



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:32 am GMT

PDB ID : 5FMZ
Title : Crystal structure of Influenza B polymerase with bound 5' vRNA
Authors : Guilligay, D.; Cusack, S.
Deposited on : 2015-11-10
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

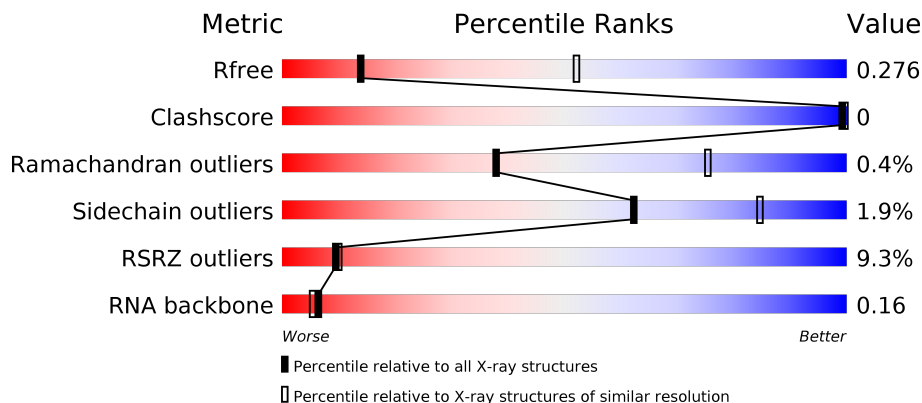
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)
RNA backbone	2435	1009 (3.96-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	751	
1	D	751	
2	B	772	
2	E	772	

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Mol	Chain	Length	Quality of chain
3	C	798	<div><div></div><div>11%</div><div>87%</div><div></div><div>11%</div></div>
3	F	798	<div><div></div><div>14%</div><div>85%</div><div></div><div>12%</div></div>
4	H	12	<div><div></div><div>58%</div><div>42%</div></div>
4	V	12	<div><div></div><div>58%</div><div>42%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34636 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 POLYMERASE ACIDIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5717	3634	957	1086	40			
1	D	715	Total	C	N	O	S	0	0	0
			5737	3646	959	1092	40			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	-12	SER	-	EXPRESSION TAG	UNP Q5V8Z9
A	-11	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-10	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-9	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-8	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-7	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-6	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-5	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
A	-3	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	-2	SER	-	EXPRESSION TAG	UNP Q5V8Z9
A	-1	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	0	SER	-	EXPRESSION TAG	UNP Q5V8Z9
A	727	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	728	SER	-	EXPRESSION TAG	UNP Q5V8Z9
A	729	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	730	SER	-	EXPRESSION TAG	UNP Q5V8Z9
A	731	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
A	732	GLU	-	EXPRESSION TAG	UNP Q5V8Z9
A	733	ASN	-	EXPRESSION TAG	UNP Q5V8Z9
A	734	LEU	-	EXPRESSION TAG	UNP Q5V8Z9
A	735	TYR	-	EXPRESSION TAG	UNP Q5V8Z9
A	736	PHE	-	EXPRESSION TAG	UNP Q5V8Z9
A	737	GLN	-	EXPRESSION TAG	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	-12	SER	-	EXPRESSION TAG	UNP Q5V8Z9
D	-11	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-10	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-9	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-8	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-7	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-6	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q5V8Z9
D	-3	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	-2	SER	-	EXPRESSION TAG	UNP Q5V8Z9
D	-1	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	0	SER	-	EXPRESSION TAG	UNP Q5V8Z9
D	727	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	728	SER	-	EXPRESSION TAG	UNP Q5V8Z9
D	729	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	730	SER	-	EXPRESSION TAG	UNP Q5V8Z9
D	731	GLY	-	EXPRESSION TAG	UNP Q5V8Z9
D	732	GLU	-	EXPRESSION TAG	UNP Q5V8Z9
D	733	ASN	-	EXPRESSION TAG	UNP Q5V8Z9
D	734	LEU	-	EXPRESSION TAG	UNP Q5V8Z9
D	735	TYR	-	EXPRESSION TAG	UNP Q5V8Z9
D	736	PHE	-	EXPRESSION TAG	UNP Q5V8Z9
D	737	GLN	-	EXPRESSION TAG	UNP Q5V8Z9

