



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:40 AM UTC

PDB ID : 4QIW / pdb_00004qiw
Title : Crystal structure of euryarchaeal RNA polymerase from *Thermococcus kodakarensis*
Authors : Jun, S.-H.; Murakami, K.S.
Deposited on : 2014-06-02
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

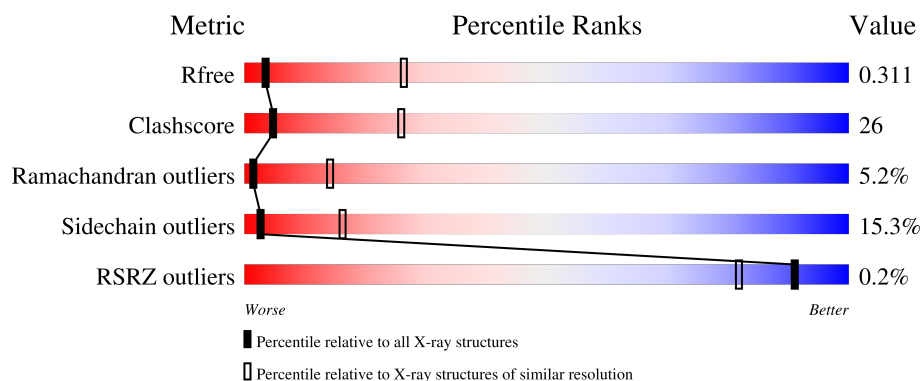
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	906	
1	I	906	
2	B	1123	
2	J	1123	
3	C	391	

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Mol	Chain	Length	Quality of chain
3	M	391	
4	D	259	
4	O	259	
5	E	190	
5	Q	190	
6	F	122	
6	R	122	
7	H	82	
7	S	82	
8	K	57	
8	T	57	
9	L	100	
9	U	100	
10	N	65	
10	V	65	
11	P	49	
11	W	49	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51069 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	0	0
			6891	4357	1221	1275	38			
1	I	862	Total	C	N	O	S	0	0	0
			6875	4347	1220	1270	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			
2	J	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	369	Total	C	N	O	S	0	0	0
			2882	1819	498	555	10			
3	M	369	Total	C	N	O	S	0	0	0
			2879	1816	498	555	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			
4	O	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			
5	Q	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			
6	R	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	expression tag	UNP Q5JI52
F	116	ASP	-	expression tag	UNP Q5JI52
F	117	GLU	-	expression tag	UNP Q5JI52
F	118	TYR	-	expression tag	UNP Q5JI52
F	119	ARG	-	expression tag	UNP Q5JI52
F	120	PRO	-	expression tag	UNP Q5JI52
F	121	LEU	-	expression tag	UNP Q5JI52
F	122	GLU	-	expression tag	UNP Q5JI52
R	115	ILE	-	expression tag	UNP Q5JI52
R	116	ASP	-	expression tag	UNP Q5JI52
R	117	GLU	-	expression tag	UNP Q5JI52
R	118	TYR	-	expression tag	UNP Q5JI52
R	119	ARG	-	expression tag	UNP Q5JI52
R	120	PRO	-	expression tag	UNP Q5JI52
R	121	LEU	-	expression tag	UNP Q5JI52
R	122	GLU	-	expression tag	UNP Q5JI52

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	76	Total	C	N	O	0	0	0
			627	408	105	114			
7	S	76	Total	C	N	O	0	0	0
			627	408	105	114			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	56	Total 433	C 284	N 75	O 73	S 1	0	0	0
8	T	56	Total 433	C 284	N 75	O 73	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	94	Total 775	C 493	N 134	O 146	S 2	0	0	0
9	U	94	Total 775	C 493	N 134	O 146	S 2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	HIS	-	expression tag	UNP Q5JE88
L	96	HIS	-	expression tag	UNP Q5JE88
L	97	HIS	-	expression tag	UNP Q5JE88
L	98	HIS	-	expression tag	UNP Q5JE88
L	99	HIS	-	expression tag	UNP Q5JE88
L	100	HIS	-	expression tag	UNP Q5JE88
U	95	HIS	-	expression tag	UNP Q5JE88
U	96	HIS	-	expression tag	UNP Q5JE88
U	97	HIS	-	expression tag	UNP Q5JE88
U	98	HIS	-	expression tag	UNP Q5JE88
U	99	HIS	-	expression tag	UNP Q5JE88
U	100	HIS	-	expression tag	UNP Q5JE88

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	63	Total 510	C 326	N 87	O 91	S 6	0	0	0
10	V	63	Total 510	C 326	N 87	O 91	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	42	Total 329	C 206	N 65	O 54	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	W	42	Total	C	N	O	S	0	0	0
			329	206	65	54	4			

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mg	0	0
			2	2		
12	I	2	Total	Mg	0	0
			2	2		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	N	1	Total	Zn	0	0
			1	1		
13	P	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	V	1	Total	Zn	0	0
			1	1		
13	W	1	Total	Zn	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	O	0	0
			1	1		
14	B	1	Total	O	0	0
			1	1		
14	C	1	Total	O	0	0
			1	1		
14	I	1	Total	O	0	0
			1	1		

