wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:16 AM GMT

PDB ID	:	3HOV
Title	:	Complete RNA polymerase II elongation complex II
Authors	:	Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on	:	2009-06-03
Resolution	:	3.50 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:

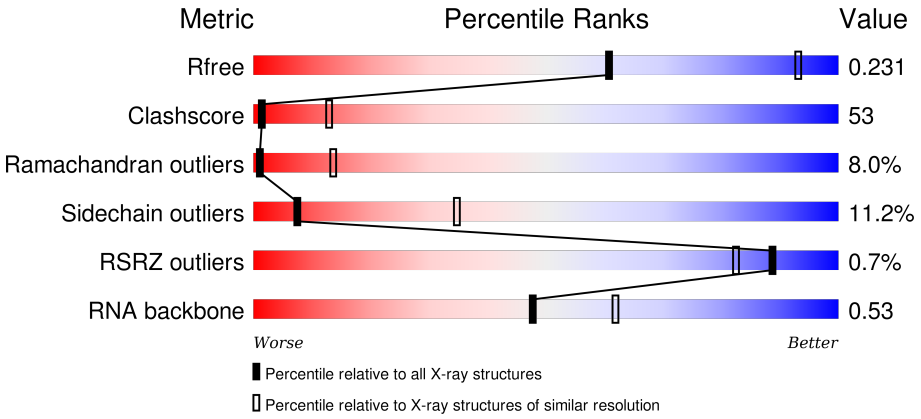
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	% 27% 44% 9% • 18%
2	B	1224	% 25% 52% 12% 10%
3	C	318	26% 46% 11% 16%
4	D	221	25% 44% 10% • 19%

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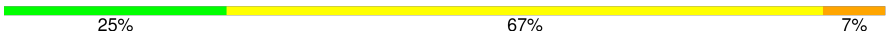
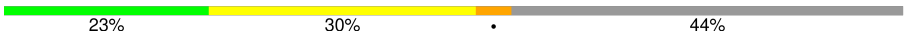
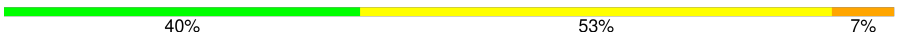
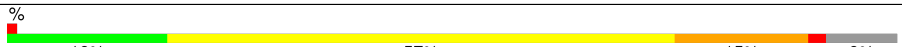
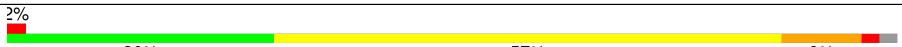
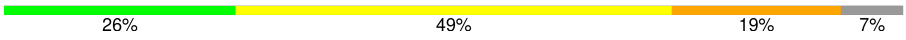
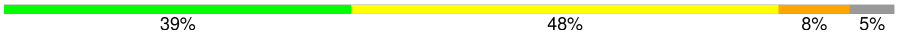
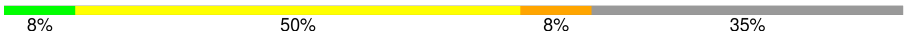
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	13	
15	P	17	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31777 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	1416	11143	7021	1949	2111	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	1104	8779	5560	1537	1627	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	178	1434	887	257	288	2	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	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	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	114	Total	C	N	O	S	0	0	0
			919	590	156	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 5'-D(*AP*GP*CP*TP*CP*AP*A*GP*TP*AP*GP*TP *TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	17	Total	Br	C	N	O	P	0	0	0
			347	1	166	61	103	16			

- Molecule 14 is a DNA chain called 5'-D(*T*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP *T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	5	Total	C	N	O	P	0	0	0
			97	48	18	27	4			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*AP*CP*C P*AP*GP*GP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			215	96	42	67	10			

- 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).

