1384	374	362	10	0	0

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	CY	123	979	592	195	189	3	0	0

- Molecule 60 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	CZ	44	376	235	76	64	1	0	0

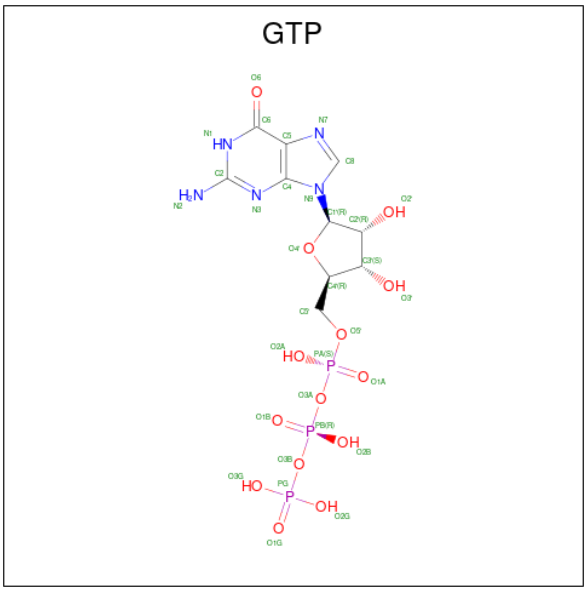
- Molecule 61 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	UP	54	422	264	88	70	0	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	UX	1	1	1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	CI	1	32	10	5	14	3	0

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
64	CI	1	1	1	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	UA	0.47	0/6521	0.65	5/8867 (0.1%)
2	UB	0.33	0/4154	0.54	2/5583 (0.0%)
3	UC	0.40	0/595	0.52	0/786
4	UD	0.38	0/6211	0.56	2/8408 (0.0%)
5	UF	0.35	0/2657	0.54	1/3596 (0.0%)
6	UG	0.47	0/3790	0.62	3/5120 (0.1%)
7	UJ	0.34	0/8567	0.61	5/11619 (0.0%)
8	UK	0.41	0/1701	0.52	1/2251 (0.0%)
9	UL	0.37	0/6299	0.63	4/8531 (0.0%)
10	UM	0.33	0/5755	0.61	2/7827 (0.0%)
11	UN	0.39	0/1425	0.55	1/1913 (0.1%)
12	UO	0.41	0/3903	0.61	3/5312 (0.1%)
13	UQ	0.40	0/6136	0.63	4/8348 (0.0%)
14	UR	0.43	0/3564	0.59	1/4816 (0.0%)
15	UU	0.45	1/6903 (0.0%)	0.60	2/9392 (0.0%)
16	UX	0.42	0/1493	0.59	0/2011
17	UZ	0.34	0/1861	0.61	1/2531 (0.0%)
18	CA	0.46	0/1814	0.60	0/2456
18	CB	0.34	0/1853	0.54	0/2511
19	CC	0.37	0/2911	0.58	1/3937 (0.0%)
20	CD	0.36	0/3205	0.60	3/4338 (0.1%)
21	CE	0.45	0/891	0.66	2/1214 (0.2%)
21	CF	0.41	0/876	0.64	1/1195 (0.1%)
22	CG	0.36	0/3307	0.59	0/4462
23	CH	0.38	0/2939	0.58	1/3988 (0.0%)
24	CI	0.42	0/6631	0.58	1/8943 (0.0%)
25	CJ	0.48	0/1462	0.56	0/1967
26	CK	0.45	0/2376	0.64	2/3214 (0.1%)
27	CL	0.37	0/1812	0.51	0/2437
28	CM	0.48	0/3573	0.60	0/4829
29	CN	0.36	0/1797	0.56	1/2443 (0.0%)
29	CO	0.31	0/1714	0.55	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.34	0/1923	0.56	0/2577
31	CQ	0.30	0/1379	0.57	0/1850
32	CR	0.40	0/6108	0.80	14/8266 (0.2%)
32	CS	0.40	0/6108	0.80	14/8266 (0.2%)
33	CT	0.43	0/1053	0.58	0/1413
34	Ca	0.35	0/1850	0.61	0/2486
35	Cb	0.32	0/1890	0.61	1/2548 (0.0%)
36	Cc	0.40	0/1485	0.54	0/2008
37	Cd	0.34	0/1850	0.55	0/2474
38	Ce	0.34	0/1298	0.66	3/1750 (0.2%)
39	Cf	0.33	0/1429	0.54	0/1915
40	Cg	0.39	0/1259	0.55	0/1687
41	Ch	0.32	0/557	0.51	0/749
42	Ci	0.34	0/819	0.54	0/1107
43	Cj	0.49	0/958	0.60	0/1293
44	Ck	0.30	0/1190	0.54	0/1592
45	Cm	0.41	0/1001	0.57	0/1345
46	Cn	0.44	0/712	0.56	0/954
47	Co	0.32	0/754	0.59	0/1011
48	Cp	0.44	0/458	0.61	1/617 (0.2%)
49	CU	0.32	0/1350	0.53	0/1810
50	C1	0.61	1/37546 (0.0%)	1.24	401/58475 (0.7%)
51	C2	0.64	0/5459	1.40	72/8498 (0.8%)
52	CW	0.33	0/2996	0.67	2/4075 (0.0%)
53	UT	0.34	0/16371	0.63	10/22154 (0.0%)
54	UH	0.33	0/2852	0.56	0/3846
55	UE	0.31	0/980	0.58	0/1316
55	UI	0.26	0/980	0.52	0/1316
56	US	0.33	0/3765	0.57	1/5100 (0.0%)
57	Cl	0.30	0/638	0.60	0/857
58	CX	0.28	0/2180	0.55	1/2956 (0.0%)
59	CY	0.36	0/986	0.53	0/1303
60	CZ	0.39	0/384	0.68	0/511
61	UP	0.34	0/428	0.60	0/570
All	All	0.44	2/219692 (0.0%)	0.80	569/305865 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	UD	0	1
7	UJ	0	2
9	UL	0	2
10	UM	0	4
12	UO	0	1
13	UQ	0	4
14	UR	0	1
15	UU	0	3
17	UZ	0	3
18	CB	0	1
21	CF	0	1
22	CG	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cb	0	1
36	Cc	0	1
37	Cd	0	1
38	Ce	0	1
52	CW	0	2
53	UT	0	10
55	UE	0	1
56	US	0	1
57	Cl	0	1
59	CY	0	1
All	All	0	59

