wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2017 – 11:18 PM EDT

PDB ID	:	3PO2
Title	:	Arrested RNA Polymerase II elongation complex
Authors	:	Cheung, A.C.M.; Cramer, P.
Deposited on	:	unknown
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

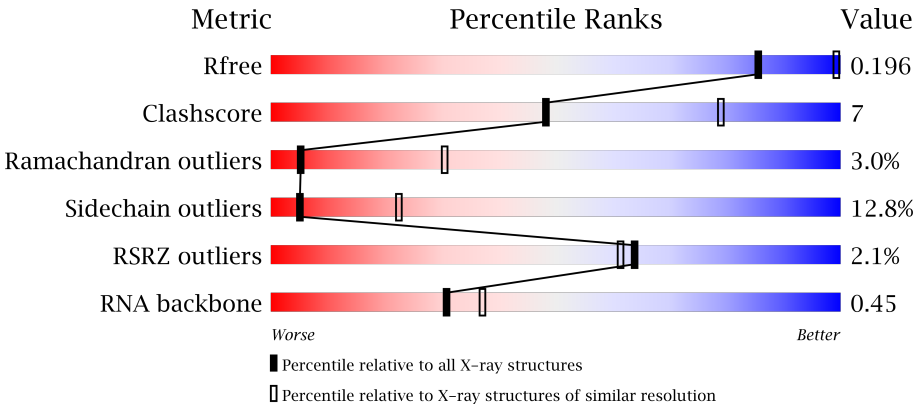
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	.% 59% 19% • • 18%
2	B	1224	2% 68% 20% • 8%
3	C	318	.% 57% 23% • • 16%
4	D	221	.% 62% 17% • 19%

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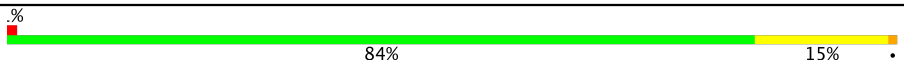
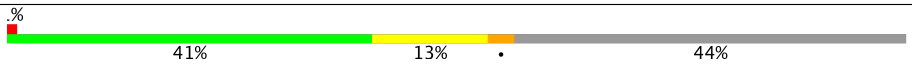
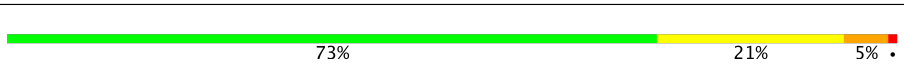
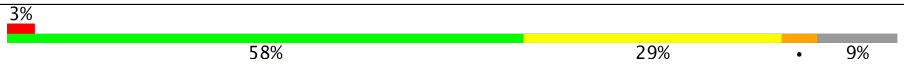
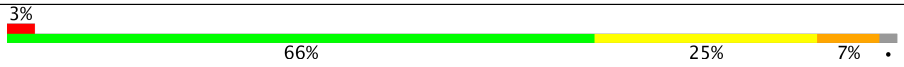
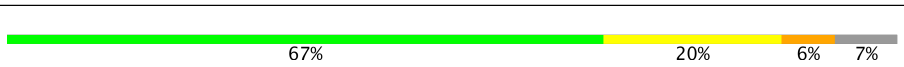
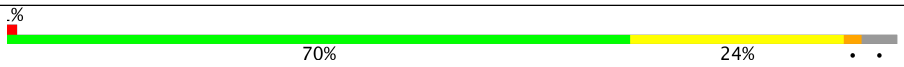
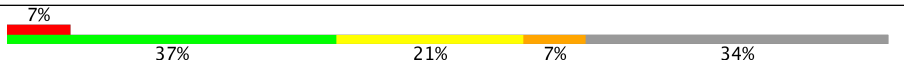
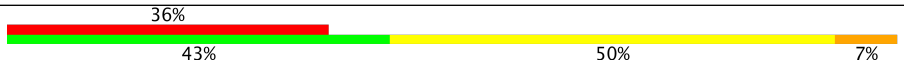
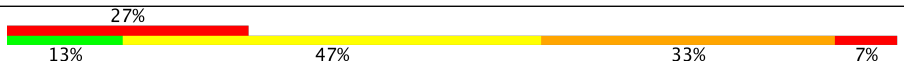
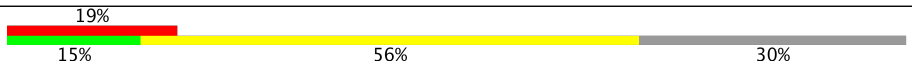
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	15	
15	T	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	ACT	A	1734	-	-	-	X
20	PEG	G	172	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32287 atoms, of which 0 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
			Total	C	N	O	S			
1	A	1421	11190	7052	1957	2119	62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1121	8899	5632	1563	1649	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	180	1440	890	256	291	3	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- 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 RPABC3.

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 RPABC5.

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 RPABC4.

