



## wwPDB EM Validation Summary Report

Mar 6, 2025 – 03:06 pm GMT

PDB ID : 8S1P  
EMDB ID : EMD-19638  
Title : YlmH bound to PtRNA-50S  
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.  
Deposited on : 2024-02-15  
Resolution : 1.96 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](mailto: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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, 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) : 2.41



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Mol	Chain	Length	Quality of chain
8	E	207	98%
9	F	179	92% 7%
10	G	179	86% 11%
11	J	145	98%
12	K	122	98%
13	L	146	98%
14	M	144	93% 6%
15	N	120	94%
16	O	120	99%
17	P	115	97%
18	Q	119	97%
19	R	102	100%
20	S	113	96%
21	T	95	96%
22	U	103	98%
23	W	94	84% 15%
24	X	62	95%
25	Y	66	98%
26	Z	59	98%
27	b	4	100%
28	V	275	88% 9%
29	a	76	61% 30% 9%
30	0	59	88% 10%
31	1	49	100%
32	2	44	98%

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 91097 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 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	64	512	321	107	82	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	37	297	186	60	46	5	0	0

- Molecule 3 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	46	356	222	63	66	5	0	0

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	A	2733	58713	26198	10859	18924	2732	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	B	112	2392	1068	435	778	111	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	273	2094	1302	412	374	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	207	1575	988	290	292	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	206	1567	983	290	292	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	178	1405	893	245	260	7	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	175	1342	835	248	257	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	143	1131	714	207	205	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	122	921	571	173	173	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	146	1082	671	207	202	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	135	1076	690	205	176	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	119	954	583	186	181	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	120	913	564	176	172	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	113	922	588	177	156	1	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	118	950	597	191	158	4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	102	795	506	140	148	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	110	850	530	165	151	4	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace	
23	W	80	Total	C	N	O		0	0
			611	378	119	114			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	61	Total	C	N	O	S	0	0
			468	289	98	79	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 27 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
27	b	4	Total	C	N	O		0	0
			20	12	4	4			

- Molecule 28 is a protein called Putative RNA-binding protein YlmH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	249	1988	1256	350	376	6	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	258	GLY	-	expression tag	UNP P71020
V	259	SER	-	expression tag	UNP P71020
V	260	GLY	-	expression tag	UNP P71020
V	261	SER	-	expression tag	UNP P71020
V	262	GLY	-	expression tag	UNP P71020
V	263	SER	-	expression tag	UNP P71020
V	264	GLY	-	expression tag	UNP P71020
V	265	SER	-	expression tag	UNP P71020
V	266	GLY	-	expression tag	UNP P71020
V	267	SER	-	expression tag	UNP P71020
V	268	ASP	-	expression tag	UNP P71020
V	269	TYR	-	expression tag	UNP P71020
V	270	LYS	-	expression tag	UNP P71020
V	271	ASP	-	expression tag	UNP P71020
V	272	ASP	-	expression tag	UNP P71020
V	273	ASP	-	expression tag	UNP P71020
V	274	ASP	-	expression tag	UNP P71020
V	275	LYS	-	expression tag	UNP P71020

- Molecule 29 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	a	69	1477	657	268	483	69	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	0	53	418	258	84	69	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	1	49	411	250	82	75	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	2	44	368	222	89	55	2	0	0

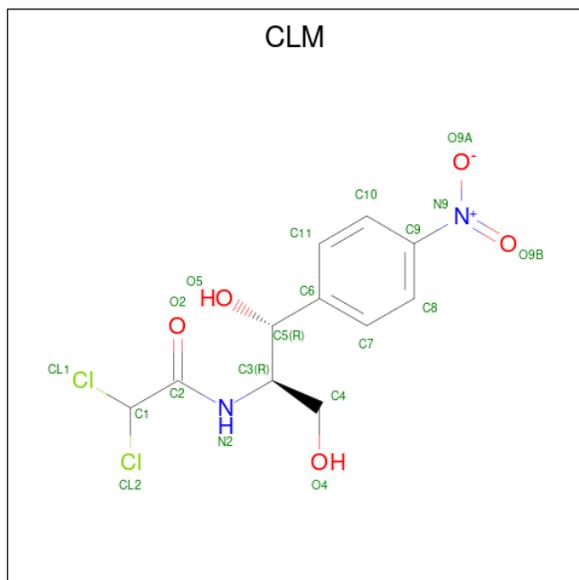
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	4	1	Total	Zn	0
			1	1	
33	6	1	Total	Zn	0
			1	1	
33	0	1	Total	Zn	0
			1	1	
33	1	1	Total	Zn	0
			1	1	

