wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 01:42 pm BST

PDB ID	:	3I4N
Title	:	8-oxoguanine containing RNA polymerase II elongation complex E
Authors	:	Damsma, G.E.; Cramer, P.
Deposited on	:	2009-07-02
Resolution	:	3.90 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:

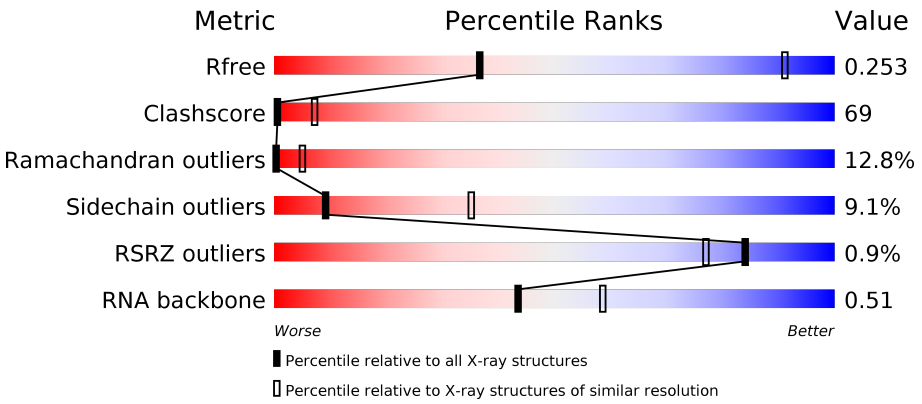
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.90 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	17% 52% 12% • 18%
2	B	1224	% 21% 56% 13% • 8%
3	C	324	19% 52% 12% • 17%
4	D	221	% 19% 48% 14% • 18%

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Mol	Chain	Length	Quality of chain
5	E	215	23% 63% 13%
6	F	155	10% 39% 6% 43%
7	G	171	35% 57% 8%
8	H	146	5% 16% 58% 18% 6%
9	I	122	3% 29% 52% 15%
10	J	70	16% 51% 26% 7%
11	K	120	2% 26% 63% 8%
12	L	70	39% 26% 33%
13	T	26	77% 23%
14	N	12	25% 67% 8%
15	P	16	13% 44% 6% 38%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32307 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	1429	11240	7079	1966	2133	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	1125	8942	5659	1571	1657	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	270	2125	1336	353	422	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- 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	182	1465	904	262	296	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	88	712	455	120	134	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	137	1101	693	185	218	5	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	117	952	586	173	182	11	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	116	929	596	158	173	2	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	47	370	228	73	65	4	0	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
13	T	20	407	1	194	72	121	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	N	11	224	108	42	64	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	P	10	207	94	35	69	9	0	0	0

