



Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 10:50 AM JST

PDB ID : 8I9Y
EMDB ID : EMD-35288
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- Ytm1-2
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation 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 ⓘ 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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

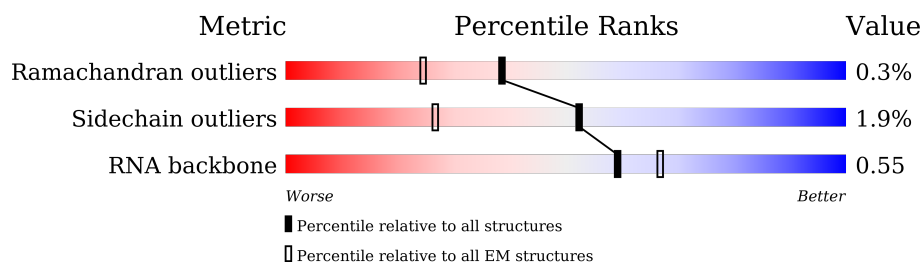
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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.



















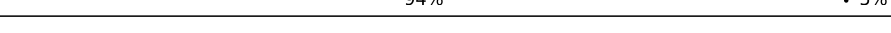




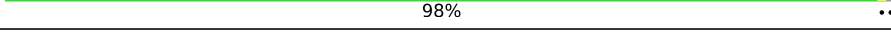


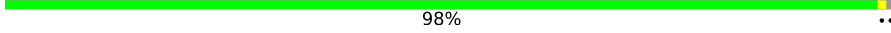
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	C1	3341	
2	C2	319	
3	CA	316	
4	CB	391	
5	CC	801	
6	CD	495	
7	CE	598	
8	CF	270	
9	CG	184	




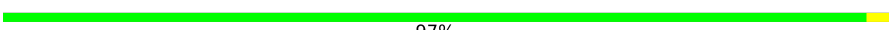






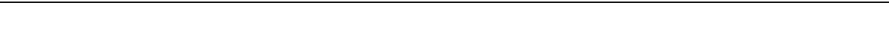

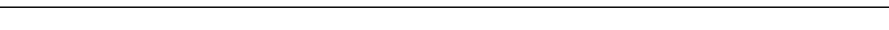
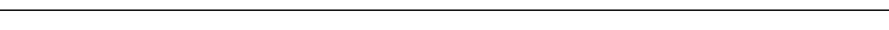
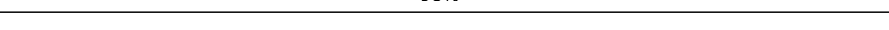


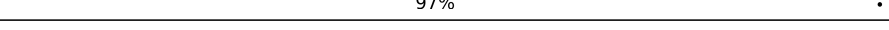
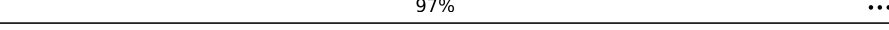
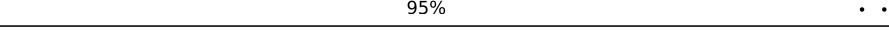





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Mol	Chain	Length	Quality of chain
10	CH	661	
11	CI	414	
12	CJ	679	
13	CK	261	
14	CL	558	
15	CM	249	
15	LF	249	
16	CN	246	
17	CO	120	
18	CP	751	
19	CQ	225	
20	CR	237	
21	CS	834	
22	CT	688	
23	CU	451	
24	CV	147	
25	CX	203	
26	CY	788	
27	Cz	123	
28	LB	392	
29	LC	365	
30	LE	200	
31	LG	262	
32	LH	192	
33	LK	165	

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Mol	Chain	Length	Quality of chain
34	LL	213	
35	LM	142	
36	LN	203	
37	LO	204	
38	LP	187	
39	LQ	213	
40	LR	2898	
41	LS	174	
42	LT	160	
43	LU	127	
44	LV	139	
45	LX	156	
46	LY	138	
47	LZ	135	
48	Lc	108	
49	Ld	120	
50	Le	131	
51	Lf	109	
52	Lg	119	
53	Lh	935	
54	Li	110	
55	Lj	95	
56	Lk	81	
57	Ll	51	
58	Lq	217	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 156553 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 RNA chain called RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	2609	Total	C	N	O	P	0	0
			55815	24911	10105	18190	2609		

- Molecule 2 is a RNA chain called RNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	256	Total	C	N	O	P	0	0
			5456	2435	974	1791	256		

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	251	Total	C	N	O	S	0	0
			2069	1324	381	357	7		

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CB	260	Total	C	N	O	S	0	0
			2063	1322	367	371	3		

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	CC	658	Total	C	N	O	P	S	0	0
			5297	3368	931	983	2	13		

- Molecule 6 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CD	460	Total	C	N	O	S	0	0
			3468	2173	610	679	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	88	ASP	GLU	conflict	UNP G0SFB5

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CE	462	Total	C	N	O	S	0	0
			3669	2350	642	666	11		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 8 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CF	245	Total	C	N	O	S	0	0
			1945	1222	352	362	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CG	177	Total	C	N	O	S	0	0
			1396	884	247	253	12		

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CH	542	Total	C	N	O	S	0	0
			4388	2784	770	818	16		

- Molecule 11 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CJ	494	Total	C	N	O	S	0	0
			4040	2575	719	734	12		

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CK	229	Total	C	N	O	S	0	0
			1835	1149	362	320	4		

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	CL	397	Total	C	N	O	0	0
			2239	1350	459	430		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CM	223	Total	C	N	O	S	0	0
			1820	1169	340	308	3		
15	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 17 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	356	Total	C	N	O	S	0	0
			2798	1777	495	510	16		

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	179	Total	C	N	O	S	0	0
			1485	926	304	245	10		

- Molecule 20 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CS	262	Total	C	N	O	S	0	0
			2105	1322	399	377	7		

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CT	488	Total	C	N	O	S	0	0
			3911	2486	690	719	16		

- Molecule 23 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

- Molecule 24 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	CV	139	Total	C	N	O		
			1073	672	213	188	0	0

- Molecule 25 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CX	88	Total	C	N	O	S		
			701	435	128	135	3	0	0

- Molecule 26 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CY	420	Total	C	N	O	S		
			3399	2181	616	590	12	0	0

- Molecule 27 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Cz	70	Total	C	N	O	S		
			592	368	120	101	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LB	356	Total	C	N	O	S		
			2829	1798	518	501	12	0	0

- Molecule 29 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LC	362	Total	C	N	O	S		
			2752	1738	526	479	9	0	0

- Molecule 30 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LE	179	Total	C	N	O	S		
			1403	898	255	247	3	0	0

- Molecule 31 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	204	Total	C	N	O	S	0	0
			1644	1060	297	282	5		

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 33 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LK	146	Total	C	N	O	S	0	0
			1112	701	203	206	2		

- Molecule 34 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 35 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 36 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 37 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 38 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	169	Total	C	N	O	S	0	0
			1345	835	273	234	3		

- Molecule 39 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 40 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LR	119	Total	C	N	O	S	0	0
			969	610	196	159	4		

- Molecule 41 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 42 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 43 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LU	105	Total	C	N	O	S	0	0
			850	551	147	151	1		

- Molecule 44 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 45 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LX	137	Total	C	N	O		
			1062	678	194	190	0	0

- Molecule 46 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LY	134	Total	C	N	O	S		
			1065	664	215	184	2	0	0

- Molecule 47 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LZ	135	Total	C	N	O	S		
			1112	713	207	188	4	0	0

- Molecule 48 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lc	98	Total	C	N	O	S		
			731	463	126	137	5	0	0

- Molecule 49 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ld	109	Total	C	N	O	S		
			890	563	171	155	1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Le	127	Total	C	N	O	S		
			1025	645	209	164	7	0	0

- Molecule 51 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lf	108	Total	C	N	O	S		
			862	546	171	144	1	0	0

- Molecule 52 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lg	117	Total	C	N	O	S	0	0
			930	578	189	159	4		

- Molecule 53 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lh	121	Total	C	N	O	S	0	0
			995	633	196	166			

- Molecule 54 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 55 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 56 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lk	75	Total	C	N	O	S	0	0
			620	394	117	107	2		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	SER	deletion	UNP G0SG89
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89