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	A	45	Total	K	0
			45	45	
34	C	2	Total	K	0
			2	2	

- Molecule 35 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C<sub>11</sub>H<sub>12</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
35	A	1	20	11	2	2	5	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	154	Total	Mg	0
			154	154	
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	N	1	Total	Mg	0
			1	1	
36	a	1	Total	Mg	0
			1	1	

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	3	15	Total	O	0
			15	15	
37	4	3	Total	O	0
			3	3	
37	A	2422	Total	O	0
			2422	2422	
37	B	10	Total	O	0
			10	10	
37	C	55	Total	O	0
			55	55	
37	D	28	Total	O	0
			28	28	
37	E	28	Total	O	0
			28	28	
37	J	13	Total	O	0
			13	13	
37	K	15	Total	O	0
			15	15	
37	L	25	Total	O	0
			25	25	
37	M	12	Total	O	0
			12	12	
37	N	20	Total	O	0
			20	20	

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Mol	Chain	Residues	Atoms		AltConf
37	P	15	Total 15	O 15	0
37	Q	24	Total 24	O 24	0
37	R	16	Total 16	O 16	0
37	S	13	Total 13	O 13	0
37	T	8	Total 8	O 8	0
37	U	3	Total 3	O 3	0
37	W	7	Total 7	O 7	0
37	X	6	Total 6	O 6	0
37	Z	4	Total 4	O 4	0
37	a	2	Total 2	O 2	0
37	0	14	Total 14	O 14	0
37	2	13	Total 13	O 13	0

### 3 Residue-property plots [i](#)

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: 50S ribosomal protein L35

Chain 3:  92% 5% .



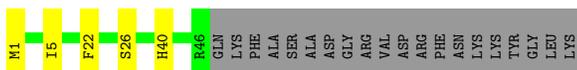
- Molecule 2: 50S ribosomal protein L36

Chain 4:  100%

There are no outlier residues recorded for this chain.