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

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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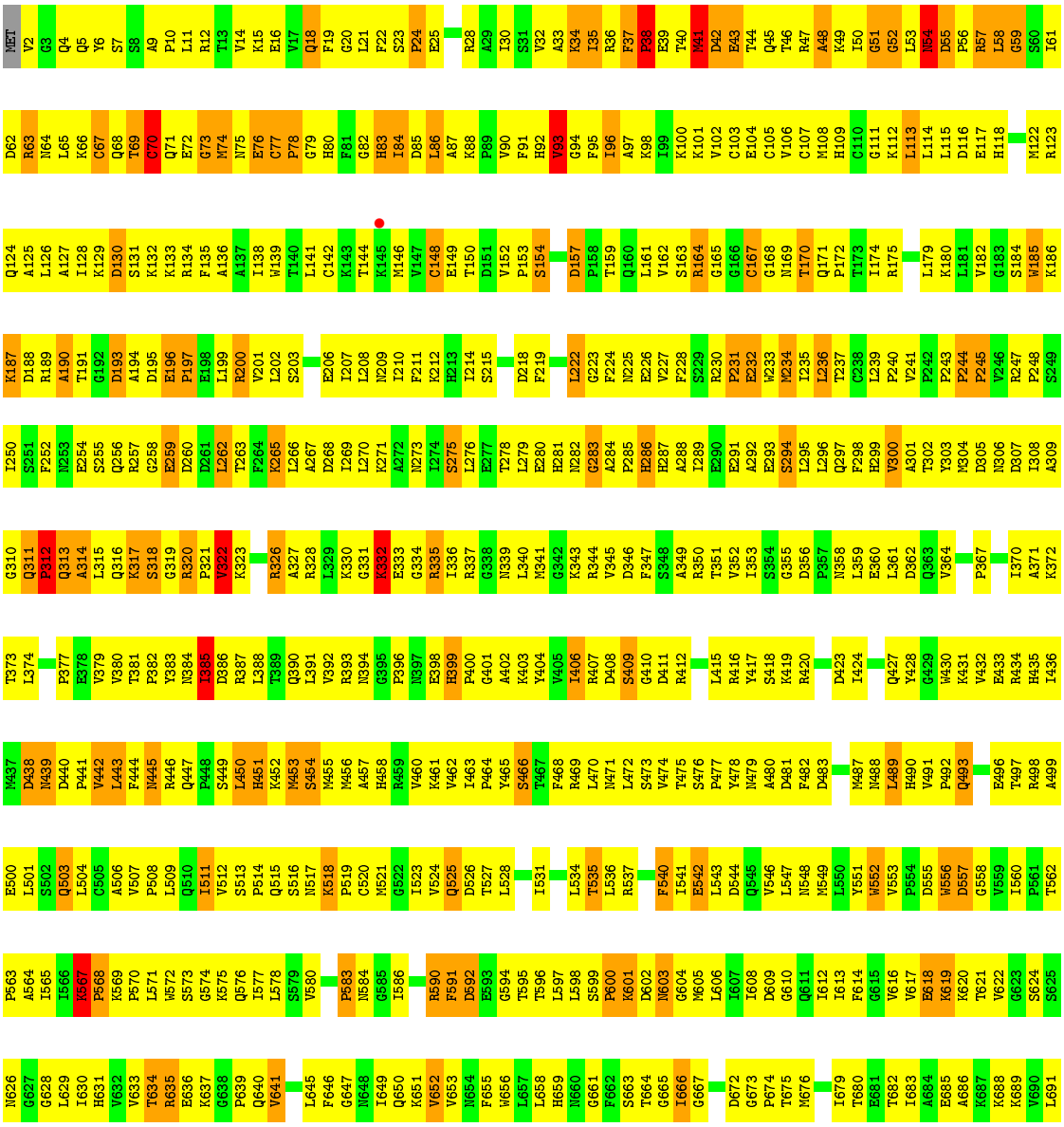
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
17	A	2	2	2	0	0
			Total	Zn		
17	L	1	1	1	0	0

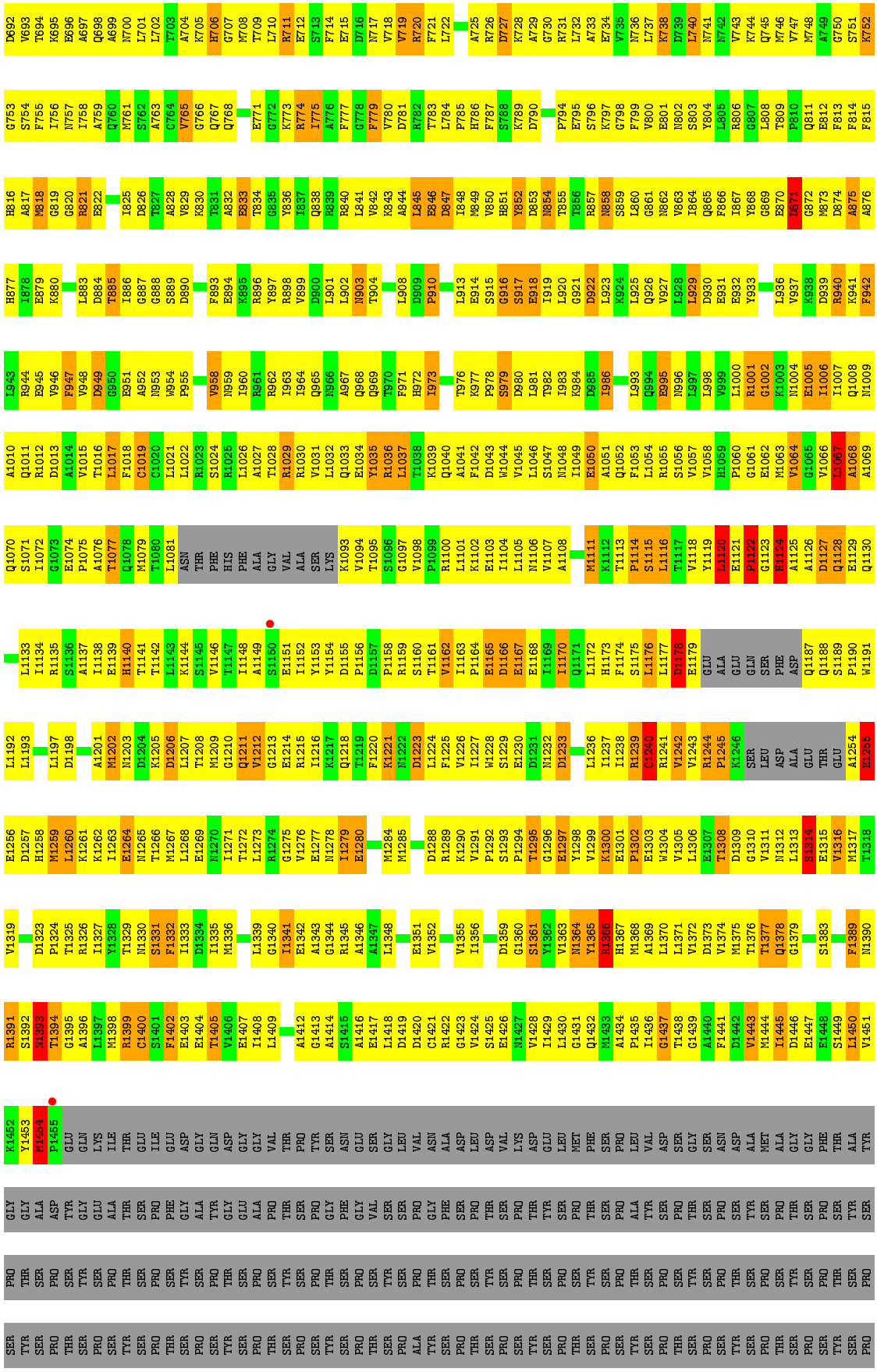
3 Residue-property plots (i)