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	708	Total	C	N	O	S	0	0	0
			5547	3500	953	1042	52			
2	E	733	Total	C	N	O	S	0	0	0
			5755	3633	996	1074	52			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	-7	SER	-	EXPRESSION TAG	UNP Q5V8Y6
B	-6	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	-5	SER	-	EXPRESSION TAG	UNP Q5V8Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	-3	SER	-	EXPRESSION TAG	UNP Q5V8Y6
B	-2	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	-1	SER	-	EXPRESSION TAG	UNP Q5V8Y6
B	0	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	753	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	754	SER	-	EXPRESSION TAG	UNP Q5V8Y6
B	755	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	756	SER	-	EXPRESSION TAG	UNP Q5V8Y6
B	757	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
B	758	GLU	-	EXPRESSION TAG	UNP Q5V8Y6
B	759	ASN	-	EXPRESSION TAG	UNP Q5V8Y6
B	760	LEU	-	EXPRESSION TAG	UNP Q5V8Y6
B	761	TYR	-	EXPRESSION TAG	UNP Q5V8Y6
B	762	PHE	-	EXPRESSION TAG	UNP Q5V8Y6
B	763	GLN	-	EXPRESSION TAG	UNP Q5V8Y6
E	-8	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	-7	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	-6	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	-5	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	-4	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	-3	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	-2	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	-1	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	0	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	753	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	754	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	755	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	756	SER	-	EXPRESSION TAG	UNP Q5V8Y6
E	757	GLY	-	EXPRESSION TAG	UNP Q5V8Y6
E	758	GLU	-	EXPRESSION TAG	UNP Q5V8Y6
E	759	ASN	-	EXPRESSION TAG	UNP Q5V8Y6
E	760	LEU	-	EXPRESSION TAG	UNP Q5V8Y6
E	761	TYR	-	EXPRESSION TAG	UNP Q5V8Y6
E	762	PHE	-	EXPRESSION TAG	UNP Q5V8Y6
E	763	GLN	-	EXPRESSION TAG	UNP Q5V8Y6

- Molecule 3 is a protein called POLYMERASE BASIC PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	714	Total	C	N	O	S	0	0	0
			5719	3640	999	1040	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	703	Total	C	N	O	S	0	0	0
			5637	3591	982	1024	40			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	-7	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	-6	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	-5	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	-4	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	-3	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	-2	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	-1	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	0	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	771	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	772	TRP	-	EXPRESSION TAG	UNP Q5V8X3
C	773	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	774	HIS	-	EXPRESSION TAG	UNP Q5V8X3
C	775	PRO	-	EXPRESSION TAG	UNP Q5V8X3
C	776	GLN	-	EXPRESSION TAG	UNP Q5V8X3
C	777	PHE	-	EXPRESSION TAG	UNP Q5V8X3
C	778	GLU	-	EXPRESSION TAG	UNP Q5V8X3
C	779	LYS	-	EXPRESSION TAG	UNP Q5V8X3
C	780	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	781	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	782	GLY	-	EXPRESSION TAG	UNP Q5V8X3
C	783	SER	-	EXPRESSION TAG	UNP Q5V8X3
C	784	GLU	-	EXPRESSION TAG	UNP Q5V8X3
C	785	ASN	-	EXPRESSION TAG	UNP Q5V8X3
C	786	LEU	-	EXPRESSION TAG	UNP Q5V8X3
C	787	TYR	-	EXPRESSION TAG	UNP Q5V8X3
C	788	PHE	-	EXPRESSION TAG	UNP Q5V8X3
C	789	GLN	-	EXPRESSION TAG	UNP Q5V8X3
F	-8	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	-7	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	-6	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	-5	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	-4	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	-3	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	-2	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	-1	SER	-	EXPRESSION TAG	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	771	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	772	TRP	-	EXPRESSION TAG	UNP Q5V8X3
F	773	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	774	HIS	-	EXPRESSION TAG	UNP Q5V8X3
F	775	PRO	-	EXPRESSION TAG	UNP Q5V8X3
F	776	GLN	-	EXPRESSION TAG	UNP Q5V8X3
F	777	PHE	-	EXPRESSION TAG	UNP Q5V8X3
F	778	GLU	-	EXPRESSION TAG	UNP Q5V8X3
F	779	LYS	-	EXPRESSION TAG	UNP Q5V8X3
F	780	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	781	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	782	GLY	-	EXPRESSION TAG	UNP Q5V8X3
F	783	SER	-	EXPRESSION TAG	UNP Q5V8X3
F	784	GLU	-	EXPRESSION TAG	UNP Q5V8X3
F	785	ASN	-	EXPRESSION TAG	UNP Q5V8X3
F	786	LEU	-	EXPRESSION TAG	UNP Q5V8X3
F	787	TYR	-	EXPRESSION TAG	UNP Q5V8X3
F	788	PHE	-	EXPRESSION TAG	UNP Q5V8X3
F	789	GLN	-	EXPRESSION TAG	UNP Q5V8X3

