



## wwPDB EM Validation Summary Report ⓘ

Jun 26, 2025 – 12:40 AM JST

PDB ID : 9IM3 / pdb\_00009im3  
EMDB ID : EMD-60684  
Title : The Cryo-EM structure of MPXV E5 head-to-head double hexamer conformation  
Authors : Cheng, Y.X.; Han, P.; Wang, H.  
Deposited on : 2024-07-01  
Resolution : 3.31 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>  
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>.

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

EMDB validation analysis : **FAILED**  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

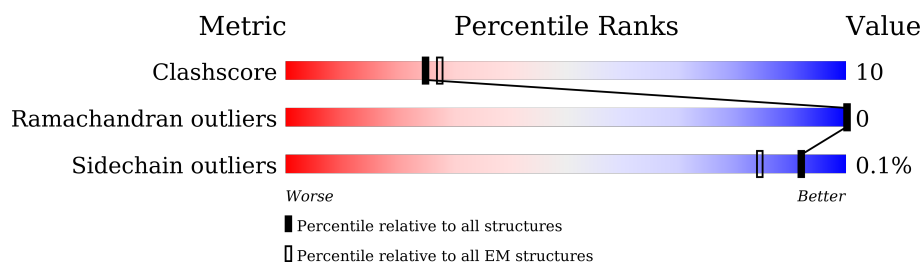
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.31 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	785	48% 17% 35%
1	B	785	49% 16% 35%
1	C	785	49% 16% 35%
1	E	785	52% 13% 35%
1	F	785	46% 18% 35%
1	J	785	45% 20% 35%
1	M	785	46% 18% 35%
1	N	785	52% 13% 35%
1	O	785	48% 17% 35%

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Mol	Chain	Length	Quality of chain
1	Q	785	 49% 16% 35%
1	R	785	 50% 15% 35%
1	S	785	 48% 17% 35%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Primase D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	B	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	C	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	E	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	F	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	J	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	M	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	N	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	O	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	Q	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	R	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	S	510	Total 4141	C 2665	N 696	O 761	S 19	0	0





Chain E:



L671	ASN	E459	T247	ARG	SER	ALA	MET
K674	ASN	E595	R248	VAL	THR	TYR	ASP
K677	HS97	M462	V250	THR	GLY	ALA	ALA
I681	I602	Q469	I263	ARG	THR	ARG	ILE
P682	K607	P470	L284	ASN	ASN	PHE	GLY
L686	K607	N475	R288	ASN	LYS	ASP	ASP
P684	R612	K476	E299	CYS	THR	VAL	ILE
V707	R613	K477	I306	ASP	THR	ASP	PHE
V711	M618	R479	I305	THR	HIS	LEU	VAL
V714	A622	T485	N310	VAL	ILE	ALA	LYS
I714	R625	L486	P311	MET	PHE	THR	ILE
M717	R626	L490	K317	GLN	LEU	ASP	GLY
T718	R627	C491	R342	GLU	GLU	VAL	VAL
D719	T828	G492	L334	PRO	THR	ILE	THR
K723	H629	G492	I334	HIS	TYR	ASP	SER
L734	PHE	K495	L340	ASN	THR	TYR	ALA
L736	SER	G496	L341	ILE	THR	LEU	CYS
E757	GLN	F500	T342	GLU	MET	THR	ARG
S758	SER	E513	E343	ASP	ASP	ALA	GLN
I760	GLY	K513	K356	TYR	LEU	GLN	GLU
E767	ARG	R514	V349	PHE	ILE	ASP	ASP
S768	GLU	L515	V350	THR	MET	PHE	PRO
I769	ALA	S518	I351	TYR	LYS	ILE	ARG
H763	ALA	A519	W355	VAL	ARG	GLU	PHE
N768	GLU	A519	K356	MET	THR	VAL	GLU
D771	ASN	L536	F357	ASN	LEU	SER	ALA
E772	ASP	D537	S358	ASN	GLU	ASN	PHE
Y773	ALA	S359	E360	ASN	LEU	VAL	CYS
I779	ALA	I544	E360	ASN	ARG	ALA	LYS
S782	TYR	L547	L363	TYR	SER	PHE	ARG
S782	ASP	H548	K377	THR	GLU	THR	GLY
S782	VAL	L549	I396	PHE	ASN	TYR	ILE
I779	LYS	K950	V401	SER	GLU	GLY	ASN
S782	LEU	R551	V404	ARG	THR	CYS	ASN
S782	ASP	K576	V404	ARG	THR	GLY	ASN
S782	GLY	L577	V404	LEU	SER	ILE	PRO
PRO	L655	T578	V404	GLU	ILE	ALA	ASN
		V582	K412	LEU	ASP	HIS	PRO
		ILE	M417	VAL	THR	GLU	CYS
		GLY	M417	PRO	ALA	VAL	LEU
		ARG	D421	ASP	ILE	VAL	PHE
		PRO	M426	LYS	THR	LYS	GLU
		CYS	M426	ARG	ARG	THR	SER
		PHE	F427	THR	ARG	LEU	GLY
		SER	F428	LYS	THR	ARG	ASP
		ASN	Y428	THR	THR	SER	ARG
		LYS	E244	THR	THR	ASN	GLU

