



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:07 AM UTC

PDB ID : 4BY7 / pdb_00004by7
Title : elongating RNA Polymerase II-Bye1 TLD complex
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-18
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

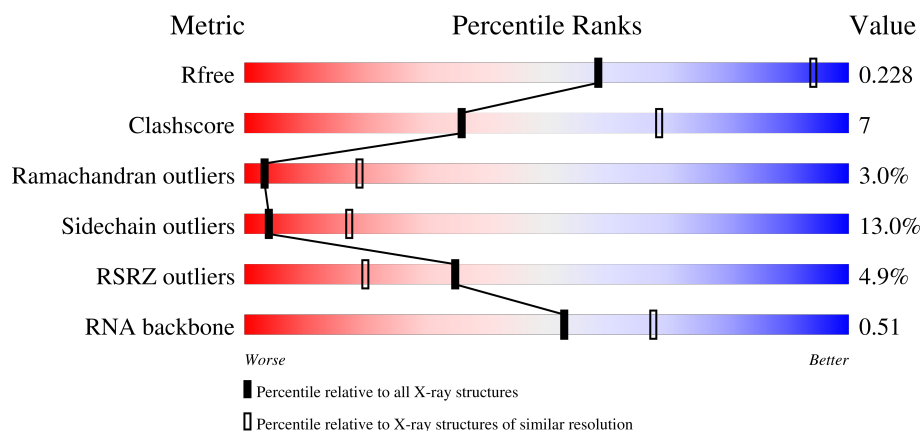
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	2% 58% 19% 5% 18%
2	B	1224	5% 65% 21% • 9%
3	C	318	57% 22% 5% 16%
4	D	221	5% 58% 19% • 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	26	
16	X	146	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33261 atoms, of which 34 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0	0
			11223	7068	1959	2134	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1387	860	246	279	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called , 5'-D(*DAP*AP*AP*GP*TP*AP*CP*TP*TP*GP*A

P*GP*CP*DTP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	13	Total	C	N	O	P	0	0	0
			269	128	52	76	13			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			215	96	41	68	10			

- Molecule 15 is a DNA chain called 5'-D(*DAP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DAP *TP*TP*CP*CP*BP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	25	Total	Br	C	N	O	P	0	0
			504	1	240	83	155	25		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	119	Total	C	N	O	S	0	0	0
			977	628	162	184	3			

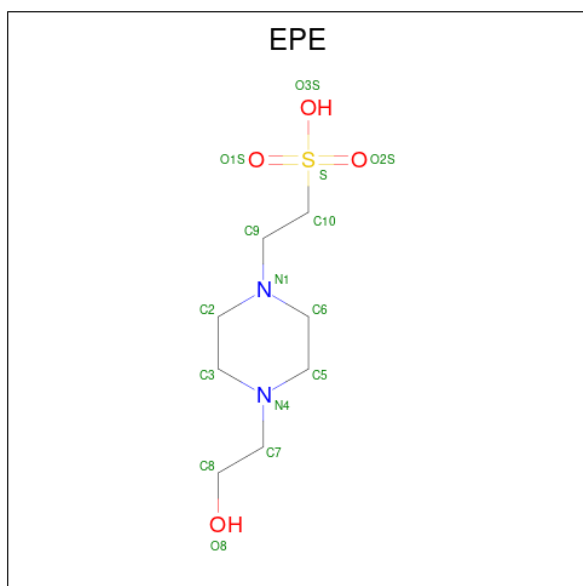
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		
17	B	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		
17	J	1	Total	Zn	0	0
			1	1		
17	L	1	Total	Zn	0	0
			1	1		

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Mg 1 1	0	0

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).