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Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	THR	deletion	UNP G0SG89

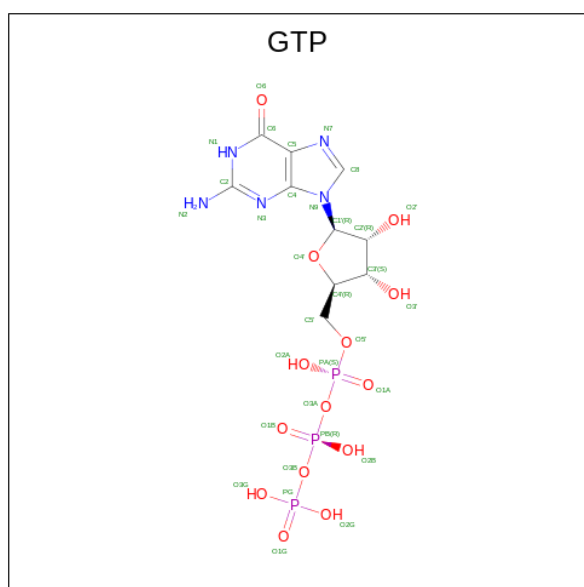
- Molecule 57 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Ll	38	Total	C	N	O	0	0
			322	204	68	50		

- Molecule 58 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Lq	207	Total	C	N	O	S	0	0
			1600	1016	285	291	8		

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



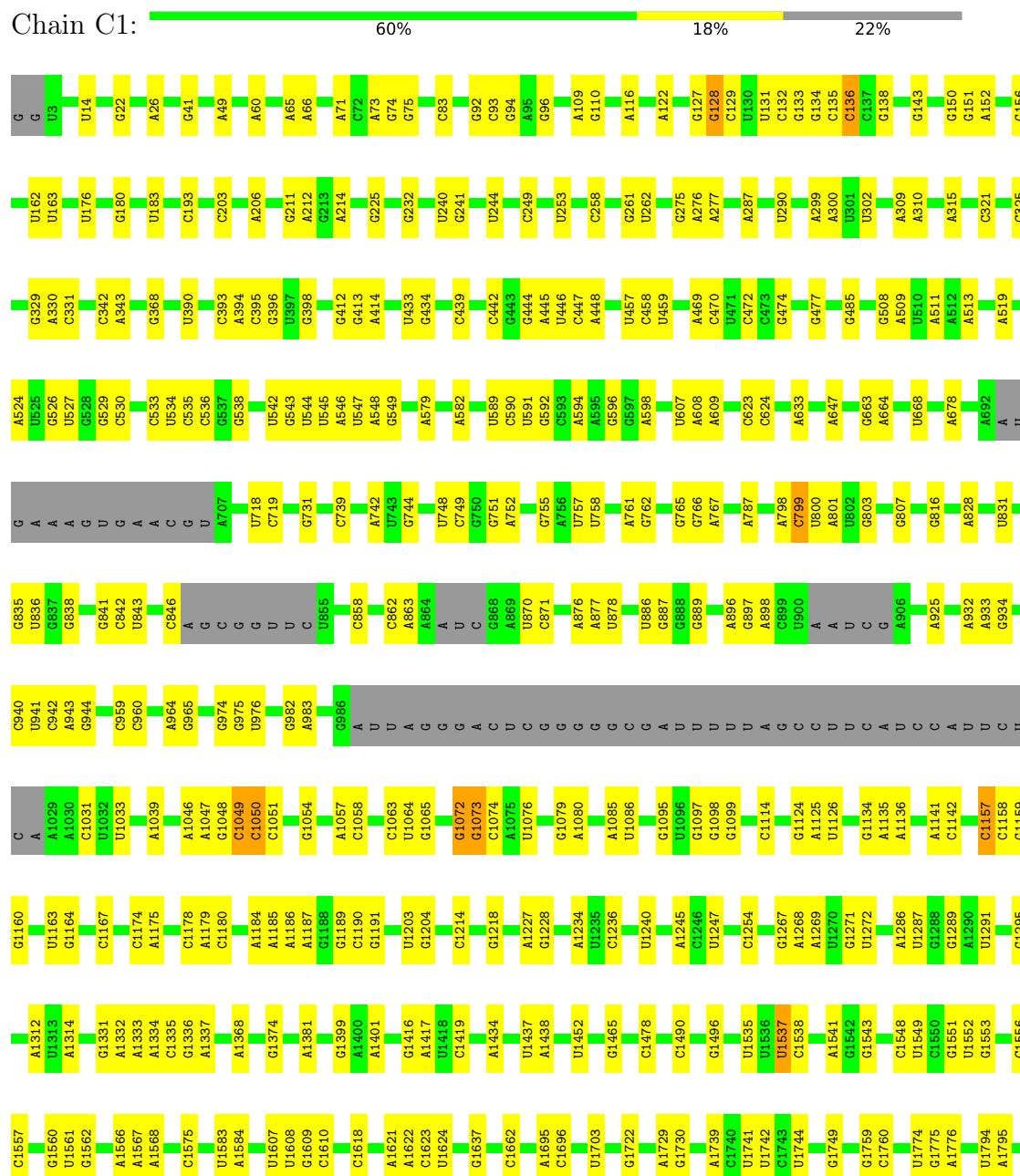
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	Lj	1	1	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (3341-MER)









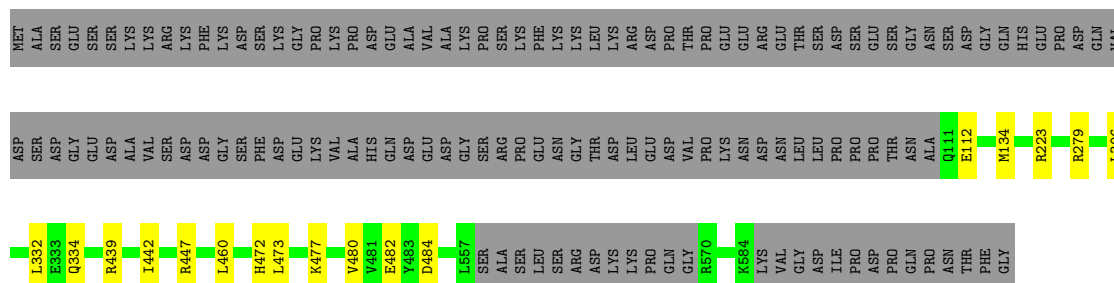
- Molecule 6: Ribosome biogenesis protein YTM1

Chain CD: 93% 7%



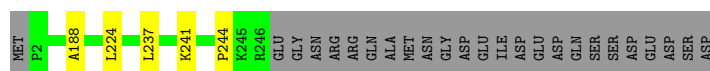
- Molecule 7: RNA helicase

Chain CE: 74% 23%



- Molecule 8: Ribosome assembly factor mrt4

Chain CF: 89% 9%



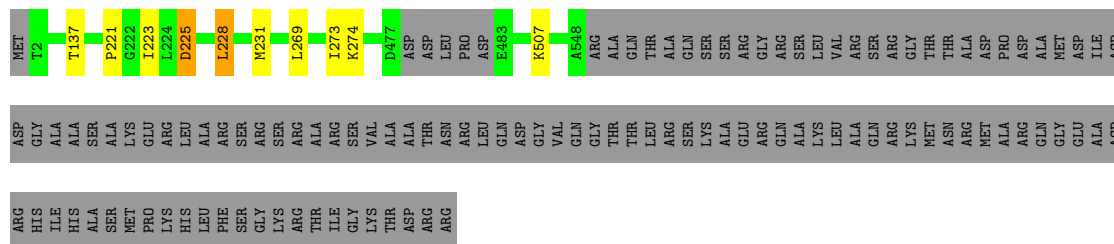
- Molecule 9: 60S ribosome subunit biogenesis protein NIP7

Chain CG: 94% 2%



- Molecule 10: Nucleolar GTP-binding protein 1

Chain CH: 80% 18%



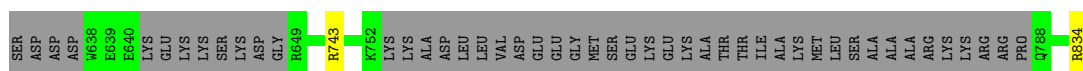
- Molecule 11: Putative RNA-binding protein

