



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 4, 2021 – 12:14 PM JST

PDB ID : 7EH2
Title : Thermus thermophilus transcription initiation complex containing a template-strand pyrimidine at position TSS-2 and GpG RNA primer
Authors : Li, L.; Zhang, Y.
Deposited on : 2021-03-27
Resolution : 3.34 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 ⓘ symbol.

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 : 2.22
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) : 2.22

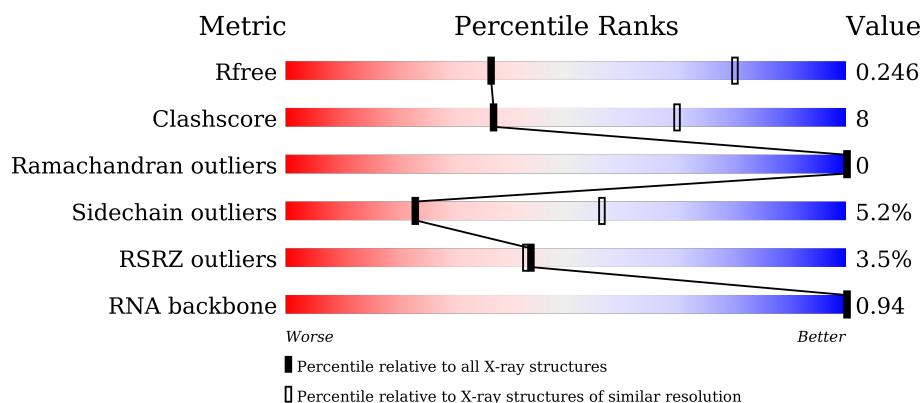
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

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 of 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 $\leq 5\%$. 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	315	<div> <div>3%</div> <div>52%</div> <div>20%</div> <div>•</div> <div>27%</div> </div>
1	B	315	<div> <div>5%</div> <div>53%</div> <div>16%</div> <div>•</div> <div>30%</div> </div>
1	K	315	<div> <div>6%</div> <div>54%</div> <div>16%</div> <div>•</div> <div>28%</div> </div>
1	L	315	<div> <div>6%</div> <div>53%</div> <div>17%</div> <div>•</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	1119	 77% 21% ..
2	M	1119	 74% 23% ..
3	D	1524	 77% 18% ..
3	N	1524	 75% 21% ..
4	E	99	 72% 22% • 5%
4	O	99	 76% 19% 5%
5	F	443	 65% 12% • 22%
5	P	443	 63% 15% 22%
6	G	27	 44% 48% 7%
6	J	27	 33% 59% 7%
7	H	19	 37% 53% 11%
7	Q	19	 42% 47% 11%
8	I	2	 100%
8	R	2	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56841 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	229	Total	C	N	O	S	0	0	0
			1777	1136	306	333	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	227	Total	C	N	O	S	0	0	0
			1781	1138	308	333	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8742	5534	1552	1632	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8724	5520	1551	1629	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11680	7405	2051	2189	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11675	7402	2047	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2803	1768	509	522	4			
5	P	347	Total	C	N	O	S	0	0	0
			2757	1738	490	525	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			
6	J	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*CP*CP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			
7	Q	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			
8	R	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	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	D	1	Total Mg 1 1	0	0
10	L	1	Total Mg 1 1	0	0
10	N	1	Total Mg 1 1	0	0

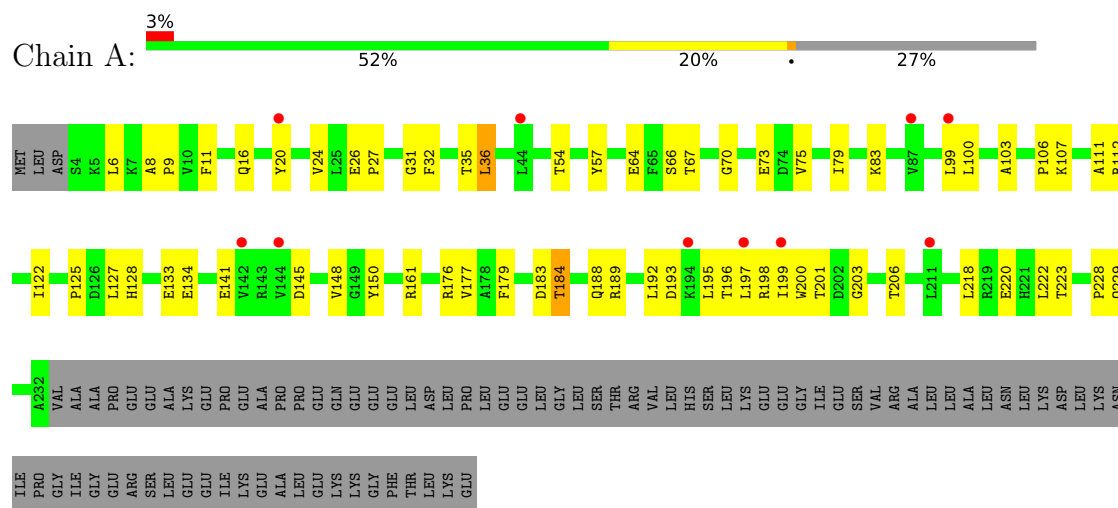
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total O 4 4	0	0
11	B	4	Total O 4 4	0	0
11	C	5	Total O 5 5	0	0
11	D	10	Total O 10 10	0	0
11	E	2	Total O 2 2	0	0
11	F	1	Total O 1 1	0	0
11	K	2	Total O 2 2	0	0
11	L	1	Total O 1 1	0	0
11	M	1	Total O 1 1	0	0
11	N	9	Total O 9 9	0	0
11	O	2	Total O 2 2	0	0
11	G	1	Total O 1 1	0	0