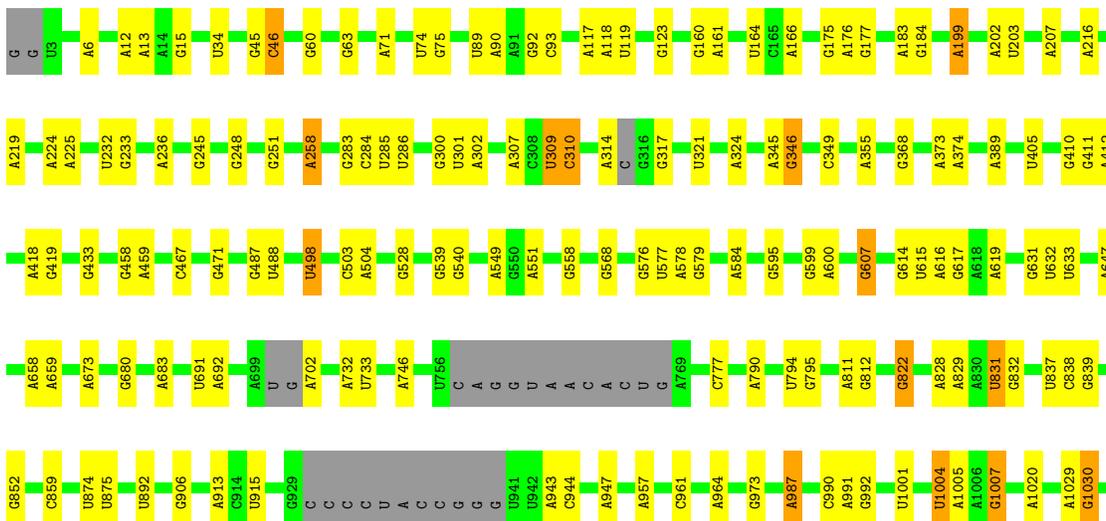
- Molecule 3: 50S ribosomal protein L31

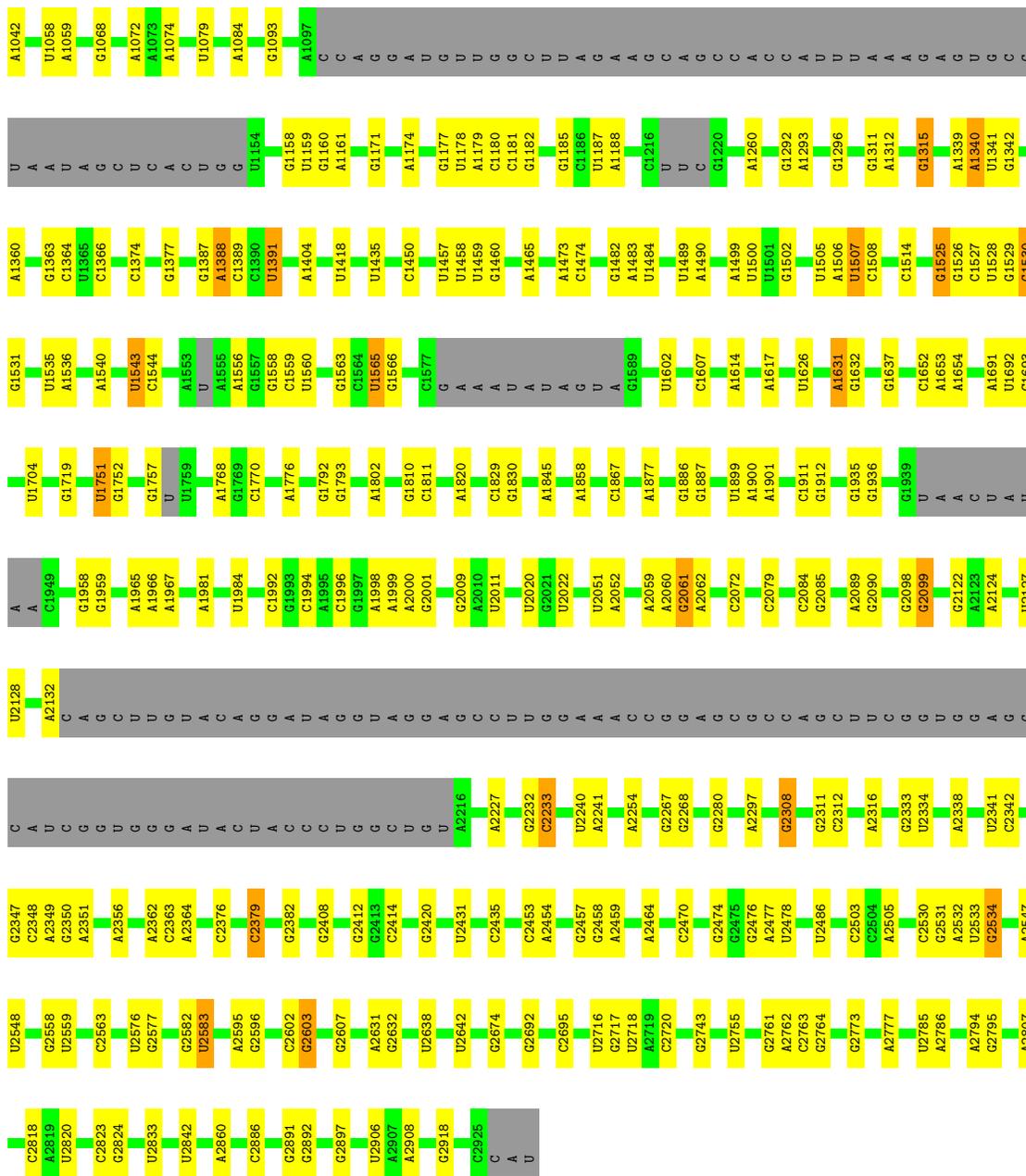
Chain 6:  62% 8% 30%



- Molecule 4: 23S rRNA

Chain A:  79% 14% 7%





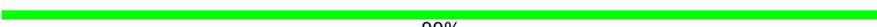
• Molecule 5: 5S rRNA



• Molecule 6: 50S ribosomal protein L2



- Molecule 7: 50S ribosomal protein L3

Chain D:  99%



- Molecule 8: 50S ribosomal protein L4

Chain E:  98%



- Molecule 9: 50S ribosomal protein L5

Chain F:  92% 7%

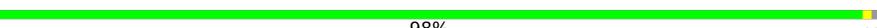


- Molecule 10: Large ribosomal subunit protein uL6

Chain G:  86% 11%

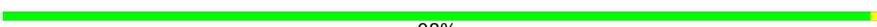


- Molecule 11: 50S ribosomal protein L13

Chain J:  98%



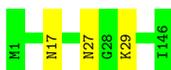
- Molecule 12: 50S ribosomal protein L14

Chain K:  98%



- Molecule 13: 50S ribosomal protein L15

Chain L:  98%



- Molecule 14: 50S ribosomal protein L16

Chain M:  93% 6%



- Molecule 15: 50S ribosomal protein L17

Chain N:  94%



- Molecule 16: 50S ribosomal protein L18

Chain O:  99%

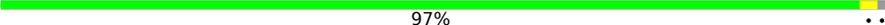


- Molecule 17: 50S ribosomal protein L19

Chain P:  97%



- Molecule 18: Large ribosomal subunit protein bL20

Chain Q:  97%