- Molecule 12: Pescadillo homolog

- Molecule 13: Ribosome biogenesis protein NSA2 homolog

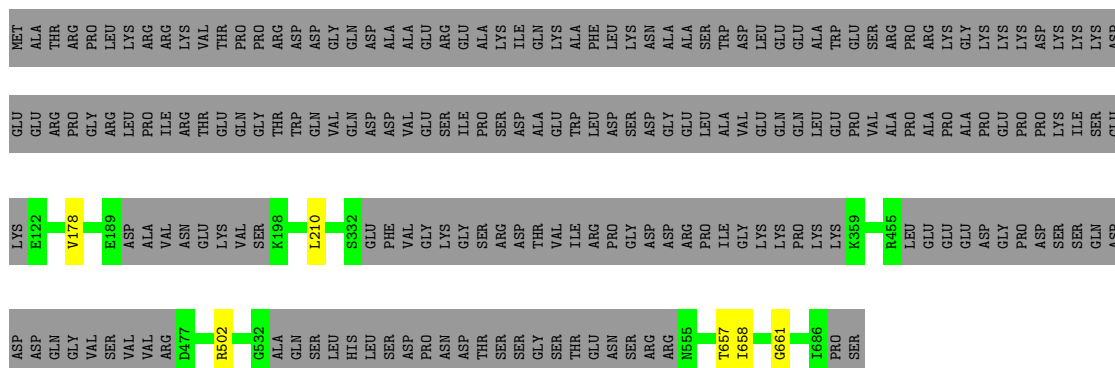
- Molecule 14: Putative GTP binding protein





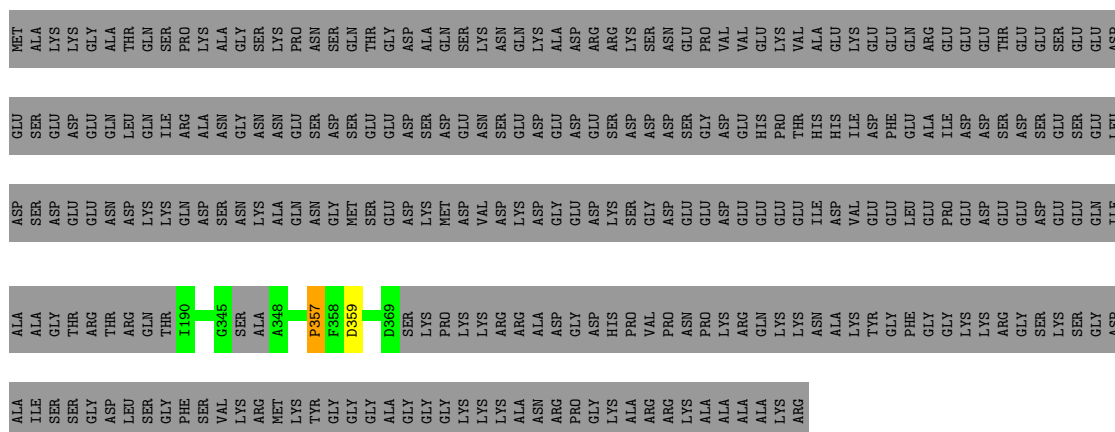
• Molecule 22: Nucleolar complex-associated protein 3

Chain CT: 70% 29%



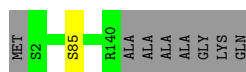
• Molecule 23: rRNA-processing protein EBP2

Chain CU: 39% 61%



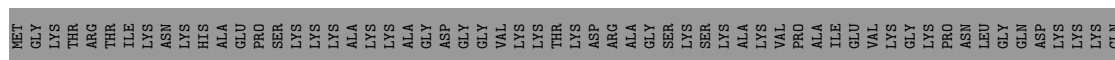
• Molecule 24: Putative 60S ribosomal protein

Chain CV: 94% 5%



• Molecule 25: 60S ribosomal subunit-like protein

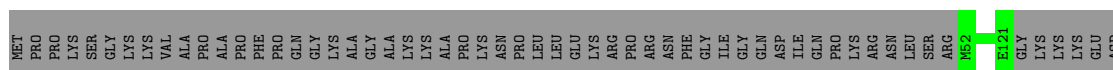
Chain CX: 43% 57%





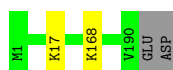
- Molecule 31: 60S ribosomal protein L8

Chain LG: 77% 22%



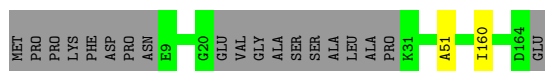
- Molecule 32: 60S ribosomal protein I9-like protein

Chain LH: 98% ..



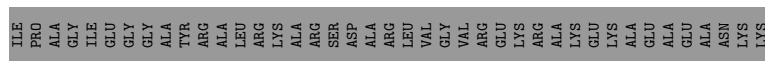
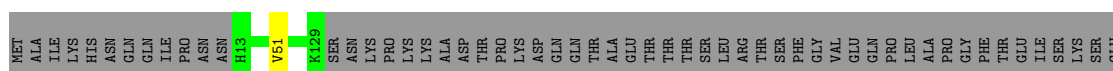
- Molecule 33: 60S ribosomal protein L12-like protein

Chain LK: 87% 12%



- Molecule 34: 60S ribosomal protein L13

Chain LL: 54% 45%



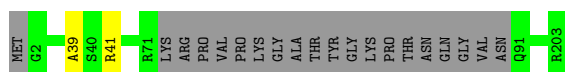
- Molecule 35: 60S ribosomal protein L14-like protein

Chain LM: 95% ..



- Molecule 36: Ribosomal protein L15

Chain LN: 89% 10%



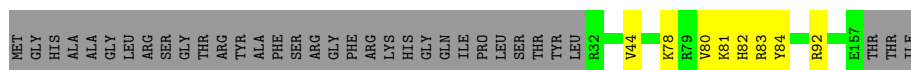






- Molecule 42: 60S ribosomal protein l21-like protein

Chain LT: 74% 5% 21%



- Molecule 43: 60S ribosomal protein L22-like protein

Chain LU: 76% 6% 17%



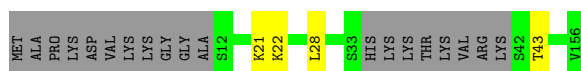
- Molecule 44: 60S ribosomal protein l23-like protein

Chain LV: 96% ..



- Molecule 45: 60S ribosomal protein L25-like protein

Chain LX: 85% . 12%



- Molecule 46: 60S ribosomal protein L26-like protein

Chain LY: 97% .



- Molecule 47: 60S ribosomal protein L27

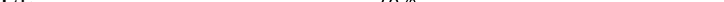
Chain LZ: 98% .



- Molecule 48: 60S ribosomal protein l30-like protein

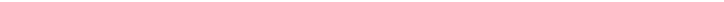
Chain Lc: 88% . 9%

- Molecule 54: 60S ribosomal protein L36

Chain Li:  78% 20%

MET	SER	GLU	ASP	ALA	THR	PRO	LYS	ALA	PRO	VAL	GLU	ARG	THR	GLY	LEU	ILE	ARG	GLY	LEU	ASN	LYS	G23	K25	H24	R37	H110
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Molecule 55: Ribosomal protein L37

Chain Lj:  77% . 22%

MET	THR	LYS	GLY	THR	SER	SER	PHE	GLY	LYS	ARG	HIS	ASN	K14	L18	R87	GLY	PRO	ALA	VAL	SER	THR	SER	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 56: 60S ribosomal protein L38-like protein

Chain Lk: 93% 7%

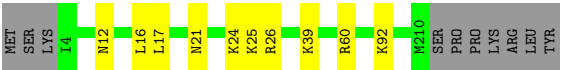
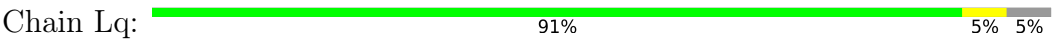
MET
 P2
 K76
 ARG
 LYS
 SER
 SER
 ALA