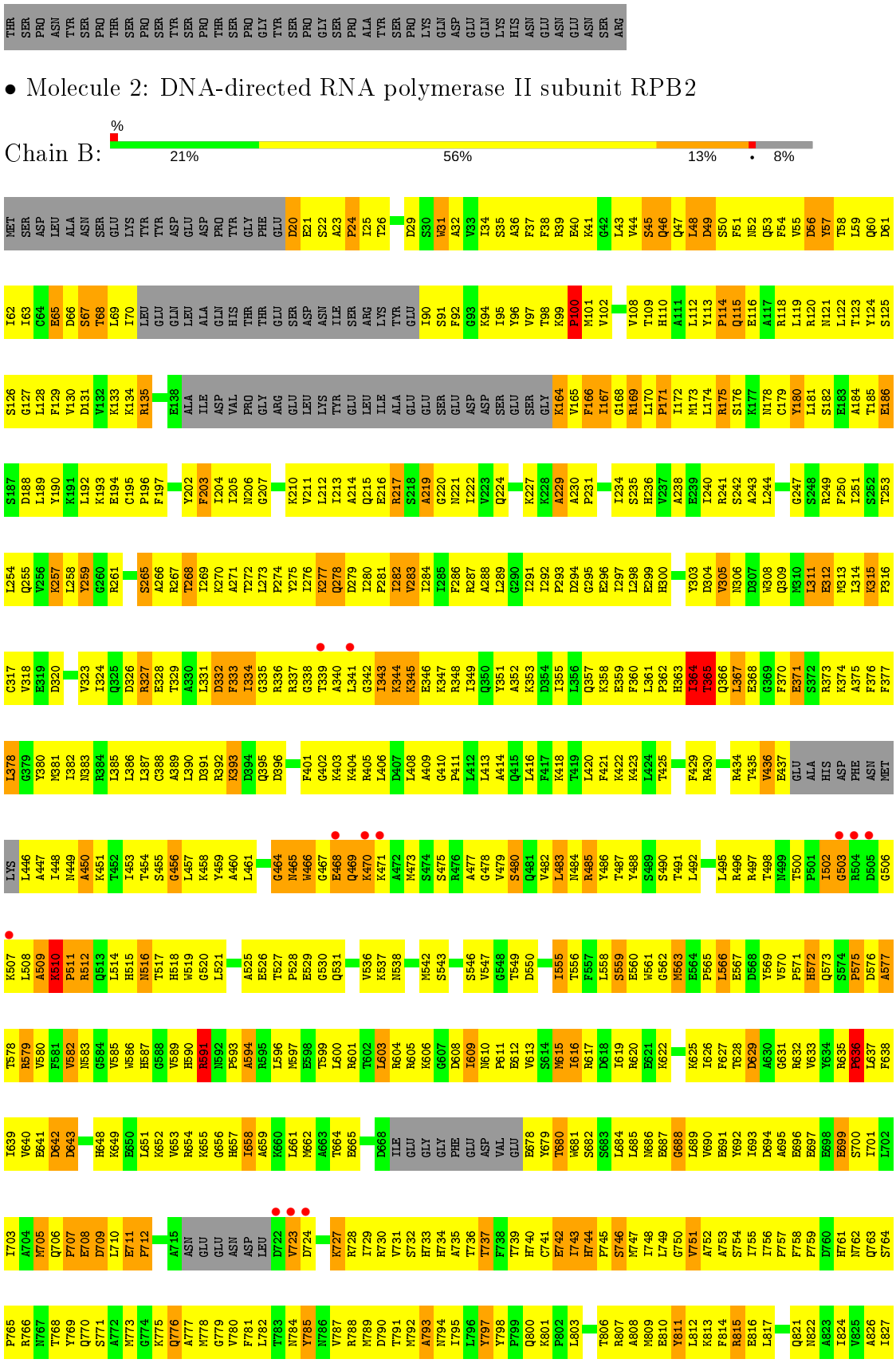
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