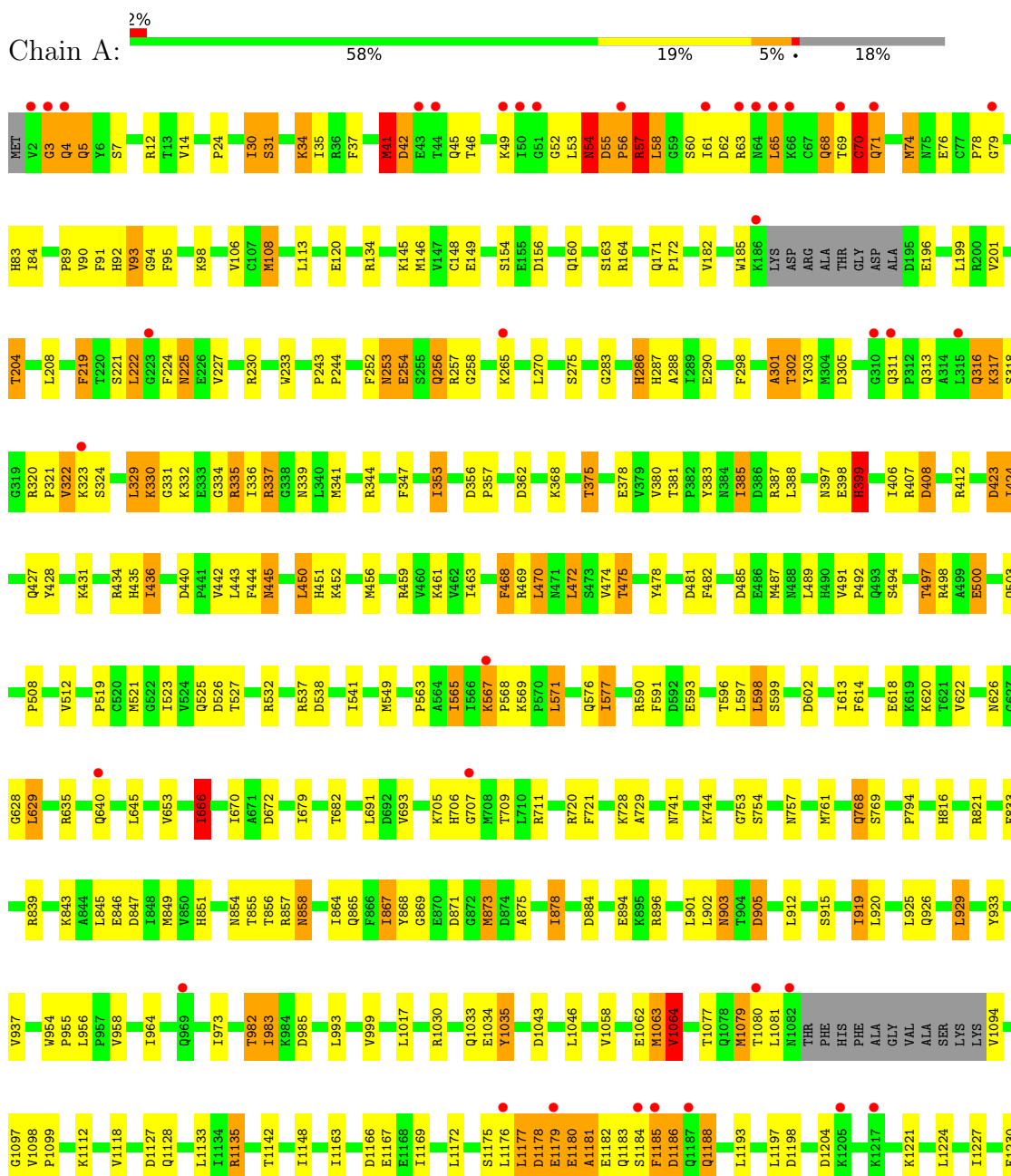


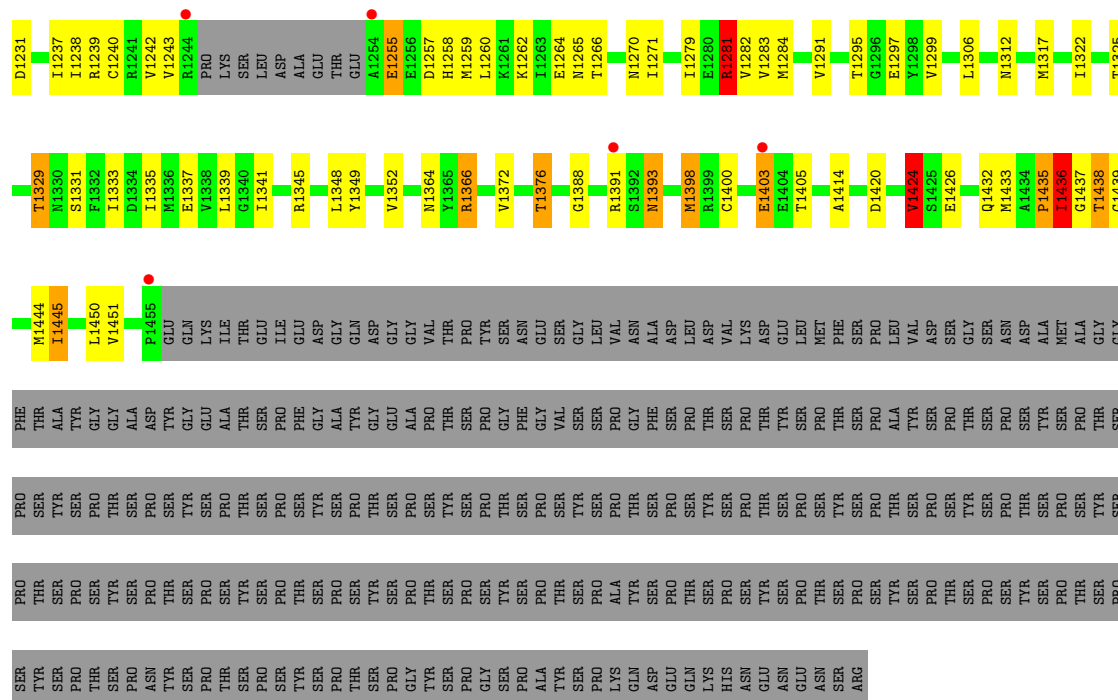
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
19	G	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