- Molecule 57: 60S ribosomal protein L39

Chain L1: 75% 25%

MET
P2
A39
LYS
ARG
ARG
HIS
TRP
ARG
LYS
THR
ARG
LEU
GLY
LEU

- Molecule 58: Ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70516	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	C1	0.34	0/62448	0.82	37/97346 (0.0%)
2	C2	0.30	0/6097	0.77	0/9499
3	CA	0.35	0/2115	0.63	1/2840 (0.0%)
4	CB	0.36	0/2109	0.65	0/2866
5	CC	0.31	0/5423	0.59	0/7380
6	CD	0.26	0/3543	0.58	0/4824
7	CE	0.33	0/3739	0.58	0/5040
8	CF	0.30	0/1982	0.58	0/2671
9	CG	0.31	0/1422	0.57	0/1920
10	CH	0.32	0/4468	0.57	0/6029
11	CI	0.32	0/1225	0.63	0/1645
12	CJ	0.31	0/4125	0.58	0/5548
13	CK	0.27	0/1863	0.55	0/2494
14	CL	0.29	0/2247	0.51	0/3076
15	CM	0.31	0/1851	0.58	0/2481
15	LF	0.31	0/2055	0.59	1/2758 (0.0%)
16	CN	0.31	0/1881	0.62	0/2560
17	CO	0.26	0/470	0.52	0/619
18	CP	0.32	0/2859	0.59	0/3870
19	CQ	0.32	0/1507	0.64	0/1996
20	CR	0.27	0/1369	0.59	0/1828
21	CS	0.26	0/2127	0.53	0/2817
22	CT	0.29	0/3974	0.57	0/5357
23	CU	0.31	0/1428	0.59	0/1910
24	CV	0.26	0/1091	0.54	0/1468
25	CX	0.29	0/705	0.55	0/938
26	CY	0.31	0/3454	0.63	0/4637
27	Cz	0.30	0/598	0.62	0/785
28	LB	0.32	0/2885	0.61	0/3872
29	LC	0.30	0/2809	0.55	0/3787
30	LE	0.28	0/1428	0.53	0/1921
31	LG	0.32	0/1667	0.55	0/2230

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
32	LH	0.28	0/1516	0.56	0/2038
33	LK	0.25	0/1124	0.54	0/1507
34	LL	0.30	0/983	0.63	0/1318
35	LM	0.32	0/1120	0.59	0/1507
36	LN	0.30	0/1595	0.62	1/2132 (0.0%)
37	LO	0.33	0/1652	0.58	0/2215
38	LP	0.26	0/1367	0.59	0/1838
39	LQ	0.28	0/1033	0.58	0/1391
40	LR	0.26	0/985	0.55	0/1318
41	LS	0.30	0/1468	0.58	0/1975
42	LT	0.29	0/1033	0.53	0/1389
43	LU	0.34	0/863	0.57	0/1155
44	LV	0.29	0/1013	0.54	0/1361
45	LX	0.30	0/1078	0.52	0/1451
46	LY	0.26	0/1079	0.56	0/1443
47	LZ	0.30	0/1135	0.61	0/1519
48	Lc	0.35	0/740	0.59	0/995
49	Ld	0.33	0/904	0.59	0/1209
50	Le	0.25	0/1043	0.54	0/1389
51	Lf	0.33	0/883	0.62	0/1187
52	Lg	0.34	0/943	0.61	0/1258
53	Lh	0.25	0/1006	0.54	0/1338
54	Li	0.28	0/738	0.62	0/971
55	Lj	0.34	0/606	0.68	0/803
56	Lk	0.26	0/628	0.57	0/835
57	Ll	0.24	0/329	0.54	0/440
58	Lq	0.29	0/1621	0.63	0/2180
All	All	0.32	0/165449	0.70	40/237174 (0.0%)

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
58	Lq	0	1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1050	C	N3-C2-O2	-12.25	113.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1050	C	N1-C2-O2	10.69	125.31	118.90
1	C1	1583	U	C2-N1-C1'	8.47	127.87	117.70
1	C1	136	C	N3-C2-O2	-8.14	116.20	121.90
1	C1	2723	C	N3-C2-O2	-7.78	116.46	121.90
1	C1	2452	C	N3-C2-O2	-7.68	116.52	121.90
1	C1	1583	U	N1-C2-O2	7.50	128.05	122.80
1	C1	1051	C	N3-C2-O2	-7.22	116.84	121.90
1	C1	1537	U	C2-N1-C1'	7.15	126.28	117.70
1	C1	1051	C	C6-N1-C2	-6.89	117.54	120.30
1	C1	1583	U	N3-C2-O2	-6.64	117.55	122.20
1	C1	1537	U	N3-C2-O2	-6.54	117.62	122.20
1	C1	1537	U	N1-C2-O2	6.44	127.31	122.80
3	CA	236	PRO	N-CA-CB	-6.39	95.58	102.60
1	C1	799	C	N3-C2-O2	-6.38	117.43	121.90
1	C1	1050	C	C6-N1-C2	-6.32	117.77	120.30
1	C1	83	C	C2-N3-C4	-6.08	116.86	119.90
15	LF	13	LEU	CA-CB-CG	6.05	129.21	115.30
1	C1	1157	C	C6-N1-C2	6.00	122.70	120.30
1	C1	127	G	N3-C4-N9	5.97	129.58	126.00
1	C1	1583	U	C6-N1-C1'	-5.74	113.17	121.20
1	C1	249	C	N3-C2-O2	-5.73	117.89	121.90
1	C1	128	G	C5-C6-O6	5.50	131.90	128.60
1	C1	799	C	N1-C2-O2	5.43	122.16	118.90
1	C1	2745	G	N1-C6-O6	-5.41	116.66	119.90
1	C1	2752	G	C5-C6-O6	5.38	131.83	128.60
1	C1	940	C	O4'-C1'-N1	5.36	112.48	108.20
1	C1	83	C	N1-C2-N3	5.32	122.92	119.20
36	LN	39	ALA	O-C-N	5.28	131.14	122.70
1	C1	1073	G	N1-C2-N2	-5.26	111.47	116.20
1	C1	128	G	N3-C4-N9	-5.24	122.86	126.00
1	C1	442	C	C2-N1-C1'	5.19	124.51	118.80
1	C1	2752	G	N1-C6-O6	-5.16	116.80	119.90
1	C1	398	G	O4'-C1'-N9	5.14	112.31	108.20
1	C1	127	G	C4-N9-C1'	5.11	133.14	126.50
1	C1	127	G	C8-N9-C1'	-5.10	120.37	127.00
1	C1	2745	G	C5-C6-O6	5.08	131.65	128.60
1	C1	1072	G	N1-C2-N2	-5.06	111.64	116.20
1	C1	1049	C	N1-C2-O2	5.05	121.93	118.90
1	C1	2413	G	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	Lq	60	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 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	
3	CA	247/316 (78%)	228 (92%)	16 (6%)	3 (1%)	11	38
4	CB	256/391 (66%)	228 (89%)	28 (11%)	0	100	100
5	CC	648/801 (81%)	606 (94%)	38 (6%)	4 (1%)	22	53
6	CD	450/495 (91%)	416 (92%)	34 (8%)	0	100	100
7	CE	458/598 (77%)	428 (93%)	30 (7%)	0	100	100
8	CF	243/270 (90%)	227 (93%)	14 (6%)	2 (1%)	16	48
9	CG	175/184 (95%)	163 (93%)	11 (6%)	1 (1%)	22	53
10	CH	538/661 (81%)	511 (95%)	25 (5%)	2 (0%)	30	63
11	CI	144/414 (35%)	135 (94%)	9 (6%)	0	100	100
12	CJ	484/679 (71%)	462 (96%)	21 (4%)	1 (0%)	44	74
13	CK	223/261 (85%)	212 (95%)	11 (5%)	0	100	100
14	CL	393/558 (70%)	366 (93%)	25 (6%)	2 (0%)	25	58
15	CM	219/249 (88%)	210 (96%)	9 (4%)	0	100	100
15	LF	245/249 (98%)	238 (97%)	7 (3%)	0	100	100
16	CN	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	354/751 (47%)	330 (93%)	24 (7%)	0	100	100
19	CQ	173/225 (77%)	165 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CR	159/237 (67%)	157 (99%)	2 (1%)	0	100	100
21	CS	246/834 (30%)	238 (97%)	8 (3%)	0	100	100
22	CT	478/688 (70%)	452 (95%)	24 (5%)	2 (0%)	30	63
23	CU	174/451 (39%)	170 (98%)	3 (2%)	1 (1%)	22	53
24	CV	137/147 (93%)	135 (98%)	1 (1%)	1 (1%)	19	51
25	CX	86/203 (42%)	84 (98%)	2 (2%)	0	100	100
26	CY	406/788 (52%)	371 (91%)	33 (8%)	2 (0%)	25	58
27	Cz	68/123 (55%)	64 (94%)	4 (6%)	0	100	100
28	LB	352/392 (90%)	333 (95%)	19 (5%)	0	100	100
29	LC	360/365 (99%)	344 (96%)	16 (4%)	0	100	100
30	LE	175/200 (88%)	163 (93%)	11 (6%)	1 (1%)	22	53
31	LG	200/262 (76%)	189 (94%)	11 (6%)	0	100	100
32	LH	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
33	LK	142/165 (86%)	129 (91%)	11 (8%)	2 (1%)	9	34
34	LL	115/213 (54%)	107 (93%)	7 (6%)	1 (1%)	14	45
35	LM	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
36	LN	179/203 (88%)	170 (95%)	9 (5%)	0	100	100
37	LO	202/204 (99%)	190 (94%)	9 (4%)	3 (2%)	8	33
38	LP	165/187 (88%)	160 (97%)	5 (3%)	0	100	100
39	LQ	127/213 (60%)	121 (95%)	6 (5%)	0	100	100
40	LR	115/2898 (4%)	115 (100%)	0	0	100	100
41	LS	172/174 (99%)	160 (93%)	12 (7%)	0	100	100
42	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	16	48
43	LU	103/127 (81%)	96 (93%)	7 (7%)	0	100	100
44	LV	133/139 (96%)	128 (96%)	5 (4%)	0	100	100
45	LX	133/156 (85%)	129 (97%)	4 (3%)	0	100	100
46	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
47	LZ	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
48	Lc	96/108 (89%)	93 (97%)	3 (3%)	0	100	100
49	Ld	107/120 (89%)	101 (94%)	6 (6%)	0	100	100
50	Le	125/131 (95%)	123 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	Lf	106/109 (97%)	99 (93%)	5 (5%)	2 (2%)	6	27
52	Lg	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
53	Lh	119/935 (13%)	113 (95%)	6 (5%)	0	100	100
54	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
55	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
56	Lk	73/81 (90%)	67 (92%)	6 (8%)	0	100	100
57	Ll	36/51 (71%)	33 (92%)	3 (8%)	0	100	100
58	Lq	205/217 (94%)	179 (87%)	25 (12%)	1 (0%)	25	58
All	All	11829/19680 (60%)	11173 (94%)	624 (5%)	32 (0%)	38	68

