



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 07:48 PM UTC

PDB ID : 8WB0 / pdb_00008wb0
EMDB ID : EMD-37411
Title : De novo transcribing complex 17 (TC17), the early elongation complex with Pol II positioned 17nt downstream of TSS
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-08
Resolution : 2.94 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

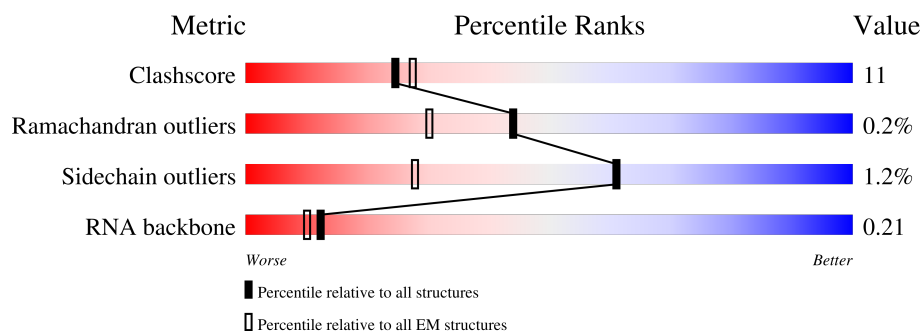
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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.



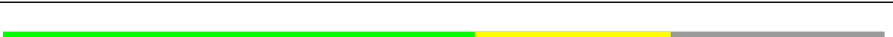
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	N	8	38% 38% 25%
2	S	517	22% 5% 73%
3	T	249	35% 6% 59%
4	X	99	15% 28% 57%
5	Y	99	30% 24% 45%
6	Z	13	31% 46% 15% 8%
7	o	1970	55% 18% 26%

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Mol	Chain	Length	Quality of chain
8	p	1174	
9	q	275	
10	r	142	
11	s	210	
12	t	127	
13	u	172	
14	v	150	
15	w	125	
16	x	67	
17	y	117	
18	z	58	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 35758 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	8	Total	C	H	N	O	S	
			94	39	30	10	14	1	
								0	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	138	Total	C	N	O	S		
			1138	719	208	208	3		
								0	0

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	103	Total	C	N	O	S		
			789	492	142	154	1		
								0	0

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P		
			876	416	160	257	43		
								0	0

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P		
			1115	528	210	323	54		
								0	0

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	13	Total	C	N	O	P		
			270	122	42	93	13		
								0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	y	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 18 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

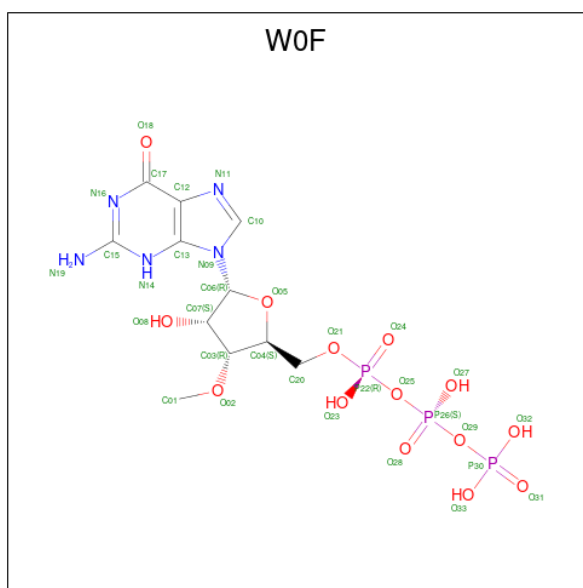
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	o	2	Total	Zn	0
			2	2	
19	p	1	Total	Zn	0
			1	1	
19	q	1	Total	Zn	0
			1	1	
19	w	2	Total	Zn	0
			2	2	
19	x	1	Total	Zn	0
			1	1	
19	z	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	o	1	Total	Mg	0
			1	1	

- Molecule 21 is [(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	p	1	Total	C	N	O	P	0
			33	11	5	14	3	

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.

