



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:40 am BST

PDB ID : 4XLN  
Title : Crystal structure of T. aquaticus transcription initiation complex containing bubble promoter and RNA  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

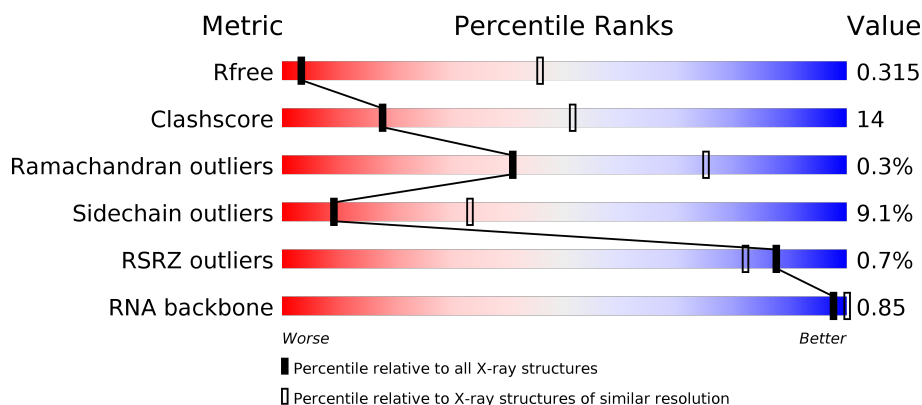
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	G	314	
1	H	314	

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	48	
6	R	48	
7	P	48	
7	S	48	
8	Q	4	
8	T	4	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 58255 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			
5	L	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
6	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
7	S	43	Total	C	N	O	P	0	0	0
			882	421	164	255	42			

- Molecule 8 is a RNA chain called RNA (5'-D(P\*UP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
8	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	2	Total	Zn	0	0
			2	2		
9	D	2	Total	Zn	0	0
			2	2		

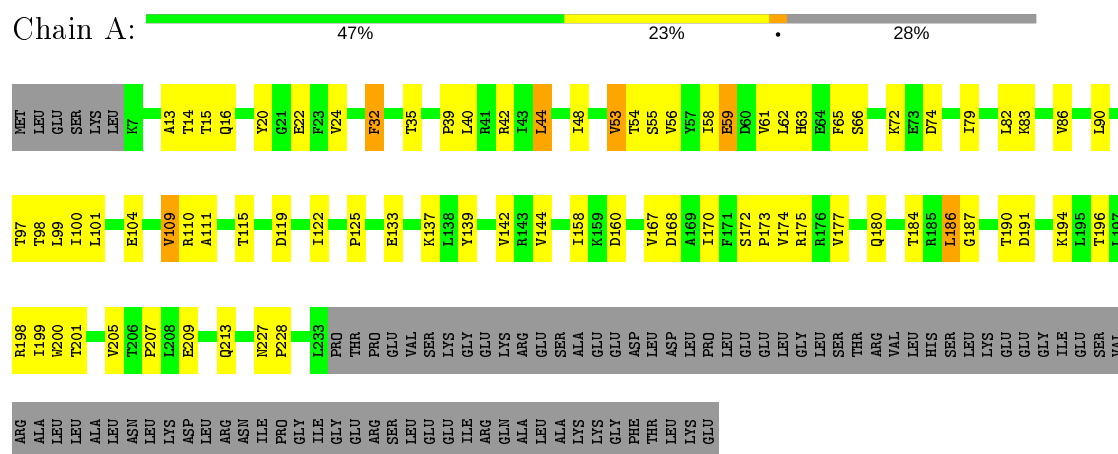
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	1	Total 1	Mg 1	0	0
10	D	1	Total 1	Mg 1	0	0

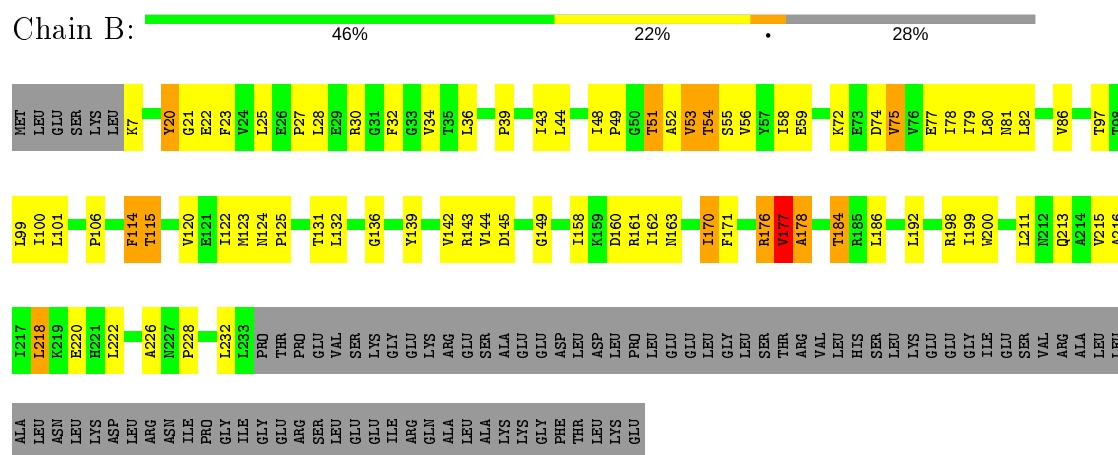
### 3 Residue-property plots

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.