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	CA	236	PRO
5	CC	161	ASP
22	CT	502	ARG
26	CY	692	ALA
26	CY	707	PHE
34	LL	51	VAL
9	CG	43	ASP
5	CC	440	PRO
10	CH	225	ASP
10	CH	228	LEU
14	CL	439	ASP
22	CT	661	GLY
24	CV	85	SER
30	LE	191	LYS
33	LK	51	ALA
37	LO	190	LYS
3	CA	123	MET
3	CA	124	GLU
8	CF	188	ALA
37	LO	191	VAL
58	Lq	16	LEU
14	CL	446	ASP
33	LK	160	ILE
51	Lf	3	SER
51	Lf	4	GLU
12	CJ	216	GLN

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Mol	Chain	Res	Type
37	LO	65	TYR
42	LT	44	VAL
8	CF	244	PRO
5	CC	120	PRO
23	CU	357	PRO
5	CC	567	GLY

5.3.2 Protein sidechains ⓘ

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	
3	CA	223/276 (81%)	213 (96%)	10 (4%)	23	53
4	CB	222/329 (68%)	210 (95%)	12 (5%)	18	47
5	CC	578/708 (82%)	566 (98%)	12 (2%)	48	72
6	CD	381/410 (93%)	381 (100%)	0	100	100
7	CE	398/517 (77%)	381 (96%)	17 (4%)	25	55
8	CF	214/236 (91%)	211 (99%)	3 (1%)	62	81
9	CG	150/155 (97%)	147 (98%)	3 (2%)	50	74
10	CH	481/575 (84%)	471 (98%)	10 (2%)	48	72
11	CI	121/336 (36%)	119 (98%)	2 (2%)	56	78
12	CJ	428/579 (74%)	425 (99%)	3 (1%)	81	90
13	CK	195/225 (87%)	193 (99%)	2 (1%)	73	86
14	CL	72/458 (16%)	71 (99%)	1 (1%)	62	81
15	CM	191/215 (89%)	190 (100%)	1 (0%)	86	92
15	LF	213/215 (99%)	212 (100%)	1 (0%)	86	92
16	CN	206/206 (100%)	200 (97%)	6 (3%)	37	65
17	CO	48/99 (48%)	48 (100%)	0	100	100
18	CP	302/632 (48%)	295 (98%)	7 (2%)	45	70
19	CQ	150/192 (78%)	145 (97%)	5 (3%)	33	62
20	CR	144/206 (70%)	143 (99%)	1 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CS	209/716 (29%)	207 (99%)	2 (1%)	73	86
22	CT	427/600 (71%)	423 (99%)	4 (1%)	75	88
23	CU	149/376 (40%)	147 (99%)	2 (1%)	65	82
24	CV	109/112 (97%)	109 (100%)	0	100	100
25	CX	76/172 (44%)	76 (100%)	0	100	100
26	CY	364/686 (53%)	358 (98%)	6 (2%)	58	79
27	Cz	60/107 (56%)	58 (97%)	2 (3%)	33	62
28	LB	301/331 (91%)	293 (97%)	8 (3%)	40	67
29	LC	283/285 (99%)	278 (98%)	5 (2%)	54	76
30	LE	151/166 (91%)	151 (100%)	0	100	100
31	LG	175/222 (79%)	173 (99%)	2 (1%)	70	84
32	LH	167/169 (99%)	165 (99%)	2 (1%)	67	83
33	LK	121/136 (89%)	121 (100%)	0	100	100
34	LL	99/176 (56%)	99 (100%)	0	100	100
35	LM	115/117 (98%)	113 (98%)	2 (2%)	56	78
36	LN	164/180 (91%)	163 (99%)	1 (1%)	84	91
37	LO	163/163 (100%)	158 (97%)	5 (3%)	35	63
38	LP	137/152 (90%)	135 (98%)	2 (2%)	60	80
39	LQ	110/178 (62%)	109 (99%)	1 (1%)	75	88
40	LR	104/2396 (4%)	104 (100%)	0	100	100
41	LS	154/154 (100%)	151 (98%)	3 (2%)	52	75
42	LT	109/135 (81%)	102 (94%)	7 (6%)	14	42
43	LU	93/108 (86%)	85 (91%)	8 (9%)	8	31
44	LV	99/102 (97%)	98 (99%)	1 (1%)	73	86
45	LX	114/129 (88%)	110 (96%)	4 (4%)	31	61
46	LY	117/119 (98%)	117 (100%)	0	100	100
47	LZ	121/121 (100%)	118 (98%)	3 (2%)	42	69
48	Lc	79/88 (90%)	76 (96%)	3 (4%)	28	59
49	Ld	95/105 (90%)	94 (99%)	1 (1%)	70	84
50	Le	110/114 (96%)	110 (100%)	0	100	100
51	Lf	89/90 (99%)	88 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	Lg	101/102 (99%)	97 (96%)	4 (4%)	27	58
53	Lh	108/781 (14%)	108 (100%)	0	100	100
54	Li	75/93 (81%)	73 (97%)	2 (3%)	40	67
55	Lj	61/78 (78%)	60 (98%)	1 (2%)	58	79
56	Lk	71/76 (93%)	71 (100%)	0	100	100
57	Ll	34/46 (74%)	34 (100%)	0	100	100
58	Lq	179/189 (95%)	171 (96%)	8 (4%)	23	53
All	All	10010/16639 (60%)	9824 (98%)	186 (2%)	52	75