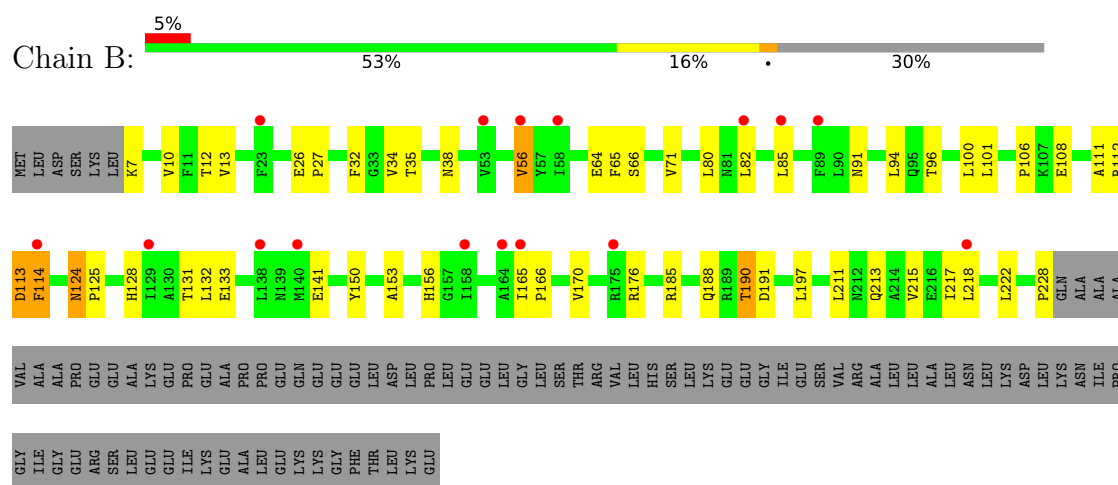
3 Residue-property plots [i](#)