3 Residue-property plots

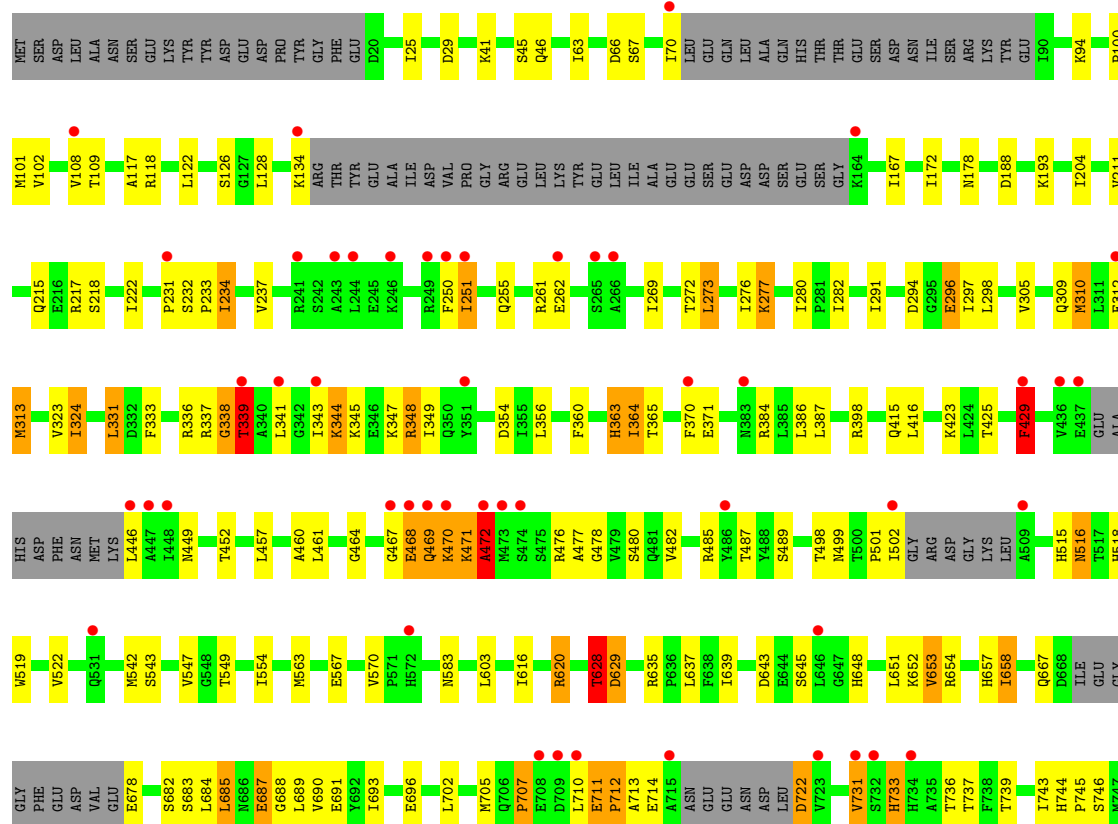
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