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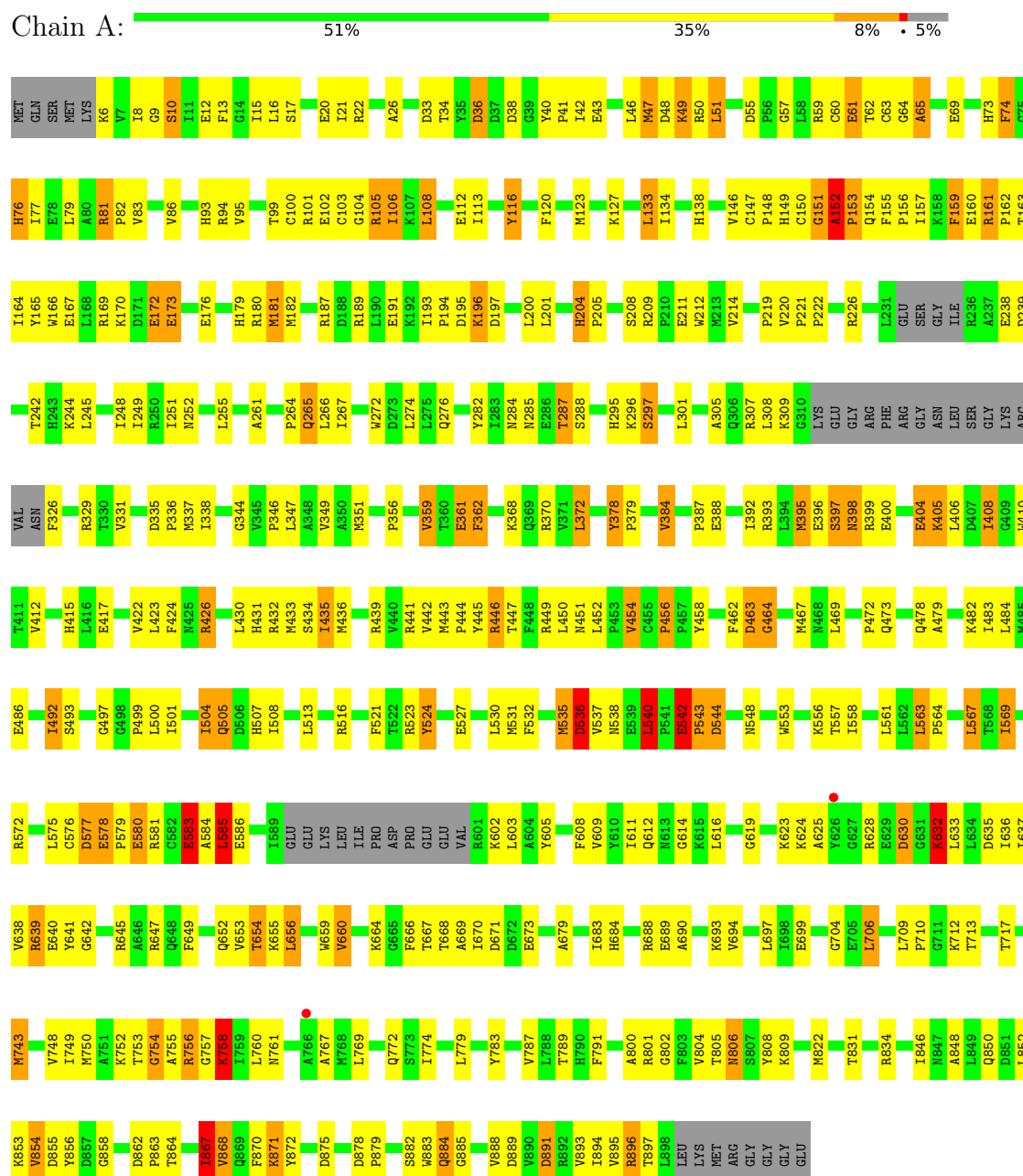
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	O	0	0
			1	1		
14	M	1	Total	O	0	0
			1	1		