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 DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			288	138	57	80	13			

- Molecule 14 is a RNA chain called RNA product strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	15	Total	C	N	O	P	0	0	0
			300	135	45	105	15			

- Molecule 15 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0	0
			389	1	185	66	118	19			

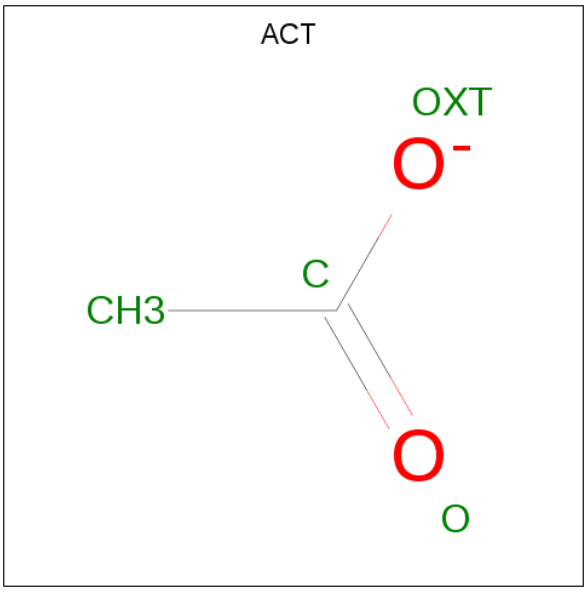
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

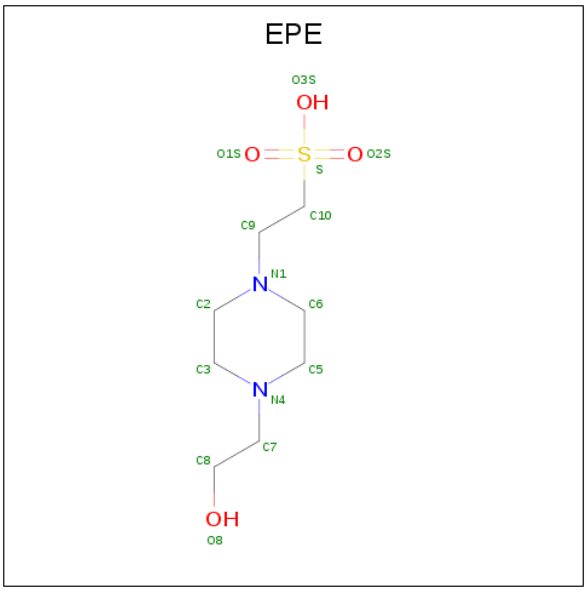
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



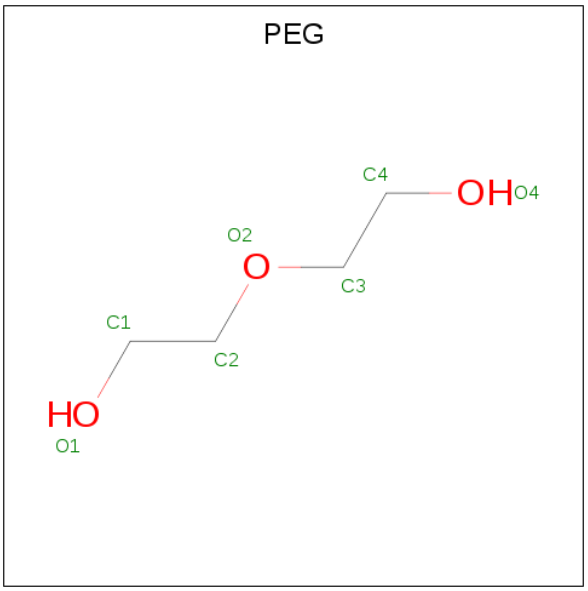
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 20 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