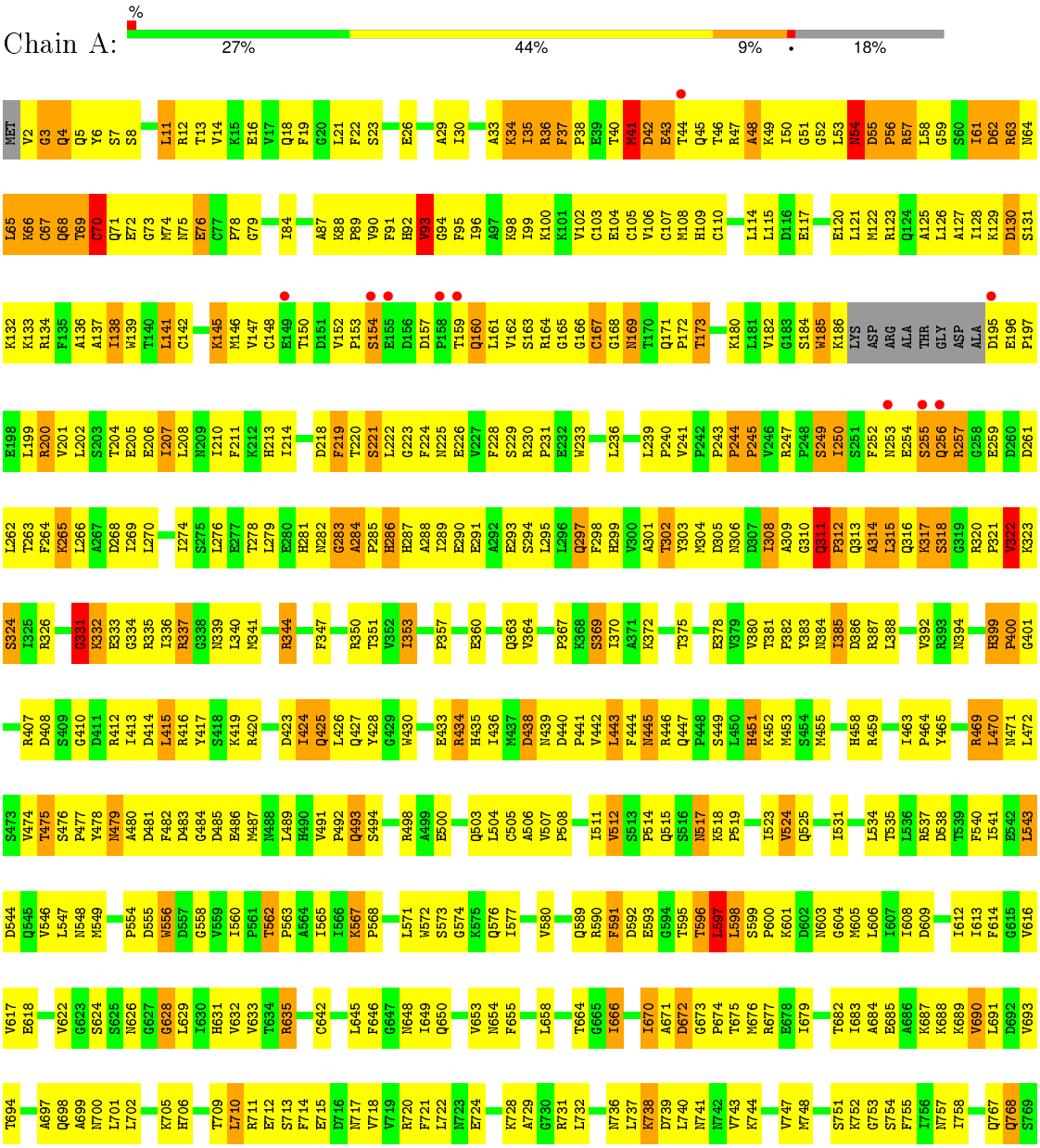
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