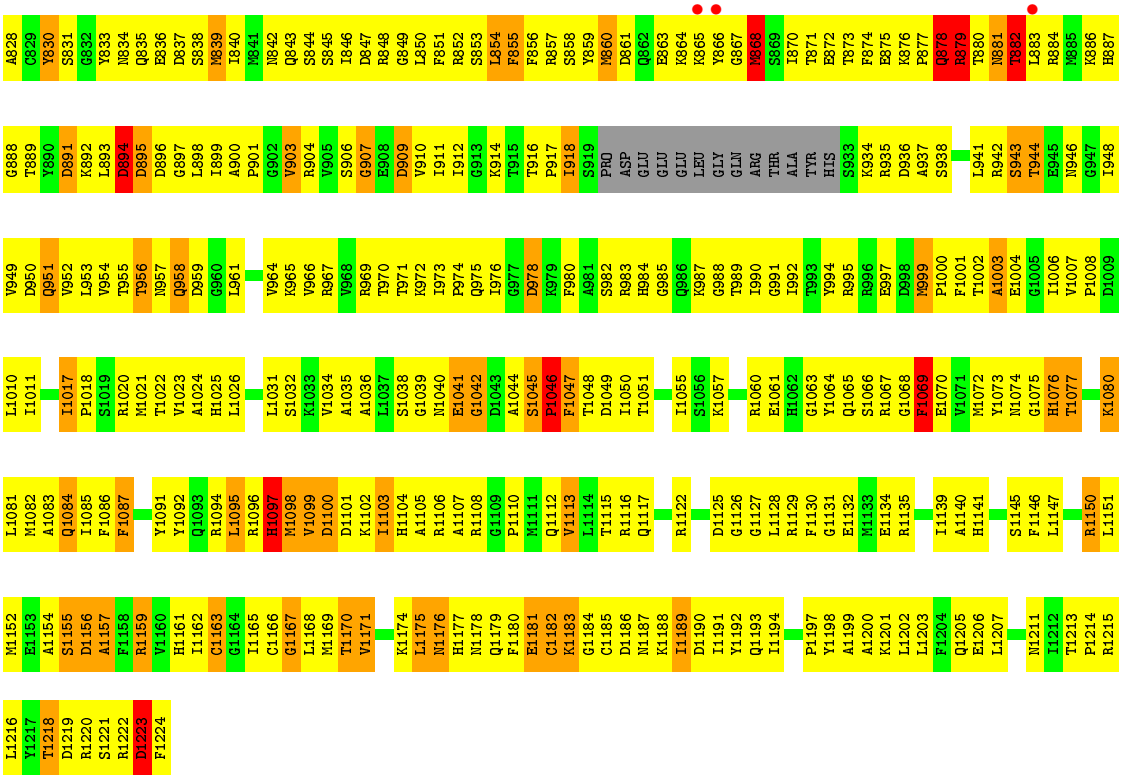
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A: 17% 52% 12% • 18%



