wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2018 – 09:24 pm GMT

PDB ID	:	2R92
Title	:	Elongation complex of RNA polymerase II with artificial RdRP scaffold
Authors	:	Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on	:	2007-09-12
Resolution	:	3.80 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 (i) symbol.

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

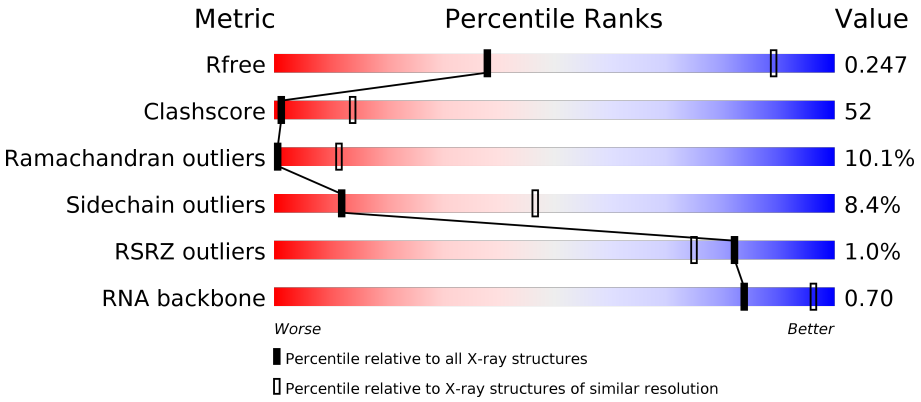
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

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 3.80 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}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)
RNA backbone	2636	1083 (4.70-2.90)

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 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	P	16	13% 13% 38% 6% 44%
2	T	17	41% 6% 29% 6% 18% 41%
3	A	1733	27% 44% 9% • 18%
4	B	1224	% 27% 53% 10% 9%

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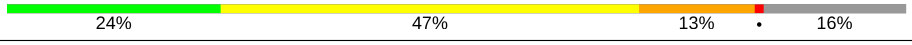
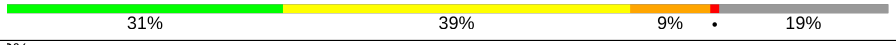
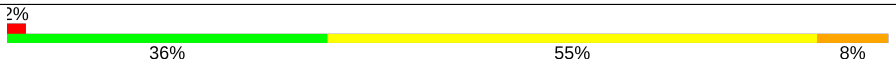
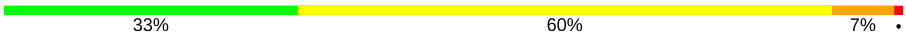
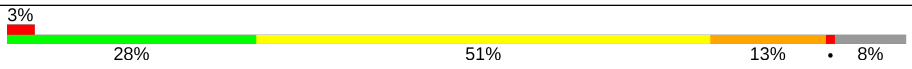
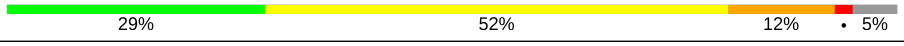
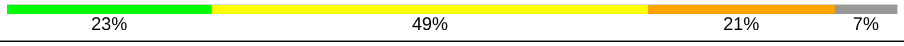
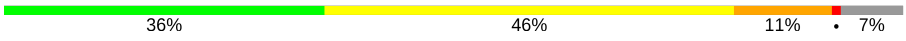
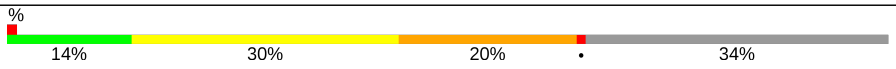
Mol	Chain	Length	Quality of chain
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 31611 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 RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	9	192	87	39	58	8	0	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	10	208	94	36	69	9	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1422	11194	7054	1959	2119	62	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	1112	8841	5596	1550	1640	55	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	267	2101	1320	349	419	13	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

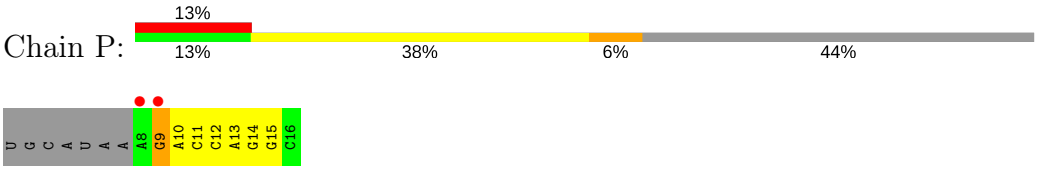
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

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 geometryand 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.