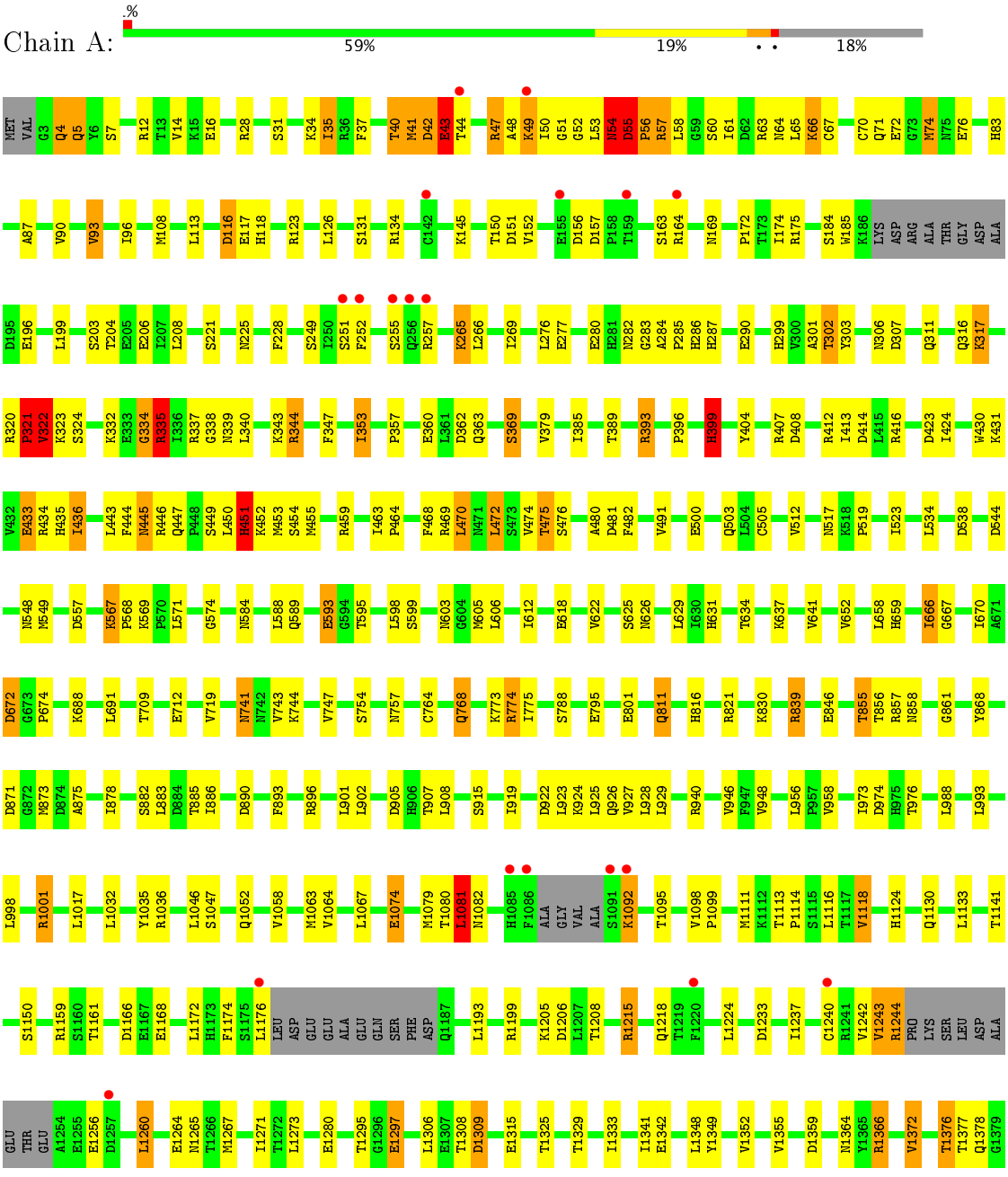


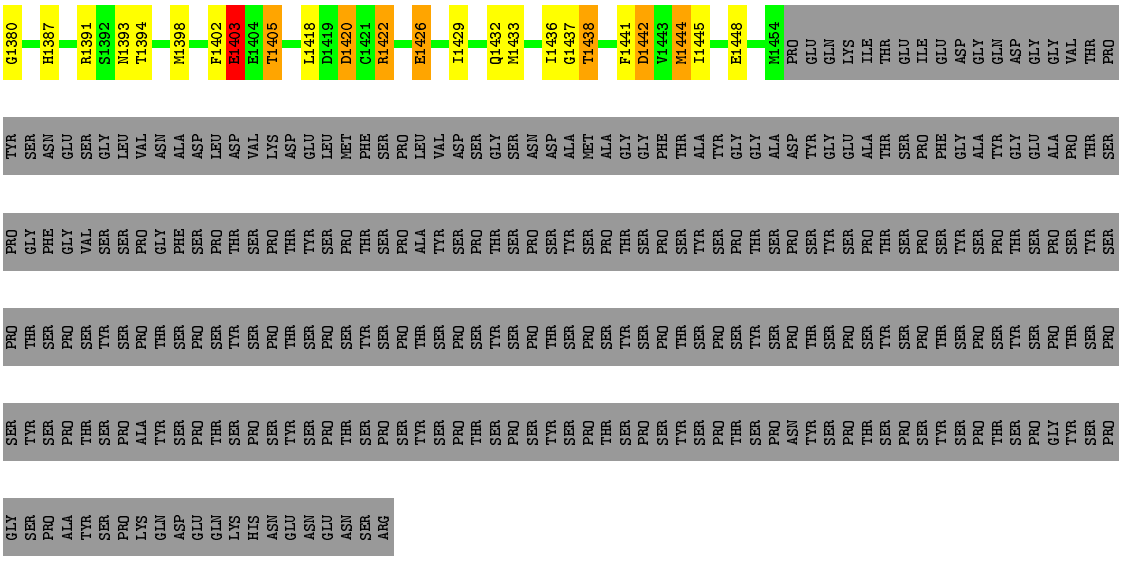
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	G	1	7	4	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