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C1	1081	G	C2-N3	-5.49	1.28	1.32
15	UU	640	CYS	CB-SG	-5.31	1.73	1.81

The worst 5 of 569 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	C2	2	G	O5'-P-OP1	-30.49	74.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C2	2	G	OP1-P-OP2	-27.27	78.70	119.60
51	C2	2	G	O5'-P-OP2	18.13	132.46	110.70
51	C2	1	A	OP1-P-O3'	13.81	135.58	105.20
51	C2	1	A	OP2-P-O3'	-13.14	76.29	105.20

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide
7	UJ	1661	ASP	Peptide
7	UJ	1662	GLN	Peptide
9	UL	153	ASP	Peptide

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	UA	835/904 (92%)	768 (92%)	67 (8%)	0	100 100
2	UB	502/907 (55%)	470 (94%)	32 (6%)	0	100 100
3	UC	72/648 (11%)	64 (89%)	8 (11%)	0	100 100
4	UD	754/884 (85%)	722 (96%)	32 (4%)	0	100 100
5	UF	325/414 (78%)	310 (95%)	14 (4%)	1 (0%)	41 75
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	34 72
7	UJ	1062/1802 (59%)	1010 (95%)	52 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	711 (93%)	56 (7%)	0	100	100
10	UM	705/912 (77%)	656 (93%)	48 (7%)	1 (0%)	51	84
11	UN	171/938 (18%)	167 (98%)	3 (2%)	1 (1%)	25	64
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	41	75
14	UR	437/618 (71%)	416 (95%)	21 (5%)	0	100	100
15	UU	890/1049 (85%)	832 (94%)	58 (6%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	212 (93%)	16 (7%)	1 (0%)	34	72
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	220 (94%)	15 (6%)	0	100	100
19	CC	383/523 (73%)	367 (96%)	16 (4%)	0	100	100
20	CD	416/582 (72%)	393 (94%)	23 (6%)	0	100	100
21	CE	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	19	58
22	CG	402/630 (64%)	375 (93%)	27 (7%)	0	100	100
23	CH	383/411 (93%)	344 (90%)	38 (10%)	1 (0%)	41	75
24	CI	812/1163 (70%)	761 (94%)	49 (6%)	2 (0%)	47	81
25	CJ	177/183 (97%)	166 (94%)	11 (6%)	0	100	100
26	CK	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
27	CL	225/785 (29%)	212 (94%)	12 (5%)	1 (0%)	34	72
28	CM	443/446 (99%)	417 (94%)	26 (6%)	0	100	100
29	CN	222/252 (88%)	210 (95%)	12 (5%)	0	100	100
29	CO	211/252 (84%)	197 (93%)	12 (6%)	2 (1%)	17	56
30	CP	227/322 (70%)	221 (97%)	6 (3%)	0	100	100
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	68
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	29	68
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	211 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Cb	230/264 (87%)	204 (89%)	26 (11%)	0	100	100
36	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
37	Cd	224/239 (94%)	211 (94%)	13 (6%)	0	100	100
38	Ce	155/203 (76%)	140 (90%)	15 (10%)	0	100	100
39	Cf	170/202 (84%)	164 (96%)	6 (4%)	0	100	100
40	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
42	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
43	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
44	Ck	136/161 (84%)	129 (95%)	7 (5%)	0	100	100
45	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
46	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
47	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
48	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
49	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100
52	CW	380/668 (57%)	349 (92%)	31 (8%)	0	100	100
53	UT	1987/2612 (76%)	1871 (94%)	110 (6%)	6 (0%)	41	75
54	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100	100
55	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100	100
55	UI	121/410 (30%)	121 (100%)	0	0	100	100
56	US	443/549 (81%)	415 (94%)	28 (6%)	0	100	100
57	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
58	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100	100
59	CY	119/381 (31%)	109 (92%)	10 (8%)	0	100	100
60	CZ	42/609 (7%)	34 (81%)	8 (19%)	0	100	100
61	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	8	40
All	All	21864/32830 (67%)	20513 (94%)	1321 (6%)	30 (0%)	54	84