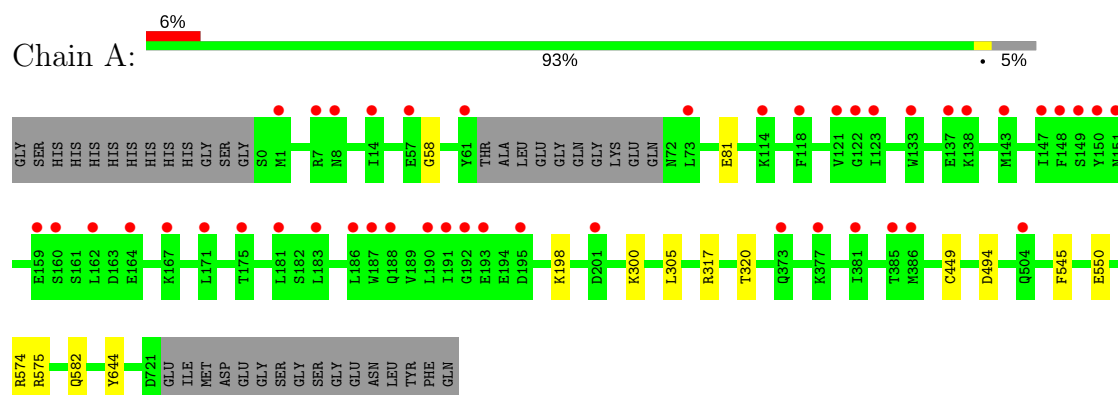
- Molecule 4 is a RNA chain called 5'-R(*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			
4	V	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			

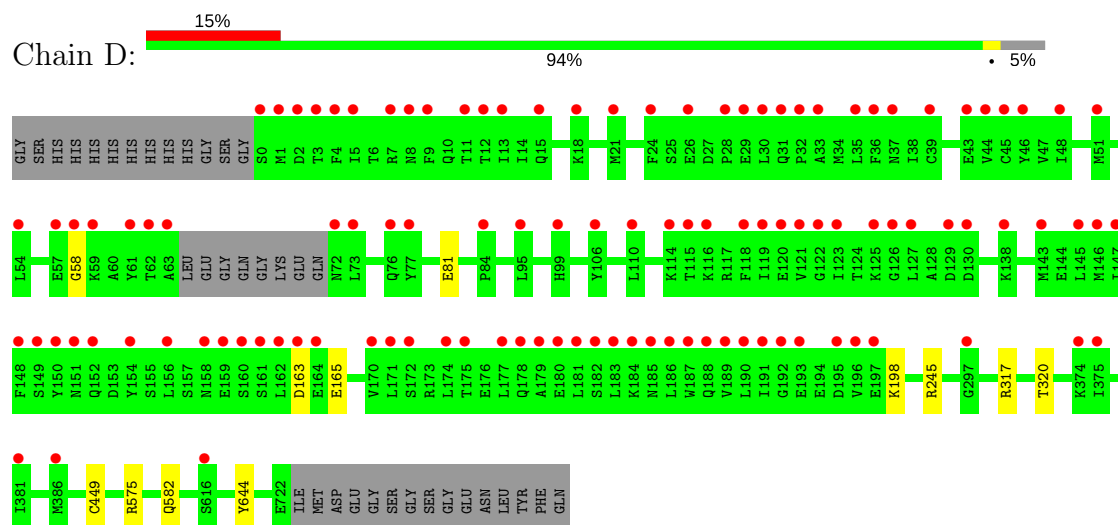
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