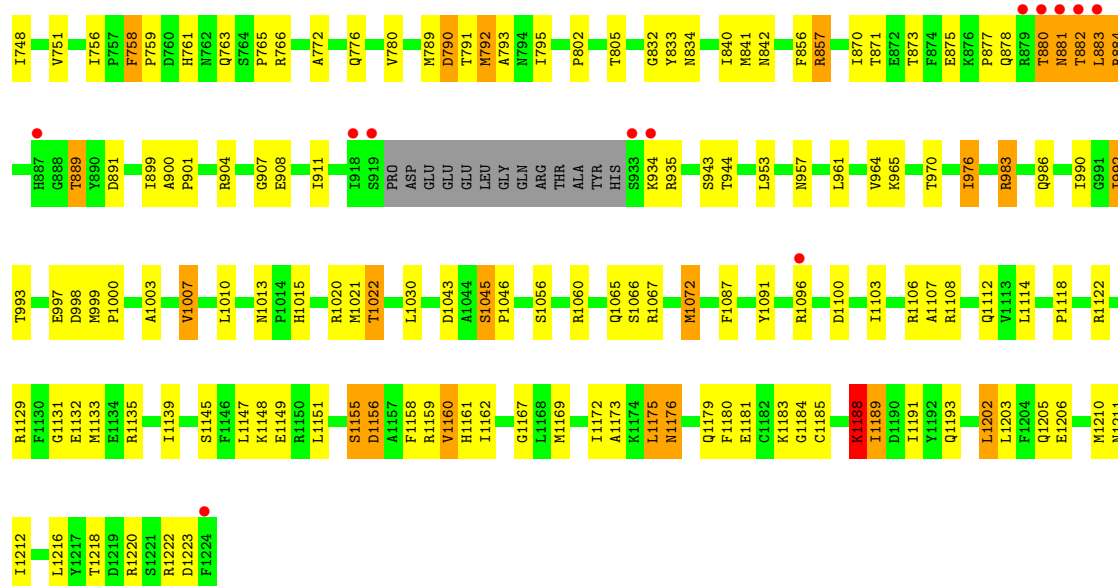
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





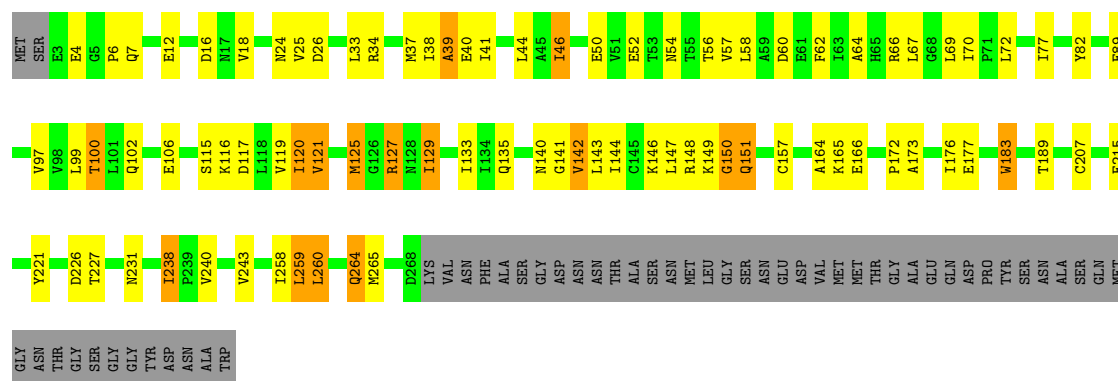
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





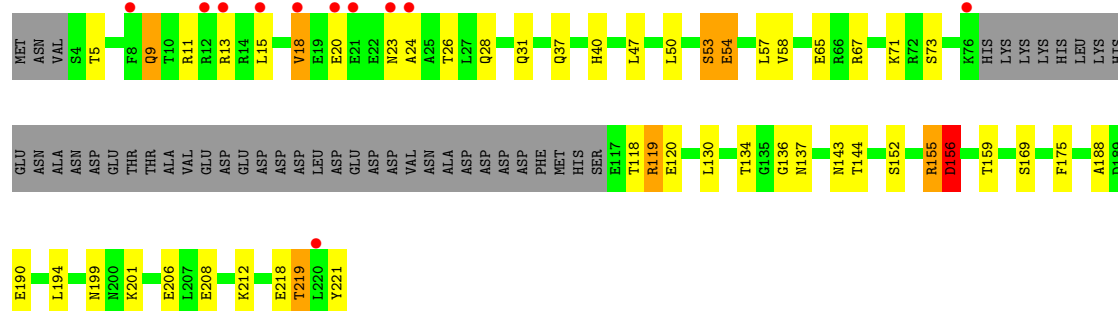
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 57% 22% 5% 16%