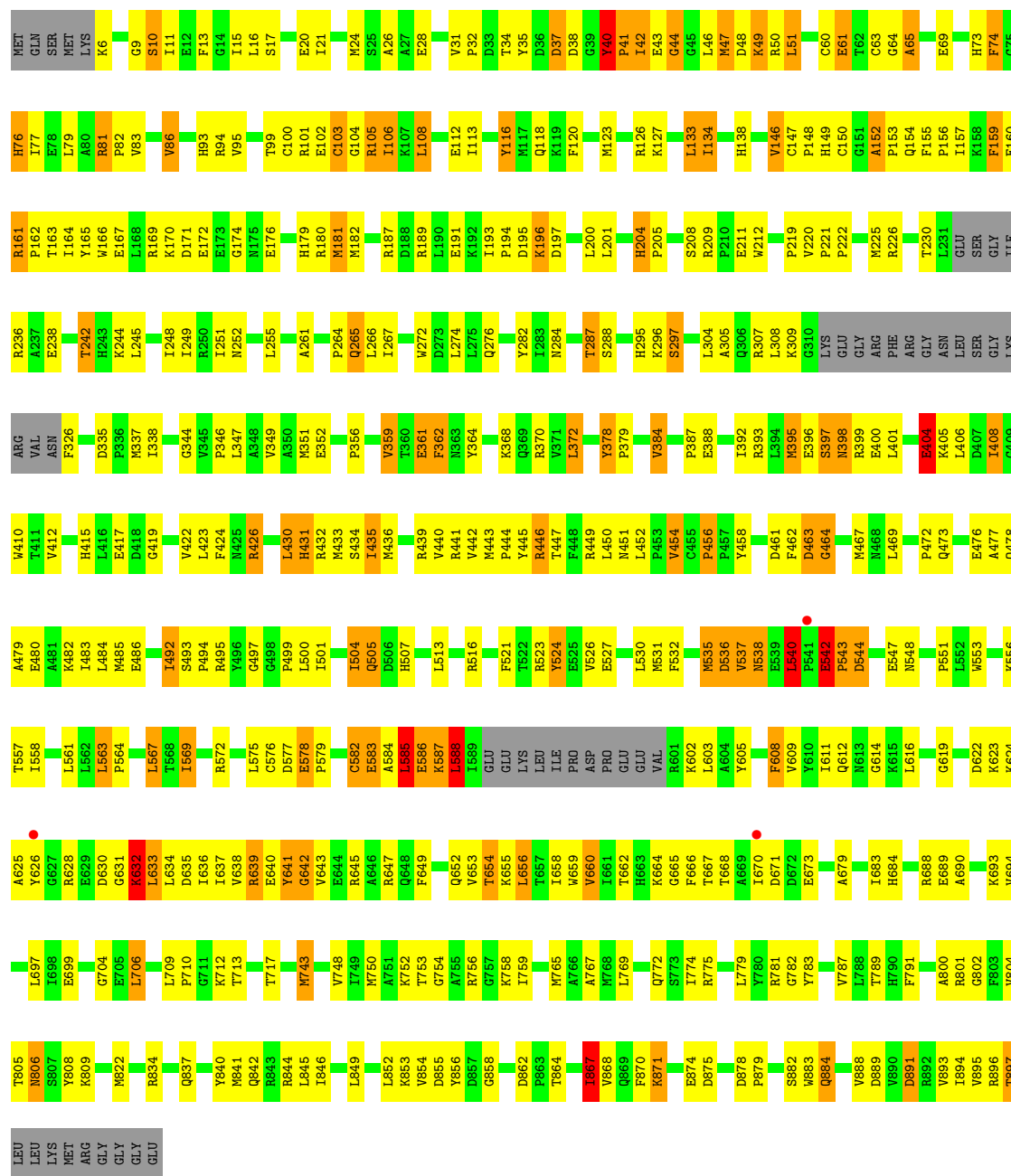
3 Residue-property plots

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

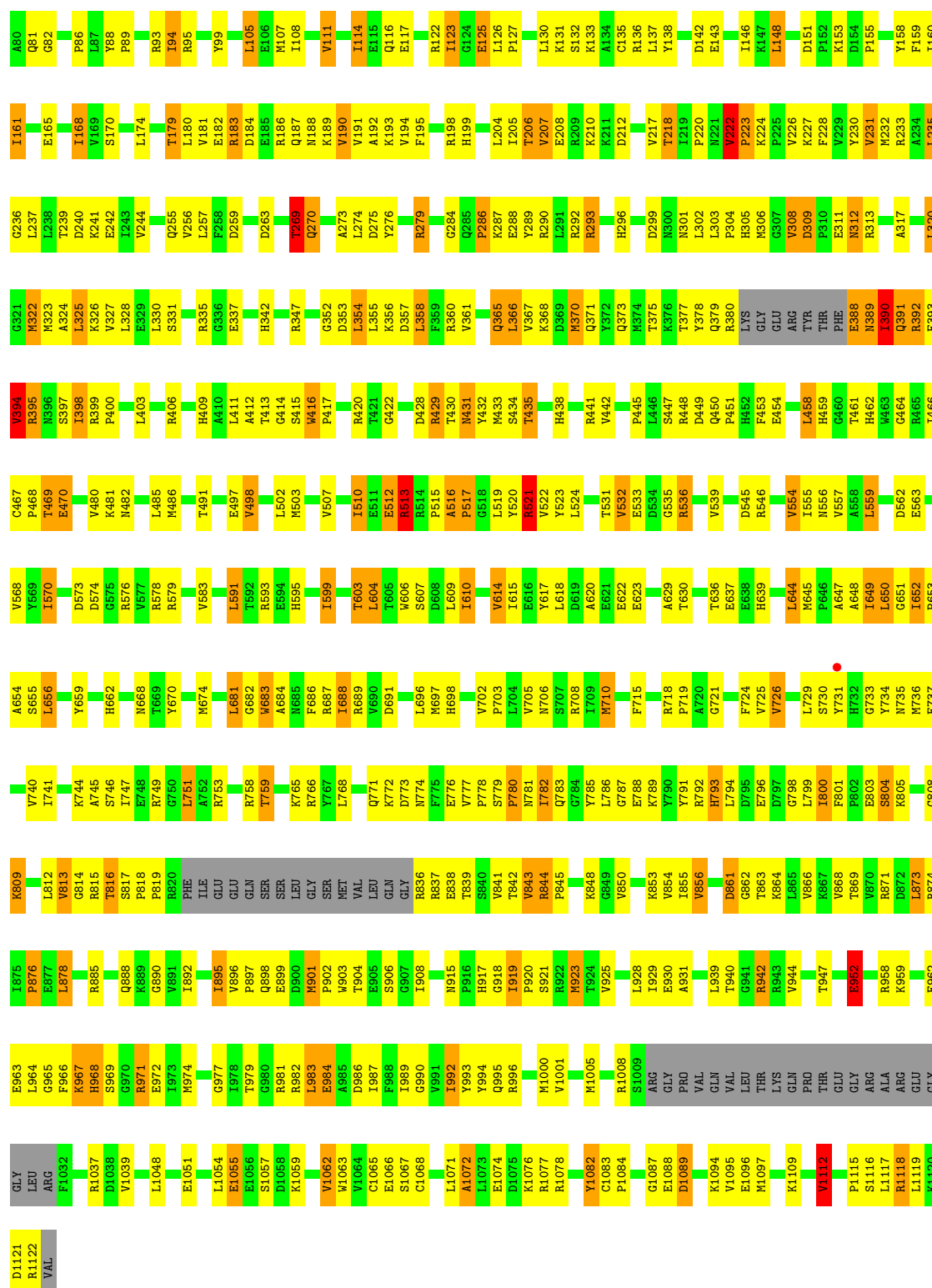


Chain I: 48% 37% 9% • 5%