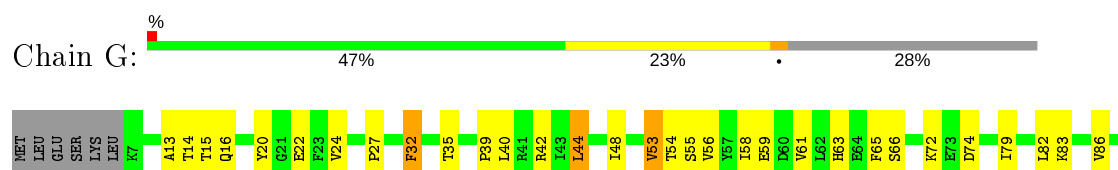
- Molecule 1: DNA-directed RNA polymerase subunit alpha

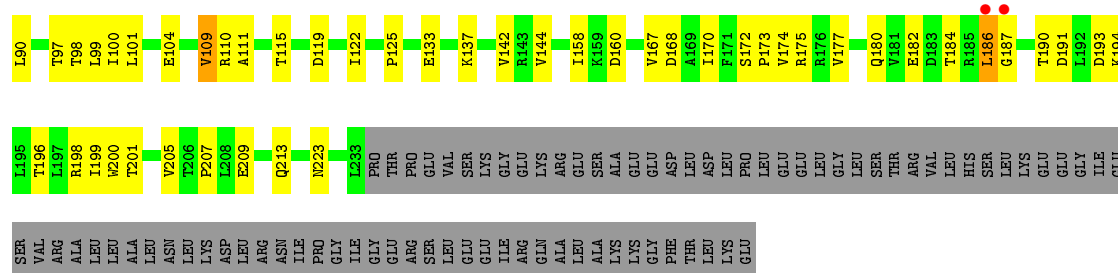


- Molecule 1: DNA-directed RNA polymerase subunit alpha

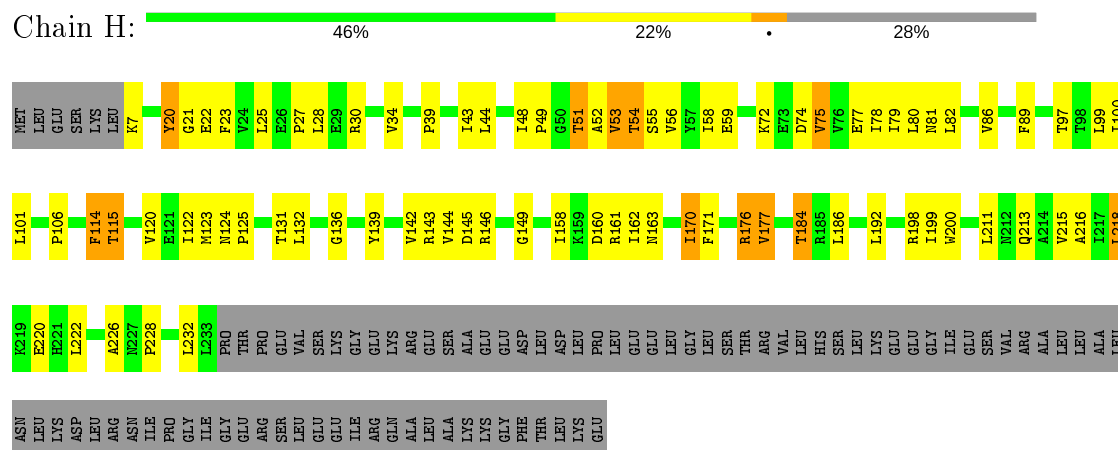


- Molecule 1: DNA-directed RNA polymerase subunit alpha