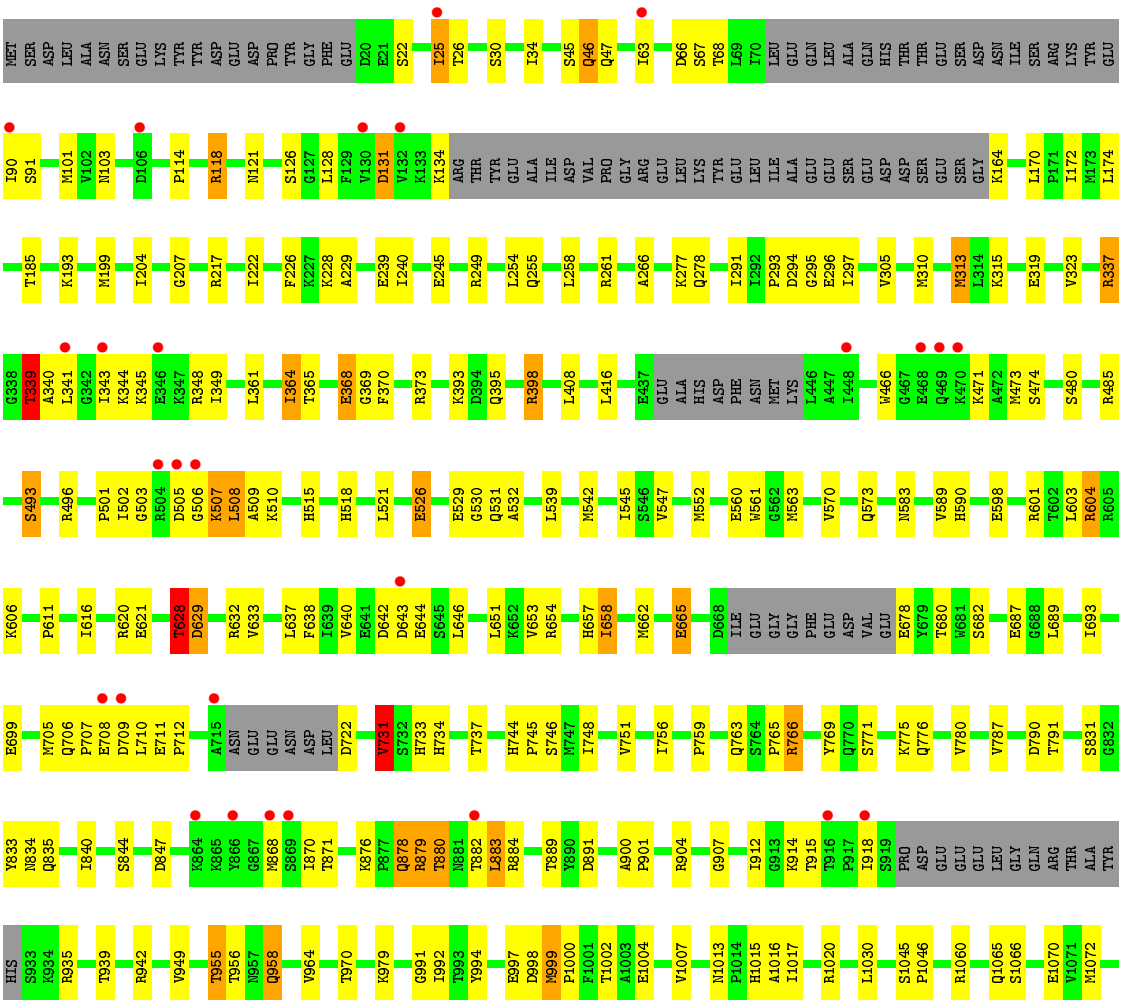
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