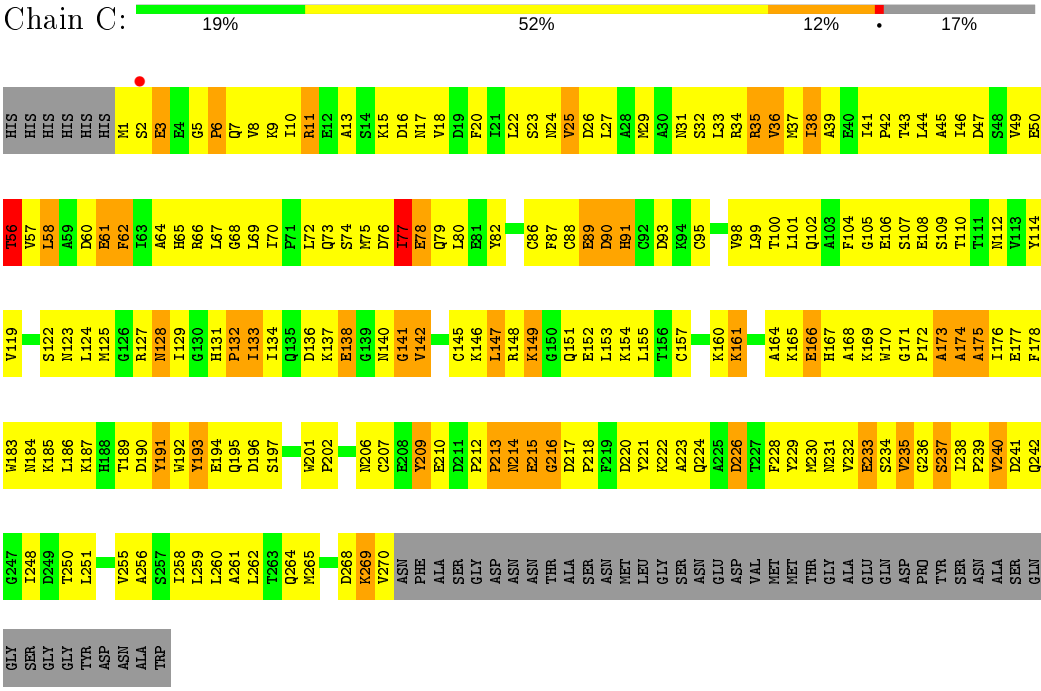



THR SER PRO ASN TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO GLY TYR SER PRO GLY SER PRO ALA TYR SER PRO LYS GLN ASP GLU GLN LYS HIS ASN GLU ASN GLU ASN SER ARG
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2
Chain B:
%
21%
56%
13%
8%



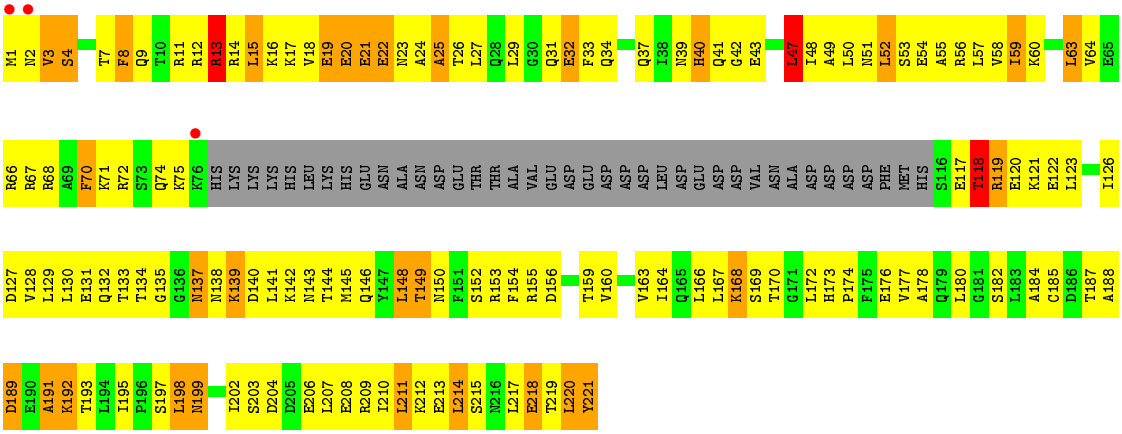
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



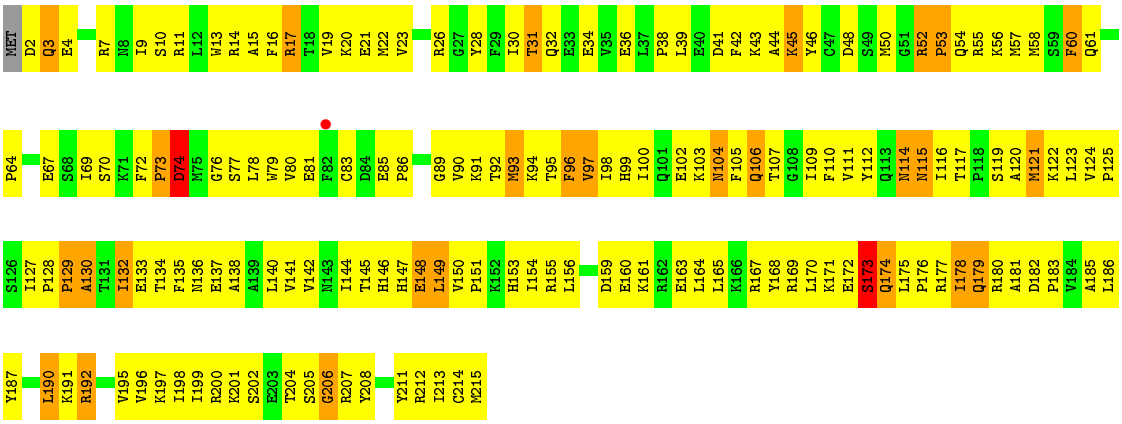
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