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
53	UT	487	ILE

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Mol	Chain	Res	Type
6	UG	580	GLU
13	UQ	708	SER
17	UZ	293	ILE

4.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	648 (100%)	3 (0%)	88	94
2	UB	425/788 (54%)	423 (100%)	2 (0%)	88	94
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	652 (100%)	1 (0%)	93	98
5	UF	248/341 (73%)	248 (100%)	0	100	100
6	UG	373/474 (79%)	370 (99%)	3 (1%)	81	91
7	UJ	898/1526 (59%)	893 (99%)	5 (1%)	86	94
8	UK	159/227 (70%)	159 (100%)	0	100	100
9	UL	667/821 (81%)	666 (100%)	1 (0%)	93	98
10	UM	606/770 (79%)	602 (99%)	4 (1%)	84	93
11	UN	146/765 (19%)	146 (100%)	0	100	100
12	UO	404/456 (89%)	402 (100%)	2 (0%)	88	94
13	UQ	650/817 (80%)	649 (100%)	1 (0%)	93	98
14	UR	360/524 (69%)	359 (100%)	1 (0%)	92	97
15	UU	672/863 (78%)	669 (100%)	3 (0%)	91	96
16	UX	150/167 (90%)	150 (100%)	0	100	100
17	UZ	187/329 (57%)	183 (98%)	4 (2%)	53	79
18	CA	175/228 (77%)	173 (99%)	2 (1%)	73	88
18	CB	195/228 (86%)	194 (100%)	1 (0%)	88	94
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	319/489 (65%)	319 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	87 (99%)	1 (1%)	73	88
22	CG	331/525 (63%)	330 (100%)	1 (0%)	92	97
23	CH	303/320 (95%)	301 (99%)	2 (1%)	84	93
24	CI	661/1009 (66%)	656 (99%)	5 (1%)	81	91
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	239 (98%)	6 (2%)	49	76
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	362 (100%)	2 (0%)	88	94
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	191 (99%)	2 (1%)	76	88
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	145/215 (67%)	144 (99%)	1 (1%)	84	93
32	CR	654/916 (71%)	449 (69%)	205 (31%)	0	2
32	CS	654/916 (71%)	449 (69%)	205 (31%)	0	2
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	147 (99%)	2 (1%)	69	86
37	Cd	192/204 (94%)	191 (100%)	1 (0%)	88	94
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	122/162 (75%)	120 (98%)	2 (2%)	62	83
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	126/143 (88%)	126 (100%)	0	100	100
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	79 (100%)	0	100	100
48	Cp	46/61 (75%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	CU	137/260 (53%)	135 (98%)	2 (2%)	65	84
52	CW	309/587 (53%)	306 (99%)	3 (1%)	76	88
53	UT	1732/2276 (76%)	1719 (99%)	13 (1%)	81	91
54	UH	301/788 (38%)	297 (99%)	4 (1%)	69	86
55	UE	105/346 (30%)	105 (100%)	0	100	100
55	UI	105/346 (30%)	105 (100%)	0	100	100
56	US	404/493 (82%)	403 (100%)	1 (0%)	93	98
57	Cl	71/135 (53%)	70 (99%)	1 (1%)	67	85
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	100/322 (31%)	92 (92%)	8 (8%)	12	41
60	CZ	38/519 (7%)	37 (97%)	1 (3%)	46	74
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	18216/27810 (66%)	17715 (97%)	501 (3%)	46	72