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

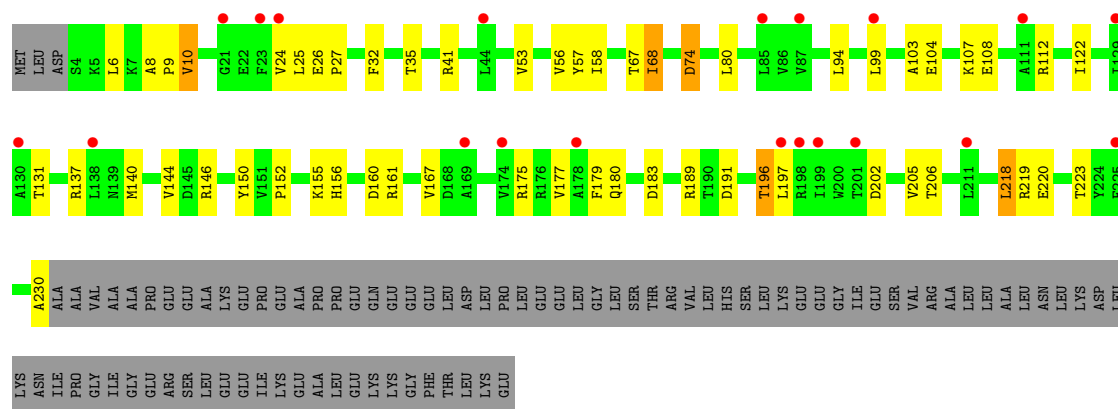


• Molecule 1: DNA-directed RNA polymerase subunit alpha

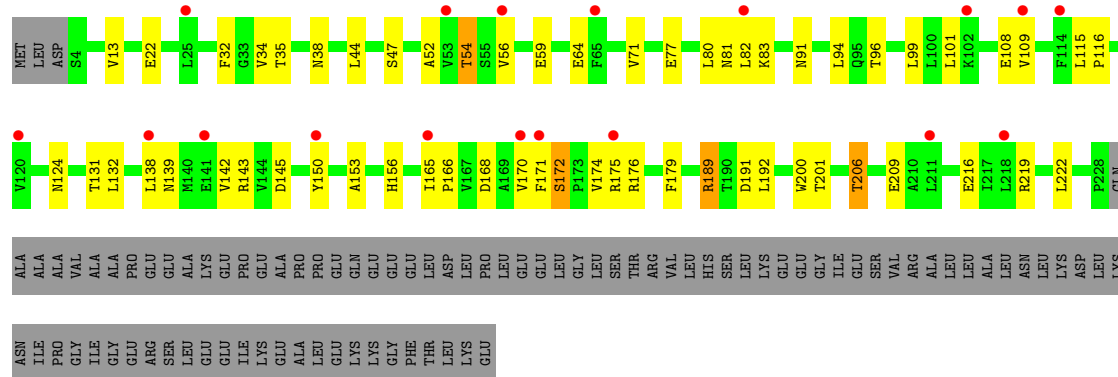


• Molecule 1: DNA-directed RNA polymerase subunit alpha

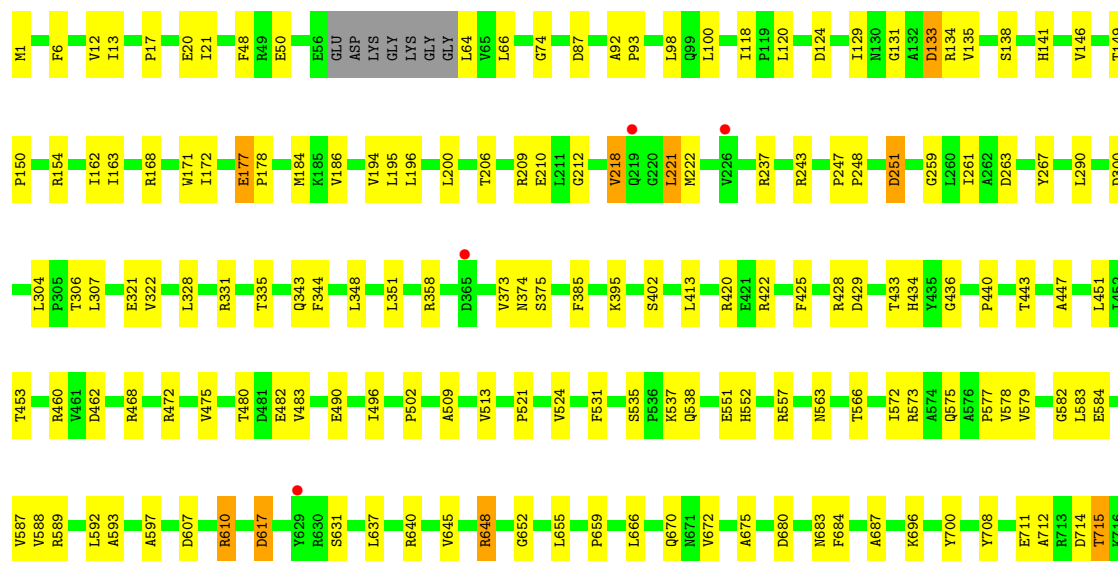
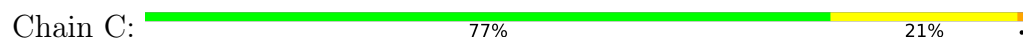