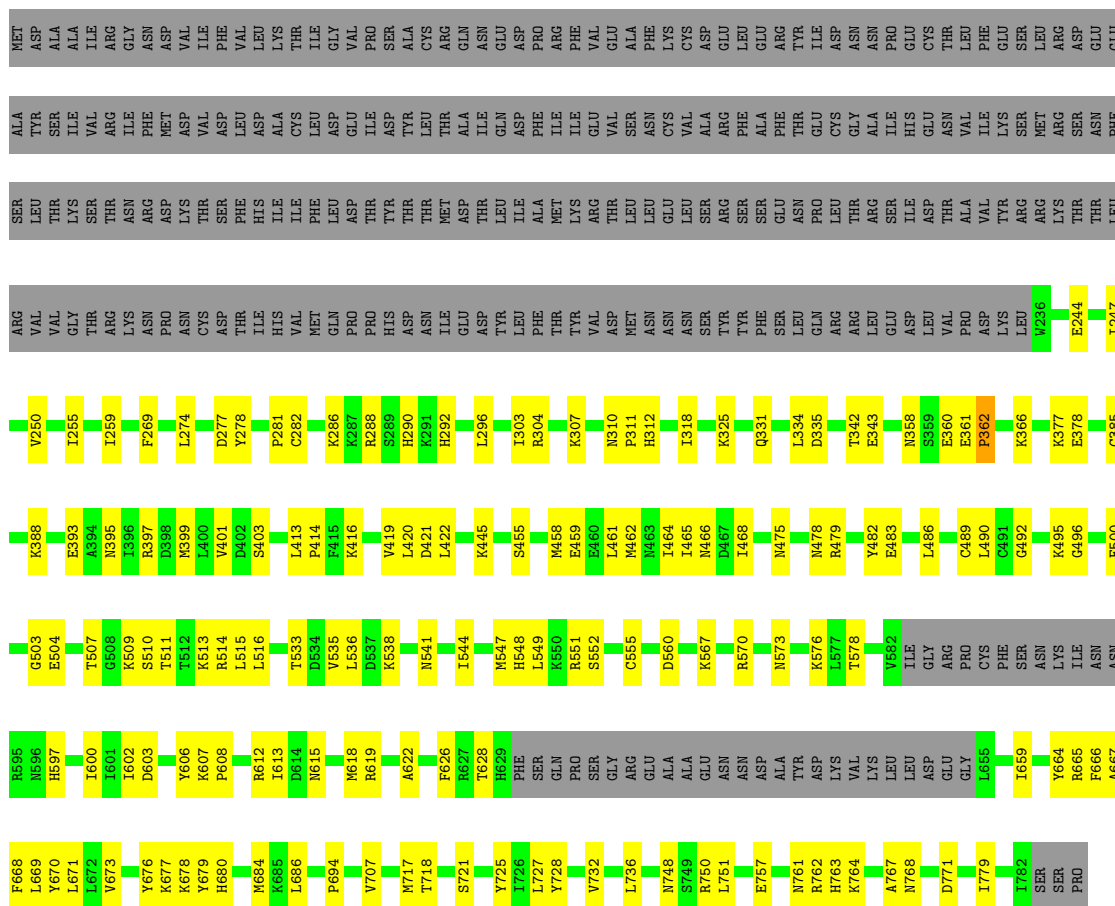
Chain F:



N478	N479	N355	I247	ARG	SER	ALA	MET
E480	E480	K356	K248	VAL	LEU	TYR	ASP
N481	N481	K357	R249	VAL	THR	THR	ALA
N482	N482	K358	Y250	GLY	LYS	ILE	ALA
E483	E483	K359	S251	THR	SER	VAL	ILE
K484	K484	E360	K252	ARG	THR	ARG	ARG
N485	N485	E361	I253	LYS	ASN	ILE	GLY
L486	L486	K362	F254	ASN	ASP	PHE	ASN
		K363	N255	PRO	ASP	MET	ASN
C491	C491	I364	N256	ASN	LYS	VAL	VAL
C492	C492	K365	S257	CYS	THR	ASP	PHE
A493	A493	K366	I258	ASP	SER	ASP	THR
T494	T494	K367	I259	THR	PHE	LEU	VAL
			F260	ILE	ILE	ASP	LEU
L498	L498	K377	F261	HIS	ILE	ALA	LYS
T499	T499			VAL	ILE	CYS	THR
F500	F500	C385	F269	MET	PHE	LEU	ILE
F501	F501	P386	T270	GLN	LEU	ASP	GLY
F502	F502	K387		PRO	ASP	GLU	VAL
G503	G503		P273	THR	THR	ILE	PRO
		E393		HIS	TYR	ASP	SER
L536	L536		D277	ASP	THR	TYR	ALA
		R397	Y278	ASN	THR	LEU	CYS
N541	N541			ILE	MET	THR	ARG
I544	I544	V401	T280	GLU	ASP	ALA	GLN
		L413	P281	ASP	THR	ILE	ASN
C555	C555		C282	TYR	LEU	GLN	GLU
		K416	A283	LEU	ILE	ASP	ASP
				PHE	ALA	PHE	PRO
K568	K568	L420	R288	THR	MET	ILE	ARG
D572	D572	L421		TYR	LYS	ILE	PHE
		L422	H292	VAL	ARG	VAL	GLU
K576	K576	T439	P293	ASP	LYS	VAL	GLU
L577	L577		H294	MET	LEU	SER	ALA
P580	P580	K445	Q295	ASN	LEU	ASN	PHE
C581	C581	F446	L296	ASN	GLU	CYS	LYS
V682	V682	D447	S297	ASN	LEU	VAL	CYS
			E299	THR	SER	ASP	ASP
ILE	ILE	K450	I303	THR	SER	PHE	LEU
GLY	GLY		R304	PHE	SER	ALA	GLU
ARG	ARG	S455	I305	SER	GLU	PHE	ARG
CYS	CYS	P456	Y306	LEU	ASN	THR	TYR
PHE	PHE	E457		GLN	PRO	GLU	ILE
SER	SER	M458	G309	ARG	THR	CYS	ASP
ASN	ASN	E459		ARG	LEU	GLY	ASN
ILE	ILE	E460	H312	GLU	SER	ILE	ASN
ASN	ASN	L461	K317	ASP	THR	ALA	PRO
ASN	ASN	M462	I318	VAL	THR	VAL	CYS
R595	R595	I464	A319	PRO	ALA	VAL	THR
N596	N596		L340	ASP	VAL	ILE	PHE
H597	H597	P470	L341	LYS	TYR	LYS	GLU
		L471	T342	LEU	ARG	SER	SER
				W236	ARG	MET	LEU
I600	I600		I348	LYS	LYS	ARG	ASP
		M475	V349		THR	SER	GLU
Y606	Y606	K476	H350	D245	THR	ASN	