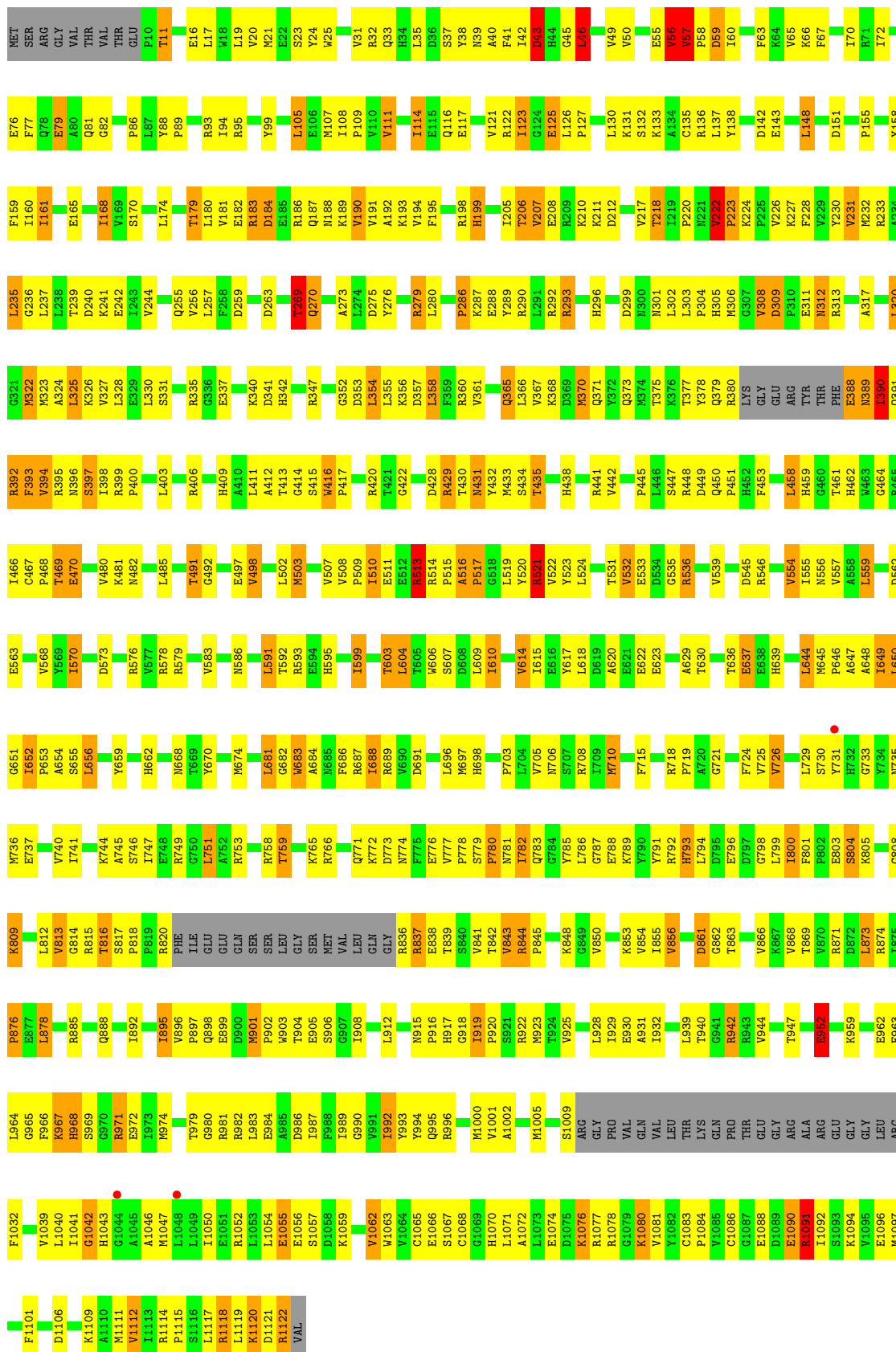
Chain B: 46% 38% 10% 5%



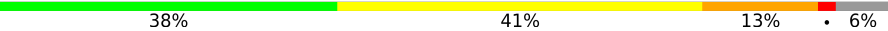


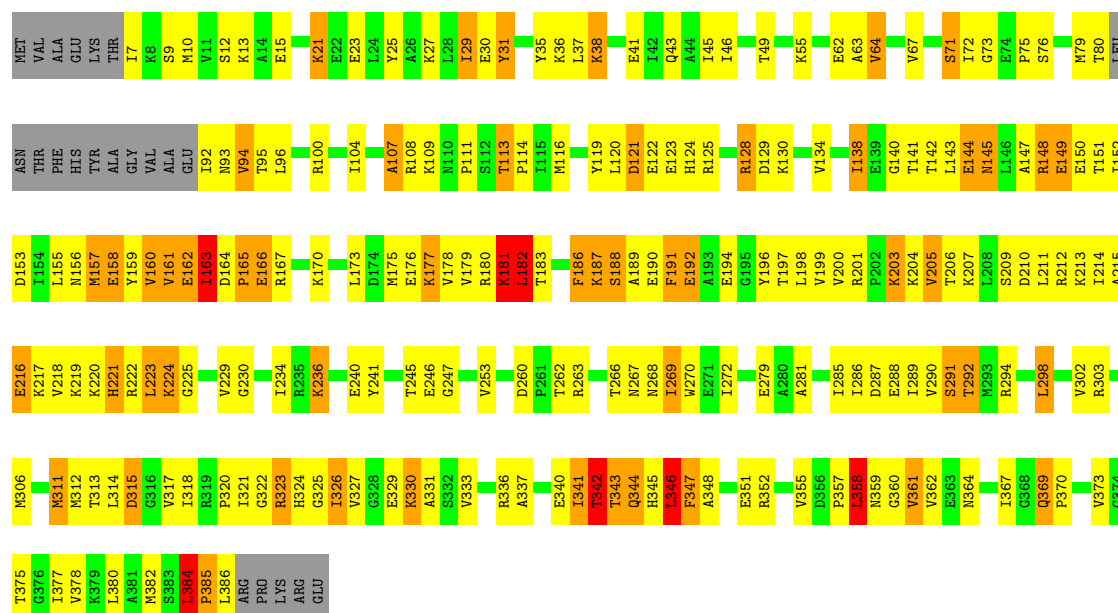
• Molecule 2: DNA-directed RNA polymerase