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	63	ARG
3	CA	64	LYS
3	CA	83	LEU
3	CA	120	LEU
3	CA	124	GLU
3	CA	192	ARG
3	CA	233	GLU
3	CA	236	PRO
3	CA	237	ARG
3	CA	278	ARG
4	CB	46	LYS
4	CB	47	GLN
4	CB	65	THR
4	CB	67	THR
4	CB	69	LYS
4	CB	71	HIS
4	CB	245	VAL
4	CB	274	LYS
4	CB	279	ARG
4	CB	281	PHE
4	CB	293	ILE
4	CB	295	GLN
5	CC	161	ASP
5	CC	164	ASP
5	CC	353	SER
5	CC	386	LYS
5	CC	388	ASP
5	CC	390	LEU

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Mol	Chain	Res	Type
5	CC	392	LYS
5	CC	437	GLU
5	CC	438	LEU
5	CC	439	LYS
5	CC	564	GLU
5	CC	626	GLN
7	CE	112	GLU
7	CE	134	MET
7	CE	223	ARG
7	CE	279	ARG
7	CE	306	LEU
7	CE	332	LEU
7	CE	334	GLN
7	CE	439	ARG
7	CE	442	ILE
7	CE	447	ARG
7	CE	460	LEU
7	CE	472	HIS
7	CE	473	LEU
7	CE	477	LYS
7	CE	480	VAL
7	CE	482	GLU
7	CE	484	ASP
8	CF	224	LEU
8	CF	237	LEU
8	CF	241	LYS
9	CG	61	ARG
9	CG	63	LYS
9	CG	64	LEU
10	CH	137	THR
10	CH	221	PRO
10	CH	223	ILE
10	CH	225	ASP
10	CH	228	LEU
10	CH	231	MET
10	CH	269	LEU
10	CH	273	ILE
10	CH	274	LYS
10	CH	507	LYS
11	CI	215	ARG
11	CI	295	ARG
12	CJ	193	LYS

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Mol	Chain	Res	Type
12	CJ	195	ILE
12	CJ	217	ARG
13	CK	49	LEU
13	CK	53	GLN
14	CL	18	THR
15	CM	52	LYS
16	CN	109	VAL
16	CN	111	ASN
16	CN	152	MET
16	CN	154	LEU
16	CN	160	LEU
16	CN	223	ARG
18	CP	289	PRO
18	CP	290	PRO
18	CP	436	CYS
18	CP	439	ASP
18	CP	441	ARG
18	CP	443	PHE
18	CP	481	MET
19	CQ	134	LEU
19	CQ	137	LEU
19	CQ	138	ARG
19	CQ	144	ARG
19	CQ	162	GLU
20	CR	60	LYS
21	CS	743	ARG
21	CS	834	ARG
22	CT	178	VAL
22	CT	210	LEU
22	CT	657	THR
22	CT	658	ILE
23	CU	357	PRO
23	CU	359	ASP
26	CY	637	ILE
26	CY	640	PRO
26	CY	690	ARG
26	CY	693	LYS
26	CY	707	PHE
26	CY	747	ARG
27	Cz	52	VAL
27	Cz	53	LYS
28	LB	17	LEU

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Mol	Chain	Res	Type
28	LB	19	ARG
28	LB	126	LYS
28	LB	283	ILE
28	LB	349	ARG
28	LB	350	LYS
28	LB	354	LYS
28	LB	355	VAL
29	LC	22	VAL
29	LC	25	LYS
29	LC	262	ILE
29	LC	264	GLN
29	LC	266	ASP
15	LF	116	GLN
31	LG	160	VAL
31	LG	164	GLU
32	LH	17	LYS
32	LH	168	LYS
35	LM	112	LEU
35	LM	122	ARG
36	LN	41	ARG
37	LO	64	ARG
37	LO	190	LYS
37	LO	194	LYS
37	LO	196	SER
37	LO	199	LEU
38	LP	43	ARG
38	LP	174	ARG
39	LQ	119	ARG
41	LS	131	LYS
41	LS	133	GLU
41	LS	146	LYS
42	LT	78	LYS
42	LT	80	VAL
42	LT	81	LYS
42	LT	82	HIS
42	LT	83	ARG
42	LT	84	TYR
42	LT	92	ARG
43	LU	19	LYS
43	LU	50	ASP
43	LU	58	ASP
43	LU	59	VAL

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Mol	Chain	Res	Type
43	LU	61	LYS
43	LU	73	ILE
43	LU	76	ASN
43	LU	77	ASP
44	LV	95	LEU
45	LX	21	LYS
45	LX	22	LYS
45	LX	28	LEU
45	LX	43	THR
47	LZ	11	LEU
47	LZ	92	LYS
47	LZ	111	LYS
48	Lc	47	ILE
48	Lc	62	TYR
48	Lc	70	VAL
49	Ld	73	LYS
51	Lf	4	GLU
52	Lg	58	LEU
52	Lg	61	ARG
52	Lg	95	LEU
52	Lg	115	LYS
54	Li	25	LYS
54	Li	37	ARG
55	Lj	18	LEU
58	Lq	12	ASN
58	Lq	17	LEU
58	Lq	21	ASN
58	Lq	24	LYS
58	Lq	25	LYS
58	Lq	26	ARG
58	Lq	39	LYS
58	Lq	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	109	ASN
3	CA	178	HIS
4	CB	277	ASN
4	CB	280	ASN
5	CC	446	GLN
5	CC	626	GLN

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Mol	Chain	Res	Type
5	CC	637	GLN
5	CC	653	GLN
5	CC	716	HIS
9	CG	41	GLN
9	CG	113	ASN
10	CH	237	GLN
10	CH	258	GLN
11	CI	209	GLN
12	CJ	153	ASN
12	CJ	485	HIS
12	CJ	506	GLN
15	CM	203	GLN
16	CN	66	ASN
16	CN	82	GLN
16	CN	86	ASN
16	CN	118	HIS
17	CO	13	ASN
18	CP	437	ASN
18	CP	482	GLN
18	CP	489	GLN
21	CS	744	GLN
22	CT	215	HIS
22	CT	323	ASN
22	CT	436	GLN
23	CU	364	ASN
25	CX	113	GLN
26	CY	636	ASN
15	LF	119	ASN
15	LF	178	ASN
31	LG	212	ASN
34	LL	114	GLN
35	LM	98	ASN
38	LP	118	GLN
38	LP	120	ASN
44	LV	134	ASN
48	Lc	72	HIS
55	Lj	76	ASN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2594/3341 (77%)	571 (22%)	40 (1%)
2	C2	254/319 (79%)	49 (19%)	1 (0%)
All	All	2848/3660 (77%)	620 (21%)	41 (1%)

All (620) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	22	G
1	C1	26	A
1	C1	41	G
1	C1	49	A
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	71	A
1	C1	73	A
1	C1	74	G
1	C1	75	G
1	C1	92	G
1	C1	93	C
1	C1	94	G
1	C1	96	G
1	C1	109	A
1	C1	110	G
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	135	C
1	C1	136	C
1	C1	138	G
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G

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Mol	Chain	Res	Type
1	C1	162	U
1	C1	163	U
1	C1	176	U
1	C1	180	G
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	214	A
1	C1	225	G
1	C1	232	G
1	C1	240	U
1	C1	241	G
1	C1	244	U
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	262	U
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	299	A
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	330	A
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	390	U
1	C1	393	C
1	C1	394	A

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Mol	Chain	Res	Type
1	C1	395	C
1	C1	396	G
1	C1	412	G
1	C1	413	G
1	C1	414	A
1	C1	433	U
1	C1	434	G
1	C1	439	C
1	C1	444	G
1	C1	445	A
1	C1	446	U
1	C1	447	C
1	C1	448	A
1	C1	457	U
1	C1	458	C
1	C1	459	U
1	C1	469	A
1	C1	470	C
1	C1	472	C
1	C1	474	G
1	C1	477	G
1	C1	485	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	519	A
1	C1	524	A
1	C1	526	G
1	C1	527	U
1	C1	529	G
1	C1	530	C
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	536	C
1	C1	538	G
1	C1	542	U
1	C1	543	G
1	C1	544	U
1	C1	545	U
1	C1	546	A