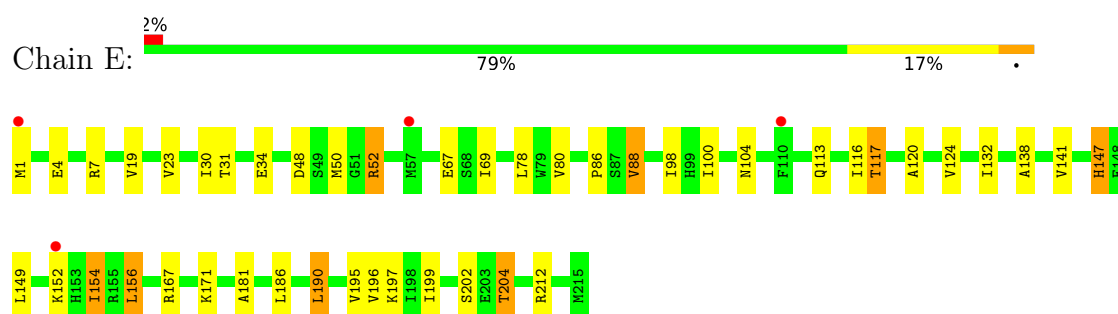


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

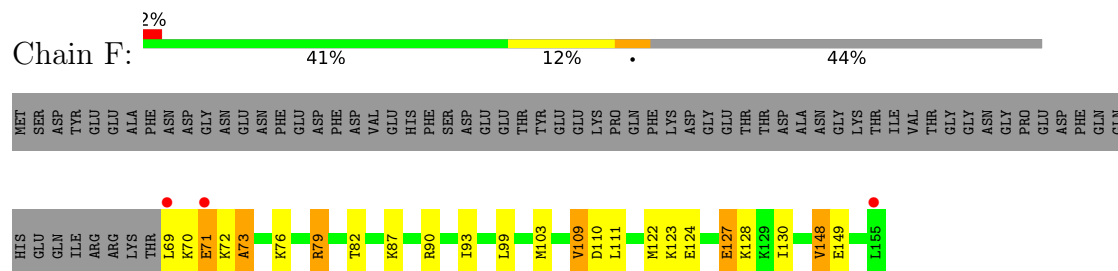
Chain D: 5% 58% 19% 19%



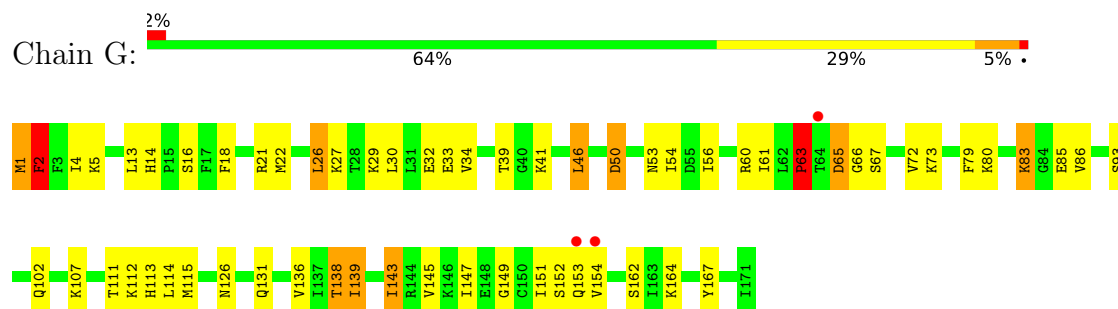
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



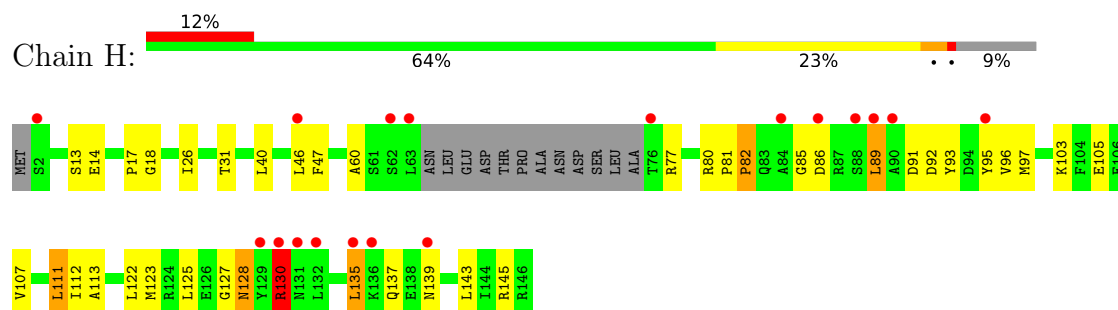
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