Chain J: 44% 40% 10% 5%



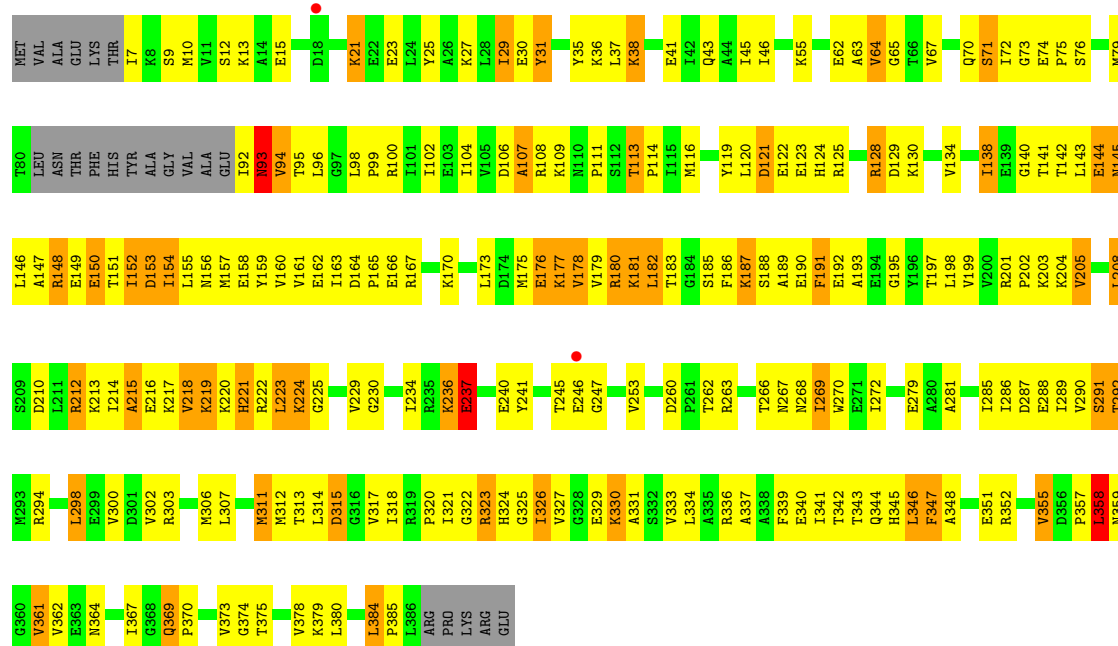
- Molecule 3: DNA-directed RNA polymerase subunit A''

Chain C:  38% 41% 13% 6%



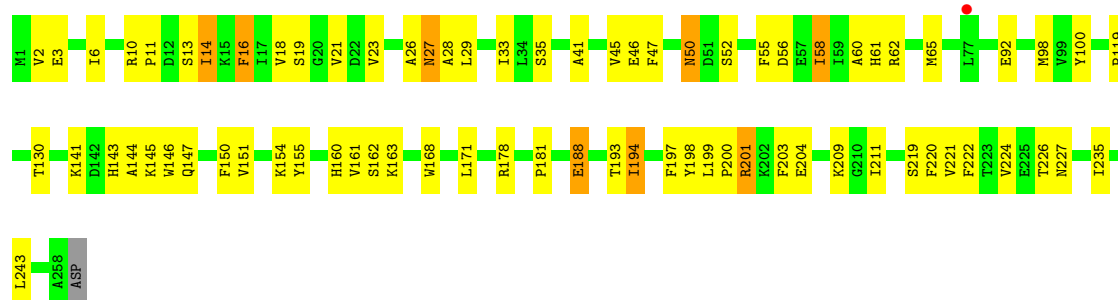
• Molecule 3: DNA-directed RNA polymerase subunit A''

Chain M:  36% 44% 13% 6%



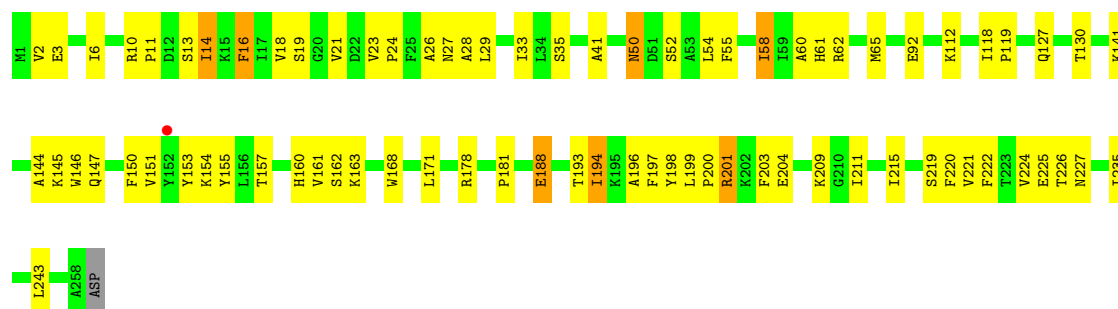
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain D:  71% 26% 3% 0%



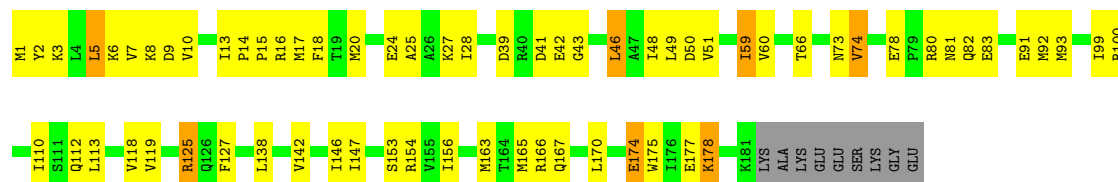
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain O: 69% 27% .