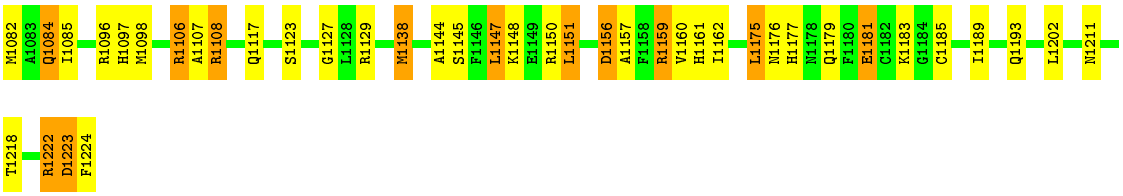




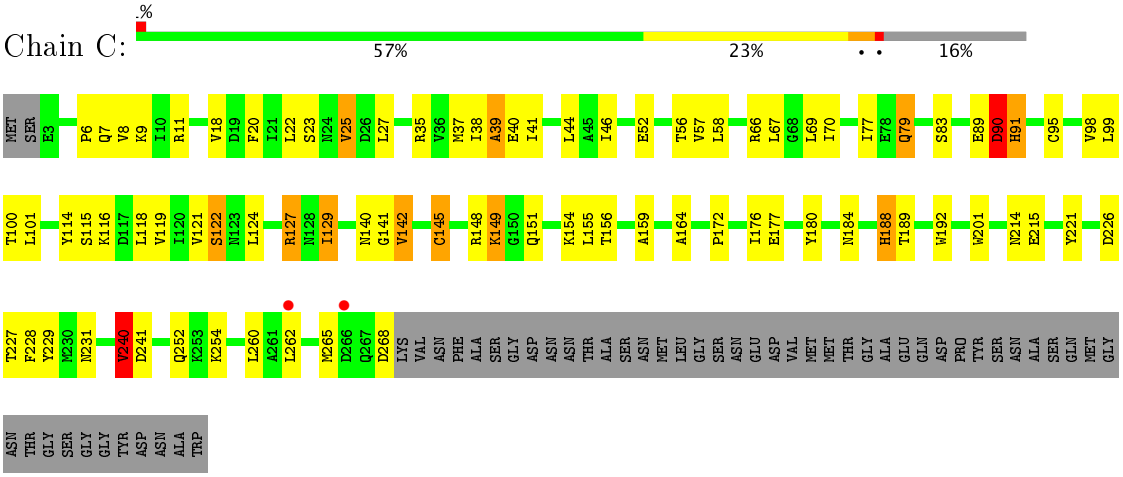
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

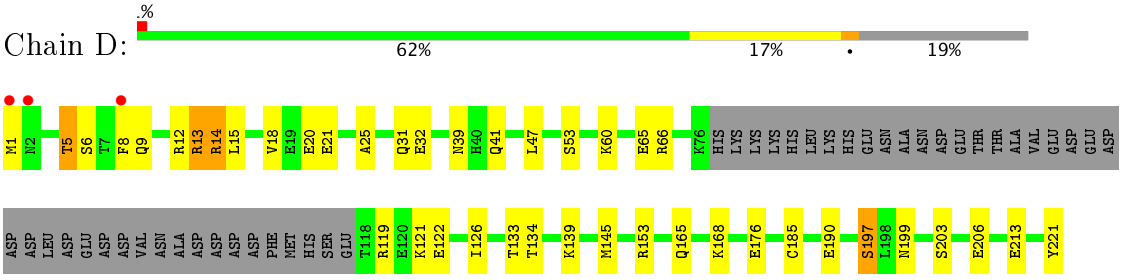




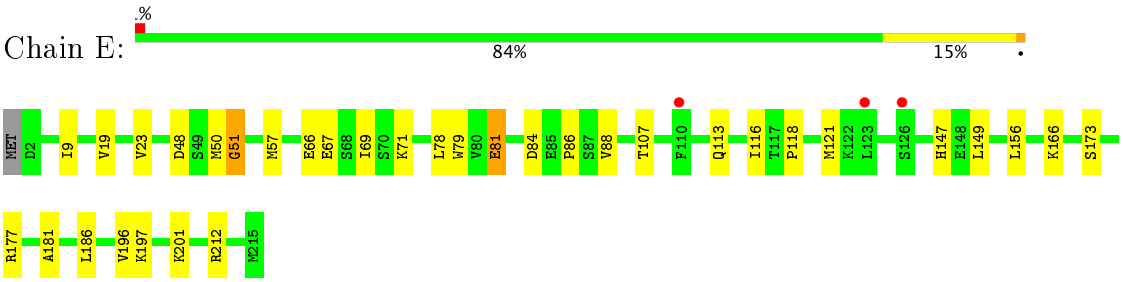
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



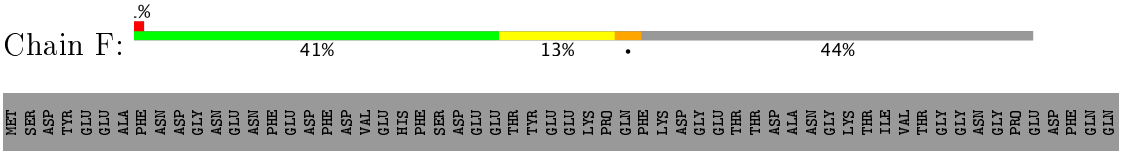
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