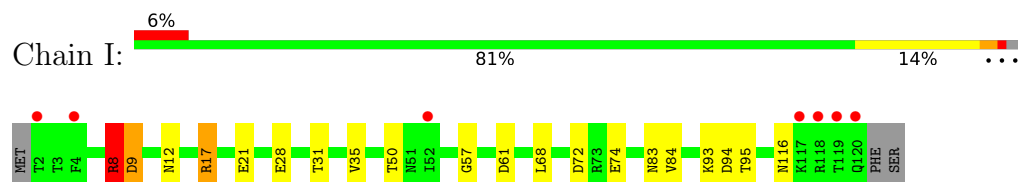
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



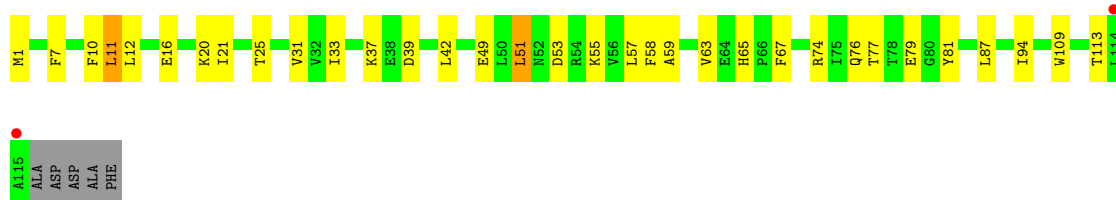
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



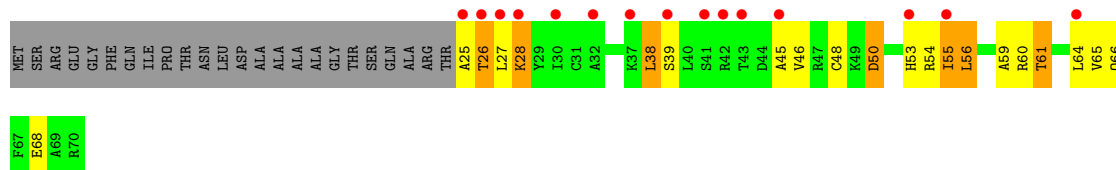
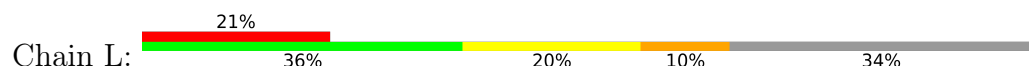
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



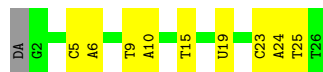
- Molecule 13: , 5'-D(*DAP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*DTP)-3'



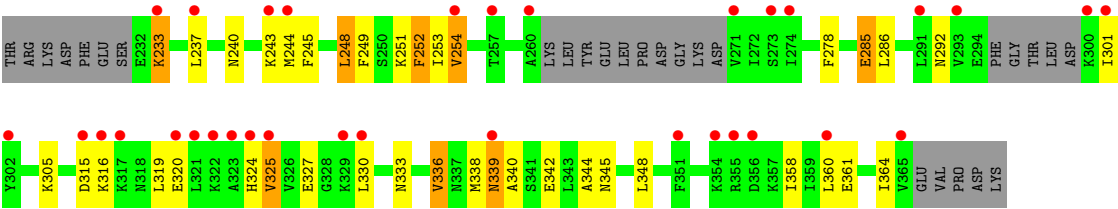
- Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'



- Molecule 15: 5'-D(*DAP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*DAP *TP*TP*CP*CP*BP*GP*GP*TP*CP*AP*TP*T)-3'