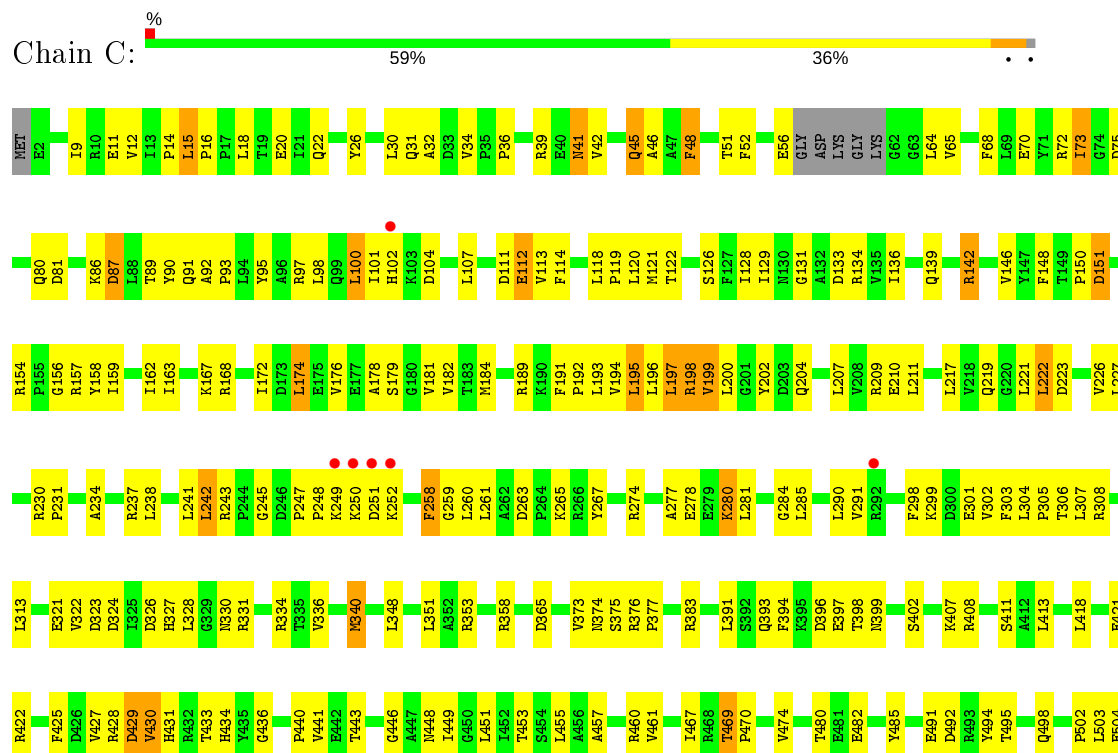




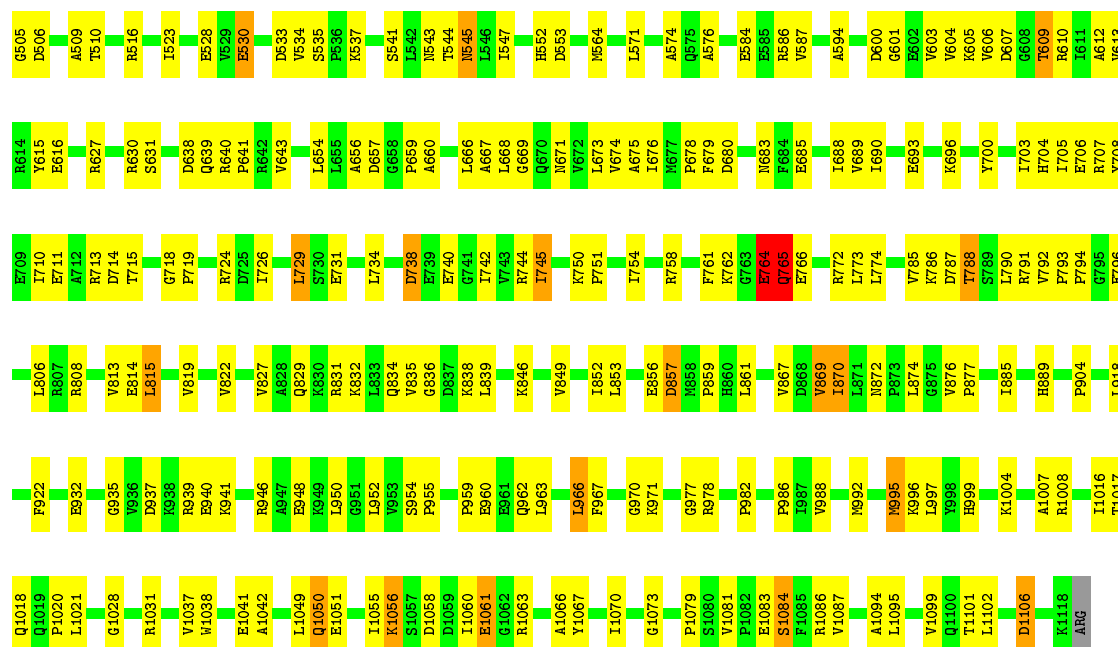
- Molecule 1: DNA-directed RNA polymerase subunit alpha



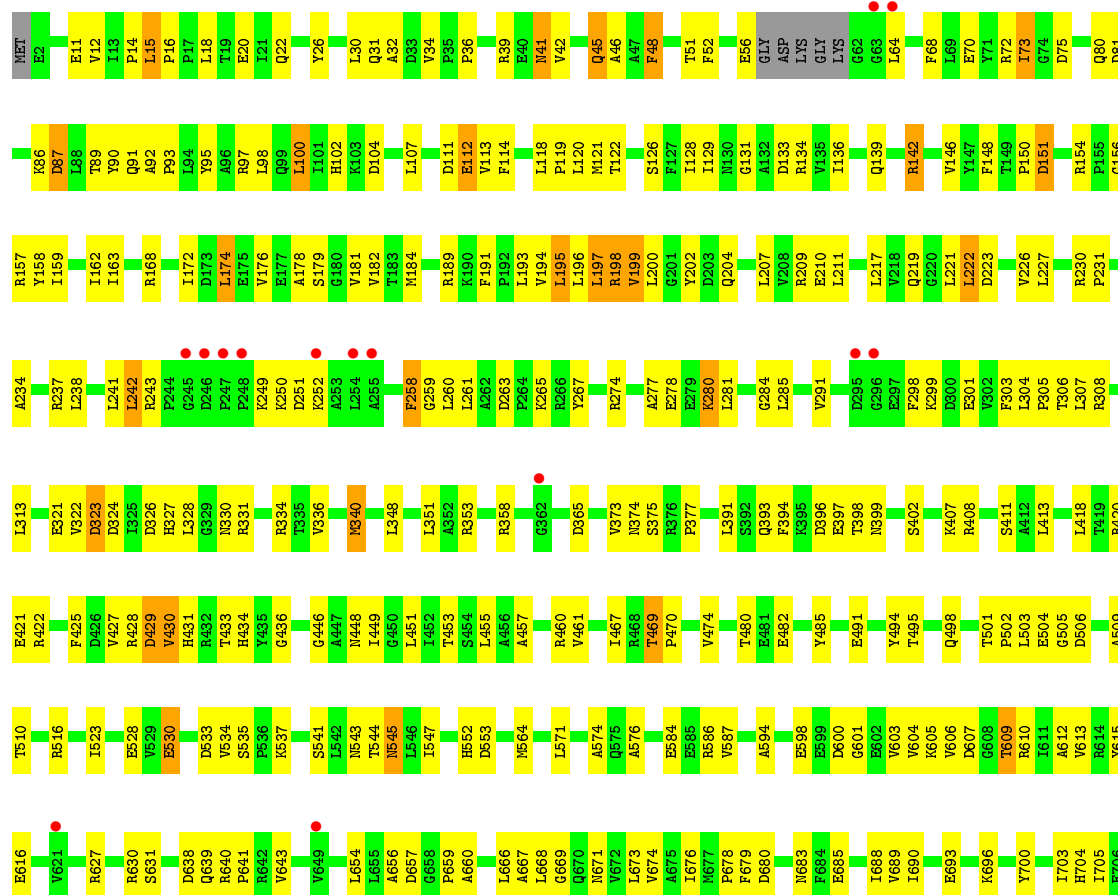
- Molecule 2: DNA-directed RNA polymerase subunit beta