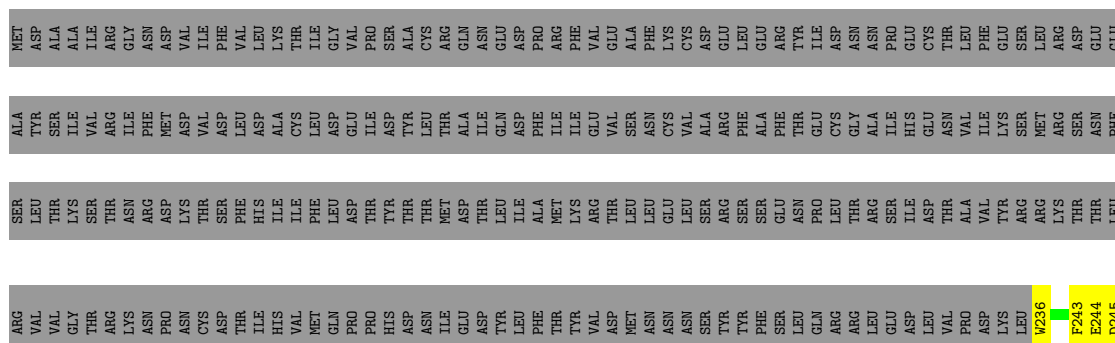
- Molecule 1: Primase D5

Chain J:  45% 20% 35%

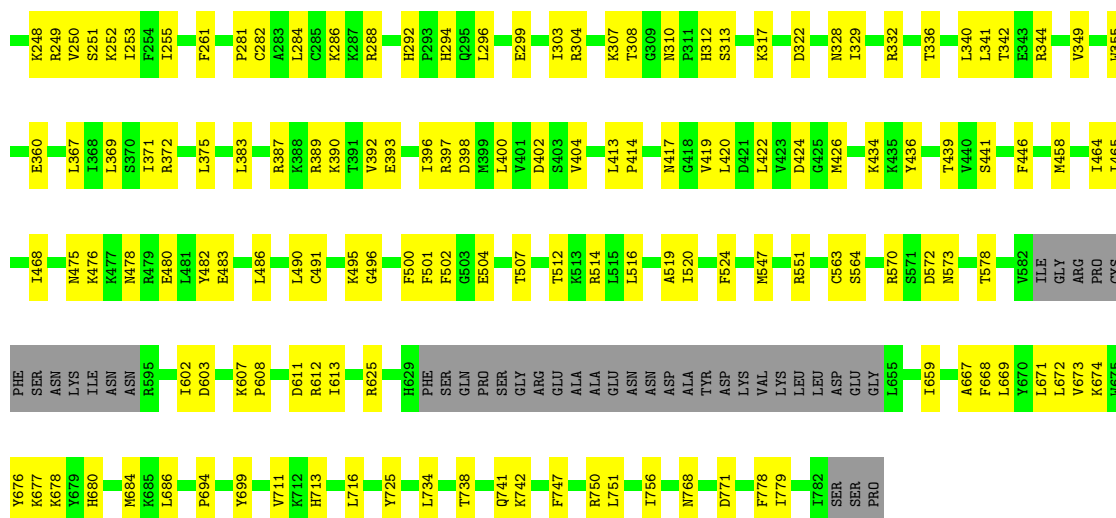


- Molecule 1: Primase D5

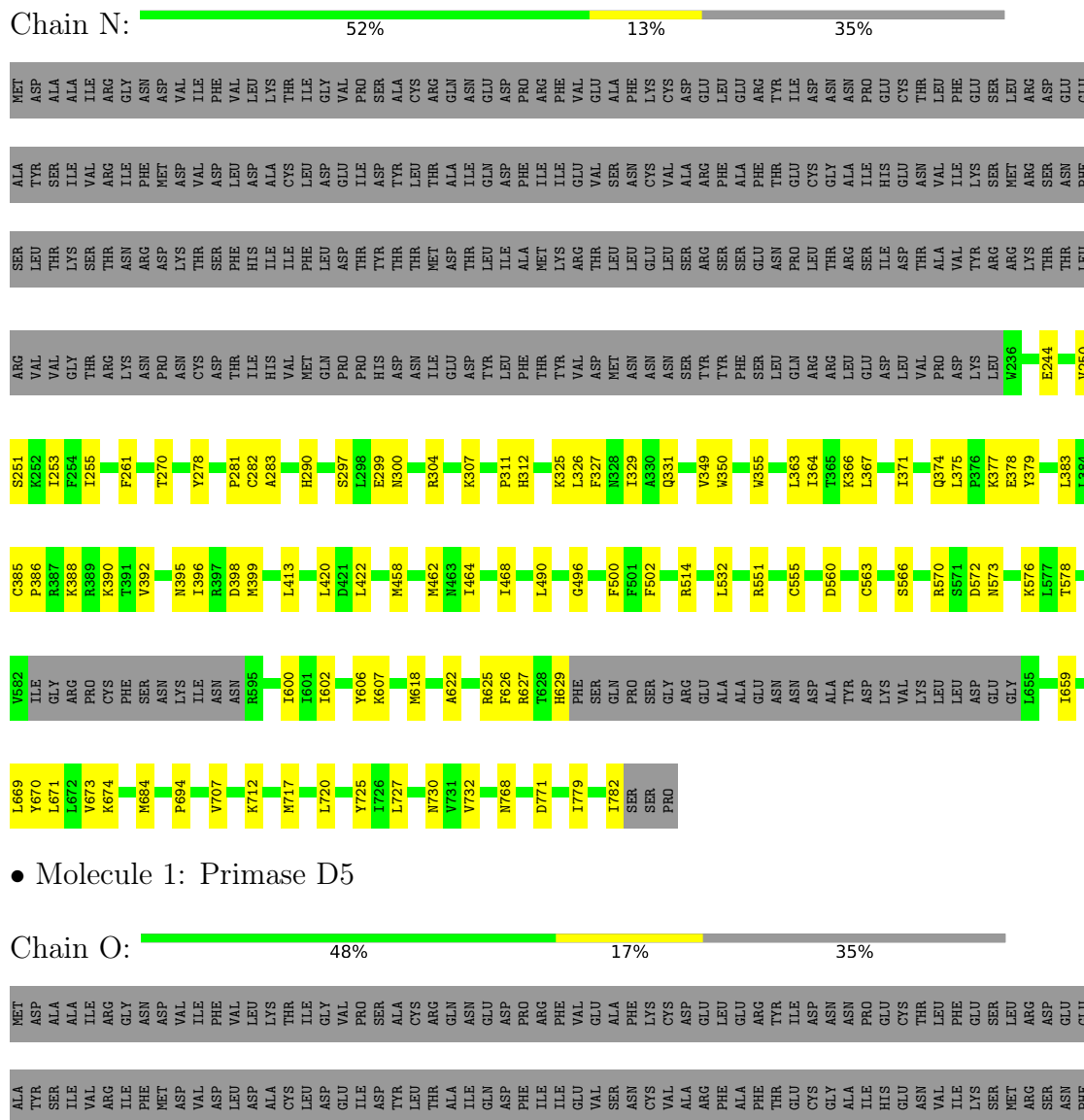
Chain M:  46% 18% 35%



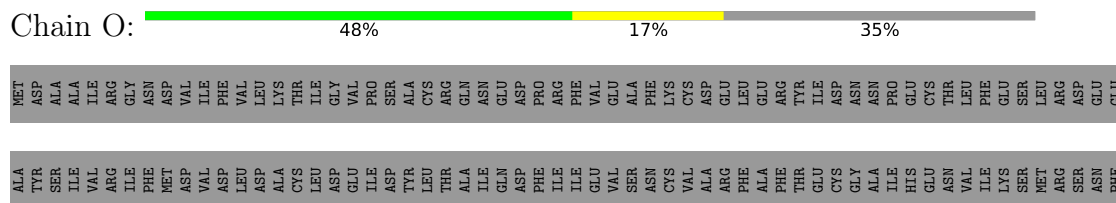




### • Molecule 1: Primase D5



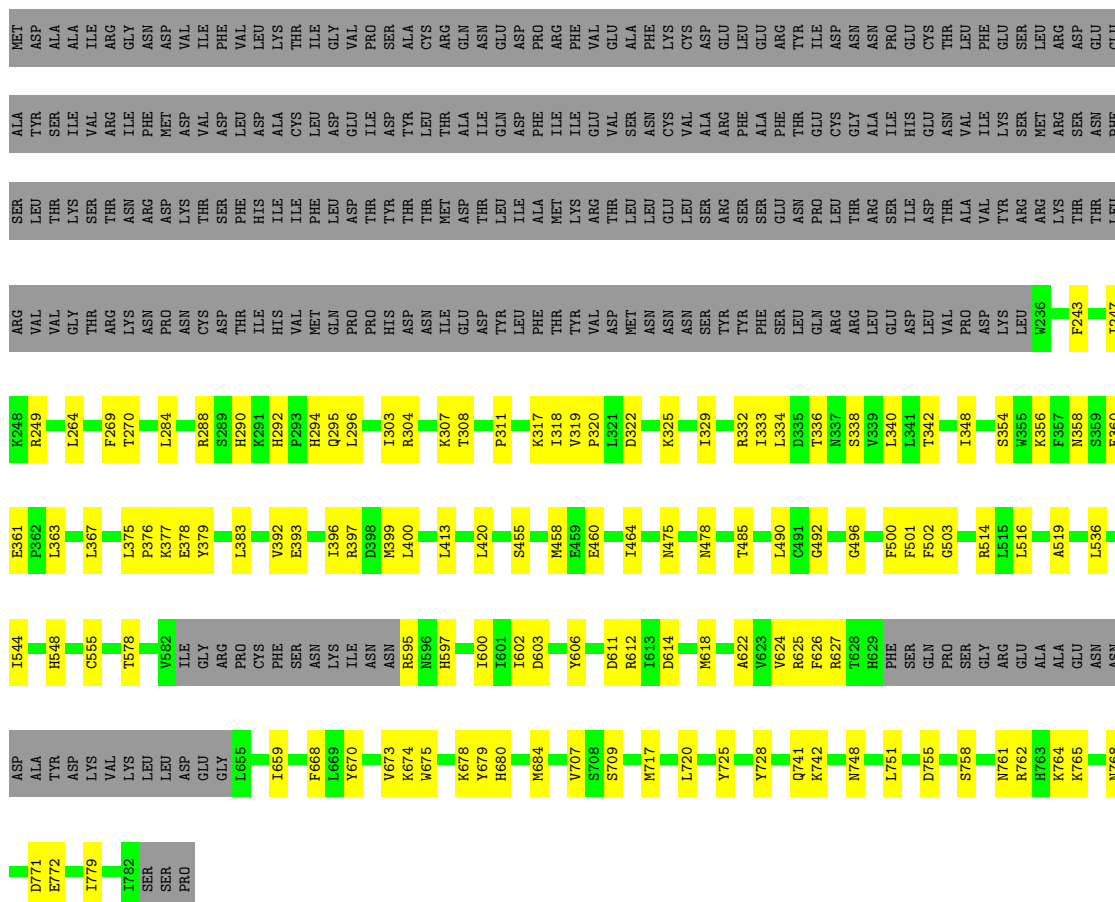
### • Molecule 1: Primase D5





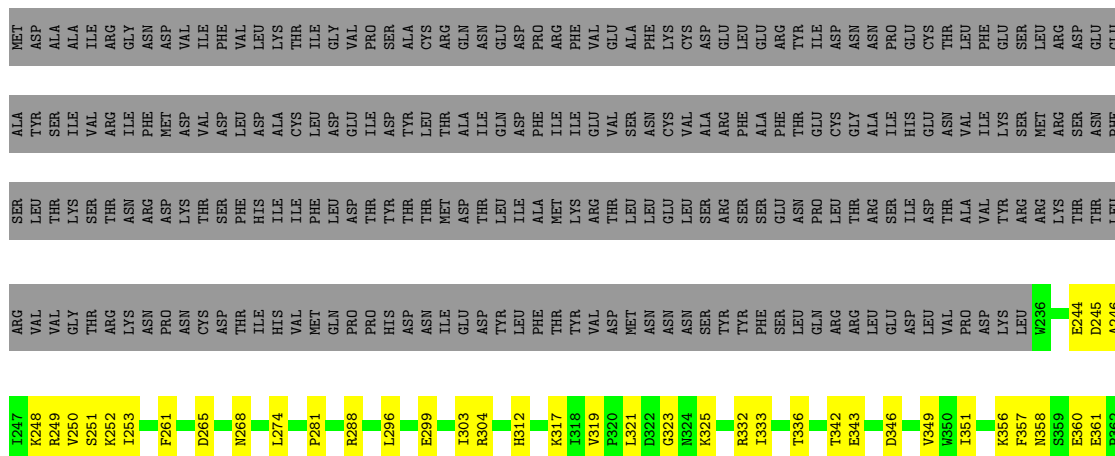
- Molecule 1: Primase D5