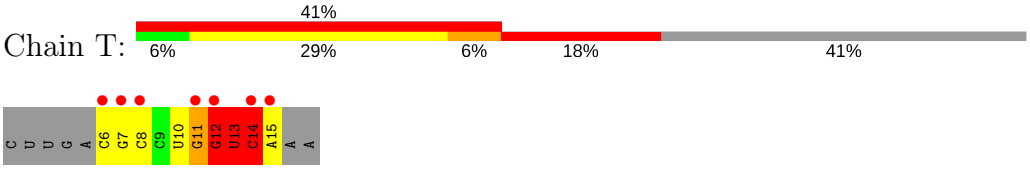
• Molecule 1: RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')

Chain P:



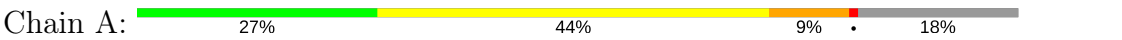
• Molecule 2: RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3')

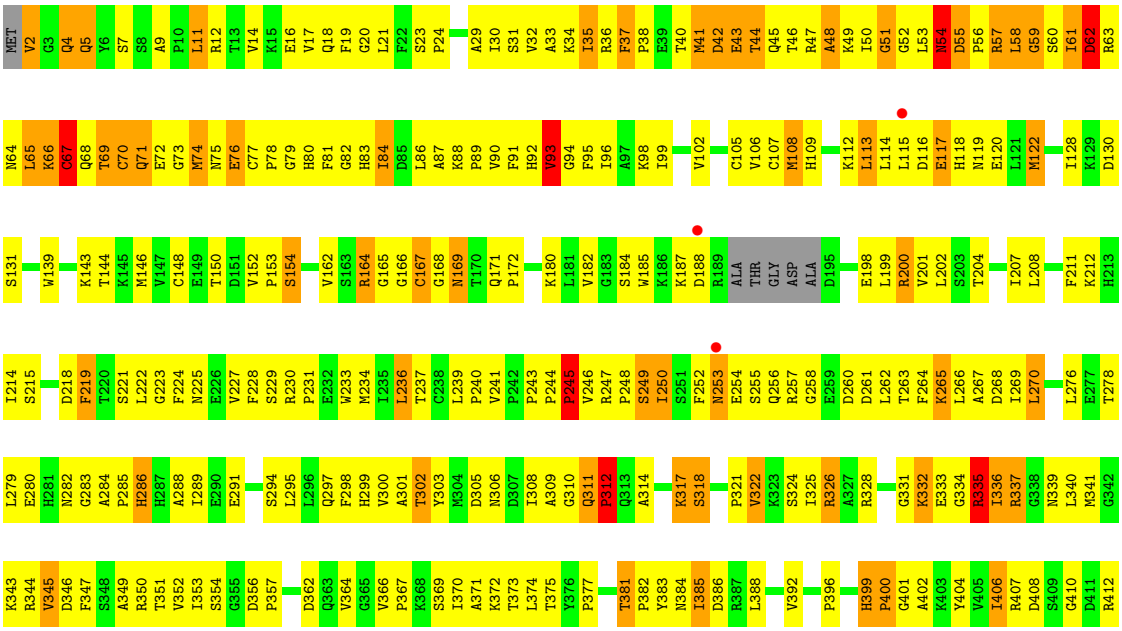
Chain T:

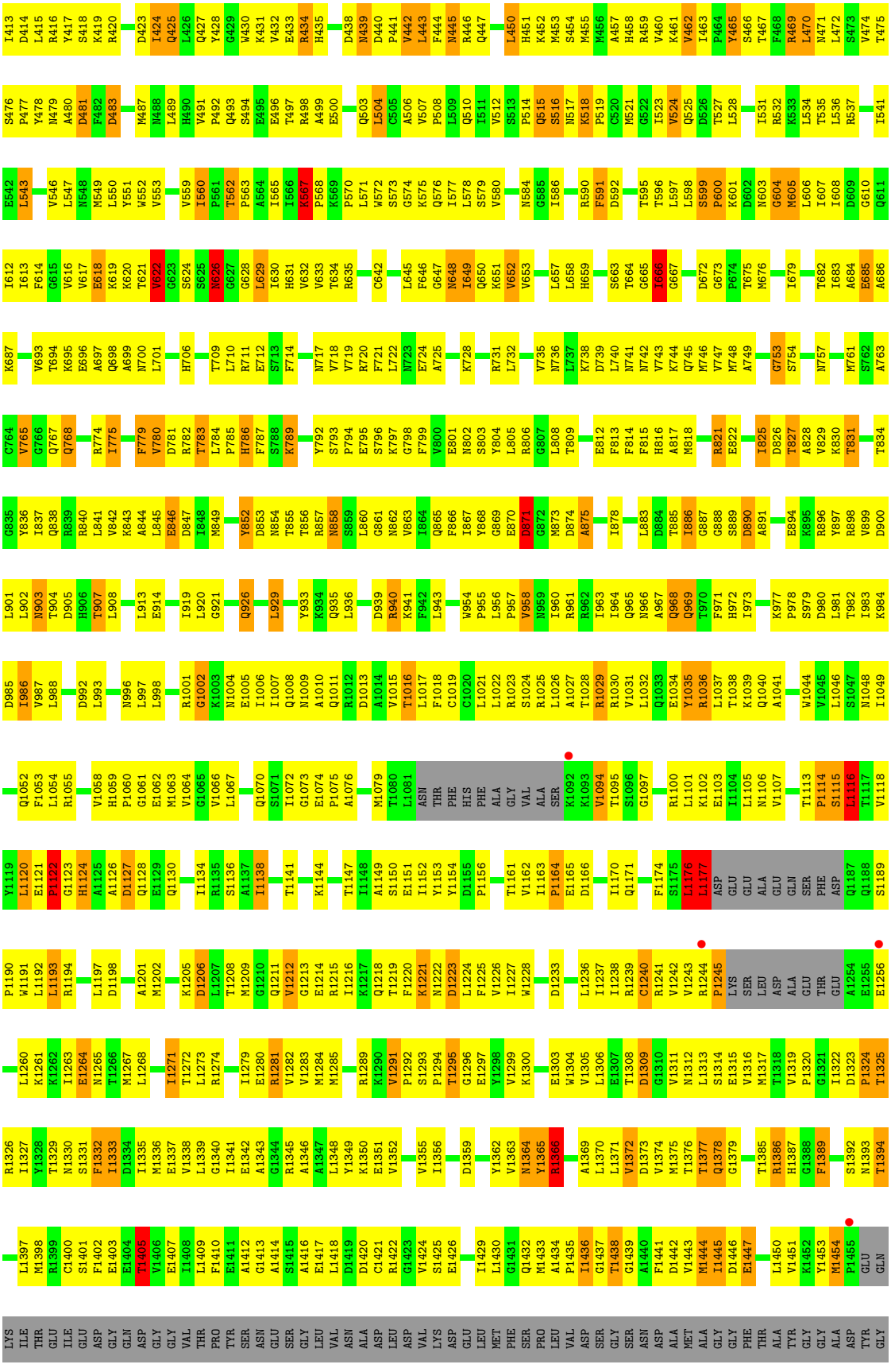


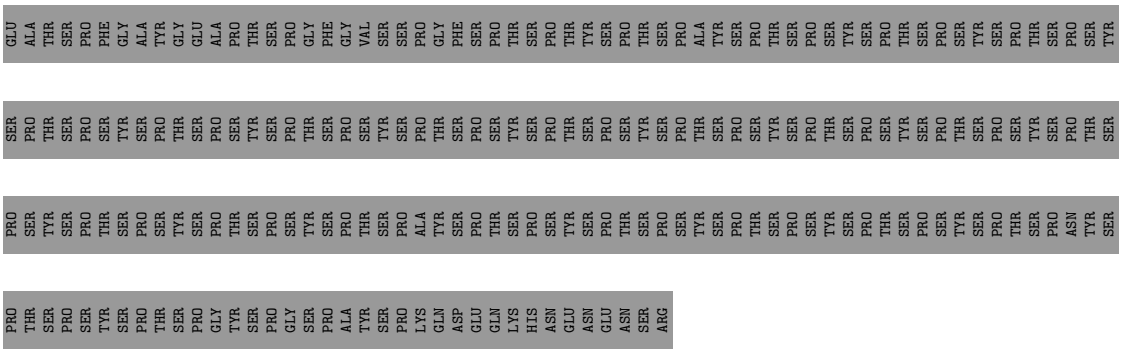
• Molecule 3: DNA-directed RNA polymerase II subunit RPB1

Chain A:



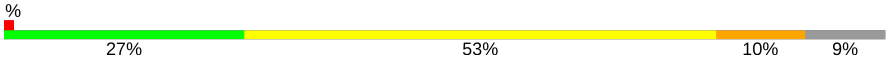


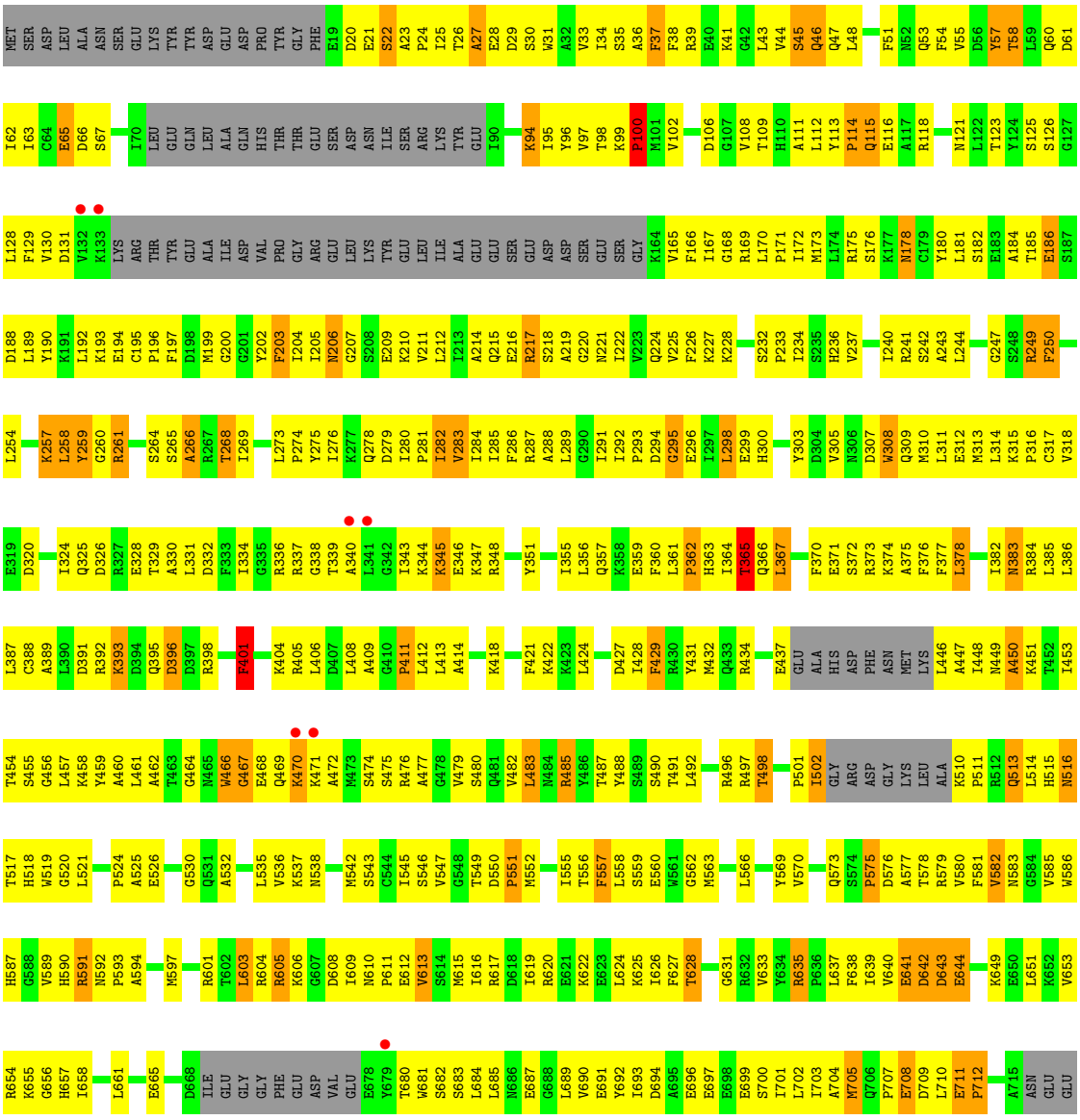


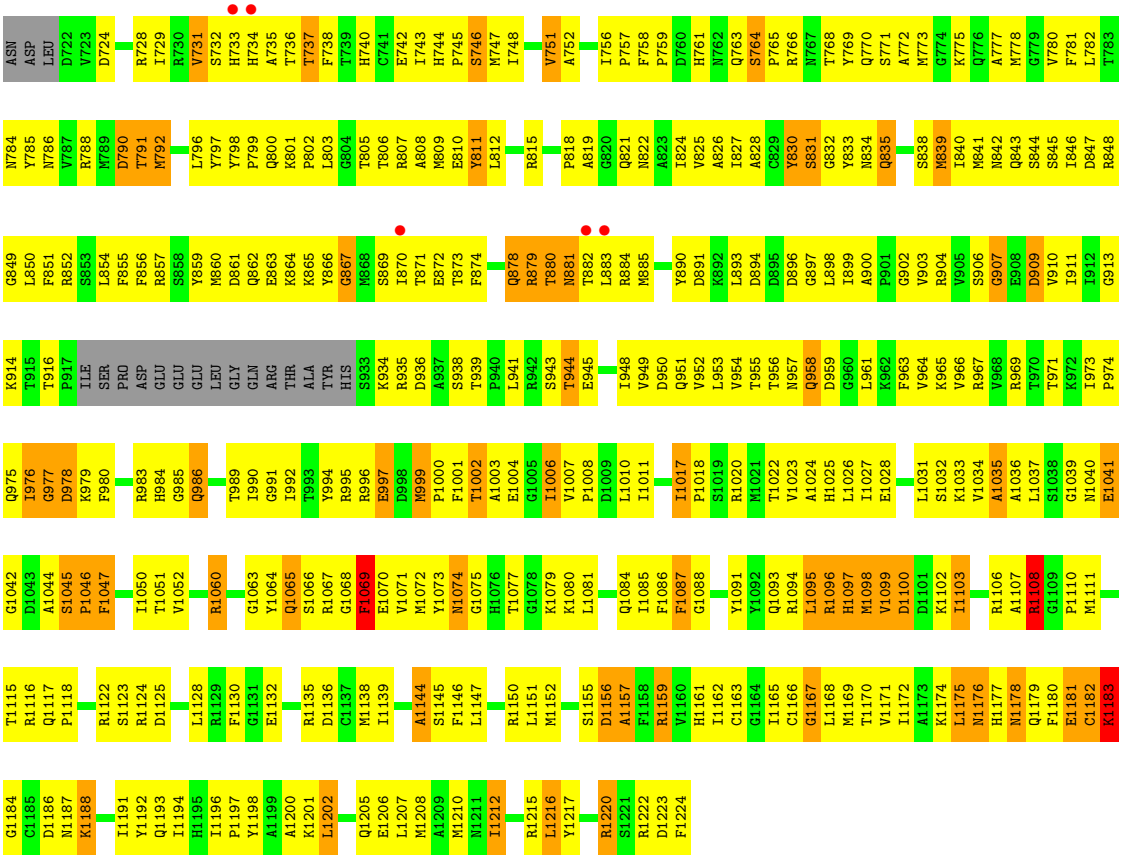


• Molecule 4: DNA-directed RNA polymerase II subunit RPB2

Chain B:

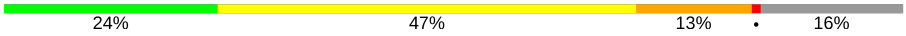


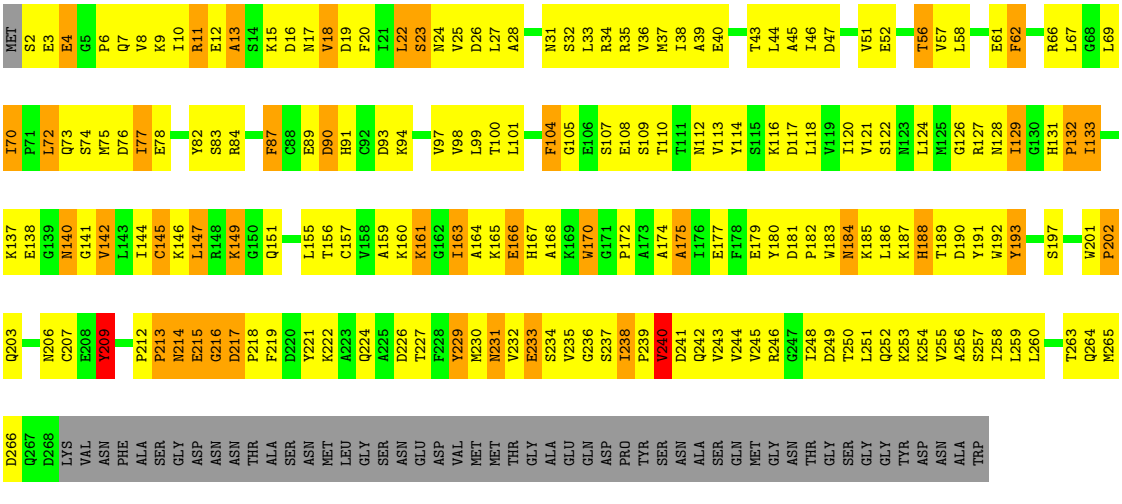




• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

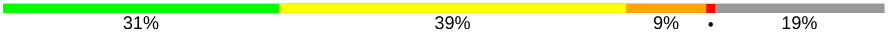
Chain C:

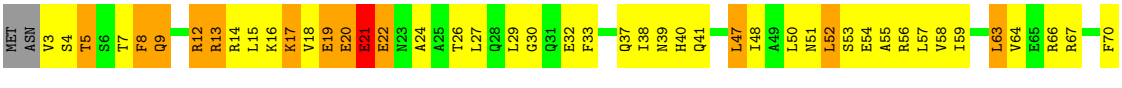


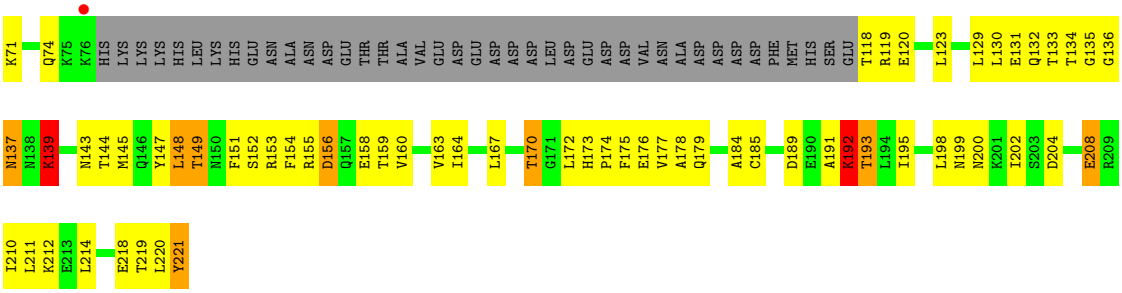


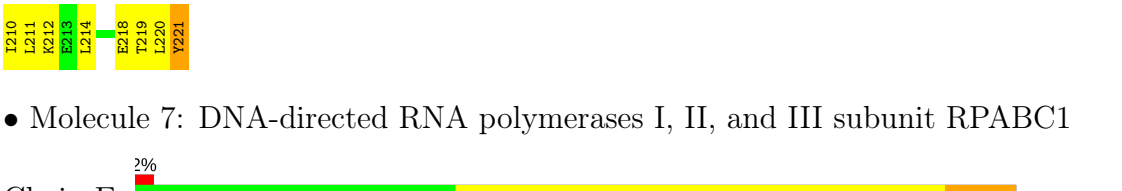
• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