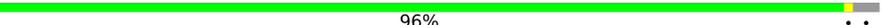


- Molecule 19: 50S ribosomal protein L21

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: 50S ribosomal protein L22

Chain S:  96%



- Molecule 21: Large ribosomal subunit protein uL23

Chain T:  96%



- Molecule 22: 50S ribosomal protein L24

Chain U: 98%



- Molecule 23: Large ribosomal subunit protein bL27

Chain W: 84% 15%



- Molecule 24: 50S ribosomal protein L28

Chain X: 95%



- Molecule 25: 50S ribosomal protein L29

Chain Y: 98%



- Molecule 26: Large ribosomal subunit protein uL30

Chain Z: 98%



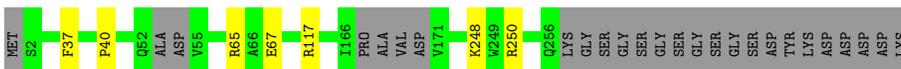
- Molecule 27: Nascent chain

Chain b: 100%

There are no outlier residues recorded for this chain.

- Molecule 28: Putative RNA-binding protein YlmH

Chain V: 88% 9%



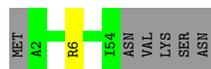
- Molecule 29: P-tRNA

Chain a:  61% 30% 9%



- Molecule 30: 50S ribosomal protein L32

Chain 0:  88% 10%

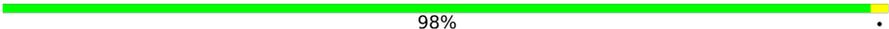


- Molecule 31: 50S ribosomal protein L33 1

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L34

Chain 2:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66113	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, H2U, G7M, MG, PSU, ZN, K, 5MU, 2MG, 2MA, OMG