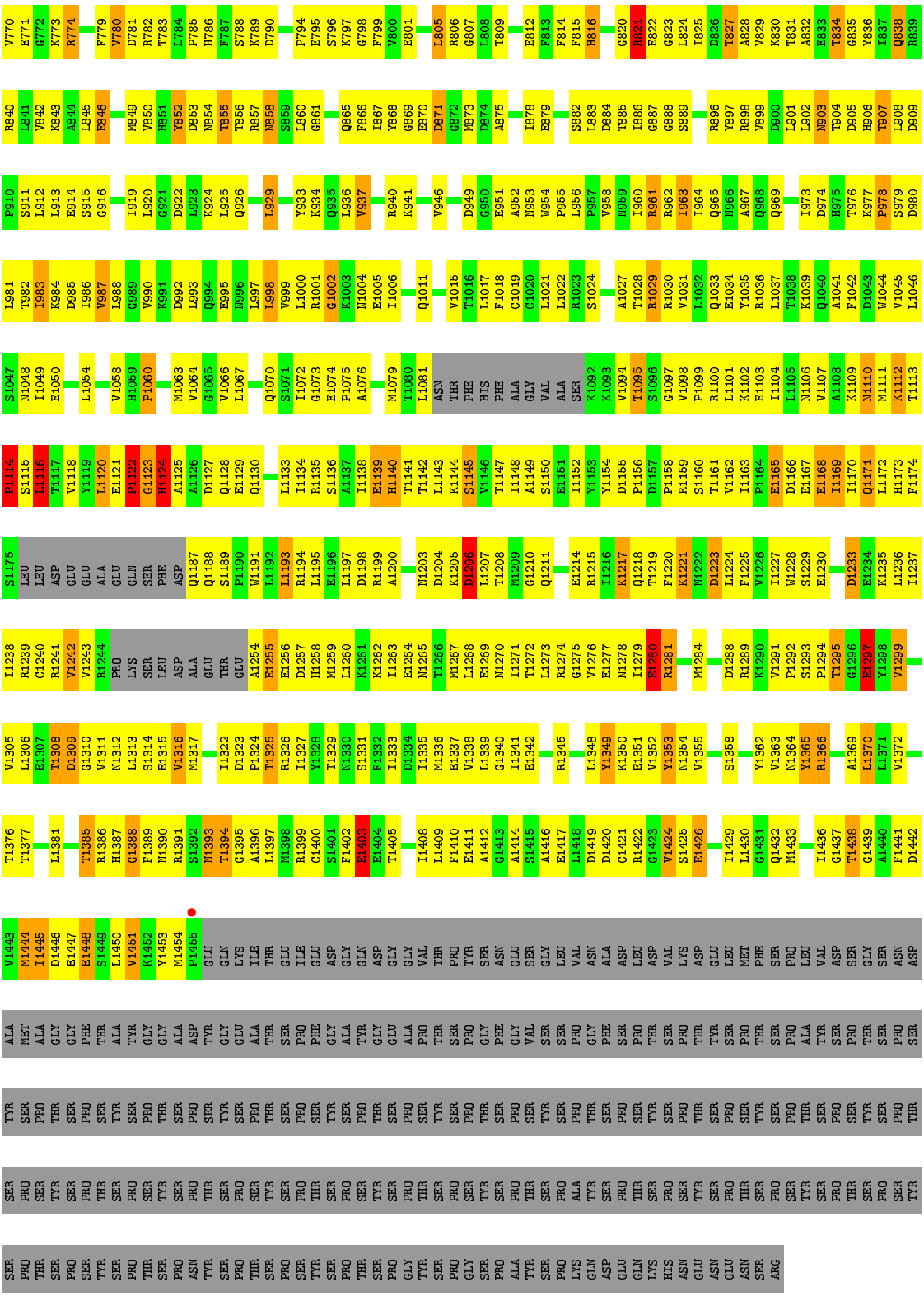
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