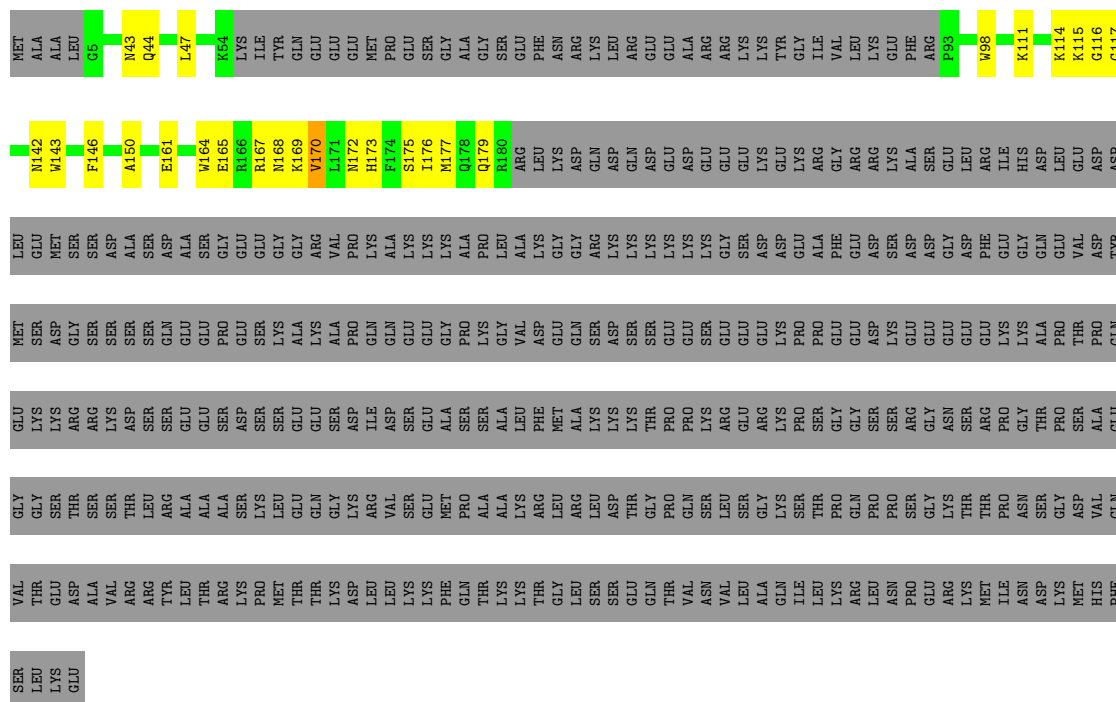
- Molecule 1: Alpha-amanitin

Chain N: 



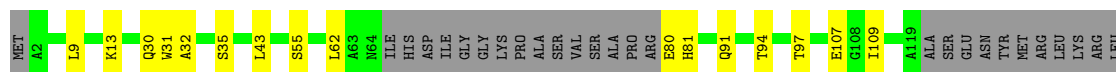
- Molecule 2: General transcription factor IIF subunit 1

Chain S: 

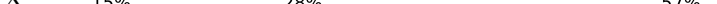


- Molecule 3: General transcription factor IIF subunit 2

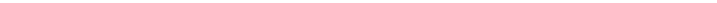
Chain T: 



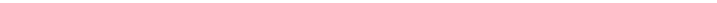
PHE GLU LYS HIS GLN TYR TYR ASN ASP ILE THR LYS GLN PRO VAL VAL TYR LYS LEU LEU GLU ILE LEU LYS GLY VAL GLN ASN VAL LYS GLY ILE ILE LYS ASN TRP TRP THP TRP GLU LYS LYS PRO GLU TYR ARG HIS TYR GLN GLY GLU LYS SER ASP