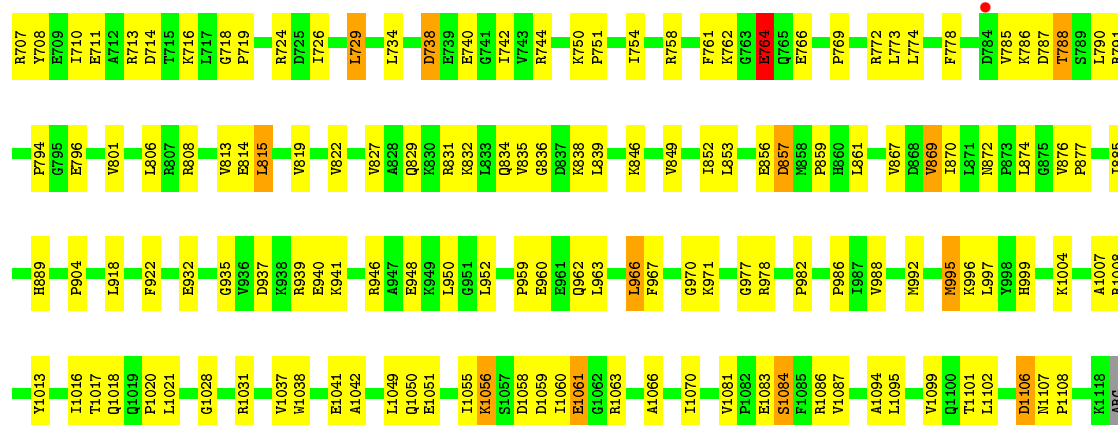






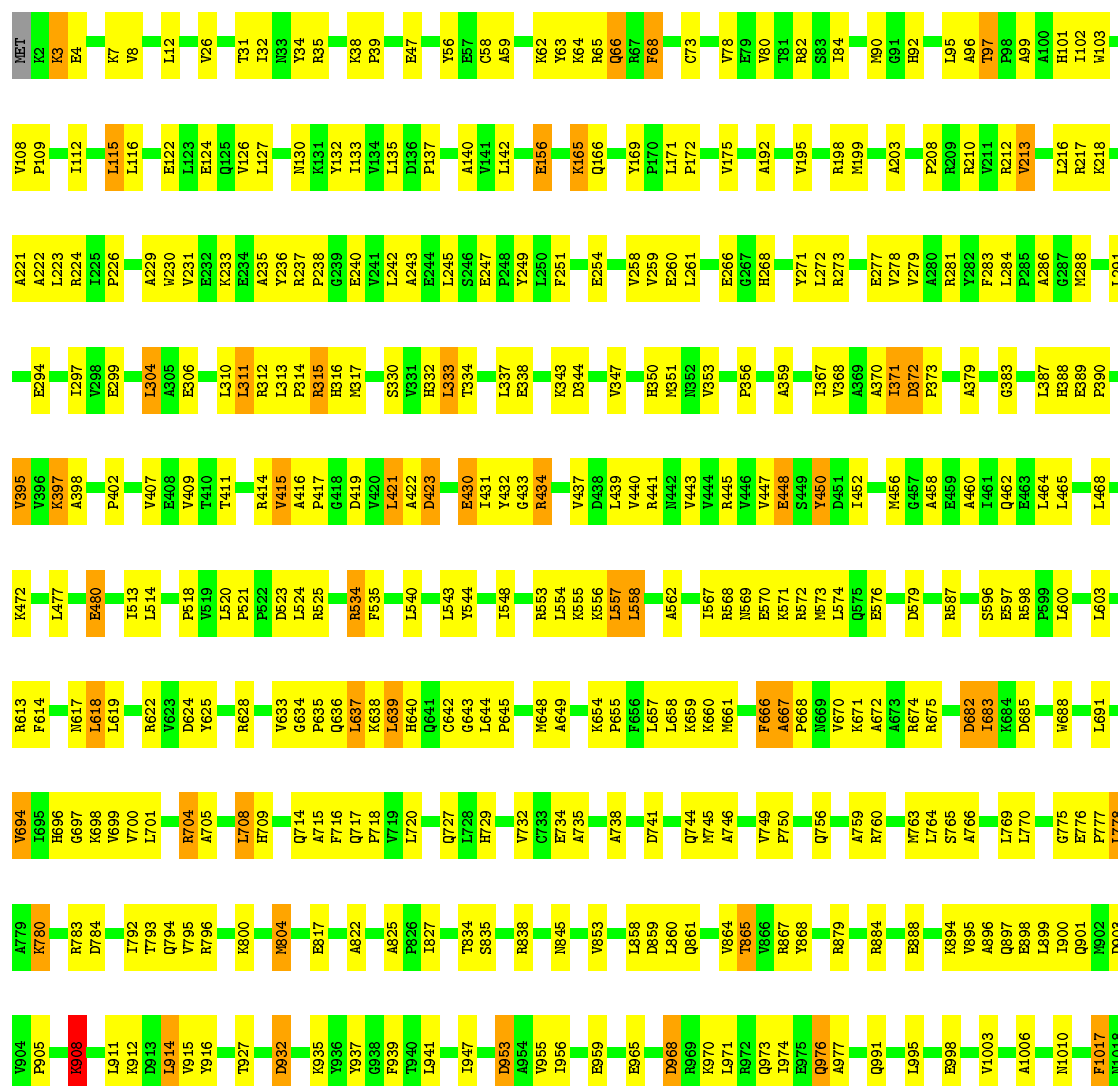
• Molecule 2: DNA-directed RNA polymerase subunit beta