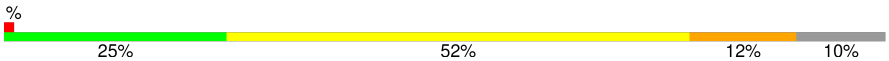
Chain A:

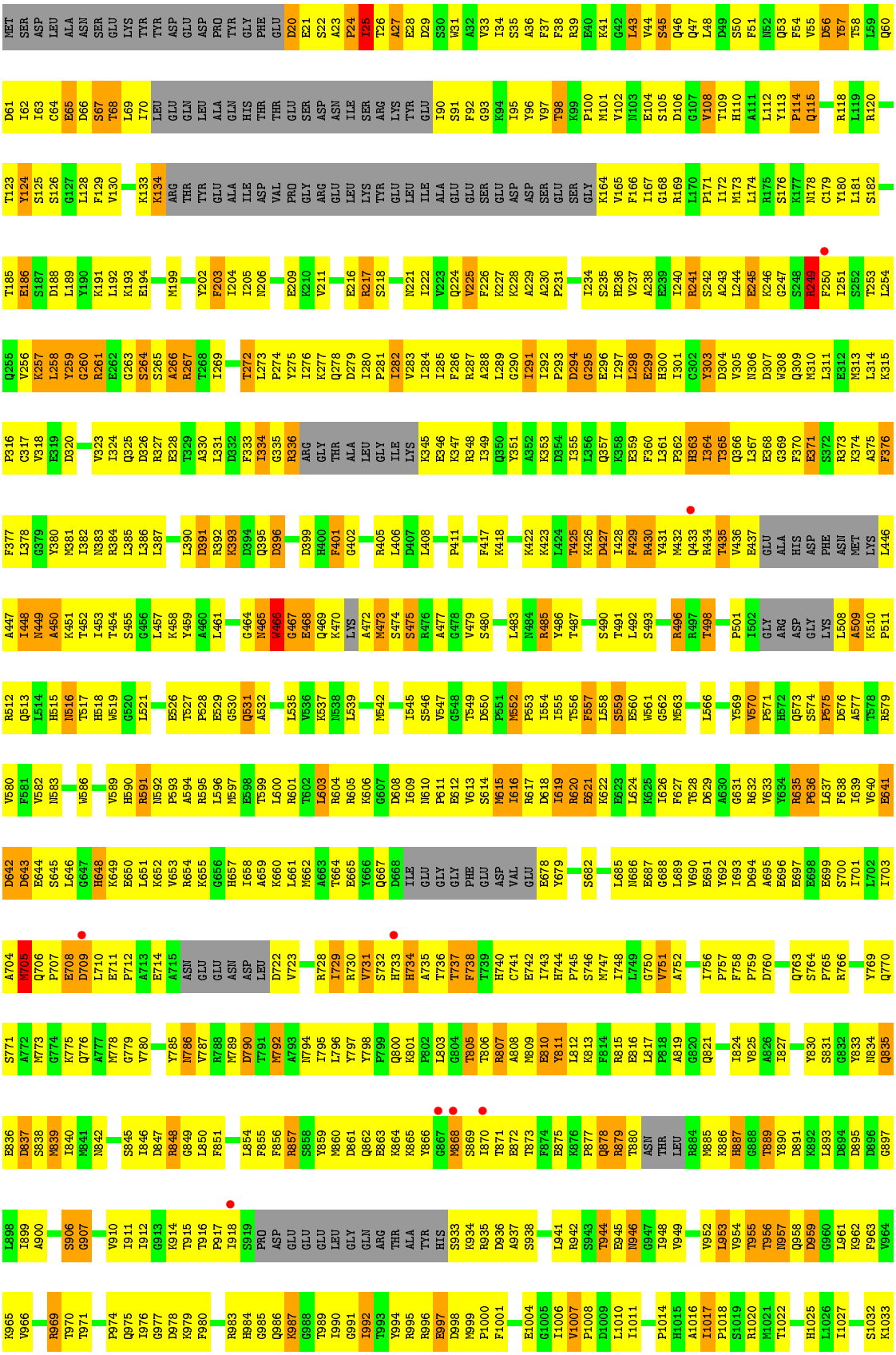


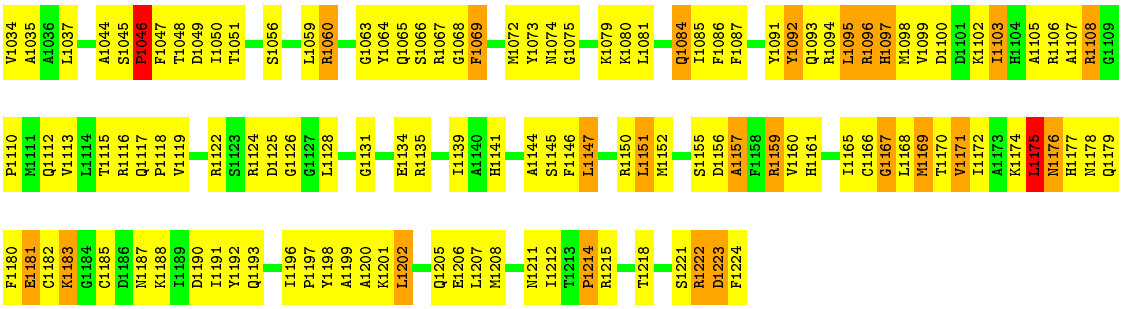


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

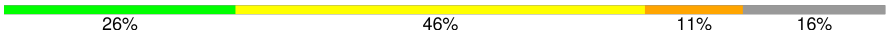


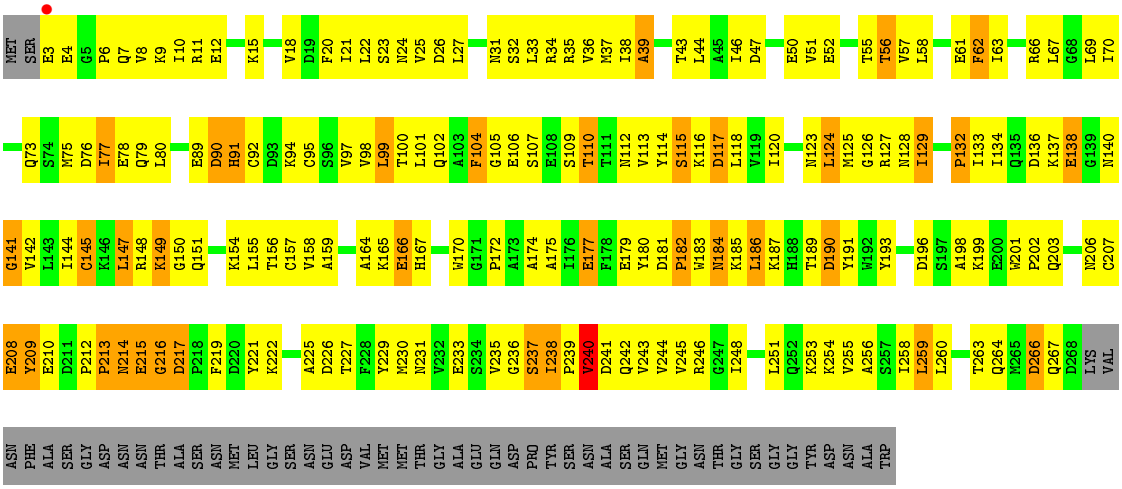




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

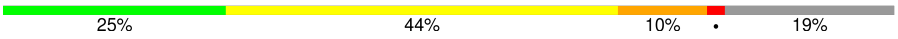
Chain C:

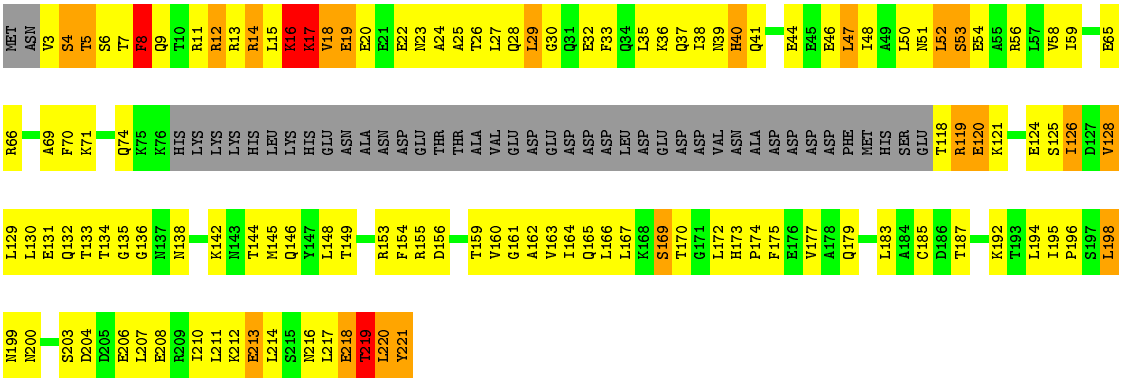




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

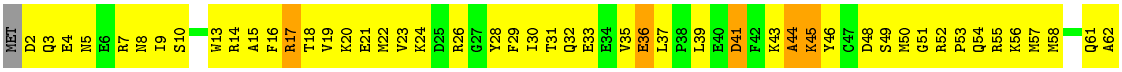
Chain D:

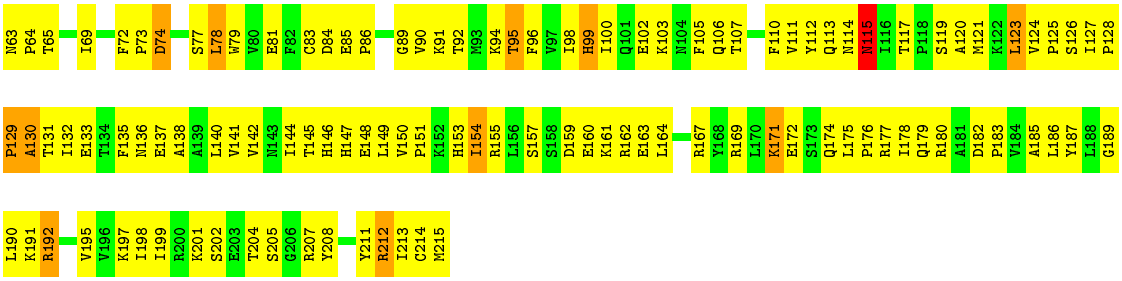




• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

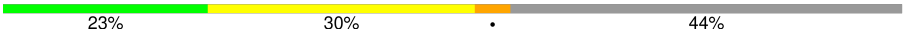
Chain E:

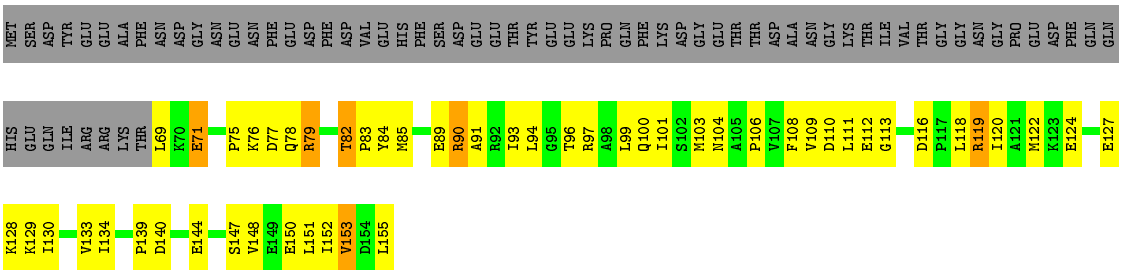




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

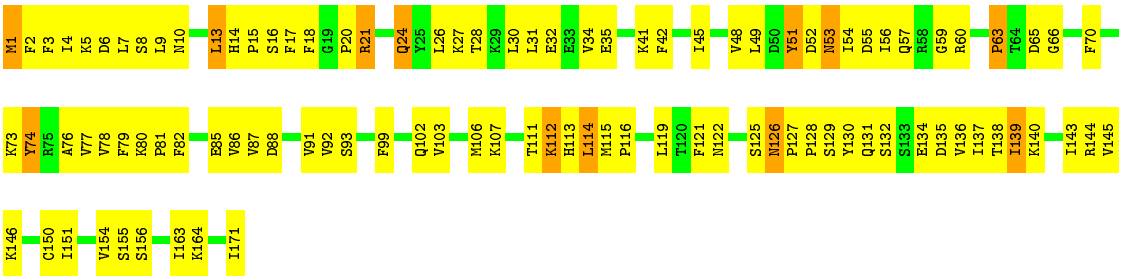
Chain F:





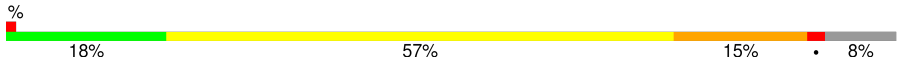
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

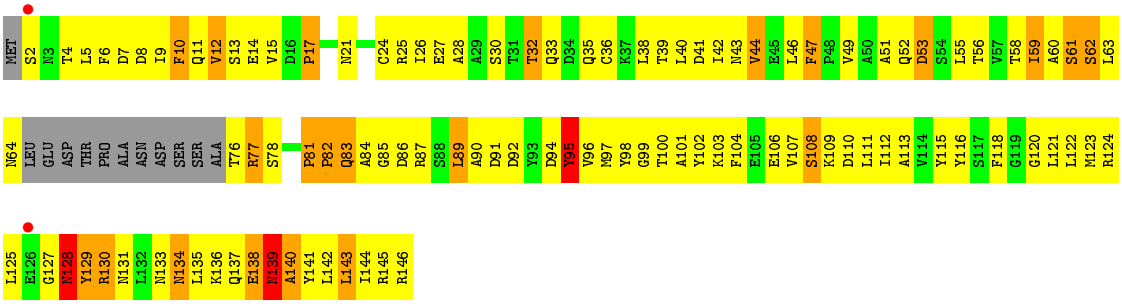
Chain G:



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

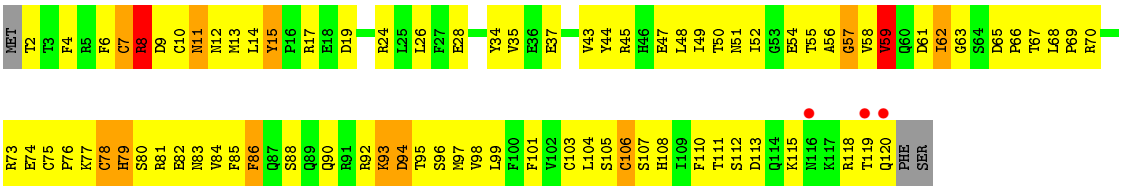
Chain H:





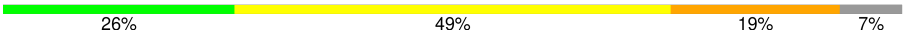
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

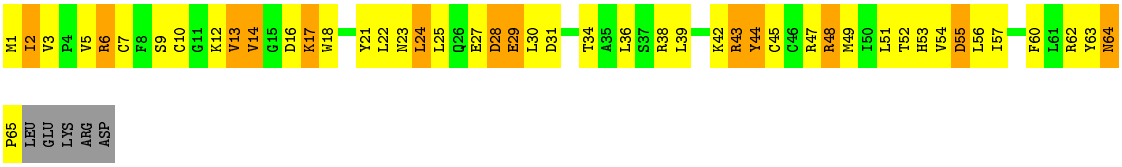
Chain I:



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

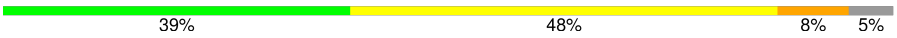
Chain J:

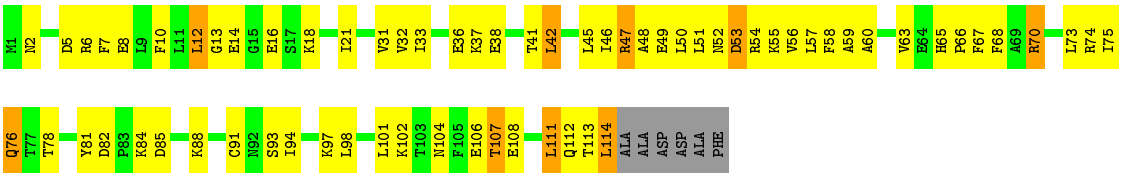




• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

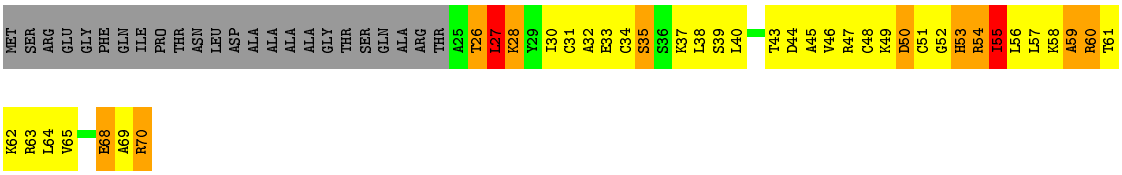
Chain K:





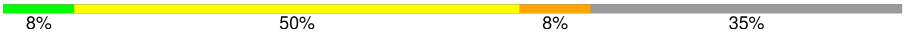
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