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	3	0.40	0/519	0.78	1/680 (0.1%)
2	4	0.34	0/300	0.77	0/393
3	6	0.37	0/363	0.67	1/485 (0.2%)
4	A	0.48	0/65469	1.12	58/102117 (0.1%)
5	B	0.55	0/2675	1.13	3/4170 (0.1%)
6	C	0.34	0/2131	0.73	1/2859 (0.0%)
7	D	0.33	0/1597	0.72	0/2140
8	E	0.32	0/1586	0.69	0/2139
9	F	0.35	0/1424	0.69	1/1910 (0.1%)
10	G	0.33	0/1360	0.65	0/1832
11	J	0.33	0/1154	0.69	0/1552
12	K	0.33	0/928	0.73	0/1245
13	L	0.35	0/1094	0.74	0/1457
14	M	0.34	0/1099	0.71	0/1468
15	N	0.31	0/961	0.74	1/1284 (0.1%)
16	O	0.33	0/922	0.70	0/1236
17	P	0.32	0/935	0.79	0/1251
18	Q	0.33	0/962	0.77	1/1277 (0.1%)
19	R	0.32	0/806	0.67	0/1080
20	S	0.33	0/859	0.76	0/1156
21	T	0.33	0/739	0.74	0/985
22	U	0.34	0/780	0.69	0/1043
23	W	0.37	0/619	0.79	0/824
24	X	0.33	0/472	0.71	0/627
25	Y	0.30	0/531	0.71	0/707
26	Z	0.32	0/458	0.72	0/613
28	V	0.35	0/2016	0.71	0/2709
29	a	0.62	0/1648	1.19	2/2564 (0.1%)
30	0	0.35	0/425	0.80	0/563
31	1	0.34	0/416	0.75	0/551
32	2	0.36	0/371	0.81	0/483
All	All	0.45	0/95619	1.04	69/143400 (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
6	C	0	1
9	F	0	3
10	G	0	1
14	M	0	1
17	P	0	1
24	X	0	1
28	V	0	1
30	0	0	1
32	2	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	558	G	O4'-C1'-N9	8.72	115.18	108.20
4	A	2583	U	O5'-P-OP1	-8.25	98.27	105.70
4	A	46	C	O5'-P-OP2	-8.07	98.44	105.70
4	A	987	A	O5'-P-OP1	-8.03	98.47	105.70
4	A	2061	G	O5'-P-OP1	-7.95	98.55	105.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	238	ARG	Sidechain
9	F	80	ARG	Sidechain
9	F	92	ARG	Sidechain
9	F	95	ARG	Sidechain
10	G	172	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	512	0	564	1	0
2	4	297	0	339	0	0
3	6	356	0	346	3	0
4	A	58713	0	29543	27	0
5	B	2392	0	1213	2	0
6	C	2094	0	2181	0	0
7	D	1575	0	1642	0	0
8	E	1567	0	1652	2	0
9	F	1405	0	1467	6	0
10	G	1342	0	1388	10	0
11	J	1131	0	1169	1	0
12	K	921	0	977	2	0
13	L	1082	0	1132	1	0
14	M	1076	0	1145	0	0
15	N	954	0	983	5	0
16	O	913	0	947	1	0
17	P	922	0	994	0	0
18	Q	950	0	1018	3	0
19	R	795	0	838	0	0
20	S	850	0	911	0	0
21	T	733	0	781	0	0
22	U	770	0	824	1	0
23	W	611	0	618	1	0
24	X	468	0	514	0	0
25	Y	530	0	568	0	0
26	Z	456	0	491	0	0
27	b	20	0	7	0	0
28	V	1988	0	2006	0	0
29	a	1477	0	750	0	0
30	0	418	0	435	0	0
31	1	411	0	423	0	0
32	2	368	0	410	0	0
33	0	1	0	0	0	0
33	1	1	0	0	0	0
33	4	1	0	0	0	0
33	6	1	0	0	0	0
34	A	45	0	0	0	0
34	C	2	0	0	0	0
35	A	20	0	11	1	0
36	A	154	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
37	0	14	0	0	0	0
37	2	13	0	0	0	0
37	3	15	0	0	0	0
37	4	3	0	0	0	0
37	A	2422	0	0	0	0
37	B	10	0	0	0	0
37	C	55	0	0	0	0
37	D	28	0	0	0	0
37	E	28	0	0	0	0
37	J	13	0	0	0	0
37	K	15	0	0	0	0
37	L	25	0	0	0	0
37	M	12	0	0	0	0
37	N	20	0	0	0	0
37	P	15	0	0	0	0
37	Q	24	0	0	0	0
37	R	16	0	0	0	0
37	S	13	0	0	0	0
37	T	8	0	0	0	0
37	U	3	0	0	0	0
37	W	7	0	0	0	0
37	X	6	0	0	0	0
37	Z	4	0	0	0	0
37	a	2	0	0	0	0
All	All	91097	0	58287	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 50 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:607:G:H21	18:Q:37:GLN:HE22	1.33	0.77
10:G:122:ILE:HD11	10:G:141:ARG:HB3	1.68	0.76
4:A:1292:G:H1	18:Q:37:GLN:HE21	1.32	0.75
4:A:2534:G:O4'	35:A:3032:CLM:CL1	2.48	0.68
4:A:790:A:O2'	4:A:1704:U:OP1	2.11	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	3	62/66 (94%)	62 (100%)	0	0	100	100
2	4	35/37 (95%)	35 (100%)	0	0	100	100
3	6	44/66 (67%)	44 (100%)	0	0	100	100
6	C	271/277 (98%)	263 (97%)	8 (3%)	0	100	100
7	D	205/209 (98%)	199 (97%)	6 (3%)	0	100	100
8	E	204/207 (99%)	197 (97%)	7 (3%)	0	100	100
9	F	176/179 (98%)	173 (98%)	3 (2%)	0	100	100
10	G	173/179 (97%)	167 (96%)	6 (4%)	0	100	100
11	J	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
12	K	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	L	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	19	10
14	M	133/144 (92%)	130 (98%)	3 (2%)	0	100	100
15	N	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
16	O	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
17	P	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
18	Q	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
19	R	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
20	S	108/113 (96%)	108 (100%)	0	0	100	100
21	T	89/95 (94%)	87 (98%)	2 (2%)	0	100	100
22	U	100/103 (97%)	94 (94%)	6 (6%)	0	100	100
23	W	78/94 (83%)	75 (96%)	3 (4%)	0	100	100
24	X	59/62 (95%)	55 (93%)	3 (5%)	1 (2%)	7	2
25	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
26	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
28	V	243/275 (88%)	220 (90%)	19 (8%)	4 (2%)	8	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	0	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
31	1	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
32	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
All	All	3206/3372 (95%)	3099 (97%)	101 (3%)	6 (0%)	45	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	X	3	ARG
28	V	65	ARG
28	V	37	PHE
13	L	29	LYS
28	V	67	GLU