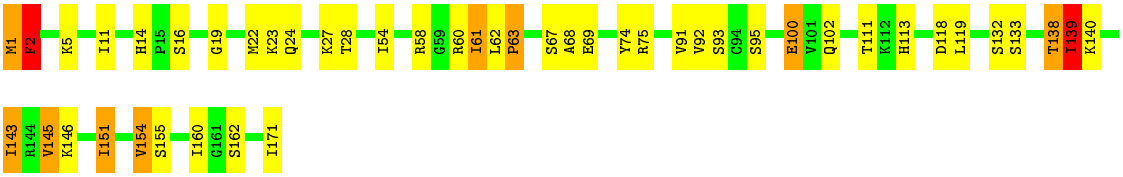


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



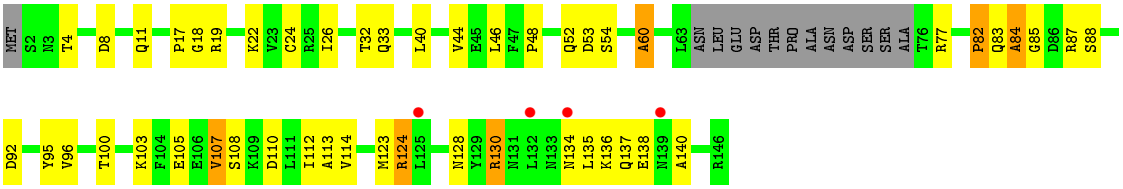
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



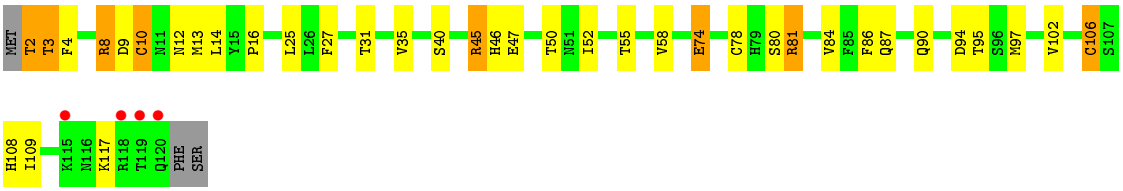
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



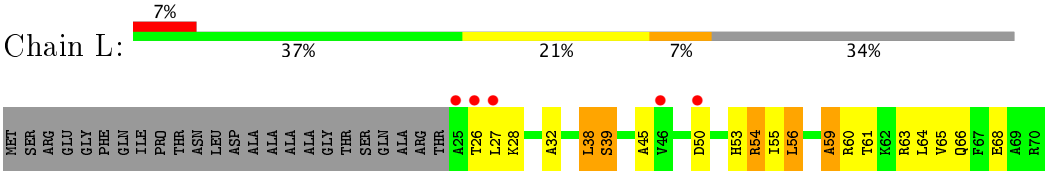
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

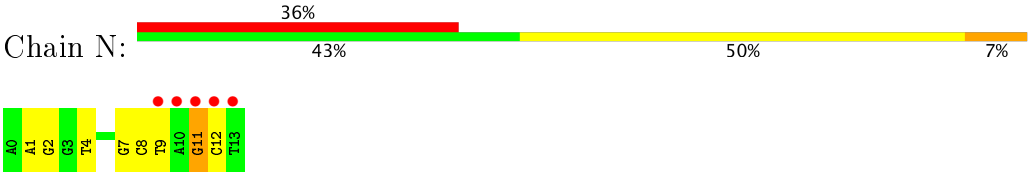
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:

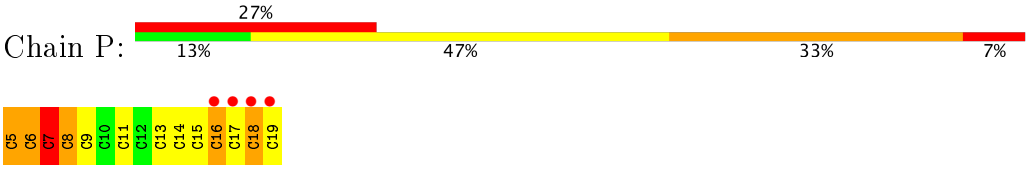
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



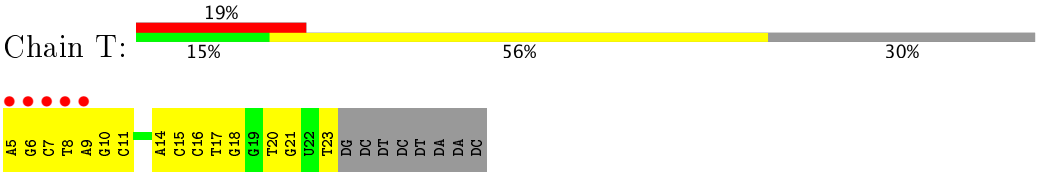
- Molecule 13: DNA non-template strand



- Molecule 14: RNA product strand



- Molecule 15: DNA template strand



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	224.57Å 394.55Å 282.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.30 48.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.98-3.30) 99.9 (48.98-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.153 , 0.178 0.173 , 0.196	Depositor DCC
R_{free} test set	3687 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	109.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 97.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 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	32287	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, PEG, BRU, ZN, ACT, EPE