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Mol	Chain	Res	Type
1	C1	547	U
1	C1	548	A
1	C1	549	G
1	C1	579	A
1	C1	582	A
1	C1	589	U
1	C1	590	C
1	C1	591	U
1	C1	592	G
1	C1	594	A
1	C1	596	G
1	C1	598	A
1	C1	607	U
1	C1	608	A
1	C1	609	A
1	C1	623	C
1	C1	624	C
1	C1	633	A
1	C1	647	A
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	718	U
1	C1	719	C
1	C1	731	G
1	C1	739	C
1	C1	742	A
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	755	G
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	766	G
1	C1	767	A
1	C1	787	A

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Mol	Chain	Res	Type
1	C1	798	A
1	C1	799	C
1	C1	800	U
1	C1	801	A
1	C1	803	G
1	C1	807	G
1	C1	816	G
1	C1	828	A
1	C1	831	U
1	C1	835	G
1	C1	836	U
1	C1	838	G
1	C1	841	G
1	C1	842	C
1	C1	843	U
1	C1	846	C
1	C1	858	C
1	C1	862	C
1	C1	863	A
1	C1	871	C
1	C1	876	A
1	C1	877	A
1	C1	878	U
1	C1	887	G
1	C1	889	G
1	C1	896	A
1	C1	898	A
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	941	U
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	959	C
1	C1	960	C
1	C1	964	A
1	C1	965	G
1	C1	974	G
1	C1	975	G
1	C1	976	U

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Mol	Chain	Res	Type
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1046	A
1	C1	1047	A
1	C1	1048	G
1	C1	1049	C
1	C1	1050	C
1	C1	1054	G
1	C1	1057	A
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1065	G
1	C1	1072	G
1	C1	1073	G
1	C1	1074	C
1	C1	1076	U
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1095	G
1	C1	1097	G
1	C1	1098	G
1	C1	1099	G
1	C1	1114	C
1	C1	1124	G
1	C1	1125	A
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1157	C
1	C1	1158	C
1	C1	1159	G
1	C1	1160	G
1	C1	1163	U
1	C1	1164	G
1	C1	1167	C

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Mol	Chain	Res	Type
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1179	A
1	C1	1180	C
1	C1	1184	A
1	C1	1185	A
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1191	G
1	C1	1203	U
1	C1	1204	G
1	C1	1214	C
1	C1	1218	G
1	C1	1227	A
1	C1	1228	G
1	C1	1234	A
1	C1	1236	C
1	C1	1240	U
1	C1	1245	A
1	C1	1247	U
1	C1	1254	C
1	C1	1267	G
1	C1	1268	A
1	C1	1269	A
1	C1	1271	G
1	C1	1272	U
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1314	A
1	C1	1331	G
1	C1	1332	A
1	C1	1333	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G

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Mol	Chain	Res	Type
1	C1	1337	A
1	C1	1368	A
1	C1	1374	G
1	C1	1381	A
1	C1	1399	G
1	C1	1401	A
1	C1	1416	G
1	C1	1417	A
1	C1	1419	C
1	C1	1434	A
1	C1	1437	U
1	C1	1438	A
1	C1	1452	U
1	C1	1465	G
1	C1	1478	C
1	C1	1490	C
1	C1	1496	G
1	C1	1535	U
1	C1	1537	U
1	C1	1538	C
1	C1	1541	A
1	C1	1543	G
1	C1	1548	C
1	C1	1549	U
1	C1	1551	G
1	C1	1552	U
1	C1	1553	G
1	C1	1556	C
1	C1	1557	C
1	C1	1560	G
1	C1	1561	U
1	C1	1562	G
1	C1	1566	A
1	C1	1567	A
1	C1	1568	A
1	C1	1575	C
1	C1	1584	A
1	C1	1607	U
1	C1	1608	U
1	C1	1609	G
1	C1	1610	C
1	C1	1618	C

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Mol	Chain	Res	Type
1	C1	1621	A
1	C1	1622	A
1	C1	1623	C
1	C1	1624	U
1	C1	1637	G
1	C1	1662	C
1	C1	1695	A
1	C1	1696	C
1	C1	1703	U
1	C1	1722	G
1	C1	1729	A
1	C1	1730	G
1	C1	1739	A
1	C1	1741	U
1	C1	1742	U
1	C1	1744	U
1	C1	1749	G
1	C1	1759	G
1	C1	1760	C
1	C1	1774	U
1	C1	1775	G
1	C1	1776	A
1	C1	1794	U
1	C1	1795	A
1	C1	1798	U
1	C1	1799	C
1	C1	1800	U
1	C1	1818	A
1	C1	1819	U
1	C1	1820	A
1	C1	1821	A
1	C1	1825	C
1	C1	1828	C
1	C1	1829	A
1	C1	1837	A
1	C1	1842	G
1	C1	1843	A
1	C1	1845	C
1	C1	1857	G
1	C1	1858	A
1	C1	1859	U
1	C1	1861	G

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Mol	Chain	Res	Type
1	C1	1864	C
1	C1	1865	A
1	C1	1866	A
1	C1	1867	U
1	C1	1874	A
1	C1	1875	A
1	C1	2297	G
1	C1	2298	U
1	C1	2302	U
1	C1	2310	A
1	C1	2311	U
1	C1	2325	A
1	C1	2327	C
1	C1	2334	A
1	C1	2335	A
1	C1	2338	G
1	C1	2342	U
1	C1	2343	G
1	C1	2345	C
1	C1	2347	A
1	C1	2350	U
1	C1	2355	G
1	C1	2356	G
1	C1	2359	A
1	C1	2361	A
1	C1	2362	G
1	C1	2363	A
1	C1	2364	A
1	C1	2384	C
1	C1	2396	U
1	C1	2397	G
1	C1	2399	G
1	C1	2407	A
1	C1	2409	A
1	C1	2410	G
1	C1	2413	G
1	C1	2414	G
1	C1	2415	U
1	C1	2422	U
1	C1	2424	G
1	C1	2425	G
1	C1	2428	G

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Mol	Chain	Res	Type
1	C1	2430	A
1	C1	2434	U
1	C1	2435	C
1	C1	2436	G
1	C1	2437	G
1	C1	2438	C
1	C1	2439	G
1	C1	2442	A
1	C1	2443	G
1	C1	2444	U
1	C1	2449	U
1	C1	2453	A
1	C1	2456	A
1	C1	2464	U
1	C1	2465	G
1	C1	2466	U
1	C1	2467	U
1	C1	2484	G
1	C1	2551	A
1	C1	2553	A
1	C1	2558	C
1	C1	2560	G
1	C1	2564	G
1	C1	2730	C
1	C1	2735	G
1	C1	2736	A
1	C1	2738	A
1	C1	2739	U
1	C1	2740	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2765	U
1	C1	2775	A
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2786	G
1	C1	2806	G

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Mol	Chain	Res	Type
1	C1	2818	U
1	C1	2819	U
1	C1	2820	U
1	C1	2845	A
1	C1	2846	U
1	C1	2847	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2889	C
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2901	G
1	C1	2902	U
1	C1	2917	C
1	C1	2922	G
1	C1	2923	U
1	C1	2926	G
1	C1	2935	G
1	C1	2936	U
1	C1	2942	C
1	C1	2948	G
1	C1	2950	U
1	C1	2954	C
1	C1	2955	U
1	C1	2956	C
1	C1	2969	A
1	C1	3006	A
1	C1	3014	U
1	C1	3015	U
1	C1	3016	G
1	C1	3035	G
1	C1	3036	U
1	C1	3037	G
1	C1	3043	A
1	C1	3049	C
1	C1	3050	C
1	C1	3070	A
1	C1	3074	C

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Mol	Chain	Res	Type
1	C1	3079	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3098	A
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3110	C
1	C1	3111	U
1	C1	3112	A
1	C1	3113	C
1	C1	3118	A
1	C1	3122	U
1	C1	3124	U
1	C1	3126	G
1	C1	3127	A
1	C1	3130	U
1	C1	3131	A
1	C1	3132	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3153	U
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3168	U
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3181	C
1	C1	3183	C
1	C1	3185	A
1	C1	3188	U
1	C1	3199	A
1	C1	3205	C
1	C1	3209	U