Chain X:  15% 28% 57%

C26		A29	C30	G31	T32		C35	T36	A37	C38		C42	C43	A44	T45	G46	DT	DC	DC	DC	DG	DG	DA	DA	DA	DA	DC	DC	DT	DG	DA	DA	DC
-----	--	-----	-----	-----	-----	--	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

Chain Y:  30% 24% 45%

DA DC DC DC DC DC DT DT DT DT DT DA DT DA DG DG DC DG DC DC DC DT DT

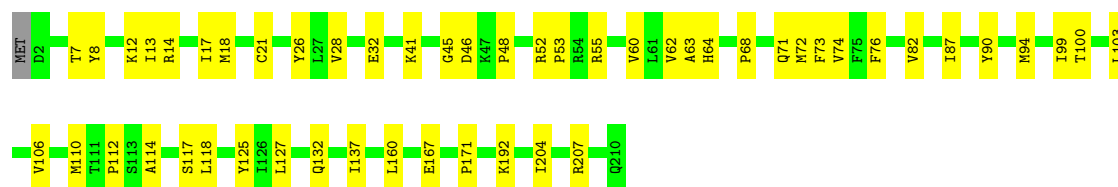
Chain Z:  31% 46% 15% 8%

A5	U8	C9	A10	U11	C12	U13		G17
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Chain o: 55% 18% 1% 26%

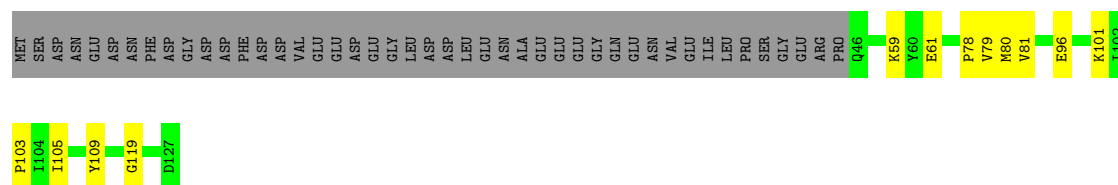
MS01 MS02 MS03 MS04 MS05 MS06 MS07 MS08 MS09 MS10 MS11 MS12 MS13 MS14 MS15 MS16 MS17 MS18 MS19 MS20 MS21 MS22 MS23 MS24 MS25 MS26 MS27 MS28 MS29 MS30 MS31 MS32 MS33 MS34 MS35 MS36 MS37 MS38 MS39 MS40 MS41 MS42 MS43 MS44 MS45 MS46 MS47 MS48 MS49 MS50 MS51 MS52 MS53 MS54 MS55 MS56 MS57 MS58 MS59 MS60 MS61 MS62 MS63 MS64 MS65 MS66 MS67 MS68 MS69 MS70 MS71 MS72 MS73 MS74 MS75 MS76 MS77 MS78 MS79 MS80 MS81 MS82 MS83 MS84 MS85 MS86 MS87 MS88 MS89 MS90 MS91 MS92 MS93 MS94 MS95 MS96 MS97 MS98 MS99 MS100

Chain s:  75% 24%



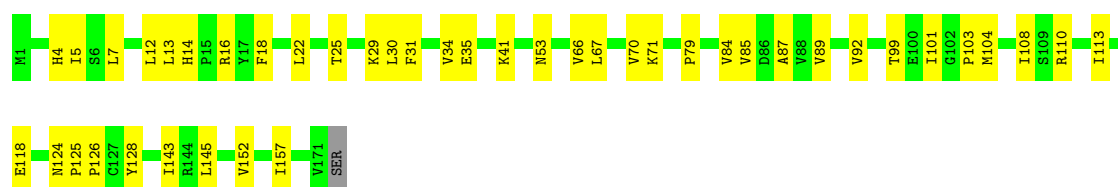
- Molecule 12: DNA-directed RNA polymerase II subunit F

Chain t:  55% 9% 35%



- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

Chain u:  74% 25%



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:  77% 20% ..



- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

Chain w:  71% 19% 9%

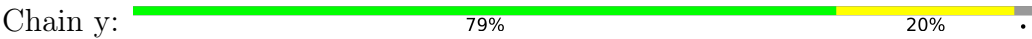


- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain x:  78% 21%



• Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a



• Molecule 18: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: CSX, ILX, HYP, TRX, G2L, W0F, MG, 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	N	0.42	0/22	0.98	0/26
2	S	0.09	0/1167	0.23	0/1576
3	T	0.09	0/799	0.25	0/1077
4	X	0.27	0/980	0.59	0/1506
5	Y	0.32	0/1252	0.55	0/1932
6	Z	0.26	0/272	0.45	0/419
7	o	0.24	0/11723	0.37	0/15830
8	p	0.26	0/9332	0.40	1/12598 (0.0%)
9	q	0.25	0/2102	0.37	0/2857
10	r	0.11	0/1064	0.22	0/1428
11	s	0.23	0/1751	0.35	1/2366 (0.0%)
12	t	0.23	0/667	0.28	0/901
13	u	0.15	0/1382	0.31	0/1874
14	v	0.23	0/1207	0.35	0/1628
15	w	0.19	0/948	0.34	0/1284
16	x	0.25	0/542	0.34	0/730
17	y	0.24	0/939	0.32	0/1271
18	z	0.20	0/377	0.36	0/500
All	All	0.24	0/36526	0.38	2/49803 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	46	ASP	CB-CA-C	-5.55	109.68	117.23
8	p	355	ASP	CB-CA-C	-5.12	110.27	117.23

There are no chirality outliers.

There are no planarity outliers.

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	N	64	30	51	11	0
2	S	1138	0	1103	19	0
3	T	789	0	795	10	0
4	X	876	0	484	24	0
5	Y	1115	0	607	25	0
6	Z	270	0	138	8	0
7	o	11510	0	11616	267	0
8	p	9149	0	9178	251	0
9	q	2059	0	2007	61	0
10	r	1050	0	1033	17	0
11	s	1720	0	1737	39	0
12	t	657	0	684	11	0
13	u	1351	0	1358	27	0
14	v	1186	0	1147	24	0
15	w	927	0	859	20	0
16	x	533	0	553	12	0
17	y	920	0	942	16	0
18	z	372	0	378	10	0
19	o	2	0	0	0	0
19	p	1	0	0	0	0
19	q	1	0	0	0	0
19	w	2	0	0	0	0
19	x	1	0	0	0	0
19	z	1	0	0	0	0
20	o	1	0	0	0	0
21	p	33	0	0	6	0
All	All	35728	30	34670	741	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 11.

The worst 5 of 741 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)
5:Y:-16:DC:O2	6:Z:17:G2L:N2	1.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:91:GLN:HB2	8:p:555:GLU:HG3	1.57	0.85
4:X:18:DG:N2	5:Y:-18:DC:O2	2.11	0.84
8:p:597:ILE:HG23	8:p:601:VAL:HB	1.61	0.82
8:p:866:ILE:HG22	8:p:867:ILE:HG13	1.61	0.80

There are no symmetry-related clashes.

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	
1	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1394 (96%)	52 (4%)	2 (0%)	48	71
8	p	1142/1174 (97%)	1074 (94%)	65 (6%)	3 (0%)	36	59
9	q	253/275 (92%)	245 (97%)	8 (3%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
13	u	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
14	v	146/150 (97%)	139 (95%)	6 (4%)	1 (1%)	18	40
15	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	3	8
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	4140/5361 (77%)	3966 (96%)	166 (4%)	8 (0%)	44	65