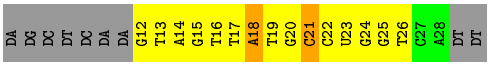
Chain L:



• Molecule 13: 5'-D(*AP*GP*CP*TP*CP*AP*A*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

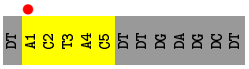
Chain T:





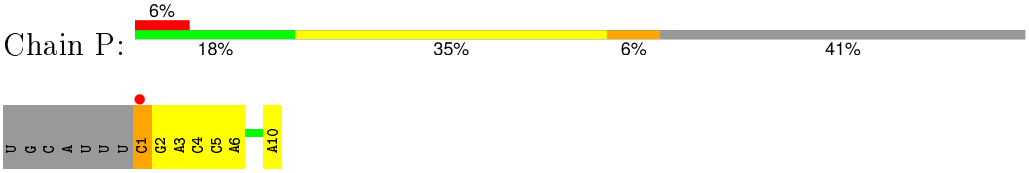
• Molecule 14: 5'-D(*T*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

Chain N:



• Molecule 15: 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*A)-3
'

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.25Å 393.38Å 283.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.17 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.9 (49.17-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.226 0.212 , 0.231	Depositor DCC
R_{free} test set	4056 reflections (2.68%)	DCC
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 99.2	EDS
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 155149 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, BRU

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	0.49	0/11342	0.77	12/15337 (0.1%)
2	B	0.48	0/8948	0.74	1/12062 (0.0%)
3	C	0.47	0/2133	0.75	1/2891 (0.0%)
4	D	0.45	0/1444	0.72	1/1935 (0.1%)
5	E	0.45	0/1788	0.68	1/2406 (0.0%)
6	F	0.56	0/717	0.80	1/967 (0.1%)
7	G	0.48	0/1368	0.76	1/1844 (0.1%)
8	H	0.43	0/1094	0.72	0/1481
9	I	0.44	0/989	0.71	0/1331
10	J	0.50	0/541	0.83	0/727
11	K	0.48	0/937	0.67	0/1265
12	L	0.57	0/365	0.84	0/485
13	T	0.54	0/365	0.85	0/560
14	N	0.57	0/108	0.78	0/164
15	P	0.45	0/240	0.82	1/372 (0.3%)
All	All	0.48	0/32379	0.75	19/43827 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
13	T	0	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	PRO	N-CA-C	-6.45	95.34	112.10
3	C	39	ALA	N-CA-C	6.38	128.24	111.00
1	A	55	ASP	N-CA-CB	6.13	121.63	110.60
1	A	3	GLY	N-CA-C	-6.04	97.99	113.10
15	P	1	C	N1-C1'-C2'	5.90	121.67	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1192	TYR	Sidechain
8	H	102	TYR	Sidechain
13	T	18	DA	Sidechain
13	T	19	DT	Sidechain
13	T	21	DC	Sidechain

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	11143	0	11217	1194	0
2	B	8779	0	8808	1069	0
3	C	2095	0	2051	259	0
4	D	1434	0	1460	156	0
5	E	1752	0	1776	193	0
6	F	705	0	731	75	0
7	G	1340	0	1357	133	0
8	H	1076	0	1046	159	0
9	I	971	0	929	118	0
10	J	532	0	542	77	0
11	K	919	0	929	82	0
12	L	363	0	388	85	0
13	T	347	0	192	20	0
14	N	97	0	58	6	0
15	P	215	0	111	7	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	31777	0	31595	3348	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 53.

The worst 5 of 3348 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)
2:B:559:SER:HA	2:B:563:MET:HB3	1.20	1.18
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.08	1.17
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.28	1.14
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.12	1.13
1:A:53:LEU:HD23	1:A:54:ASN:N	1.65	1.12

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	1406/1733 (81%)	1062 (76%)	240 (17%)	104 (7%)	1 16
2	B	1082/1224 (88%)	795 (74%)	188 (17%)	99 (9%)	1 11
3	C	264/318 (83%)	200 (76%)	45 (17%)	19 (7%)	1 17
4	D	174/221 (79%)	131 (75%)	29 (17%)	14 (8%)	1 13
5	E	212/215 (99%)	159 (75%)	40 (19%)	13 (6%)	2 21
6	F	85/155 (55%)	72 (85%)	12 (14%)	1 (1%)	16 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	169/171 (99%)	143 (85%)	20 (12%)	6 (4%)	4 37
8	H	130/146 (89%)	86 (66%)	23 (18%)	21 (16%)	0 3
9	I	117/122 (96%)	76 (65%)	31 (26%)	10 (8%)	1 13
10	J	63/70 (90%)	44 (70%)	10 (16%)	9 (14%)	0 4
11	K	112/120 (93%)	90 (80%)	19 (17%)	3 (3%)	6 44
12	L	44/70 (63%)	18 (41%)	16 (36%)	10 (23%)	0 1
All	All	3858/4565 (84%)	2876 (74%)	673 (17%)	309 (8%)	1 13