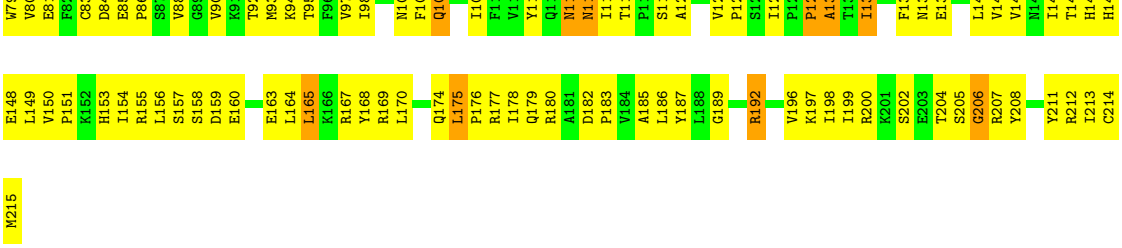
Chain D:





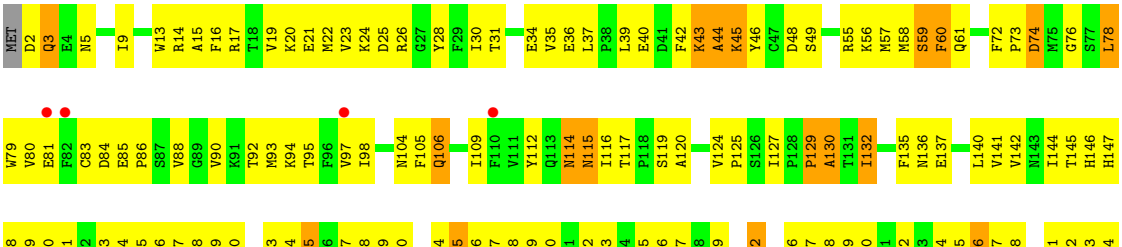






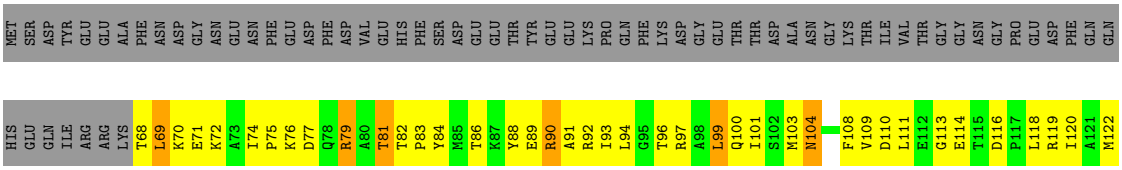
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



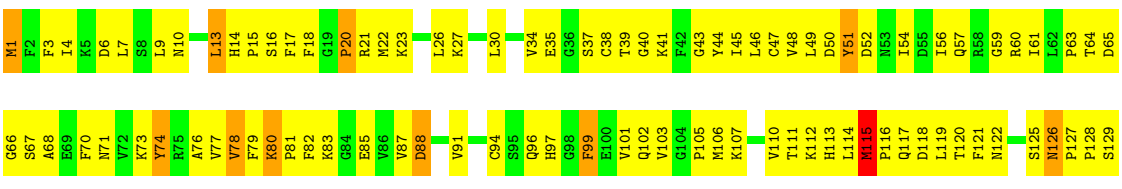
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

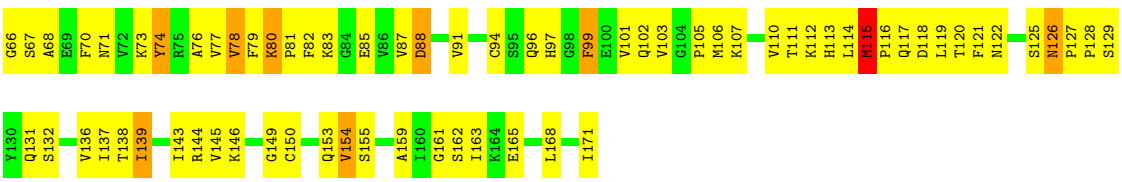
Chain F:



• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

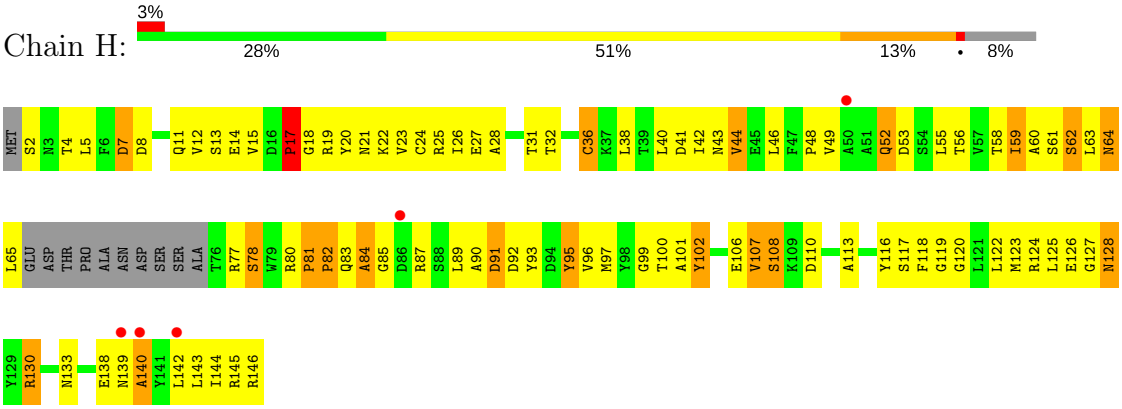
Chain G:





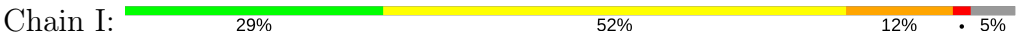
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



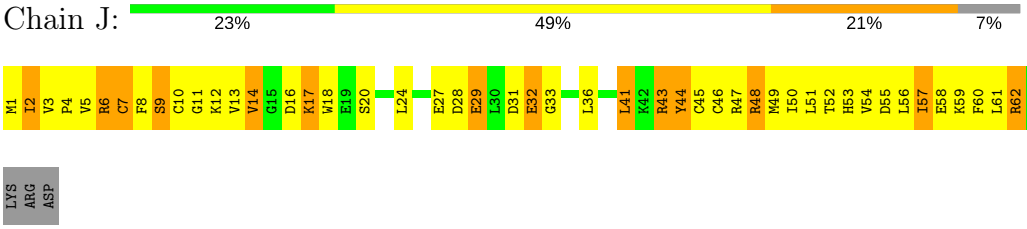
• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I:



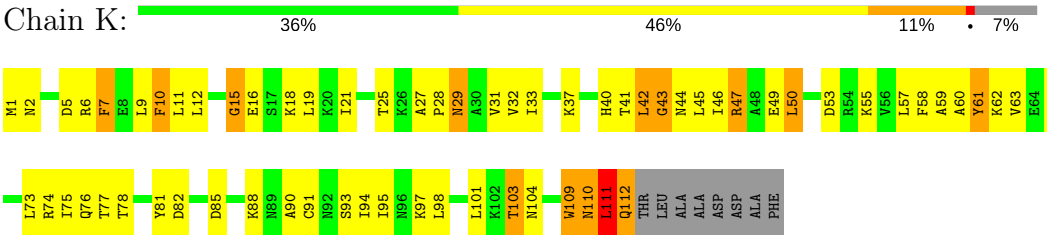
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



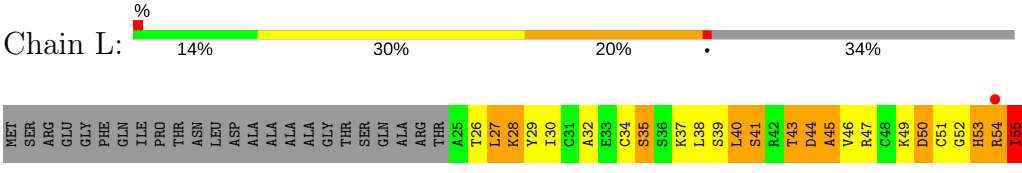
• Molecule 13: DNA-directed RNA polymerase II subunit RPB11

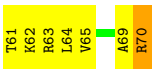
Chain K:



• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:




T61
K62
R63
L64
V65
A69
R70

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.68Å 393.85Å 283.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.9 (48.51-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.44 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.246 0.217 , 0.247	Depositor DCC
R_{free} test set	2431 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	114.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31611	wwPDB-VP
Average B, all atoms (Å^2)	128.0	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: 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	P	0.63	0/215	0.81	0/334
2	T	0.71	0/231	1.32	5/358 (1.4%)
3	A	0.42	0/11394	0.73	7/15407 (0.0%)
4	B	0.41	0/9012	0.68	1/12149 (0.0%)
5	C	0.43	0/2138	0.71	0/2896
6	D	0.39	0/1444	0.66	0/1935
7	E	0.39	0/1788	0.63	0/2406
8	F	0.45	0/724	0.76	0/977
9	G	0.45	0/1368	0.72	0/1844
10	H	0.37	0/1102	0.62	0/1492
11	I	0.38	0/962	0.65	0/1295
12	J	0.47	0/541	0.75	0/727
13	K	0.45	0/922	0.68	0/1244
14	L	0.46	0/366	0.69	0/485
All	All	0.42	0/32207	0.71	13/43549 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1176	LEU	CA-CB-CG	13.45	146.23	115.30
2	T	12	G	N9-C1'-C2'	9.04	125.76	114.00
2	T	12	G	O4'-C1'-N9	8.14	114.72	108.20
2	T	13	U	O4'-C1'-N1	7.87	114.50	108.20
3	A	1176	LEU	CB-CA-C	-7.05	96.81	110.20

There are no chirality outliers.

There are no planarity outliers.

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	P	192	0	101	6	0
2	T	208	0	110	16	0
3	A	11194	0	11278	1259	0
4	B	8841	0	8874	1006	0
5	C	2101	0	2055	275	0
6	D	1434	0	1460	146	0
7	E	1752	0	1776	163	0
8	F	712	0	738	89	0
9	G	1340	0	1357	182	0
10	H	1084	0	1057	140	0
11	I	944	0	903	120	0
12	J	532	0	542	90	0
13	K	904	0	911	93	0
14	L	364	0	388	54	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31611	0	31550	3310	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 52.