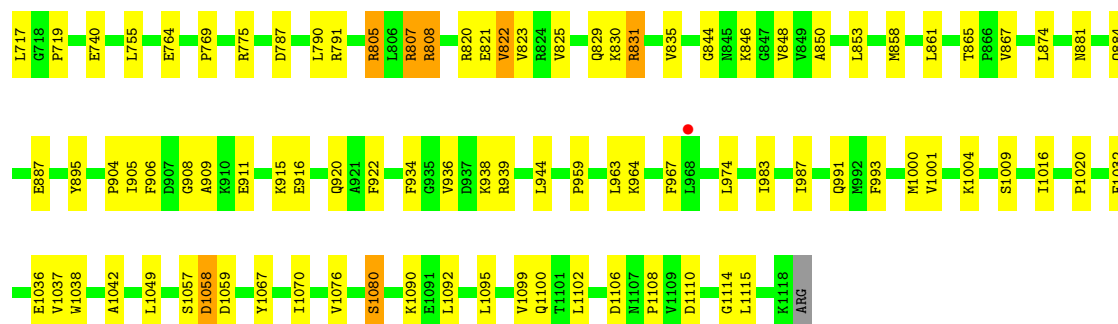


• Molecule 1: DNA-directed RNA polymerase subunit alpha

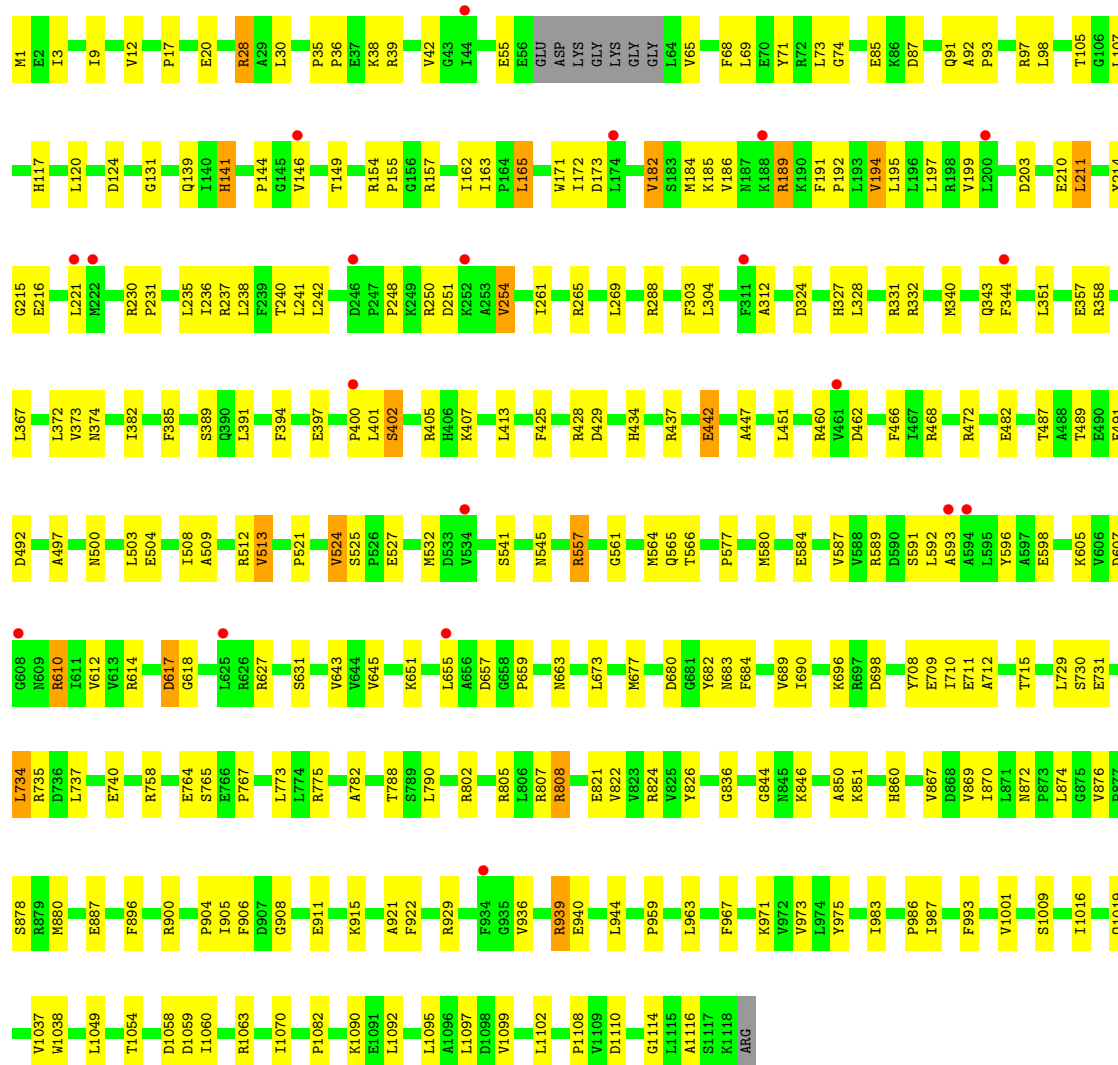
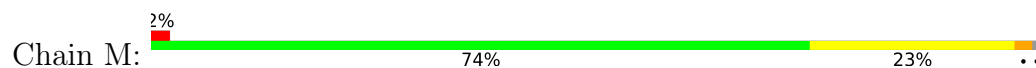