Chain R: 



- Molecule 1: Primase D5

Chain S:  48% 17% 35%



L669	ASN	L486	L363
L672	LYS	L486	K366
Y676	ILE	L490	L369
P690	ASN	C491	L369
P694	P695	C492	P376
	Y596	C496	K377
	H597	F500	E378
	L600	F500	E382
I702	L603	G503	C385
L705	D603	E504	P386
D729	Y606	T507	R387
N730	K607	G508	K388
		K509	R389
F747	F610	S510	V392
N748	D611	T511	E393
L751	G612	T512	
F752	L613	L515	L396
	K618	A519	R397
Q775	F626	T533	D398
I782	R627	D534	S403
SER	T628	V535	L413
SER	H629	L536	
PRO	PHE	D537	L420
	SER	K538	D421
	GLN		L422
	PRO		V423
	SER	T544	D424
	GLY	M547	C426
	ARG		M426
	GLU	R551	D431
	ALA	C555	
	ALA		S455
	ASN	C563	M458
	ASN		E459
	ASP	K567	E460
	ALA		L461
	TYR	R570	M462
	ASP		M463
	LYS	N573	I464
	VAL		I465
	LYS	K576	I468
	LEU	L577	
	LEU	T578	T472
	ASP		D473
	ASP		M475
	GLY		M478
	GLU	Y582	F478
	L655	I1E	
		GLY	E474
		ARG	M475
	Y664	PRO	
	R665	CYS	M478
	F666	PHE	
	F667	PRO	F478