The worst 5 of 3310 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)
3:A:58:LEU:HD12	3:A:59:GLY:H	0.99	1.11
4:B:343:ILE:HG23	4:B:347:LYS:HB2	1.25	1.09
4:B:510:LYS:HG2	4:B:511:PRO:HD3	1.22	1.08
3:A:53:LEU:HD23	3:A:54:ASN:N	1.68	1.08
5:C:43:THR:HG22	5:C:44:LEU:H	0.98	1.07

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
3	A	1412/1733 (82%)	1030 (73%)	249 (18%)	133 (9%)	1 13
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	1 14
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0 5
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	0 11
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	1 15
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	1 14
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	4 35
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0 4
11	I	114/122 (93%)	69 (60%)	30 (26%)	15 (13%)	0 5
12	J	63/70 (90%)	39 (62%)	10 (16%)	14 (22%)	0 1
13	K	110/120 (92%)	87 (79%)	15 (14%)	8 (7%)	1 20
14	L	44/70 (63%)	18 (41%)	10 (23%)	16 (36%)	0 0
All	All	3873/4565 (85%)	2744 (71%)	736 (19%)	393 (10%)	0 11

5 of 393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	4	GLN
3	A	44	THR
3	A	48	ALA
3	A	54	ASN
3	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
3	A	1245/1520 (82%)	1129 (91%)	116 (9%)	10 40
4	B	964/1061 (91%)	890 (92%)	74 (8%)	14 49
5	C	235/274 (86%)	212 (90%)	23 (10%)	9 38
6	D	160/200 (80%)	142 (89%)	18 (11%)	6 32
7	E	196/197 (100%)	188 (96%)	8 (4%)	33 66
8	F	78/137 (57%)	75 (96%)	3 (4%)	36 68
9	G	152/152 (100%)	140 (92%)	12 (8%)	13 48
10	H	119/128 (93%)	113 (95%)	6 (5%)	27 62
11	I	110/116 (95%)	99 (90%)	11 (10%)	8 37
12	J	60/65 (92%)	55 (92%)	5 (8%)	12 46
13	K	97/102 (95%)	87 (90%)	10 (10%)	8 36
14	L	40/57 (70%)	36 (90%)	4 (10%)	8 37
All	All	3456/4009 (86%)	3166 (92%)	290 (8%)	12 46

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	393	LYS
4	B	909	ASP
11	I	94	ASP
4	B	429	PHE
4	B	628	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	366	GLN
4	B	957	ASN
11	I	90	GLN
4	B	513	GLN

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Mol	Chain	Res	Type
4	B	538	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	8/16 (50%)	1 (12%)	0
2	T	9/17 (52%)	5 (55%)	2 (22%)
All	All	17/33 (51%)	6 (35%)	2 (11%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	9	G
2	T	11	G
2	T	12	G
2	T	13	U
2	T	14	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	12	G
2	T	13	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	B	1
5	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	3.04
1	B	337:ARG	C	338:GLY	N	2.61

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	P	9/16 (56%)	2.00	2 (22%) 0 0	194, 200, 200, 200	0
2	T	10/17 (58%)	2.21	7 (70%) 0 0	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.26	7 (0%) 90 86	56, 116, 175, 200	0
4	B	1112/1224 (90%)	-0.20	12 (1%) 80 72	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.29	0 100 100	74, 110, 158, 180	0
6	D	178/221 (80%)	-0.26	1 (0%) 89 84	87, 133, 184, 198	0
7	E	214/215 (99%)	-0.24	4 (1%) 66 57	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.52	0 100 100	65, 91, 129, 140	0
9	G	171/171 (100%)	-0.30	0 100 100	88, 112, 155, 163	0
10	H	135/146 (92%)	0.34	5 (3%) 41 32	139, 166, 190, 200	0
11	I	116/122 (95%)	0.06	0 100 100	114, 163, 191, 200	0
12	J	65/70 (92%)	-0.49	0 100 100	79, 108, 146, 153	0
13	K	112/120 (93%)	-0.31	0 100 100	81, 114, 139, 167	0
14	L	46/70 (65%)	0.02	1 (2%) 62 51	111, 166, 194, 196	0
All	All	3945/4598 (85%)	-0.21	39 (0%) 82 75	56, 123, 187, 200	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	471	LYS	5.2
1	P	9	G	4.6
3	A	1092	LYS	3.8
1	P	8	A	3.5
2	T	15	A	3.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	B-factors(Å^2)	Q<0.9
15	ZN	A	1506	1/1	0.95	0.08	121,121,121,121	0
15	ZN	L	105	1/1	0.97	0.11	155,155,155,155	0
16	MG	A	1	1/1	0.97	0.18	79,79,79,79	0
15	ZN	I	203	1/1	0.99	0.16	120,120,120,120	0
15	ZN	I	204	1/1	0.99	0.04	181,181,181,181	0
15	ZN	C	302	1/1	1.00	0.13	82,82,82,82	0
15	ZN	A	1508	1/1	1.00	0.14	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.25	100,100,100,100	0
15	ZN	B	1307	1/1	1.00	0.22	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.