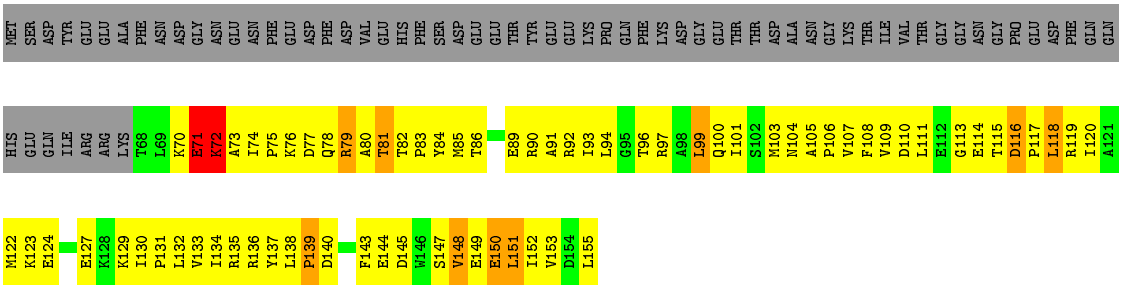
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 23% 63% 13%



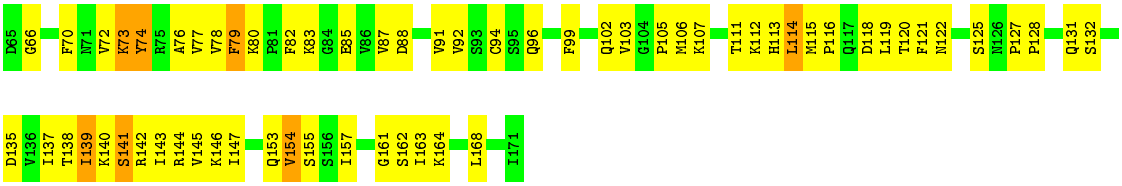
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 10% 39% 6% 43%



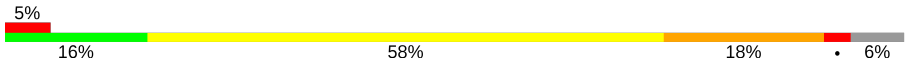
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

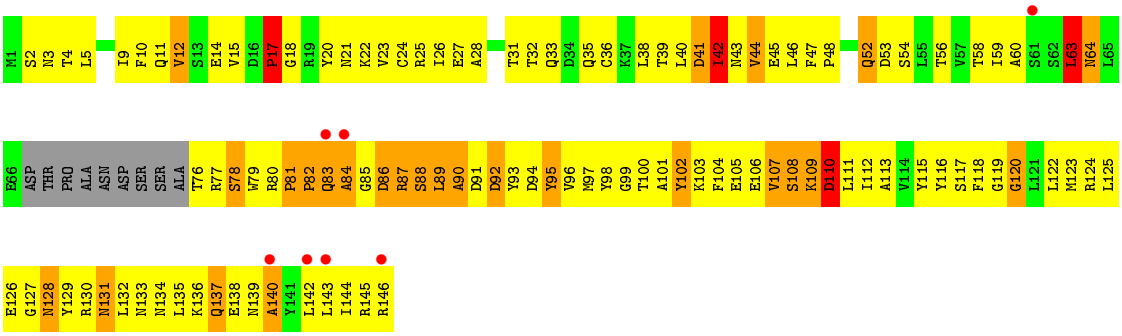
Chain G: 35% 57% 8%



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

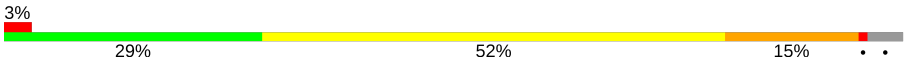
Chain H:

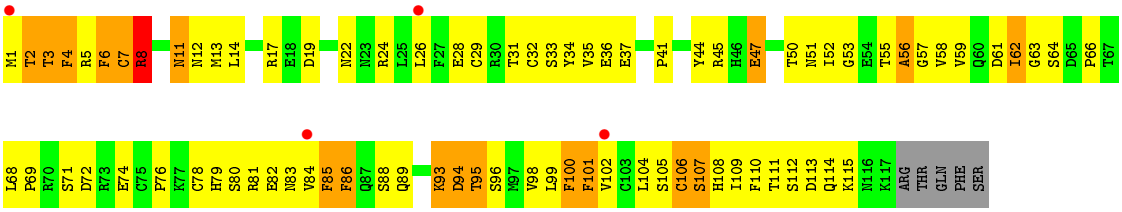




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



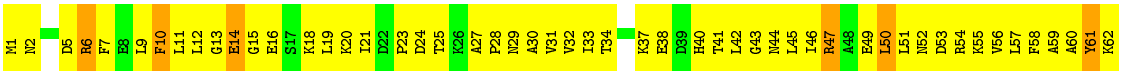


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

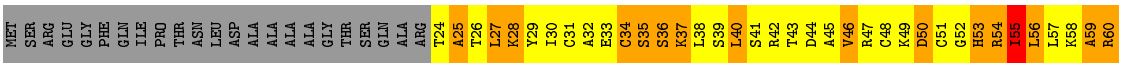
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