### 5.3.2 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	3	54/56 (96%)	53 (98%)	1 (2%)	52	47
2	4	35/35 (100%)	35 (100%)	0	100	100
3	6	39/55 (71%)	38 (97%)	1 (3%)	41	33
6	C	221/225 (98%)	221 (100%)	0	100	100
7	D	168/170 (99%)	167 (99%)	1 (1%)	84	83
8	E	169/170 (99%)	169 (100%)	0	100	100
9	F	153/154 (99%)	151 (99%)	2 (1%)	65	62
10	G	148/151 (98%)	146 (99%)	2 (1%)	62	59
11	J	121/123 (98%)	121 (100%)	0	100	100
12	K	101/101 (100%)	101 (100%)	0	100	100
13	L	110/110 (100%)	110 (100%)	0	100	100
14	M	109/116 (94%)	109 (100%)	0	100	100
15	N	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	93/93 (100%)	93 (100%)	0	100	100
17	P	98/100 (98%)	97 (99%)	1 (1%)	73	72
18	Q	97/98 (99%)	97 (100%)	0	100	100
19	R	84/84 (100%)	84 (100%)	0	100	100
20	S	91/93 (98%)	90 (99%)	1 (1%)	70	68
21	T	82/85 (96%)	82 (100%)	0	100	100
22	U	86/87 (99%)	86 (100%)	0	100	100
23	W	61/74 (82%)	61 (100%)	0	100	100
24	X	49/50 (98%)	49 (100%)	0	100	100
25	Y	56/57 (98%)	56 (100%)	0	100	100
26	Z	52/53 (98%)	52 (100%)	0	100	100
28	V	215/234 (92%)	213 (99%)	2 (1%)	75	75
30	0	47/53 (89%)	47 (100%)	0	100	100
31	1	47/47 (100%)	47 (100%)	0	100	100
32	2	39/39 (100%)	39 (100%)	0	100	100
All	All	2724/2813 (97%)	2713 (100%)	11 (0%)	88	89