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	311720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.11	0/4233	0.32	0/5721
1	B	0.11	0/4233	0.32	0/5721
1	C	0.11	0/4233	0.32	0/5721
1	E	0.10	0/4233	0.30	0/5721
1	F	0.11	0/4233	0.32	0/5721
1	J	0.14	0/4233	0.38	2/5721 (0.0%)
1	M	0.11	0/4233	0.30	0/5721
1	N	0.09	0/4233	0.27	0/5721
1	O	0.12	0/4233	0.33	1/5721 (0.0%)
1	Q	0.10	0/4233	0.28	0/5721
1	R	0.10	0/4233	0.30	0/5721
1	S	0.10	0/4233	0.30	0/5721
All	All	0.11	0/50796	0.31	3/68652 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	362	PRO	CA-N-CD	-11.03	96.55	112.00
1	O	320	PRO	CA-N-CD	-8.11	100.64	112.00
1	J	362	PRO	N-CD-CG	-5.74	94.59	103.20

There are no chirality outliers.

There are no planarity outliers.

### 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	4141	0	4187	101	0
1	B	4141	0	4187	92	0
1	C	4141	0	4187	89	0
1	E	4141	0	4187	74	0
1	F	4141	0	4187	109	0
1	J	4141	0	4187	116	0
1	M	4141	0	4187	95	0
1	N	4141	0	4187	70	0
1	O	4141	0	4187	98	0
1	Q	4141	0	4187	83	0
1	R	4141	0	4187	85	0
1	S	4141	0	4187	95	0
All	All	49692	0	50244	1031	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 10.

The worst 5 of 1031 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:M:341:LEU:HD11	1:M:400:LEU:HB3	1.65	0.79
1:F:471:LEU:HD23	1:F:479:ARG:HH12	1.47	0.78
1:F:358:ASN:ND2	1:F:361:GLU:O	2.17	0.77
1:J:483:GLU:HA	1:J:486:LEU:HD12	1.65	0.77
1:C:255:ILE:HG12	1:C:283:ALA:HB2	1.65	0.76

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	504/785 (64%)	481 (95%)	23 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	504/785 (64%)	491 (97%)	13 (3%)	0	100	100
1	C	504/785 (64%)	485 (96%)	19 (4%)	0	100	100
1	E	504/785 (64%)	492 (98%)	12 (2%)	0	100	100
1	F	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	J	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	M	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	N	504/785 (64%)	489 (97%)	15 (3%)	0	100	100
1	O	504/785 (64%)	490 (97%)	14 (3%)	0	100	100
1	Q	504/785 (64%)	485 (96%)	19 (4%)	0	100	100
1	R	504/785 (64%)	491 (97%)	13 (3%)	0	100	100
1	S	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
All	All	6048/9420 (64%)	5848 (97%)	200 (3%)	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 PDB entries followed by that with respect to all EM entries.

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	472/725 (65%)	472 (100%)	0	100	100
1	B	472/725 (65%)	472 (100%)	0	100	100
1	C	472/725 (65%)	471 (100%)	1 (0%)	92	95
1	E	472/725 (65%)	470 (100%)	2 (0%)	89	93
1	F	472/725 (65%)	472 (100%)	0	100	100
1	J	472/725 (65%)	472 (100%)	0	100	100
1	M	472/725 (65%)	471 (100%)	1 (0%)	92	95
1	N	472/725 (65%)	472 (100%)	0	100	100
1	O	472/725 (65%)	472 (100%)	0	100	100
1	Q	472/725 (65%)	472 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	472/725 (65%)	472 (100%)	0	100	100
1	S	472/725 (65%)	472 (100%)	0	100	100
All	All	5664/8700 (65%)	5660 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	426	MET
1	E	349	VAL
1	E	426	MET
1	M	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	748	ASN
1	O	292	HIS
1	S	748	ASN
1	S	312	HIS
1	M	331	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.