• Molecule 2: DNA-directed RNA polymerase subunit beta

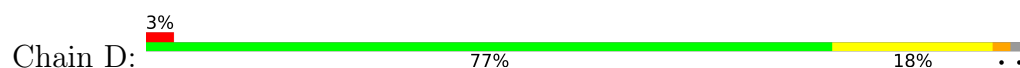


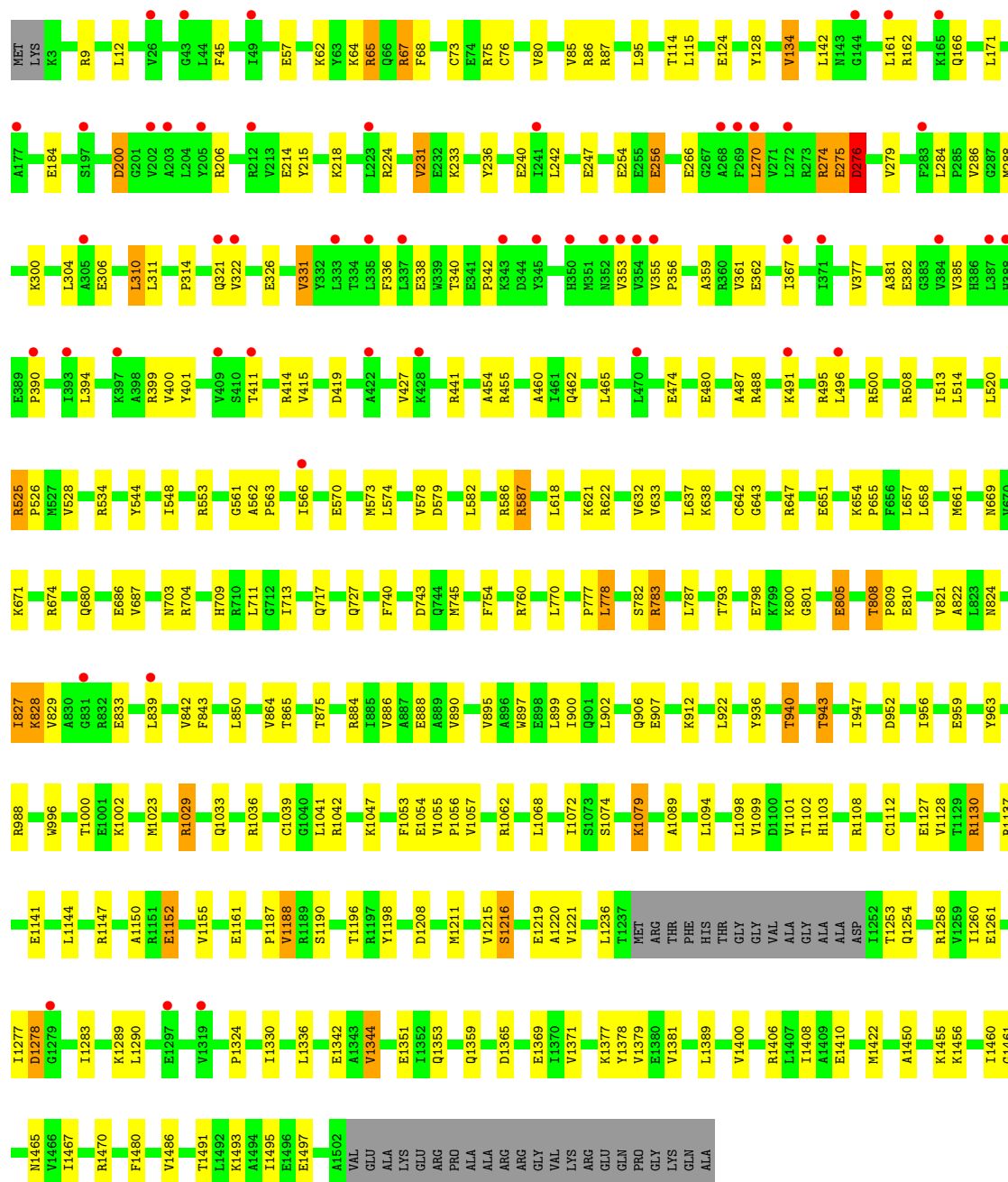