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Mol	Chain	Res	Type
1	C1	3210	U
1	C1	3213	A
1	C1	3217	U
1	C1	3227	C
1	C1	3228	G
1	C1	3229	G
1	C1	3230	G
1	C1	3244	C
1	C1	3253	U
1	C1	3255	G
1	C1	3256	A
1	C1	3258	G
1	C1	3259	U
1	C1	3270	C
1	C1	3274	U
1	C1	3280	G
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3291	U
1	C1	3293	G
1	C1	3295	U
1	C1	3298	U
1	C1	3309	G
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3325	U
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
2	C2	34	U
2	C2	35	C
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	84	C

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Mol	Chain	Res	Type
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	103	G
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	110	C
2	C2	111	A
2	C2	112	U
2	C2	113	U
2	C2	125	U
2	C2	148	G
2	C2	158	U
2	C2	163	C
2	C2	165	U
2	C2	166	C
2	C2	168	A
2	C2	173	U
2	C2	174	G
2	C2	181	U
2	C2	189	A
2	C2	195	G
2	C2	196	G
2	C2	203	G
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	219	A
2	C2	221	U
2	C2	222	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	294	A
2	C2	295	G
2	C2	300	A
2	C2	302	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	132	C
1	C1	150	G
1	C1	412	G
1	C1	445	A
1	C1	446	U
1	C1	524	A
1	C1	526	G
1	C1	543	G
1	C1	590	C
1	C1	835	G
1	C1	862	C
1	C1	870	U
1	C1	886	U
1	C1	897	G
1	C1	959	C
1	C1	964	A
1	C1	1063	C
1	C1	1134	G
1	C1	1136	A
1	C1	2301	C
1	C1	2333	G
1	C1	2360	A
1	C1	2759	A
1	C1	2777	A
1	C1	2785	U
1	C1	2817	U
1	C1	2898	A
1	C1	2925	A
1	C1	3013	U
1	C1	3014	U
1	C1	3078	U
1	C1	3131	A
1	C1	3162	A
1	C1	3204	G
1	C1	3209	U
1	C1	3229	G
1	C1	3255	G
1	C1	3257	U
1	C1	3297	U
1	C1	3330	U
2	C2	102	U

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

2 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
5	TPO	CC	163	5	8,10,11	0.76	0	10,14,16	1.32	2 (20%)
5	SEP	CC	160	5	8,9,10	1.54	1 (12%)	8,12,14	1.50	2 (25%)

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
5	TPO	CC	163	5	-	6/9/11/13	-
5	SEP	CC	160	5	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	CC	160	SEP	P-O1P	3.39	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	CC	160	SEP	P-OG-CB	-2.81	110.56	118.30
5	CC	163	TPO	O-C-CA	-2.80	117.44	124.78
5	CC	160	SEP	OG-CB-CA	2.61	110.68	108.14
5	CC	163	TPO	P-OG1-CB	2.23	129.94	123.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	N-CA-CB-OG1
5	CC	163	TPO	C-CA-CB-CG2
5	CC	163	TPO	O-C-CA-CB
5	CC	163	TPO	CG2-CB-OG1-P
5	CC	163	TPO	CB-OG1-P-O1P
5	CC	163	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 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	$\# Z > 2$
59	GTP	CH	1001	-	26,34,34	1.12	2 (7%)	32,54,54	1.49	7 (21%)

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	GTP	CH	1001	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CH	1001	GTP	C5-C6	-3.96	1.39	1.47
59	CH	1001	GTP	C2-N3	2.12	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CH	1001	GTP	C5-C6-N1	3.22	119.63	113.95
59	CH	1001	GTP	C8-N7-C5	3.08	108.85	102.99
59	CH	1001	GTP	PB-O3B-PG	-3.01	122.51	132.83
59	CH	1001	GTP	PA-O3A-PB	-2.92	122.79	132.83
59	CH	1001	GTP	C2-N1-C6	-2.85	119.85	125.10
59	CH	1001	GTP	C3'-C2'-C1'	2.56	104.83	100.98
59	CH	1001	GTP	O6-C6-C5	-2.01	120.44	124.37

There are no chirality outliers.

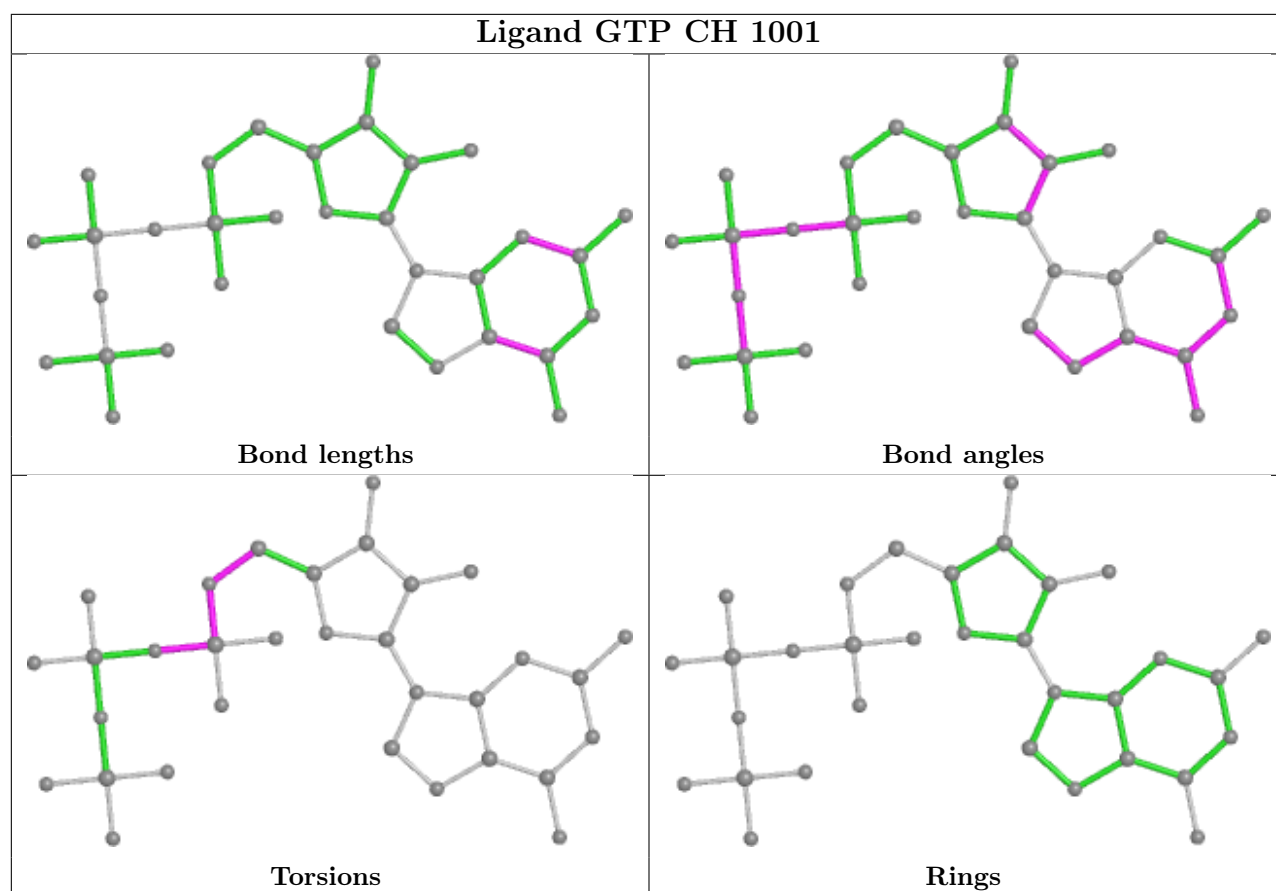
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	CH	1001	GTP	C5'-O5'-PA-O3A
59	CH	1001	GTP	PB-O3A-PA-O2A
59	CH	1001	GTP	C4'-C5'-O5'-PA
59	CH	1001	GTP	C5'-O5'-PA-O2A

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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.