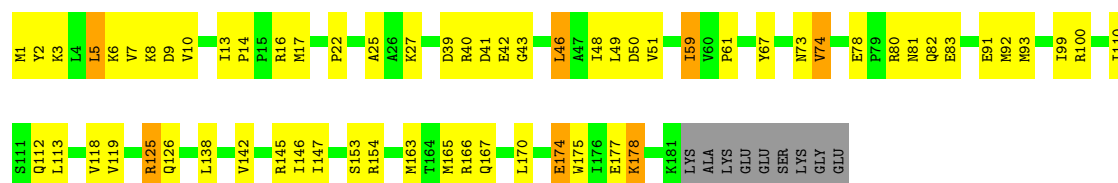
• Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain E: 60% 32% 5% .



• Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain Q: 62% 30% 5% .



• Molecule 6: DNA-directed RNA polymerase, subunit F

Chain F: 71% 25% .



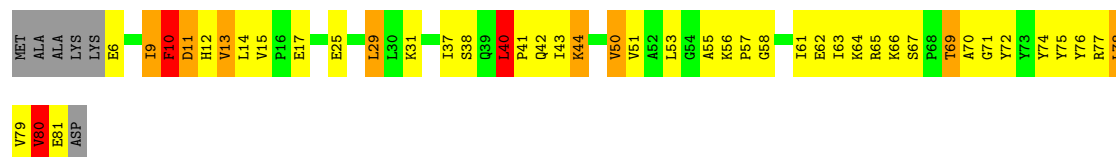
- Molecule 6: DNA-directed RNA polymerase, subunit F

Chain R:  70% 28% .

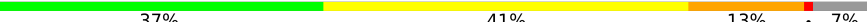


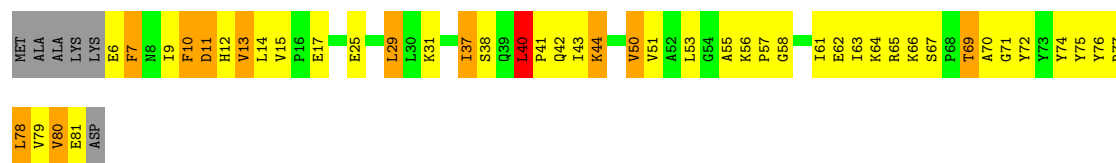
- Molecule 7: DNA-directed RNA polymerase subunit H

Chain H:  38% 41% 10% . 7%



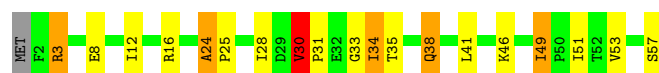
- Molecule 7: DNA-directed RNA polymerase subunit H

Chain S:  37% 41% 13% . 7%



- Molecule 8: DNA-directed RNA polymerase subunit K

Chain K:  65% 23% 9% . .



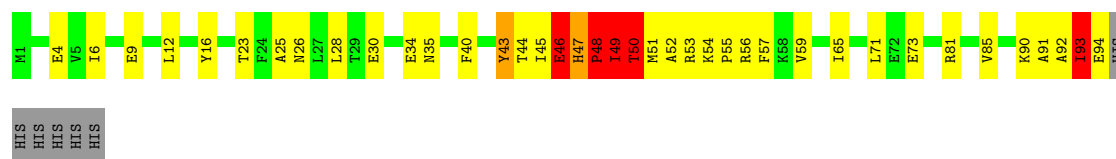
- Molecule 8: DNA-directed RNA polymerase subunit K

Chain T:  56% 33% 7% . .

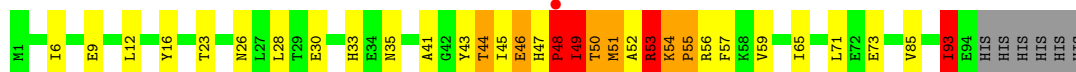


- Molecule 9: DNA-directed RNA polymerase subunit L

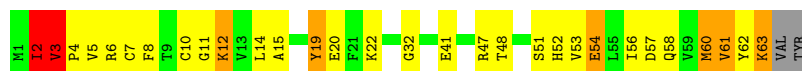
Chain L:  55% 32% . 5% 6%



- Molecule 9: DNA-directed RNA polymerase subunit L



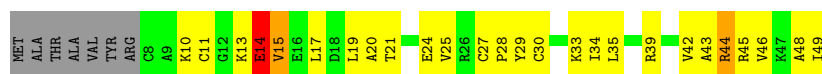
- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 11: DNA-directed RNA polymerase subunit P