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
16	x	6	ARG

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	
1	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	73	84
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1262 (99%)	18 (1%)	59	76
8	p	1001/1027 (98%)	986 (98%)	15 (2%)	57	75
9	q	234/252 (93%)	231 (99%)	3 (1%)	61	77
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	151 (99%)	1 (1%)	76	86
14	v	129/131 (98%)	127 (98%)	2 (2%)	55	74
15	w	103/112 (92%)	102 (99%)	1 (1%)	68	81
16	x	56/56 (100%)	55 (98%)	1 (2%)	51	72
17	y	104/106 (98%)	103 (99%)	1 (1%)	68	81
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3645 (99%)	43 (1%)	61	78

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	p	598	VAL
9	q	44	ILE
8	p	860	VAL
8	p	921	ILE
13	u	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
9	q	18	ASN
17	y	49	GLN
9	q	232	ASN
12	t	46	GLN
7	o	1190	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	12/13 (92%)	6 (50%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	6	C
6	Z	7	U
6	Z	8	U
6	Z	12	C
6	Z	13	U

There are no RNA pucker outliers to report.

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

5 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	$\# Z > 2$
6	G2L	Z	17	6,5,20	23,26,30	1.20	3 (13%)	31,38,44	2.12	7 (22%)
1	HYP	N	8	1	7,8,9	0.83	0	5,10,12	2.34	2 (40%)
1	CSX	N	6	1	3,6,7	1.08	0	1,6,8	2.14	1 (100%)
1	ILX	N	1	1	8,9,10	0.63	0	8,11,13	1.40	1 (12%)
1	TRX	N	2	1	15,16,17	1.11	1 (6%)	17,22,24	0.96	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
6	G2L	Z	17	6,5,20	-	2/9/27/31	0/3/3/3
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
1	CSX	N	6	1	-	2/2/5/7	-
1	ILX	N	1	1	-	7/11/12/14	-
1	TRX	N	2	1	-	2/5/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	17	G2L	C5-C4	3.18	1.47	1.38
6	Z	17	G2L	C6-N1	-2.41	1.34	1.38
1	N	2	TRX	CD2-CE2	2.40	1.44	1.41
6	Z	17	G2L	C5-N7	-2.01	1.35	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	17	G2L	C5-C4-N3	-6.22	118.49	128.39
6	Z	17	G2L	C2-N3-C4	5.04	120.98	112.30
6	Z	17	G2L	N9-C4-N3	4.57	135.09	125.95
1	N	8	HYP	CB-CG-CD	3.43	106.97	103.16
1	N	8	HYP	O-C-CA	-3.31	116.25	124.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
1	N	6	CSX	C-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	17	G2L	4	0
1	N	1	ILX	5	0
1	N	2	TRX	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
21	W0F	p	1201	-	34,35,35	4.05	14 (41%)	43,55,55	3.45	17 (39%)

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
21	W0F	p	1201	-	-	3/24/40/40	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	p	1201	W0F	P26-O29	13.80	1.74	1.59
21	p	1201	W0F	C03-C04	-9.74	1.27	1.52
21	p	1201	W0F	P22-O25	8.41	1.68	1.59
21	p	1201	W0F	O05-C04	6.90	1.60	1.45
21	p	1201	W0F	O05-C06	-5.97	1.28	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	p	1201	W0F	O05-C06-N09	-14.57	75.35	108.36
21	p	1201	W0F	C07-C06-N09	8.28	136.31	113.25
21	p	1201	W0F	O05-C04-C03	-5.80	92.69	104.92
21	p	1201	W0F	O27-P26-O25	-5.28	92.99	107.27
21	p	1201	W0F	O05-C04-C20	4.94	125.15	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