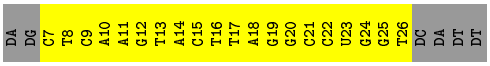
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



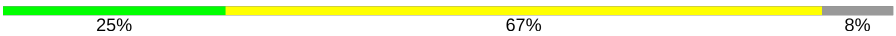
• Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')

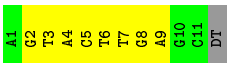
Chain T:



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

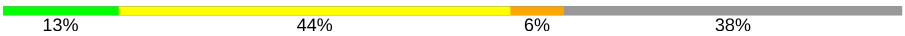
Chain N:





• Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-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	221.17Å 394.15Å 282.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 49.81 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.90) 100.0 (49.81-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.266 0.214 , 0.253	Depositor DCC
R_{free} test set	4364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	128.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 95.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32307	wwPDB-VP
Average B, all atoms (Å^2)	145.0	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 8OG, 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	0.43	0/11441	0.73	1/15473 (0.0%)
2	B	0.41	0/9116	0.69	1/12291 (0.0%)
3	C	0.42	0/2163	0.72	0/2930
4	D	0.39	0/1475	0.64	0/1976
5	E	0.39	0/1788	0.66	0/2406
6	F	0.46	0/724	0.82	0/977
7	G	0.44	0/1368	0.68	0/1844
8	H	0.38	0/1119	0.69	0/1514
9	I	0.36	0/970	0.66	0/1305
10	J	0.43	0/541	0.71	0/727
11	K	0.44	0/947	0.68	0/1279
12	L	0.45	0/372	0.75	0/495
13	T	0.61	0/405	0.84	0/618
14	N	0.67	0/251	0.93	0/386
15	P	0.54	0/230	0.82	0/356
All	All	0.42	0/32910	0.71	2/44577 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	882	THR	N-CA-C	5.61	126.14	111.00

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	567	LYS	C-N-CD	5.18	139.27	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	797	TYR	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	11240	0	11313	1726	0
2	B	8942	0	8987	1312	0
3	C	2125	0	2090	327	0
4	D	1465	0	1489	212	0
5	E	1752	0	1776	229	0
6	F	712	0	738	127	0
7	G	1340	0	1357	167	0
8	H	1101	0	1075	211	0
9	I	952	0	913	140	0
10	J	532	0	542	113	0
11	K	929	0	939	132	0
12	L	370	0	394	89	0
13	T	407	0	225	43	0
14	N	224	0	126	11	0
15	P	207	0	109	9	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	32307	0	32073	4433	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 69.

The worst 5 of 4433 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:577:ALA:HB1	2:B:589:VAL:HG11	1.19	1.14
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.07	1.14
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.12	1.13
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.25	1.12
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.06	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	1421/1733 (82%)	929 (65%)	311 (22%)	181 (13%)	0 5
2	B	1111/1224 (91%)	712 (64%)	251 (23%)	148 (13%)	0 4
3	C	268/324 (83%)	165 (62%)	69 (26%)	34 (13%)	0 5
4	D	178/221 (80%)	125 (70%)	29 (16%)	24 (14%)	0 4
5	E	212/215 (99%)	145 (68%)	42 (20%)	25 (12%)	0 6
6	F	86/155 (56%)	60 (70%)	21 (24%)	5 (6%)	1 21
7	G	169/171 (99%)	133 (79%)	25 (15%)	11 (6%)	1 19
8	H	133/146 (91%)	78 (59%)	26 (20%)	29 (22%)	0 1
9	I	115/122 (94%)	72 (63%)	29 (25%)	14 (12%)	0 6
10	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0 1
11	K	114/120 (95%)	80 (70%)	31 (27%)	3 (3%)	5 35
12	L	45/70 (64%)	18 (40%)	13 (29%)	14 (31%)	0 0
All	All	3915/4571 (86%)	2552 (65%)	861 (22%)	502 (13%)	0 5