- Molecule 11: DNA-directed RNA polymerase subunit P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.97Å 206.61Å 365.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.50 49.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.73-3.50) 95.1 (49.73-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.277 , 0.316 0.278 , 0.311	Depositor DCC
R_{free} test set	5658 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 178.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	51069	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.34	0/7028	0.83	7/9489 (0.1%)
1	I	0.37	0/7011	0.84	10/9465 (0.1%)
2	B	0.35	0/8706	0.85	17/11765 (0.1%)
2	J	0.35	0/8706	0.84	18/11765 (0.2%)
3	C	0.38	0/2917	0.82	2/3936 (0.1%)
3	M	0.35	0/2914	0.80	1/3932 (0.0%)
4	D	0.32	0/2111	0.76	0/2858
4	O	0.32	0/2111	0.77	0/2858
5	E	0.28	0/1491	0.78	2/2008 (0.1%)
5	Q	0.28	0/1491	0.78	2/2008 (0.1%)
6	F	0.30	0/1040	0.76	2/1399 (0.1%)
6	R	0.30	0/1040	0.76	2/1399 (0.1%)
7	H	0.48	0/641	0.90	4/866 (0.5%)
7	S	0.48	0/641	0.90	4/866 (0.5%)
8	K	0.36	0/441	0.89	3/598 (0.5%)
8	T	0.37	0/441	0.89	3/598 (0.5%)
9	L	0.42	1/790 (0.1%)	0.75	3/1066 (0.3%)
9	U	0.46	2/790 (0.3%)	0.82	5/1066 (0.5%)
10	N	0.34	0/518	0.89	0/695
10	V	0.34	0/518	0.89	0/695
11	P	0.38	0/333	0.96	1/445 (0.2%)
11	W	0.38	0/333	0.89	1/445 (0.2%)
All	All	0.35	3/52012 (0.0%)	0.83	87/70222 (0.1%)

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	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	4
2	J	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	55	PRO	N-CD	5.06	1.54	1.47
9	U	48	PRO	N-CD	5.05	1.54	1.47
9	L	48	PRO	N-CD	5.03	1.54	1.47

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	GLY	N-CA-C	11.30	127.23	112.77
2	J	901	MET	CA-C-N	8.46	128.39	119.85
2	J	901	MET	C-N-CA	8.46	128.39	119.85
1	I	548	ASN	N-CA-C	8.26	115.56	108.78
1	I	404	GLU	N-CA-C	-8.24	102.24	111.14

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	ASP	Peptide
1	I	582	CYS	Peptide
1	I	632	LYS	Peptide
1	I	641	TYR	Peptide
1	I	642	GLY	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	6891	0	6945	323	0
1	I	6875	0	6927	401	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8536	0	8585	487	10
2	J	8536	0	8583	601	0
3	C	2882	0	2982	315	0
3	M	2879	0	2973	258	0
4	D	2066	0	2080	60	0
4	O	2066	0	2080	70	0
5	E	1465	0	1503	73	2
5	Q	1465	0	1503	71	3
6	F	1020	0	1024	40	12
6	R	1020	0	1024	49	7
7	H	627	0	642	33	0
7	S	627	0	642	37	0
8	K	433	0	466	16	0
8	T	433	0	466	19	0
9	L	775	0	770	55	0
9	U	775	0	770	72	0
10	N	510	0	523	44	0
10	V	510	0	523	31	0
11	P	329	0	356	27	5
11	W	329	0	355	15	0
12	A	2	0	0	0	0
12	I	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	N	1	0	0	0	0
13	P	1	0	0	1	0
13	V	1	0	0	0	0
13	W	1	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	1	0	0	2	0
14	J	1	0	0	0	0
14	M	1	0	0	3	0
All	All	51069	0	51722	2636	20

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 26.

The worst 5 of 2636 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:378:TYR:CE1	2:B:388:GLU:CA	1.79	1.63
1:I:444:PRO:CG	9:U:50:THR:HG23	1.32	1.58
1:I:444:PRO:HG3	9:U:50:THR:CG2	1.09	1.56
2:J:378:TYR:CE1	2:J:388:GLU:HG3	1.38	1.56
3:C:194:GLU:HB2	3:C:196:TYR:CE2	1.41	1.55

The worst 5 of 20 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:98:LYS:NZ	5:Q:82:GLN:NE2[3_445]	1.00	1.20
2:B:61:PRO:C	6:F:31:GLU:OE1[1_655]	1.06	1.14
2:B:61:PRO:O	6:F:31:GLU:OE1[1_655]	1.11	1.09
2:B:61:PRO:CB	6:F:31:GLU:CD[1_655]	1.35	0.85
2:B:61:PRO:CA	6:F:31:GLU:OE1[1_655]	1.41	0.79

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	855/906 (94%)	689 (81%)	116 (14%)	50 (6%)	1	13
1	I	853/906 (94%)	692 (81%)	110 (13%)	51 (6%)	1	12
2	B	1061/1123 (94%)	872 (82%)	141 (13%)	48 (4%)	2	17
2	J	1061/1123 (94%)	864 (81%)	143 (14%)	54 (5%)	1	15
3	C	365/391 (93%)	258 (71%)	73 (20%)	34 (9%)	0	6
3	M	365/391 (93%)	266 (73%)	75 (20%)	24 (7%)	1	11
4	D	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	10	41
4	O	256/259 (99%)	242 (94%)	11 (4%)	3 (1%)	10	41
5	E	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
5	Q	179/190 (94%)	161 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	23
6	R	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	23
7	H	74/82 (90%)	59 (80%)	10 (14%)	5 (7%)	1	10
7	S	74/82 (90%)	60 (81%)	10 (14%)	4 (5%)	1	14
8	K	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
8	T	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
9	L	92/100 (92%)	74 (80%)	12 (13%)	6 (6%)	1	11
9	U	92/100 (92%)	75 (82%)	10 (11%)	7 (8%)	1	8
10	N	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
10	V	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
11	P	40/49 (82%)	24 (60%)	10 (25%)	6 (15%)	0	2
11	W	40/49 (82%)	22 (55%)	11 (28%)	7 (18%)	0	2
All	All	6312/6688 (94%)	5150 (82%)	832 (13%)	330 (5%)	1	14