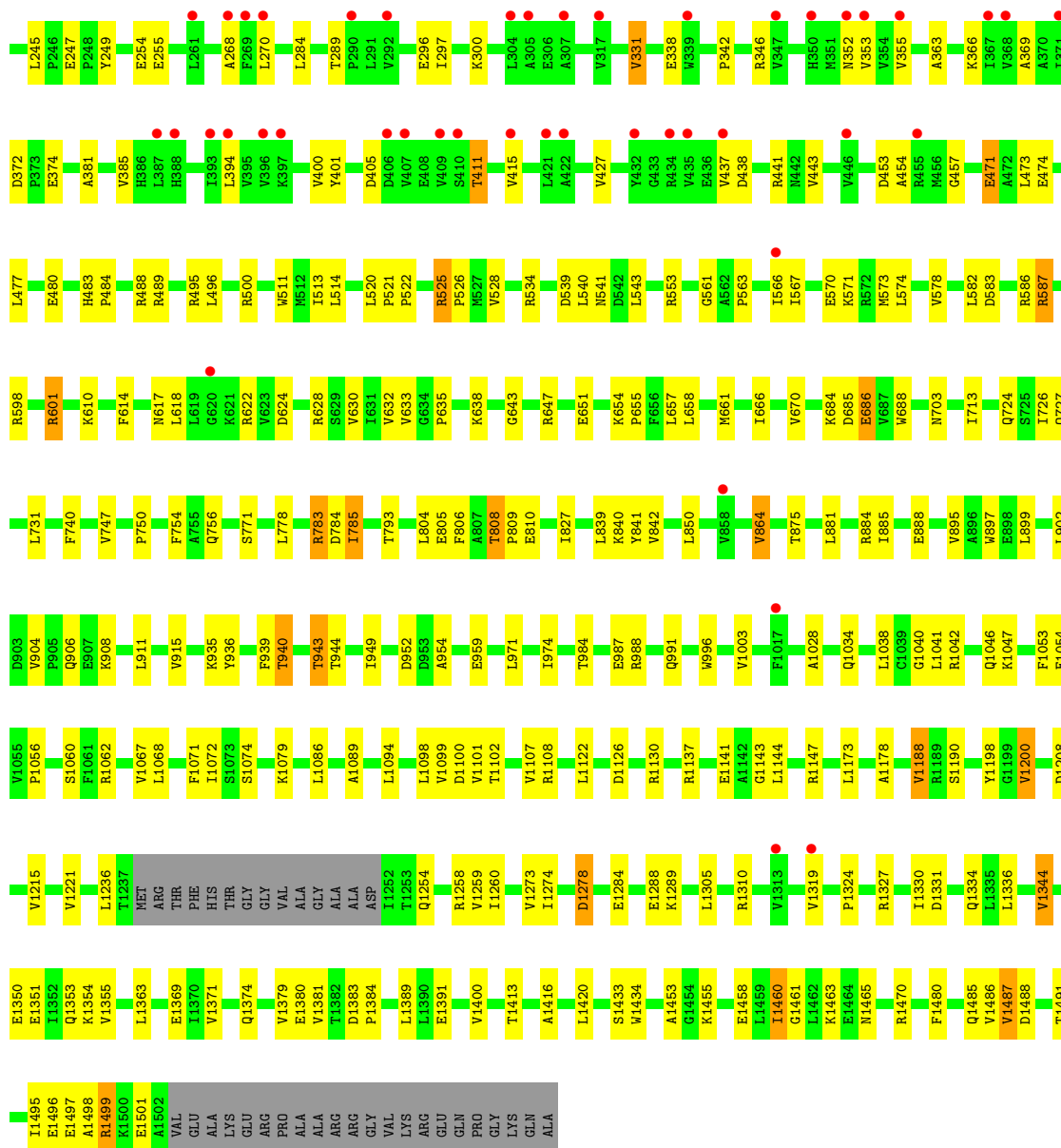
• Molecule 2: DNA-directed RNA polymerase subunit beta