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	P	80	LYS
20	S	11	ARG
28	V	250	ARG
28	V	40	PRO
9	F	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
28	V	52	GLN
24	X	23	ASN
13	L	27	ASN
22	U	20	GLN
12	K	3	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	a	66/76 (86%)	21 (31%)	0
4	A	2721/2928 (92%)	341 (12%)	53 (1%)
5	B	111/112 (99%)	18 (16%)	4 (3%)
All	All	2898/3116 (93%)	380 (13%)	57 (1%)

5 of 380 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	12	A
4	A	13	A
4	A	15	G
4	A	34	U
4	A	45	G

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	1527	C
5	B	48	G
4	A	1602	U
5	B	37	A
4	A	2631	A

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

12 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
4	2MA	A	2532	4,34,36	19,25,26	1.06	2 (10%)	21,37,40	2.10	5 (23%)
4	PSU	A	2533	4,34	18,21,22	0.92	1 (5%)	22,30,33	0.77	0
4	5MU	A	794	4	19,22,23	0.34	0	28,32,35	0.44	0
4	H2U	A	2478	4	18,21,22	0.59	0	21,30,33	0.71	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PSU	A	1001	4	18,21,22	1.03	1 (5%)	22,30,33	0.65	0
4	PSU	A	2486	4	18,21,22	1.00	1 (5%)	22,30,33	0.62	0
4	5MU	A	1968	4	19,22,23	0.34	0	28,32,35	0.42	0
4	G7M	A	2603	4,36	20,26,27	1.11	2 (10%)	17,39,42	0.32	0
4	OMG	A	2582	4	18,26,27	0.98	2 (11%)	19,38,41	0.70	0
4	2MG	A	2474	4	18,26,27	1.02	1 (5%)	16,38,41	0.84	1 (6%)
4	5MU	A	620	4,34,36	19,22,23	0.30	0	28,32,35	0.52	0
4	OMG	A	2280	29,4,34	18,26,27	0.99	2 (11%)	19,38,41	0.81	0

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
4	2MA	A	2532	4,34,36	-	2/3/25/26	0/3/3/3
4	PSU	A	2533	4,34	-	0/7/25/26	0/2/2/2
4	5MU	A	794	4	-	0/7/25/26	0/2/2/2
4	H2U	A	2478	4	-	0/7/38/39	0/2/2/2
4	PSU	A	1001	4	-	0/7/25/26	0/2/2/2
4	PSU	A	2486	4	-	0/7/25/26	0/2/2/2
4	5MU	A	1968	4	-	0/7/25/26	0/2/2/2
4	G7M	A	2603	4,36	-	0/3/25/26	0/3/3/3
4	OMG	A	2582	4	-	1/5/27/28	0/3/3/3
4	2MG	A	2474	4	-	0/5/27/28	0/3/3/3
4	5MU	A	620	4,34,36	-	0/7/25/26	0/2/2/2
4	OMG	A	2280	29,4,34	-	0/5/27/28	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2486	PSU	C6-C5	3.97	1.39	1.35
4	A	1001	PSU	C6-C5	3.97	1.39	1.35
4	A	2533	PSU	C6-C5	3.68	1.39	1.35
4	A	2603	G7M	C8-N9	3.50	1.39	1.33
4	A	2280	OMG	C5-C6	-2.62	1.42	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2532	2MA	C5-C6-N1	-6.13	116.98	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2532	2MA	CM2-C2-N1	4.56	124.28	117.15
4	A	2532	2MA	C5-C6-N6	3.84	126.18	120.35
4	A	2532	2MA	N3-C2-N1	-2.46	121.25	125.73
4	A	2532	2MA	C2-N1-C6	2.42	121.86	118.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2582	OMG	C3'-C2'-O2'-CM2
4	A	2532	2MA	O4'-C4'-C5'-O5'
4	A	2532	2MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2603	G7M	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 210 ligands modelled in this entry, 209 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	$\# Z  > 2$
35	CLM	A	3032	-	19,20,20	0.65	0	23,27,27	0.90	1 (4%)

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
35	CLM	A	3032	-	-	4/20/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3032	CLM	C5-C3-N2	3.02	115.77	110.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