5 of 330 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	151	GLY
1	A	153	PRO
1	A	154	GLN
1	A	398	ASN

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	743/779 (95%)	628 (84%)	115 (16%)	2	15
1	I	740/779 (95%)	625 (84%)	115 (16%)	2	15
2	B	923/969 (95%)	764 (83%)	159 (17%)	2	12
2	J	923/969 (95%)	761 (82%)	162 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	314/334 (94%)	250 (80%)	64 (20%)	1	7
3	M	313/334 (94%)	244 (78%)	69 (22%)	1	5
4	D	227/228 (100%)	216 (95%)	11 (5%)	23	49
4	O	227/228 (100%)	216 (95%)	11 (5%)	23	49
5	E	160/167 (96%)	144 (90%)	16 (10%)	7	28
5	Q	160/167 (96%)	144 (90%)	16 (10%)	7	28
6	F	107/107 (100%)	98 (92%)	9 (8%)	10	34
6	R	107/107 (100%)	98 (92%)	9 (8%)	10	34
7	H	68/72 (94%)	51 (75%)	17 (25%)	0	4
7	S	68/72 (94%)	50 (74%)	18 (26%)	0	3
8	K	45/46 (98%)	37 (82%)	8 (18%)	2	10
8	T	45/46 (98%)	37 (82%)	8 (18%)	2	10
9	L	81/87 (93%)	73 (90%)	8 (10%)	7	29
9	U	81/87 (93%)	74 (91%)	7 (9%)	10	33
10	N	57/59 (97%)	49 (86%)	8 (14%)	3	19
10	V	57/59 (97%)	50 (88%)	7 (12%)	4	22
11	P	35/40 (88%)	31 (89%)	4 (11%)	5	24
11	W	35/40 (88%)	31 (89%)	4 (11%)	5	24
All	All	5516/5776 (96%)	4671 (85%)	845 (15%)	3	16

5 of 845 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	393	ARG
2	J	270	GLN
6	R	100	GLU
1	I	454	VAL
1	I	388	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	162	ASN
4	O	27	ASN
1	I	265	GLN

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Mol	Chain	Res	Type
3	M	43	GLN
9	U	47	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	896:ARG	C	897:THR	N	3.01

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	863/906 (95%)	-0.44	2 (0%) 91 82	41, 157, 264, 370	0
1	I	862/906 (95%)	-0.39	3 (0%) 90 76	54, 163, 263, 381	0
2	B	1069/1123 (95%)	-0.44	1 (0%) 92 86	46, 149, 253, 402	0
2	J	1069/1123 (95%)	-0.43	3 (0%) 90 76	39, 139, 248, 360	0
3	C	369/391 (94%)	-0.41	0 100 100	68, 192, 319, 372	0
3	M	369/391 (94%)	-0.41	2 (0%) 87 68	71, 193, 327, 419	0
4	D	258/259 (99%)	-0.52	1 (0%) 88 72	71, 143, 235, 295	0
4	O	258/259 (99%)	-0.53	1 (0%) 88 72	63, 136, 226, 319	0
5	E	181/190 (95%)	-0.52	0 100 100	69, 158, 250, 398	0
5	Q	181/190 (95%)	-0.60	0 100 100	90, 163, 244, 317	0
6	F	122/122 (100%)	-0.47	0 100 100	133, 164, 244, 447	0
6	R	122/122 (100%)	-0.49	0 100 100	142, 184, 257, 324	0
7	H	76/82 (92%)	-0.52	0 100 100	105, 157, 228, 268	0
7	S	76/82 (92%)	-0.54	0 100 100	114, 166, 248, 293	0
8	K	56/57 (98%)	-0.55	0 100 100	88, 131, 196, 288	0
8	T	56/57 (98%)	-0.53	0 100 100	62, 119, 227, 330	0
9	L	94/100 (94%)	-0.44	0 100 100	78, 142, 221, 331	0
9	U	94/100 (94%)	-0.48	1 (1%) 78 54	83, 149, 223, 474	0
10	N	63/65 (96%)	-0.49	0 100 100	81, 141, 218, 281	0
10	V	63/65 (96%)	-0.41	0 100 100	69, 131, 196, 232	0
11	P	42/49 (85%)	-0.43	0 100 100	125, 173, 254, 294	0
11	W	42/49 (85%)	-0.50	0 100 100	90, 147, 201, 253	0
All	All	6385/6688 (95%)	-0.45	14 (0%) 91 82	39, 156, 270, 474	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	626	TYR	2.9
1	I	626	TYR	2.9
2	B	731	TYR	2.6
2	J	1044	GLY	2.6
1	I	541	PRO	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
13	ZN	P	1501	1/1	0.66	0.09	354,354,354,354	0
12	MG	I	1101	1/1	0.83	0.08	175,175,175,175	0
12	MG	I	1104	1/1	0.88	0.13	54,54,54,54	0
13	ZN	B	1201	1/1	0.91	0.08	364,364,364,364	0
13	ZN	A	1003	1/1	0.92	0.11	488,488,488,488	0
13	ZN	I	1103	1/1	0.93	0.10	527,527,527,527	0
13	ZN	J	1301	1/1	0.93	0.09	521,521,521,521	0
13	ZN	V	1601	1/1	0.94	0.06	210,210,210,210	0
13	ZN	N	1401	1/1	0.95	0.06	127,127,127,127	0
13	ZN	A	1002	1/1	0.95	0.05	137,137,137,137	0
13	ZN	I	1102	1/1	0.95	0.04	147,147,147,147	0
12	MG	A	1004	1/1	0.96	0.08	58,58,58,58	0
12	MG	A	1001	1/1	0.97	0.09	52,52,52,52	0
13	ZN	W	1701	1/1	0.99	0.02	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.