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	0.54	1/11391 (0.0%)	0.83	8/15402 (0.1%)
2	B	0.51	0/9072	0.79	2/12233 (0.0%)
3	C	0.50	0/2133	0.79	1/2891 (0.0%)
4	D	0.51	0/1450	0.84	1/1945 (0.1%)
5	E	0.45	0/1788	0.71	0/2406
6	F	0.59	0/717	0.85	0/967
7	G	0.51	0/1368	0.82	1/1844 (0.1%)
8	H	0.47	0/1086	0.81	0/1470
9	I	0.46	0/989	0.78	0/1331
10	J	0.48	0/541	0.84	1/727 (0.1%)
11	K	0.51	0/938	0.72	0/1267
12	L	0.59	0/365	1.05	1/485 (0.2%)
13	N	0.98	0/324	1.87	13/499 (2.6%)
14	P	1.44	2/329 (0.6%)	2.46	34/506 (6.7%)
15	T	1.20	2/411 (0.5%)	2.11	20/630 (3.2%)
All	All	0.55	5/32902 (0.0%)	0.89	82/44603 (0.2%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	5.88	1.47	1.34
14	P	5	C	C1'-N1	5.72	1.57	1.48
15	T	23	DT	C1'-N1	5.66	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	21	DG	N3-C4	5.04	1.39	1.35
14	P	6	C	C1'-N1	5.02	1.56	1.48

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	5	C	P-O3'-C3'	12.51	134.71	119.70
14	P	7	C	N1-C2-O2	11.87	126.02	118.90
15	T	8	DT	P-O3'-C3'	11.22	133.16	119.70
13	N	11	DG	O4'-C1'-N9	10.82	115.58	108.00
14	P	6	C	N1-C1'-C2'	8.75	125.38	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Mainchain

5.2 Too-close contacts (i)

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	11190	0	11255	209	0
2	B	8899	0	8940	117	0
3	C	2095	0	2051	45	0
4	D	1440	0	1456	9	0
5	E	1752	0	1776	13	0
6	F	705	0	731	12	0
7	G	1340	0	1357	23	0
8	H	1068	0	1040	16	0
9	I	971	0	927	19	0
10	J	532	0	542	11	0
11	K	920	0	929	21	0
12	L	363	0	386	6	0
13	N	288	0	159	1	0
14	P	300	0	166	1	0
15	T	389	0	214	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	A	4	0	3	0	0
19	D	15	0	17	0	0
20	G	7	0	10	0	0
All	All	32287	0	31959	445	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 445 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)
7:G:151:ILE:CD1	7:G:151:ILE:CG1	1.75	1.58
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.40	1.02
1:A:53:LEU:HD23	1:A:54:ASN:H	1.24	1.02
1:A:1081:LEU:HB2	1:A:1082:ASN:HA	1.43	0.96
10:J:48:ARG:O	10:J:52:THR:HG22	1.67	0.94

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	1411/1733 (81%)	1279 (91%)	94 (7%)	38 (3%)	6 32
2	B	1107/1224 (90%)	997 (90%)	74 (7%)	36 (3%)	4 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	264/318 (83%)	235 (89%)	23 (9%)	6 (2%)	7 36
4	D	176/221 (80%)	157 (89%)	15 (8%)	4 (2%)	7 36
5	E	212/215 (99%)	201 (95%)	9 (4%)	2 (1%)	20 55
6	F	85/155 (55%)	78 (92%)	7 (8%)	0	100 100
7	G	169/171 (99%)	157 (93%)	7 (4%)	5 (3%)	5 30
8	H	129/146 (88%)	105 (81%)	10 (8%)	14 (11%)	0 3
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	6 33
10	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	5 29
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100 100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 1
All	All	3890/4565 (85%)	3501 (90%)	271 (7%)	118 (3%)	5 30

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG

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 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	1244/1520 (82%)	1081 (87%)	163 (13%)	5 22
2	B	969/1061 (91%)	842 (87%)	127 (13%)	5 22
3	C	234/274 (85%)	205 (88%)	29 (12%)	5 24
4	D	160/200 (80%)	133 (83%)	27 (17%)	2 12
5	E	196/197 (100%)	184 (94%)	12 (6%)	22 57
6	F	77/137 (56%)	66 (86%)	11 (14%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	152/152 (100%)	132 (87%)	20 (13%)	5 21
8	H	117/128 (91%)	101 (86%)	16 (14%)	4 20
9	I	113/116 (97%)	99 (88%)	14 (12%)	5 24
10	J	60/65 (92%)	52 (87%)	8 (13%)	4 21
11	K	99/102 (97%)	91 (92%)	8 (8%)	14 44
12	L	40/57 (70%)	33 (82%)	7 (18%)	2 10
All	All	3461/4009 (86%)	3019 (87%)	442 (13%)	5 22