- Molecule 16: TRANSCRIPTION FACTOR BYE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.50Å 390.68Å 281.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 3.15 48.84 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.84-3.15) 99.9 (48.84-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.189 , 0.212 0.206 , 0.228	Depositor DCC
R_{free} test set	4003 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	99.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 115.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33261	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	9/11424 (0.1%)	1.48	103/15452 (0.7%)
2	B	0.85	1/9030 (0.0%)	1.40	71/12174 (0.6%)
3	C	0.83	0/2133	1.36	17/2891 (0.6%)
4	D	0.85	1/1397 (0.1%)	1.51	9/1878 (0.5%)
5	E	0.78	0/1796	1.32	6/2416 (0.2%)
6	F	0.93	0/717	1.38	5/967 (0.5%)
7	G	0.85	1/1368 (0.1%)	1.35	7/1844 (0.4%)
8	H	0.82	0/1085	1.24	3/1467 (0.2%)
9	I	0.82	0/989	1.26	3/1331 (0.2%)
10	J	0.84	0/541	1.51	9/727 (1.2%)
11	K	0.73	0/938	1.26	5/1267 (0.4%)
12	L	0.95	0/364	1.45	2/482 (0.4%)
13	N	0.45	0/302	0.59	0/464
14	P	0.81	1/240 (0.4%)	0.77	0/372
15	T	0.53	0/539	0.67	0/825
16	X	0.84	1/990 (0.1%)	1.59	8/1325 (0.6%)
All	All	0.85	14/33853 (0.0%)	1.40	248/45882 (0.5%)

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
15	T	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	9.31	1.46	1.33
1	A	55	ASP	CA-C	-8.63	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	7.12	1.62	1.52
4	D	24	ALA	CA-C	6.69	1.61	1.52
1	A	1403	GLU	CA-C	5.78	1.60	1.52

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASN	CA-C-N	12.87	136.73	122.83
1	A	54	ASN	C-N-CA	12.87	136.73	122.83
1	A	54	ASN	CA-CB-CG	10.10	122.69	112.60
8	H	92	ASP	N-CA-C	-9.06	101.19	112.88
1	A	1177	LEU	CA-C-N	9.05	137.99	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	15	DT	Sidechain
15	T	25	DT	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	A	11223	0	11273	195	0
2	B	8859	0	8902	127	0
3	C	2095	0	2051	37	0
4	D	1387	0	1366	21	0
5	E	1760	0	1788	24	0
6	F	705	0	731	15	0
7	G	1340	0	1357	35	0
8	H	1068	0	1039	29	0
9	I	971	0	927	6	0
10	J	532	0	542	12	0
11	K	920	0	929	15	0
12	L	363	0	385	7	0
13	N	269	0	147	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	P	215	0	109	1	0
15	T	504	0	274	4	0
16	X	977	0	996	13	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
19	A	15	17	17	1	0
19	G	15	17	17	0	0
All	All	33227	34	32850	481	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 7.

The worst 5 of 481 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)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.23	1.02
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.45	0.94
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.49	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.83	0.93
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.52	0.92

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	1418/1733 (82%)	1274 (90%)	96 (7%)	48 (3%)	3	16
2	B	1097/1224 (90%)	981 (89%)	84 (8%)	32 (3%)	3	20
3	C	264/318 (83%)	246 (93%)	14 (5%)	4 (2%)	8	33
4	D	174/221 (79%)	156 (90%)	11 (6%)	7 (4%)	2	14
5	E	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
6	F	85/155 (55%)	79 (93%)	4 (5%)	2 (2%)	4	23
7	G	169/171 (99%)	153 (90%)	12 (7%)	4 (2%)	4	23
8	H	128/146 (88%)	103 (80%)	15 (12%)	10 (8%)	1	4
9	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	7	30
10	J	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	2	11
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	42/70 (60%)	32 (76%)	5 (12%)	5 (12%)	0	1
16	X	113/146 (77%)	101 (89%)	8 (7%)	4 (4%)	3	16
All	All	3996/4711 (85%)	3603 (90%)	272 (7%)	121 (3%)	3	19

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ARG
1	A	76	GLU
1	A	253	ASN
1	A	257	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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	1248/1520 (82%)	1080 (86%)	168 (14%)	4	16
2	B	966/1061 (91%)	839 (87%)	127 (13%)	4	17
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	147/200 (74%)	131 (89%)	16 (11%)	6	23
5	E	197/197 (100%)	184 (93%)	13 (7%)	15	42
6	F	77/137 (56%)	67 (87%)	10 (13%)	4	17
7	G	152/152 (100%)	128 (84%)	24 (16%)	2	11
8	H	117/128 (91%)	106 (91%)	11 (9%)	8	29
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	24
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	8
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
16	X	109/136 (80%)	89 (82%)	20 (18%)	2	8
All	All	3559/4145 (86%)	3097 (87%)	462 (13%)	4	17

5 of 462 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	635	ARG
16	X	244	MET
2	B	1183	LYS
12	L	55	ILE
9	I	21	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	706	GLN
16	X	339	ASN
2	B	1179	GLN
16	X	318	ASN
8	H	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	3	C
14	P	5	A
14	P	9	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
15	BRU	T	19	15,14	18,21,22	1.34	3 (16%)	25,30,33	1.99	7 (28%)