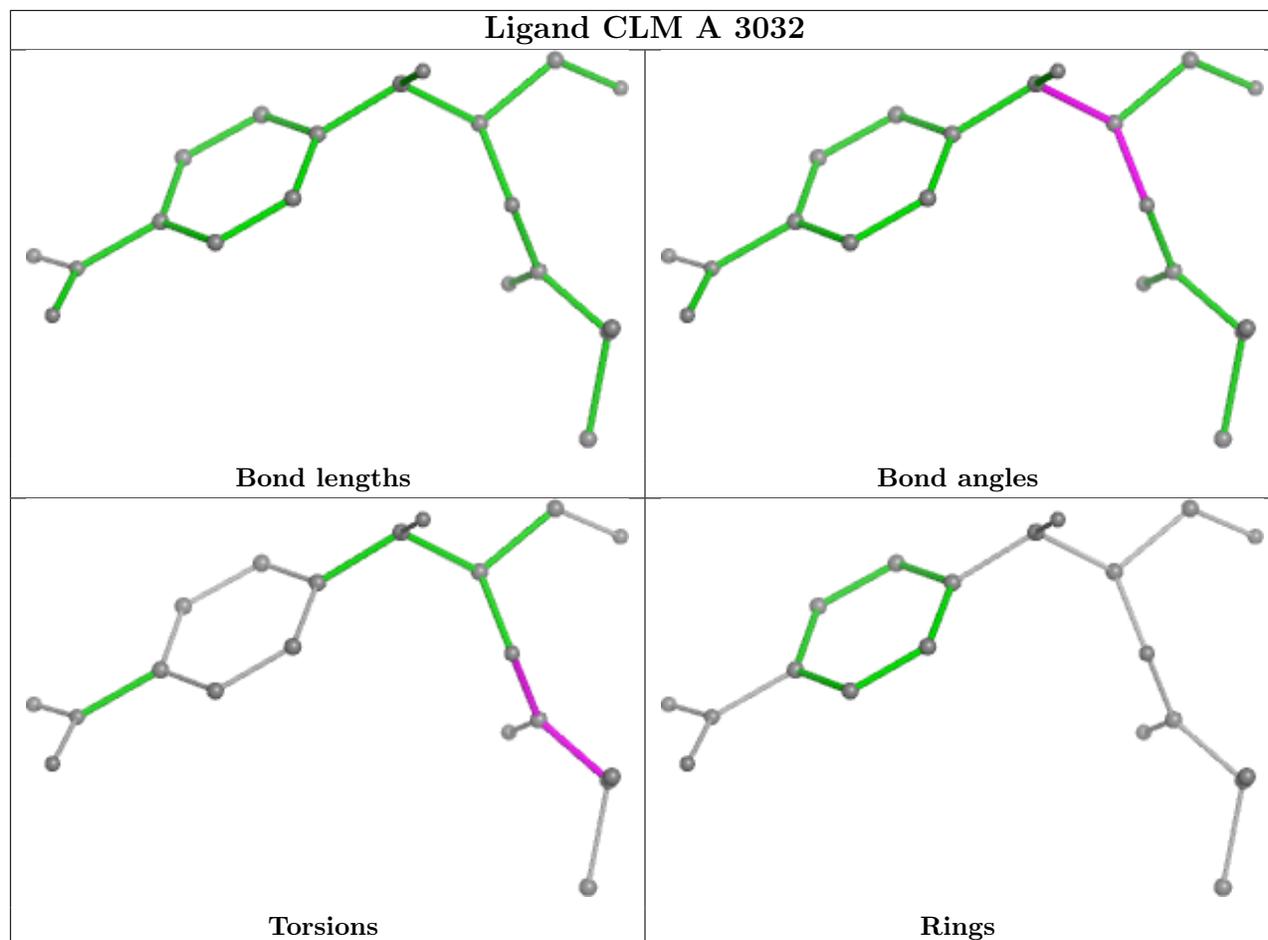
Mol	Chain	Res	Type	Atoms
35	A	3032	CLM	O2-C2-N2-C3
35	A	3032	CLM	C1-C2-N2-C3
35	A	3032	CLM	CL1-C1-C2-O2
35	A	3032	CLM	CL1-C1-C2-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3032	CLM	1	0

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.