5 of 502 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN

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	1249/1520 (82%)	1126 (90%)	123 (10%)	8	31
2	B	974/1061 (92%)	888 (91%)	86 (9%)	10	37
3	C	238/280 (85%)	219 (92%)	19 (8%)	12	41
4	D	164/200 (82%)	145 (88%)	19 (12%)	5	26
5	E	196/197 (100%)	182 (93%)	14 (7%)	14	44
6	F	78/137 (57%)	70 (90%)	8 (10%)	7	30
7	G	152/152 (100%)	144 (95%)	8 (5%)	22	52
8	H	121/128 (94%)	111 (92%)	10 (8%)	11	39
9	I	111/116 (96%)	102 (92%)	9 (8%)	11	40
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	39
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	30
12	L	41/57 (72%)	34 (83%)	7 (17%)	2	14
All	All	3483/4015 (87%)	3165 (91%)	318 (9%)	9	35

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	378	LEU
2	B	878	GLN
9	I	94	ASP
2	B	466	TRP

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Mol	Chain	Res	Type
2	B	615	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	HIS
2	B	1015	HIS
9	I	114	GLN
2	B	538	ASN
2	B	763	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	8OG	T	19	13,15	18,25,26	1.30	2 (11%)	21,37,40	2.57	5 (23%)
13	BRU	T	23	13,15	15,21,22	4.01	4 (26%)	17,30,33	4.22	5 (29%)

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	8OG	T	19	13,15	-	2/3/21/22	0/3/3/3
13	BRU	T	23	13,15	-	0/4/21/22	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-14.14	1.49	1.90
13	T	23	BRU	C4-C5	5.38	1.45	1.38
13	T	19	8OG	C6-N1	3.83	1.39	1.33
13	T	19	8OG	C8-N7	-3.11	1.30	1.34
13	T	23	BRU	C4-N3	2.64	1.37	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	23	BRU	C4-N3-C2	15.08	127.87	115.14
13	T	19	8OG	C5-C6-N1	-8.63	111.62	123.43
13	T	23	BRU	C5-C4-N3	-7.08	115.16	123.64
13	T	19	8OG	C6-N1-C2	5.84	125.21	115.93
13	T	19	8OG	C2-N3-C4	-2.86	112.08	115.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	19	8OG	O4'-C4'-C5'-O5'
13	T	19	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	19	8OG	3	0
13	T	23	BRU	2	0

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1429/1733 (82%)	-0.21	3 (0%)	95	93	73, 132, 187, 200	0
2	B	1125/1224 (91%)	-0.05	15 (1%)	77	68	79, 146, 196, 200	0
3	C	270/324 (83%)	-0.21	1 (0%)	92	87	92, 133, 183, 200	0
4	D	182/221 (82%)	-0.18	3 (1%)	72	62	122, 160, 195, 200	0
5	E	214/215 (99%)	-0.21	1 (0%)	91	85	111, 170, 198, 200	0
6	F	88/155 (56%)	-0.26	0	100	100	77, 110, 145, 175	0
7	G	171/171 (100%)	-0.16	0	100	100	113, 140, 176, 182	0
8	H	137/146 (93%)	0.28	7 (5%)	28	23	147, 178, 198, 200	0
9	I	117/122 (95%)	-0.01	4 (3%)	45	35	126, 178, 197, 200	0
10	J	65/70 (92%)	-0.30	0	100	100	112, 129, 171, 180	0
11	K	116/120 (96%)	-0.23	2 (1%)	70	60	96, 135, 160, 199	0
12	L	47/70 (67%)	-0.14	0	100	100	128, 169, 190, 200	0
13	T	18/26 (69%)	0.30	0	100	100	182, 200, 200, 200	0
14	N	11/12 (91%)	0.80	0	100	100	196, 200, 200, 200	0
15	P	10/16 (62%)	-0.14	0	100	100	199, 200, 200, 200	0
All	All	4000/4625 (86%)	-0.14	36 (0%)	84	77	73, 142, 196, 200	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	7.2
2	B	504	ARG	4.0
9	I	1	MET	3.9
4	D	76	LYS	3.5
8	H	140	ALA	3.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	BRU	T	23	20/21	0.71	0.23	198,199,200,200	0
13	8OG	T	19	23/24	0.91	0.17	186,193,198,199	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	A	2458	1/1	0.93	0.09	200,200,200,200	0
17	ZN	I	1122	1/1	0.95	0.05	198,198,198,198	0
17	ZN	A	2456	1/1	0.97	0.06	150,150,150,150	0
17	ZN	J	1066	1/1	0.99	0.27	135,135,135,135	0
17	ZN	L	1071	1/1	0.99	0.08	158,158,158,158	0
17	ZN	B	2225	1/1	0.99	0.22	106,106,106,106	0
17	ZN	A	2457	1/1	0.99	0.15	107,107,107,107	0
17	ZN	C	1269	1/1	1.00	0.14	101,101,101,101	0
17	ZN	I	1121	1/1	1.00	0.12	140,140,140,140	0

6.5 Other polymers (i)

There are no such residues in this entry.