5 of 309 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU

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	1239/1520 (82%)	1099 (89%)	140 (11%)	7 34
2	B	958/1061 (90%)	845 (88%)	113 (12%)	6 31
3	C	234/274 (85%)	205 (88%)	29 (12%)	6 29
4	D	160/200 (80%)	134 (84%)	26 (16%)	3 17
5	E	196/197 (100%)	180 (92%)	16 (8%)	14 51
6	F	77/137 (56%)	70 (91%)	7 (9%)	12 46
7	G	152/152 (100%)	138 (91%)	14 (9%)	11 45
8	H	118/128 (92%)	105 (89%)	13 (11%)	8 36
9	I	113/116 (97%)	106 (94%)	7 (6%)	23 63
10	J	60/65 (92%)	53 (88%)	7 (12%)	7 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	99/102 (97%)	91 (92%)	8 (8%)	15 52
12	L	40/57 (70%)	35 (88%)	5 (12%)	6 29
All	All	3446/4009 (86%)	3061 (89%)	385 (11%)	7 35

5 of 385 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	452	THR
2	B	889	THR
8	H	138	GLU
2	B	475	SER
2	B	645	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	484	ASN
2	B	835	GLN
8	H	128	ASN
2	B	513	GLN
2	B	573	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/17 (52%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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	$\#\|Z\| > 2$
13	BRU	T	23	13,15	13,21,22	4.59	4 (30%)	16,30,33	4.04	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
13	BRU	T	23	13,15	-	0/3/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-15.08	1.50	1.90
13	T	23	BRU	C6-N1	2.57	1.38	1.35
13	T	23	BRU	C4-N3	3.31	1.39	1.33
13	T	23	BRU	C4-C5	5.13	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	23	BRU	C5-C4-N3	-8.12	115.33	124.00
13	T	23	BRU	C5-C6-N1	2.05	123.81	119.79
13	T	23	BRU	C4-N3-C2	13.61	127.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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	1416/1733 (81%)	-0.24	11 (0%) 87 80	28, 72, 115, 145	0
2	B	1104/1224 (90%)	-0.19	8 (0%) 89 82	28, 85, 126, 140	0
3	C	266/318 (83%)	-0.21	1 (0%) 93 90	41, 71, 107, 125	0
4	D	178/221 (80%)	-0.08	0 100 100	52, 84, 120, 134	0
5	E	214/215 (99%)	-0.02	0 100 100	52, 103, 130, 138	0
6	F	87/155 (56%)	-0.53	0 100 100	32, 51, 81, 91	0
7	G	171/171 (100%)	-0.21	0 100 100	48, 71, 104, 117	0
8	H	134/146 (91%)	0.26	2 (1%) 76 67	79, 109, 127, 139	0
9	I	119/122 (97%)	0.06	3 (2%) 61 50	66, 106, 126, 144	0
10	J	65/70 (92%)	-0.36	0 100 100	49, 68, 95, 107	0
11	K	114/120 (95%)	-0.21	0 100 100	36, 76, 95, 112	0
12	L	46/70 (65%)	0.03	0 100 100	48, 111, 129, 130	0
13	T	16/26 (61%)	0.50	0 100 100	99, 137, 166, 166	0
14	N	5/13 (38%)	1.43	1 (20%) 1 2	143, 147, 156, 171	0
15	P	10/17 (58%)	0.66	1 (10%) 9 9	122, 129, 147, 153	0
All	All	3945/4621 (85%)	-0.18	27 (0%) 89 82	28, 80, 124, 171	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	4.0
2	B	918	ILE	3.2
9	I	120	GLN	3.0
14	N	1	DA	2.9
15	P	1	C	2.9

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
13	BRU	T	23	20/21	0.74	0.26	-	127,131,137,139	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
16	ZN	J	1066	1/1	0.99	0.21	-0.37	61,61,61,61	0
16	ZN	B	2225	1/1	0.99	0.17	-1.07	54,54,54,54	0
16	ZN	C	1269	1/1	0.99	0.10	-1.46	49,49,49,49	0
16	ZN	A	2457	1/1	0.99	0.14	-1.82	51,51,51,51	0
16	ZN	I	1121	1/1	0.99	0.10	-1.92	90,90,90,90	0
16	ZN	L	1071	1/1	0.91	0.08	-2.25	111,111,111,111	0
16	ZN	I	1122	1/1	0.95	0.05	-3.00	122,122,122,122	0
16	ZN	A	2456	1/1	0.97	0.06	-4.45	86,86,86,86	0
17	MG	A	2458	1/1	0.73	0.32	-	123,123,123,123	0

6.5 Other polymers (i)

There are no such residues in this entry.