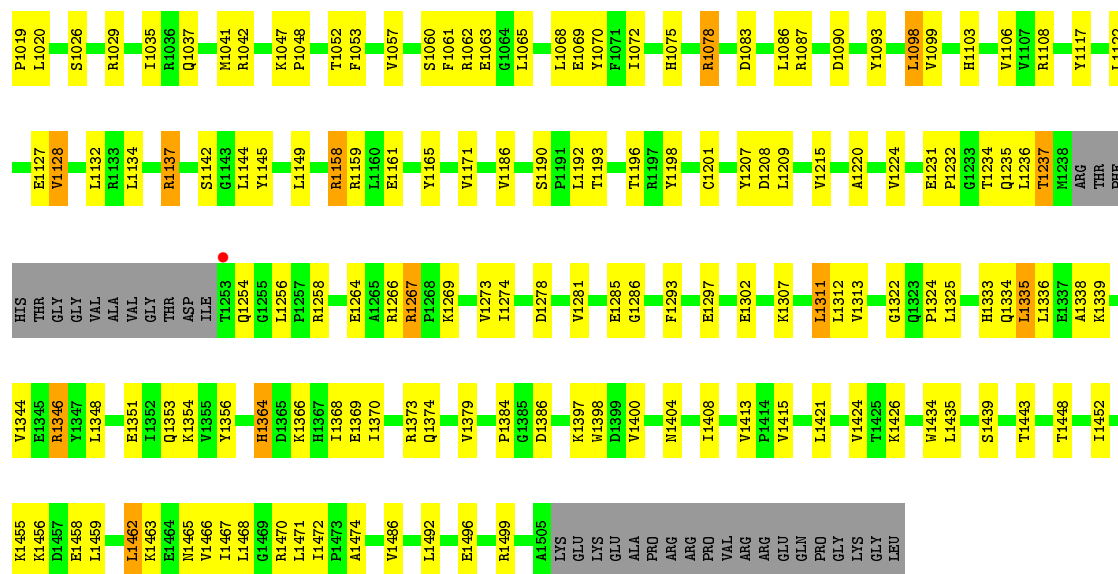




• Molecule 3: DNA-directed RNA polymerase subunit beta'