5 of 442 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	480	SER
2	B	876	LYS
9	I	10	CYS
2	B	507	LYS
2	B	628	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	178	ASN
2	B	1013	ASN
8	H	137	GLN
2	B	465	ASN
2	B	657	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	15/15 (100%)	6 (40%)	2 (13%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	6	C
14	P	7	C
14	P	8	C
14	P	17	C

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Mol	Chain	Res	Type
14	P	18	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	5	C
14	P	16	C

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

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	22	15,14	13,21,22	1.24	1 (7%)	16,30,33	2.00	3 (18%)

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	22	15,14	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	3.29	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	C5-C4-N3	-3.57	119.37	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	O4'-C1'-N1	2.29	111.65	107.78
15	T	22	BRU	C4-N3-C2	6.24	120.61	115.16

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
18	ACT	A	1734	-	1,3,3	1.53	0	0,3,3	0.00	-
19	EPE	D	222	-	15,15,15	0.64	0	18,20,20	2.28	9 (50%)
20	PEG	G	172	-	6,6,6	0.50	0	5,5,5	0.32	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
18	ACT	A	1734	-	-	0/0/0/0	0/0/0/0
19	EPE	D	222	-	-	0/9/19/19	0/1/1/1
20	PEG	G	172	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	222	EPE	O1S-S-C10	-3.04	104.18	106.79
19	D	222	EPE	C9-N1-C6	-2.37	105.18	111.26
19	D	222	EPE	C2-C3-N4	2.10	114.88	110.63
19	D	222	EPE	C6-C5-N4	2.30	115.29	110.63
19	D	222	EPE	C7-N4-C3	2.59	117.89	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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, 95^{th} 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	1421/1733 (81%)	-0.01	19 (1%) 77 75	66, 108, 173, 229	0
2	B	1121/1224 (91%)	0.11	27 (2%) 59 56	68, 119, 185, 221	0
3	C	266/318 (83%)	-0.08	2 (0%) 86 85	81, 108, 153, 188	0
4	D	180/221 (81%)	0.06	3 (1%) 70 67	90, 120, 172, 195	0
5	E	214/215 (99%)	-0.01	3 (1%) 75 73	87, 146, 197, 206	0
6	F	87/155 (56%)	-0.28	1 (1%) 80 79	71, 90, 127, 136	0
7	G	171/171 (100%)	0.08	0 100 100	83, 107, 150, 175	0
8	H	133/146 (91%)	0.36	4 (3%) 51 49	111, 154, 193, 214	0
9	I	119/122 (97%)	0.00	4 (3%) 46 42	118, 148, 190, 209	0
10	J	65/70 (92%)	-0.16	0 100 100	90, 107, 150, 161	0
11	K	115/120 (95%)	-0.10	1 (0%) 84 83	75, 108, 144, 161	0
12	L	46/70 (65%)	0.61	5 (10%) 6 5	89, 181, 199, 204	0
13	N	14/14 (100%)	1.17	5 (35%) 0 1	203, 228, 278, 279	0
14	P	15/15 (100%)	0.82	4 (26%) 1 1	151, 172, 214, 227	0
15	T	18/27 (66%)	1.00	5 (27%) 1 1	133, 199, 284, 287	0
All	All	3985/4621 (86%)	0.04	83 (2%) 64 61	66, 115, 186, 287	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	8.2
1	A	255	SER	5.9
1	A	1176	LEU	5.1
11	K	115	ALA	4.8
14	P	16	C	4.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
15	BRU	T	22	20/21	0.92	0.12	-	110,169,284,288	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
20	PEG	G	172	7/7	0.84	0.89	12.07	74,118,300,300	0
18	ACT	A	1734	4/4	0.87	0.33	10.03	67,89,129,132	0
16	ZN	B	2225	1/1	0.99	0.21	1.02	99,99,99,99	0
16	ZN	J	1066	1/1	0.99	0.23	0.04	105,105,105,105	0
16	ZN	I	1121	1/1	0.99	0.14	0.00	124,124,124,124	0
19	EPE	D	222	15/15	0.97	0.20	-0.10	53,72,130,170	0
16	ZN	A	2457	1/1	1.00	0.16	-0.74	94,94,94,94	0
16	ZN	C	1269	1/1	0.99	0.12	-0.96	93,93,93,93	0
16	ZN	A	2456	1/1	0.99	0.08	-1.42	156,156,156,156	0
17	MG	A	2458	1/1	0.99	0.13	-1.79	78,78,78,78	0
16	ZN	I	1122	1/1	0.99	0.04	-1.97	199,199,199,199	0
16	ZN	L	1071	1/1	0.96	0.03	-2.36	225,225,225,225	0

6.5 Other polymers (i)

There are no such residues in this entry.