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







- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 72% 22% 5%

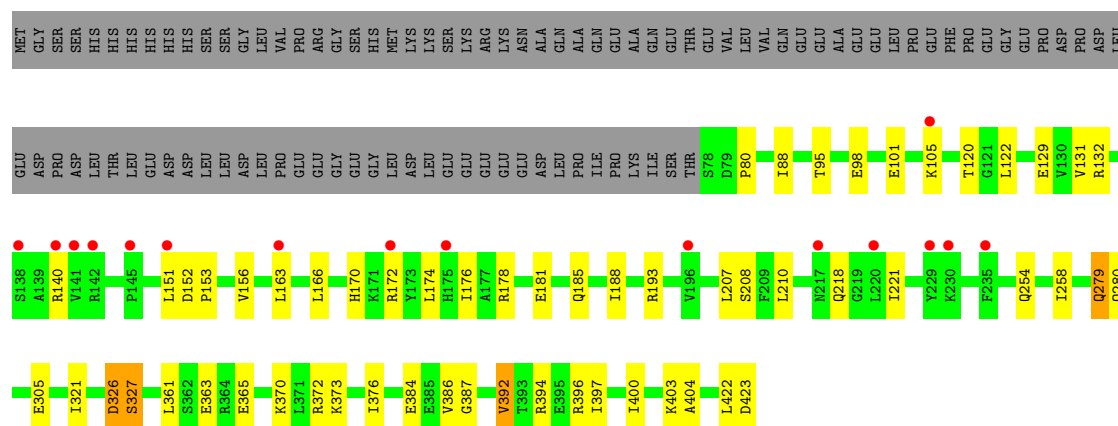


- Molecule 4: DNA-directed RNA polymerase subunit omega

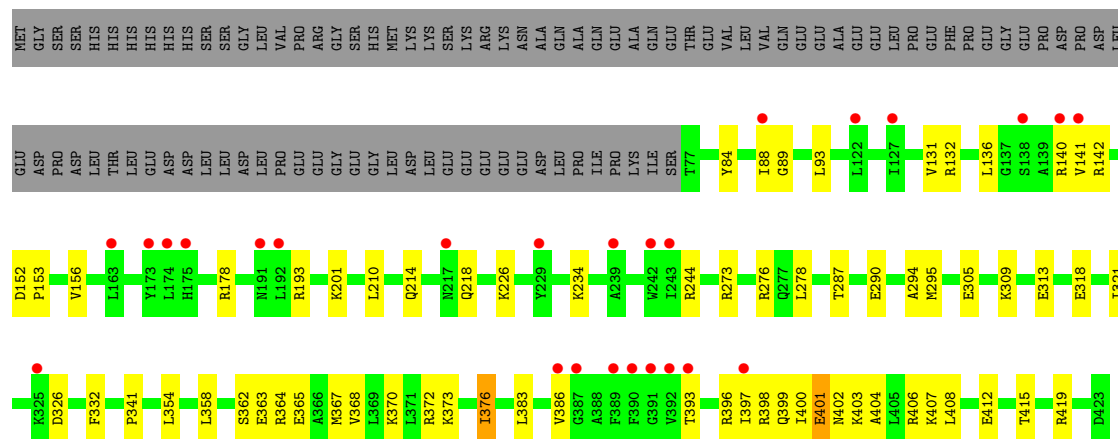
Chain O: 2% 76% 19% 5%



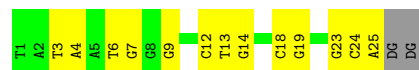
- Molecule 5: RNA polymerase sigma factor SigA



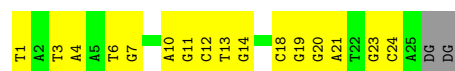
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (27-MER)



• Molecule 6: DNA (27-MER)



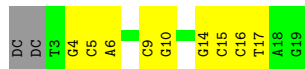
• Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*AP*G)-3')





- Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*AP*G)-3')

Chain Q: 42% 47% 11%



- Molecule 8: RNA (5'-R(*GP*G)-3')

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: RNA (5'-R(*GP*G)-3')

Chain R: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	184.85Å 104.20Å 296.65Å 90.00° 98.42° 90.00°	Depositor
Resolution (Å)	97.82 – 3.34 123.62 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.82-3.34) 99.6 (123.62-3.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.201 , 0.247 0.201 , 0.246	Depositor DCC
R_{free} test set	8256 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56841	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.25	0/1809	0.46	0/2464
1	B	0.25	0/1782	0.45	0/2424
1	K	0.26	0/1813	0.47	0/2466
1	L	0.26	0/1805	0.47	0/2454
2	C	0.26	0/8909	0.44	0/12054
2	M	0.26	0/8890	0.45	1/12030 (0.0%)
3	D	0.25	0/11885	0.44	0/16081
3	N	0.25	0/11880	0.44	0/16074
4	E	0.24	0/775	0.41	0/1045
4	O	0.25	0/775	0.40	0/1045
5	F	0.25	0/2848	0.41	0/3832
5	P	0.25	0/2800	0.41	0/3777
6	G	0.54	0/580	0.93	0/895
6	J	0.55	0/580	0.95	0/895
7	H	0.56	0/386	0.92	0/594
7	Q	0.54	0/386	0.90	0/594
8	I	0.30	0/48	0.92	0/74
8	R	0.35	0/48	1.06	0/74
All	All	0.27	0/57999	0.47	1/78872 (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
3	D	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	211	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
3	D	276	ASP	Peptide

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	1777	0	1812	42	0
1	B	1750	0	1797	31	0
1	K	1781	0	1828	32	0
1	L	1773	0	1826	35	0
2	C	8742	0	8826	138	0
2	M	8724	0	8795	165	0
3	D	11680	0	11864	187	0
3	N	11675	0	11851	203	0
4	E	761	0	778	14	0
4	O	761	0	778	12	0
5	F	2803	0	2878	39	0
5	P	2757	0	2780	47	0
6	G	516	0	283	10	0
6	J	516	0	283	15	0
7	H	345	0	193	9	0
7	Q	345	0	193	10	0
8	I	43	0	23	0	0
8	R	43	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	1	0	0	0	0
10	L	1	0	0	0	0
10	N	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	5	0	0	0	0
11	D	10	0	0	0	0
11	E	2	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	K	2	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	9	0	0	3	0
11	O	2	0	0	0	0
All	All	56841	0	56811	882	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 8.