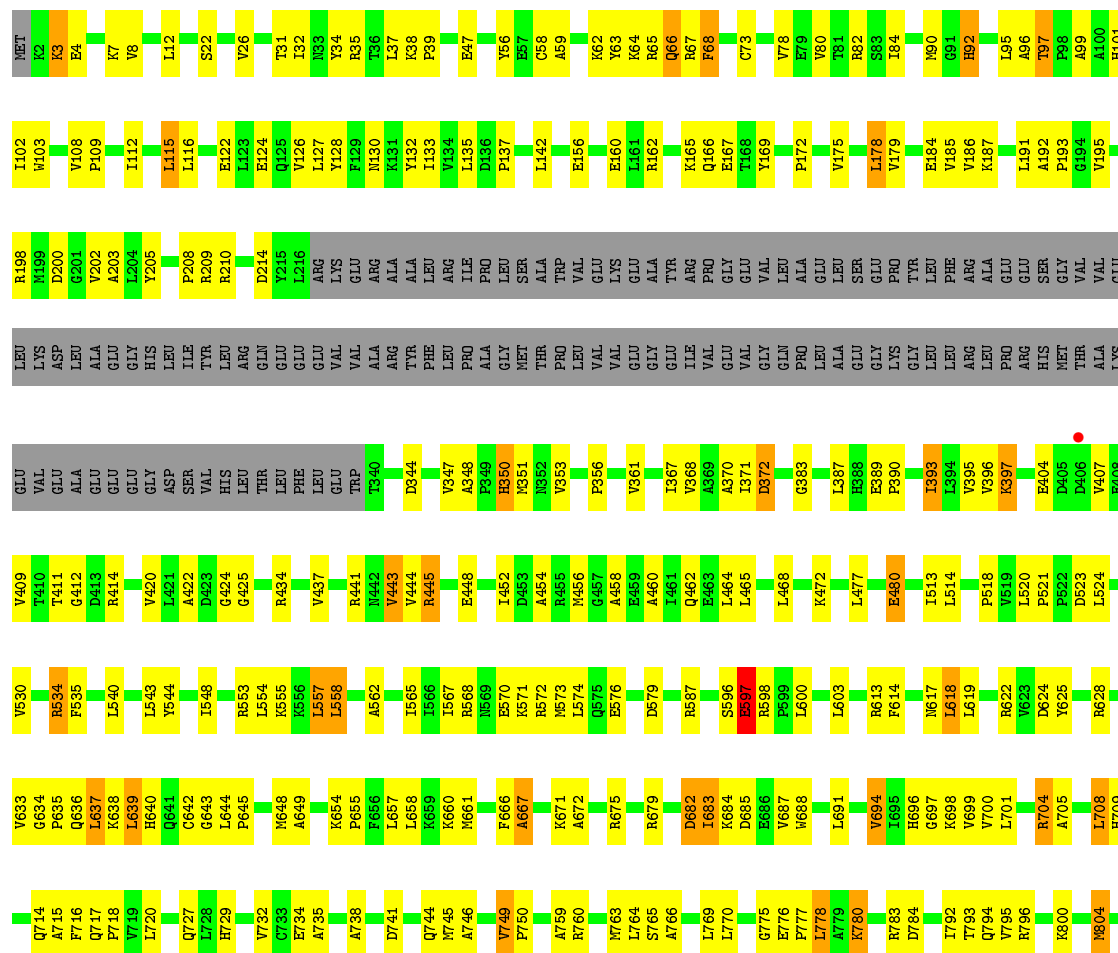
Chain D: 63% 31%

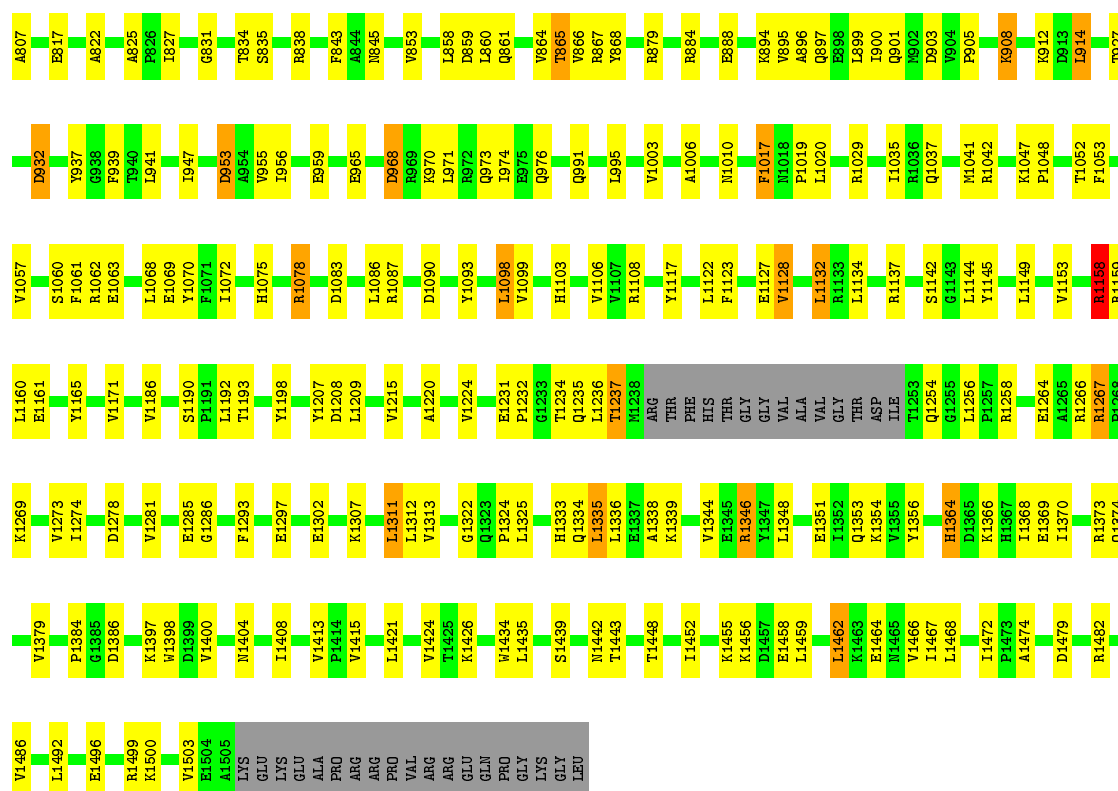




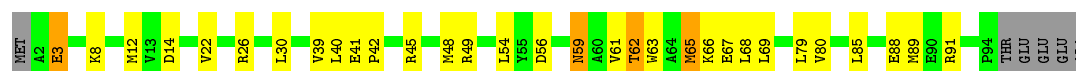
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 59% 28% 10%





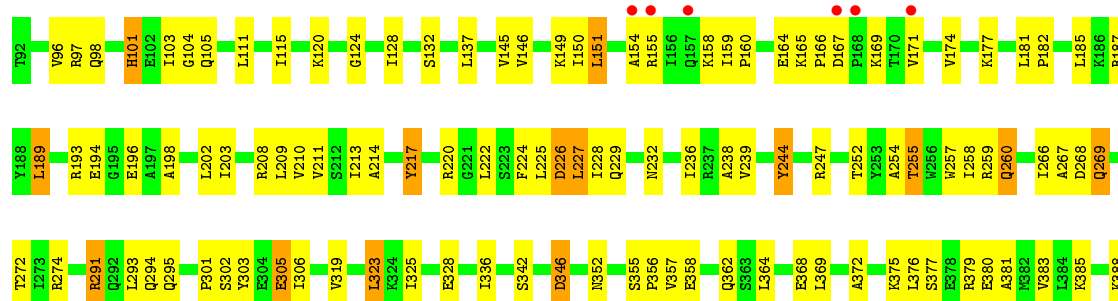
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega

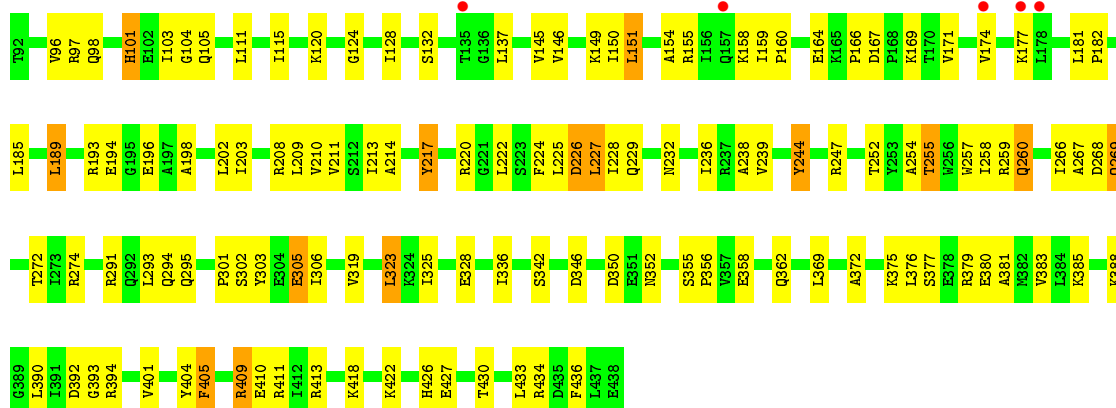


- Molecule 5: RNA polymerase sigma factor SigA

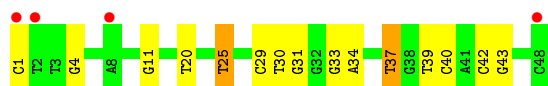




• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (48-MER)



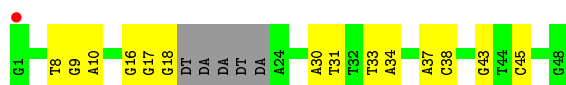
• Molecule 6: DNA (48-MER)




• Molecule 7: DNA (48-MER)



• Molecule 7: DNA (48-MER)



- Molecule 8: RNA (5'-D(P\*UP\*CP\*GP\*A)-3')

Chain Q:  75% 25%



- Molecule 8: RNA (5'-D(P\*UP\*CP\*GP\*A)-3')

Chain T:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.26 Å   289.26 Å   536.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	34.96 – 4.00 34.96 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.96-4.00) 99.0 (34.96-4.00)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 3.99 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.280   ,   0.315 0.280   ,   0.315	Depositor DCC
$R_{free}$ test set	9497 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 116.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	58255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/1804	0.46	0/2455
1	B	0.25	0/1804	0.50	1/2455 (0.0%)
1	G	0.24	0/1804	0.46	0/2455
1	H	0.24	0/1804	0.49	0/2455
2	C	0.25	1/8905 (0.0%)	0.48	3/12040 (0.0%)
2	I	0.26	1/8905 (0.0%)	0.48	2/12040 (0.0%)
3	D	0.24	0/11963	0.48	4/16165 (0.0%)
3	J	0.24	1/10959 (0.0%)	0.47	3/14802 (0.0%)
4	E	0.21	0/783	0.38	0/1054
4	K	0.21	0/783	0.38	0/1054
5	F	0.23	0/2843	0.53	4/3822 (0.1%)
5	L	0.23	0/2843	0.55	4/3822 (0.1%)
6	O	0.44	0/1109	1.07	4/1712 (0.2%)
6	R	0.44	0/1109	1.07	3/1712 (0.2%)
7	P	0.48	0/1106	1.11	5/1706 (0.3%)
7	S	0.44	0/989	1.01	0/1523
8	Q	0.15	0/94	0.67	0/144
8	T	0.16	0/94	0.67	0/144
All	All	0.26	3/59701 (0.0%)	0.55	33/81560 (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
1	B	0	2
2	C	0	2
2	I	0	1
All	All	0	5



All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	764	GLU	CD-OE2	8.42	1.34	1.25
2	C	764	GLU	CB-CG	-6.22	1.40	1.52
3	J	597	GLU	CB-CG	5.05	1.61	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	291	ARG	NE-CZ-NH2	-12.83	113.89	120.30
5	L	291	ARG	NE-CZ-NH1	12.47	126.54	120.30
5	F	291	ARG	NE-CZ-NH1	-11.97	114.31	120.30
5	F	291	ARG	NE-CZ-NH2	11.77	126.18	120.30
2	I	764	GLU	C-N-CA	8.19	142.16	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	177	VAL	Mainchain,Peptide
2	C	178	ALA	Peptide
2	C	764	GLU	Peptide
2	I	178	ALA	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1799	57	0
1	B	1770	0	1799	55	0
1	G	1770	0	1799	59	0
1	H	1770	0	1799	55	0
2	C	8739	0	8841	295	0
2	I	8739	0	8841	282	0
3	D	11761	0	11976	343	0
3	J	10779	0	10993	314	0
4	E	768	0	784	18	0
4	K	768	0	784	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2801	0	2881	97	0
5	L	2801	0	2881	87	0
6	O	988	0	544	17	0
6	R	988	0	544	16	0
7	P	985	0	543	17	0
7	S	882	0	487	14	0
8	Q	85	0	43	0	0
8	T	85	0	43	1	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58255	0	57381	1567	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 14.