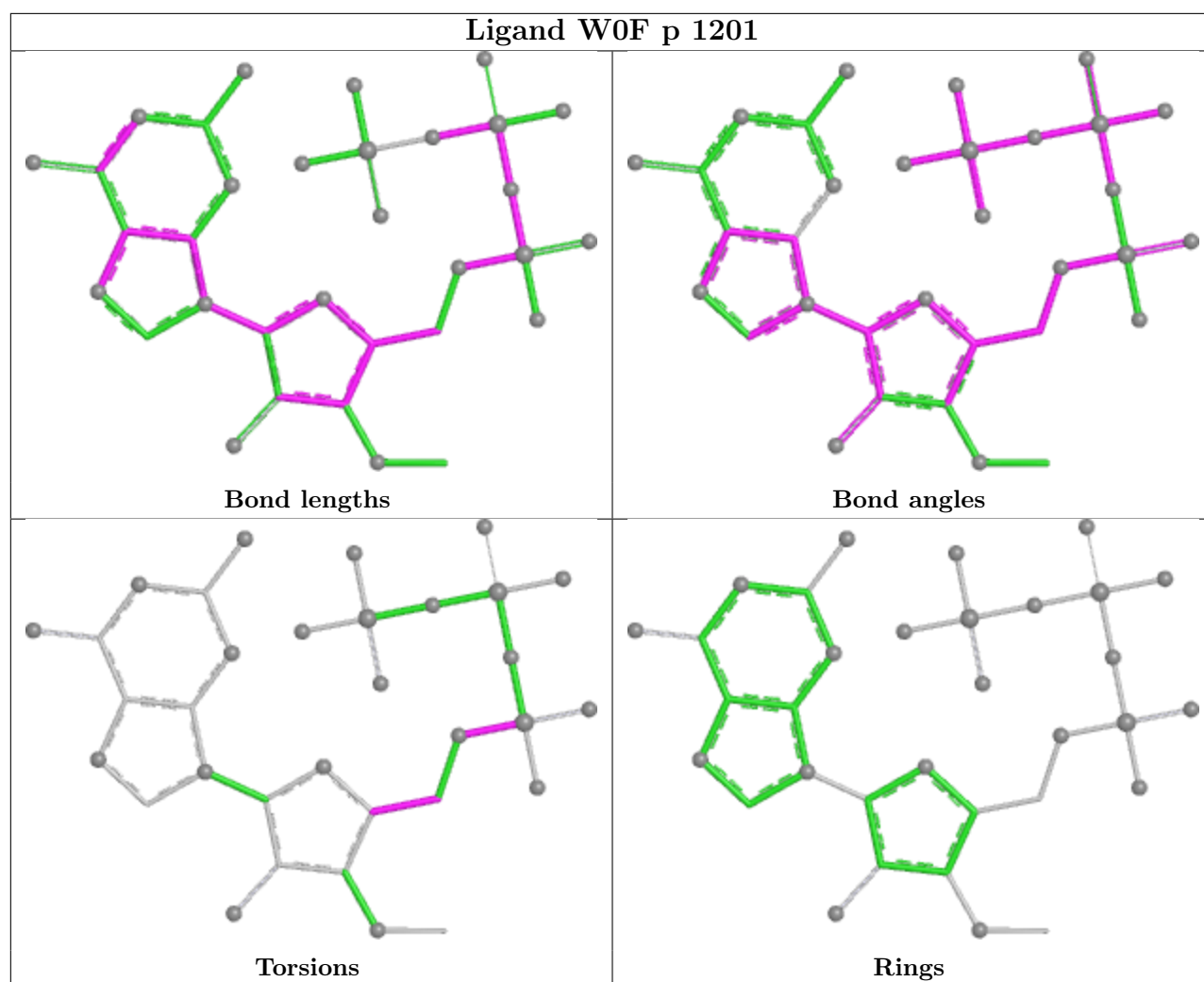
Mol	Chain	Res	Type	Atoms
21	p	1201	W0F	C20-O21-P22-O24
21	p	1201	W0F	C20-O21-P22-O25
21	p	1201	W0F	C03-C04-C20-O21

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	p	1201	W0F	6	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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37411. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.