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
15	BRU	T	19	15,14	-	0/7/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	19	BRU	C2-N1	2.71	1.42	1.38
15	T	19	BRU	C6-C5	2.63	1.39	1.34
15	T	19	BRU	C4-N3	-2.13	1.34	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	BRU	C5-C4-N3	4.38	118.38	113.34
15	T	19	BRU	O4-C4-C5	-4.09	120.59	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	BRU	N3-C2-N1	3.86	119.92	114.89
15	T	19	BRU	C4-N3-C2	-3.53	122.72	127.34
15	T	19	BRU	BR-C5-C4	3.23	121.74	118.02

There are no chirality outliers.

There are no torsion outliers.

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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
19	EPE	G	1172	-	15,15,15	1.24	1 (6%)	19,20,20	0.51	0
19	EPE	A	2459	-	15,15,15	1.02	1 (6%)	19,20,20	0.64	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
19	EPE	G	1172	-	-	3/9/19/19	0/1/1/1
19	EPE	A	2459	-	-	6/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1172	EPE	C10-S	-4.73	1.71	1.77
19	A	2459	EPE	C10-S	-3.86	1.72	1.77

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	2459	EPE	C9-C10-S-O1S
19	A	2459	EPE	C9-C10-S-O2S
19	A	2459	EPE	C8-C7-N4-C3
19	A	2459	EPE	C9-C10-S-O3S
19	G	1172	EPE	N4-C7-C8-O8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	2459	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
8	H	1
12	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	4.90
1	H	62:SER	C	63:LEU	N	3.28
1	L	59:ALA	C	60:ARG	N	2.90

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1426/1733 (82%)	0.04	42 (2%)	53	34	60, 98, 157, 213	0
2	B	1115/1224 (91%)	0.23	61 (5%)	30	17	61, 107, 165, 198	0
3	C	266/318 (83%)	-0.20	0	100	100	74, 96, 135, 164	0
4	D	178/221 (80%)	0.18	11 (6%)	26	15	79, 111, 156, 183	0
5	E	215/215 (100%)	0.08	4 (1%)	66	45	80, 134, 176, 192	0
6	F	87/155 (56%)	-0.26	3 (3%)	48	28	67, 81, 116, 141	0
7	G	171/171 (100%)	0.03	3 (1%)	67	47	77, 99, 135, 155	0
8	H	133/146 (91%)	0.71	18 (13%)	7	4	103, 140, 180, 198	0
9	I	119/122 (97%)	0.43	7 (5%)	28	16	108, 139, 175, 194	0
10	J	65/70 (92%)	-0.23	1 (1%)	72	52	82, 96, 138, 151	0
11	K	115/120 (95%)	-0.23	2 (1%)	69	48	68, 98, 135, 156	0
12	L	46/70 (65%)	1.65	15 (32%)	1	1	77, 172, 184, 191	0
13	N	13/14 (92%)	0.93	0	100	100	150, 182, 258, 261	0
14	P	10/11 (90%)	0.16	1 (10%)	12	7	85, 108, 157, 162	0
15	T	24/26 (92%)	0.67	0	100	100	98, 147, 265, 267	0
16	X	119/146 (81%)	1.41	33 (27%)	1	1	160, 190, 211, 222	0
All	All	4102/4762 (86%)	0.16	201 (4%)	35	20	60, 106, 177, 267	0

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	8.2
12	L	27	LEU	7.6
2	B	502	ILE	7.2
8	H	63	LEU	7.1
12	L	25	ALA	6.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BRU	T	19	20/21	0.96	0.08	91,98,105,114	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	EPE	G	1172	15/15	0.62	0.35	217,230,230,231	0
19	EPE	A	2459	15/15	0.72	0.38	249,261,272,273	0
18	MG	A	2458	1/1	0.94	0.10	275,275,275,275	0
17	ZN	L	1071	1/1	0.98	0.05	193,193,193,193	0
17	ZN	I	1121	1/1	0.99	0.05	117,117,117,117	0
17	ZN	I	1122	1/1	0.99	0.06	191,191,191,191	0
17	ZN	J	1066	1/1	1.00	0.03	84,84,84,84	0
17	ZN	B	2225	1/1	1.00	0.05	87,87,87,87	0
17	ZN	C	1269	1/1	1.00	0.02	88,88,88,88	0
17	ZN	A	2456	1/1	1.00	0.02	124,124,124,124	0
17	ZN	A	2457	1/1	1.00	0.06	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.