5 of 501 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	CR	842	GLU
32	CS	856	ASP
32	CS	104	ILE
32	CS	848	LEU
53	UT	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
28	CM	77	ASN
33	CT	107	GLN
57	Cl	21	ASN
29	CN	243	HIS
32	CR	655	GLN

4.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1550/2352 (65%)	483 (31%)	33 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1776/2582 (68%)	551 (31%)	37 (2%)

5 of 551 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	5	G
50	C1	7	A
50	C1	13	G
50	C1	14	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	2054	A
51	C2	91	G
50	C1	2077	C
50	C1	2219	C
50	C1	684	U

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
63	GTP	CI	1201	-	26,34,34	0.97	1 (3%)	32,54,54	1.79	5 (15%)

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
63	GTP	CI	1201	-	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	CI	1201	GTP	C6-N1	-2.87	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	CI	1201	GTP	PA-O3A-PB	-5.41	114.27	132.83
63	CI	1201	GTP	PB-O3B-PG	-4.84	116.23	132.83
63	CI	1201	GTP	C3'-C2'-C1'	2.86	105.28	100.98
63	CI	1201	GTP	C5-C6-N1	2.76	118.83	113.95
63	CI	1201	GTP	C8-N7-C5	2.50	107.75	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	O4'-C4'-C5'-O5'
63	CI	1201	GTP	C3'-C4'-C5'-O5'

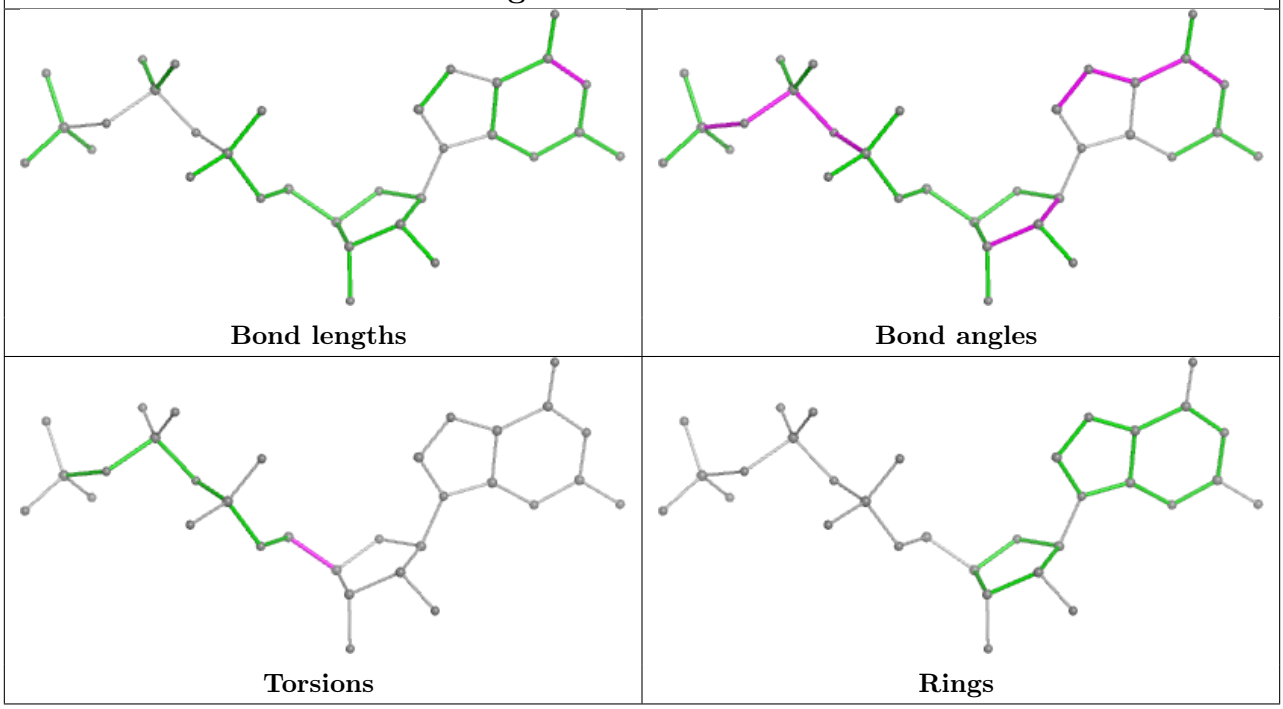
There are no ring outliers.

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 then 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 GTP CI 1201



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.77
1	C2	105:C	O3'	110:A	P	16.05
1	C2	119:C	O3'	123:A	P	11.95

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10052. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis (i)

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit (i)

This section was not generated.