The worst 5 of 882 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:M:462:ASP:HB3	2:M:468:ARG:HD2	1.58	0.84
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.62	0.81
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.61	0.81
5:P:408:LEU:O	5:P:412:GLU:HB2	1.83	0.77
3:N:60:CYS:SG	11:N:1702:HOH:O	2.43	0.76

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	227/315 (72%)	220 (97%)	7 (3%)	0	100	100
1	B	220/315 (70%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	225/315 (71%)	219 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	219 (98%)	4 (2%)	0	100	100
2	C	1107/1119 (99%)	1082 (98%)	25 (2%)	0	100	100
2	M	1107/1119 (99%)	1077 (97%)	30 (3%)	0	100	100
3	D	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100
3	N	1482/1524 (97%)	1446 (98%)	36 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	342 (99%)	2 (1%)	0	100	100
5	P	345/443 (78%)	334 (97%)	11 (3%)	0	100	100
All	All	6946/7630 (91%)	6781 (98%)	165 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	195/273 (71%)	185 (95%)	10 (5%)	24	57
1	B	195/273 (71%)	179 (92%)	16 (8%)	11	39
1	K	198/273 (72%)	182 (92%)	16 (8%)	11	39
1	L	198/273 (72%)	188 (95%)	10 (5%)	24	57
2	C	931/941 (99%)	879 (94%)	52 (6%)	21	54
2	M	927/941 (98%)	879 (95%)	48 (5%)	23	56
3	D	1241/1279 (97%)	1175 (95%)	66 (5%)	22	56
3	N	1240/1279 (97%)	1181 (95%)	59 (5%)	25	59
4	E	83/88 (94%)	79 (95%)	4 (5%)	25	59
4	O	83/88 (94%)	81 (98%)	2 (2%)	49	75
5	F	300/388 (77%)	289 (96%)	11 (4%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	P	291/388 (75%)	281 (97%)	10 (3%)	37 67
All	All	5882/6484 (91%)	5578 (95%)	304 (5%)	23 56

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	939	ARG
3	N	1413	THR
3	N	142	LEU
3	N	686	GLU
5	P	376	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	704	HIS
3	D	973	GLN
2	M	141	HIS
2	M	704	HIS
3	N	994	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	R	1/2 (50%)	0	0
All	All	2/4 (50%)	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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, 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	229/315 (72%)	0.39	10 (4%) 34 35	63, 82, 107, 131	0
1	B	222/315 (70%)	0.55	16 (7%) 15 16	66, 96, 127, 148	0
1	K	227/315 (72%)	0.55	20 (8%) 10 10	70, 92, 113, 130	0
1	L	225/315 (71%)	0.47	18 (8%) 12 12	68, 99, 133, 152	0
2	C	1111/1119 (99%)	0.17	5 (0%) 91 91	46, 80, 132, 163	0
2	M	1111/1119 (99%)	0.28	20 (1%) 68 67	51, 100, 161, 179	0
3	D	1486/1524 (97%)	0.32	53 (3%) 42 41	48, 83, 143, 186	1 (0%)
3	N	1486/1524 (97%)	0.34	62 (4%) 36 36	52, 90, 142, 196	1 (0%)
4	E	94/99 (94%)	0.23	0 100 100	63, 85, 122, 130	0
4	O	94/99 (94%)	0.14	2 (2%) 63 63	71, 100, 137, 144	0
5	F	346/443 (78%)	0.35	16 (4%) 32 33	58, 91, 135, 158	0
5	P	347/443 (78%)	0.53	26 (7%) 14 14	70, 108, 173, 191	0
6	G	25/27 (92%)	-0.08	0 100 100	87, 128, 187, 196	0
6	J	25/27 (92%)	0.13	0 100 100	90, 134, 190, 196	0
7	H	17/19 (89%)	0.04	0 100 100	77, 110, 182, 190	0
7	Q	17/19 (89%)	0.04	0 100 100	93, 122, 186, 189	0
8	I	2/2 (100%)	0.75	0 100 100	79, 79, 79, 85	2 (100%)
8	R	2/2 (100%)	0.30	0 100 100	88, 88, 88, 93	2 (100%)
All	All	7066/7726 (91%)	0.32	248 (3%) 44 43	46, 91, 148, 196	6 (0%)

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	392	VAL	8.5
1	B	138	LEU	5.2
5	P	391	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
3	N	394	LEU	4.8
5	P	389	PHE	4.4

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 monosaccharides 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(\AA^2)	Q<0.9
10	MG	L	401	1/1	0.77	0.17	77,77,77,77	0
9	ZN	N	1601	1/1	0.95	0.24	93,93,93,93	0
10	MG	N	1603	1/1	0.98	0.23	61,61,61,61	0
10	MG	D	2003	1/1	0.99	0.24	54,54,54,54	0
9	ZN	D	2001	1/1	0.99	0.23	78,78,78,78	0
9	ZN	N	1602	1/1	0.99	0.15	129,129,129,129	0
9	ZN	D	2002	1/1	1.00	0.17	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.