The worst 5 of 1567 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:THR:HB	1:G:22:GLU:HB2	1.54	0.90
1:A:14:THR:HB	1:A:22:GLU:HB2	1.54	0.89
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.54	0.88
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.56	0.88
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.85

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	225/314 (72%)	206 (92%)	18 (8%)	1 (0%)	34	71
1	B	225/314 (72%)	205 (91%)	17 (8%)	3 (1%)	12	48
1	G	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
1	H	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
2	C	1108/1119 (99%)	1011 (91%)	94 (8%)	3 (0%)	41	75
2	I	1108/1119 (99%)	1012 (91%)	94 (8%)	2 (0%)	47	79
3	D	1486/1524 (98%)	1340 (90%)	141 (10%)	5 (0%)	41	75
3	J	1361/1524 (89%)	1235 (91%)	123 (9%)	3 (0%)	47	79
4	E	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	345/347 (99%)	316 (92%)	29 (8%)	0	100	100
5	L	345/347 (99%)	314 (91%)	31 (9%)	0	100	100
All	All	6835/7434 (92%)	6214 (91%)	602 (9%)	19 (0%)	41	75

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	765	GLN
3	D	1128	VAL
3	J	1128	VAL
1	A	53	VAL
1	B	178	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	186 (96%)	8 (4%)	30	57
1	B	194/270 (72%)	179 (92%)	15 (8%)	13	40
1	G	194/270 (72%)	186 (96%)	8 (4%)	30	57
1	H	194/270 (72%)	179 (92%)	15 (8%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	931/936 (100%)	837 (90%)	94 (10%)	7	29
2	I	931/936 (100%)	838 (90%)	93 (10%)	7	29
3	D	1252/1281 (98%)	1128 (90%)	124 (10%)	8	29
3	J	1150/1281 (90%)	1048 (91%)	102 (9%)	9	34
4	E	83/88 (94%)	77 (93%)	6 (7%)	14	42
4	K	83/88 (94%)	77 (93%)	6 (7%)	14	42
5	F	297/299 (99%)	269 (91%)	28 (9%)	8	31
5	L	297/299 (99%)	269 (91%)	28 (9%)	8	31
All	All	5800/6288 (92%)	5273 (91%)	527 (9%)	9	33

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1448	THR
1	H	177	VAL
3	J	1397	LYS
4	E	62	THR
5	F	328	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	232	ASN
1	H	156	HIS
5	L	101	HIS
5	F	260	GLN
1	G	81	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Q	3/4 (75%)	1 (33%)	0
8	T	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Q	2	C
8	T	2	C

There are no RNA pucker outliers to report.

## 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 6 ligands modelled in this entry, 6 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/314 (72%)	-0.33	0  	68, 121, 176, 228	0
1	B	227/314 (72%)	-0.49	0  	42, 95, 150, 180	0
1	G	227/314 (72%)	-0.01	2 (0%)  	96, 156, 194, 223	0
1	H	227/314 (72%)	-0.29	0  	80, 131, 171, 192	0
2	C	1112/1119 (99%)	-0.30	6 (0%)  	30, 123, 203, 260	0
2	I	1112/1119 (99%)	-0.17	15 (1%)  	60, 146, 214, 259	0
3	D	1490/1524 (97%)	-0.42	1 (0%)  	22, 88, 155, 231	0
3	J	1367/1524 (89%)	-0.33	1 (0%)  	29, 112, 177, 240	0
4	E	93/99 (93%)	-0.41	0  	23, 89, 154, 187	0
4	K	93/99 (93%)	-0.24	0  	67, 126, 181, 236	0
5	F	347/347 (100%)	-0.20	6 (1%)  	52, 131, 221, 275	0
5	L	347/347 (100%)	-0.12	5 (1%)  	81, 151, 225, 270	0
6	O	48/48 (100%)	0.40	4 (8%)  	86, 193, 267, 293	0
6	R	48/48 (100%)	0.08	1 (2%)  	109, 184, 277, 300	0
7	P	48/48 (100%)	0.61	4 (8%)  	77, 199, 251, 283	0
7	S	43/48 (89%)	0.14	1 (2%)  	100, 195, 234, 248	0
8	Q	4/4 (100%)	0.06	0  	116, 124, 128, 150	0
8	T	4/4 (100%)	0.05	0  	122, 130, 143, 154	0
All	All	7064/7634 (92%)	-0.28	46 (0%)  	22, 120, 200, 300	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	5.3
5	L	177	LYS	4.4
2	I	246	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	1253	THR	3.6
7	P	48	DG	3.2

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
10	MG	D	2003	1/1	0.94	0.07	180,180,180,180	0
9	ZN	J	2002	1/1	0.95	0.07	166,166,166,166	0
10	MG	J	2003	1/1	0.95	0.25	188,188,188,188	0
9	ZN	D	2002	1/1	0.96	0.07	79,79,79,79	0
9	ZN	D	2001	1/1	0.97	0.12	79,79,79,79	0
9	ZN	J	2001	1/1	0.99	0.12	97,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.