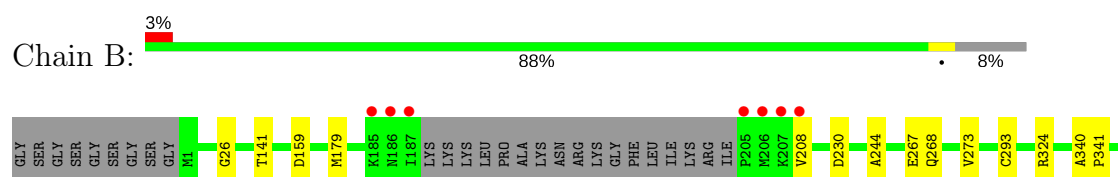
• Molecule 1: POLYMERASE ACIDIC PROTEIN

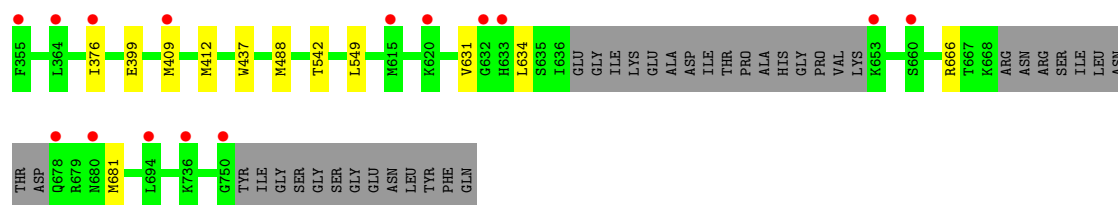


• Molecule 1: POLYMERASE ACIDIC PROTEIN

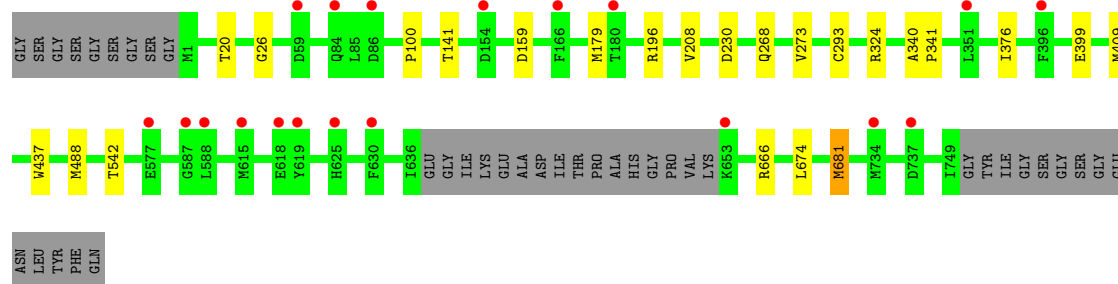


• Molecule 2: RNA-DIRECTED RNA POLYMERASE CATALYTIC SUBUNIT

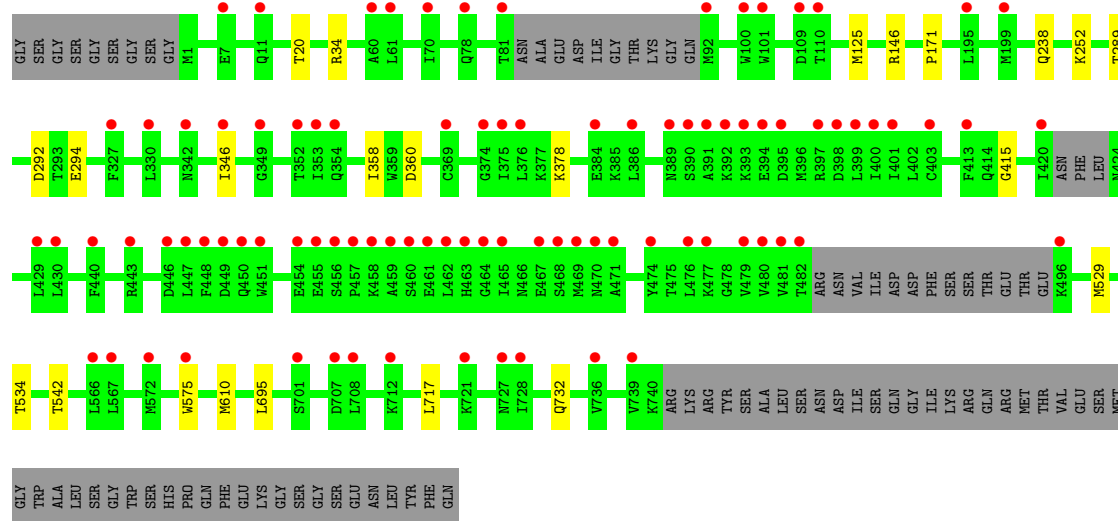
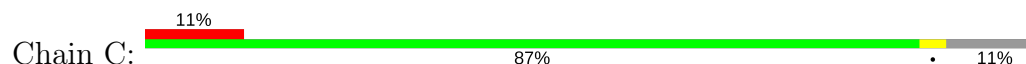




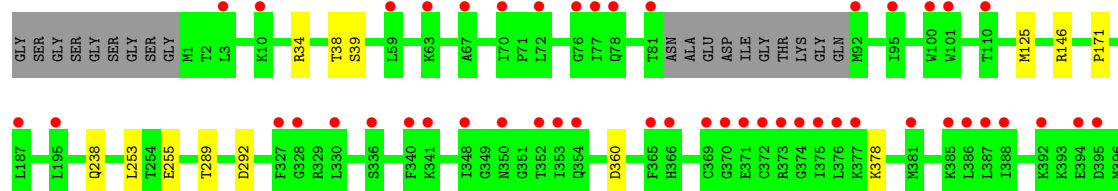
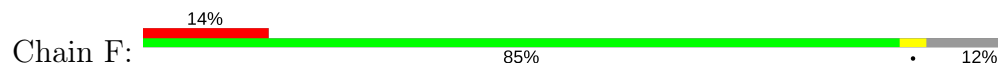
• Molecule 2: RNA-DIRECTED RNA POLYMERASE CATALYTIC SUBUNIT

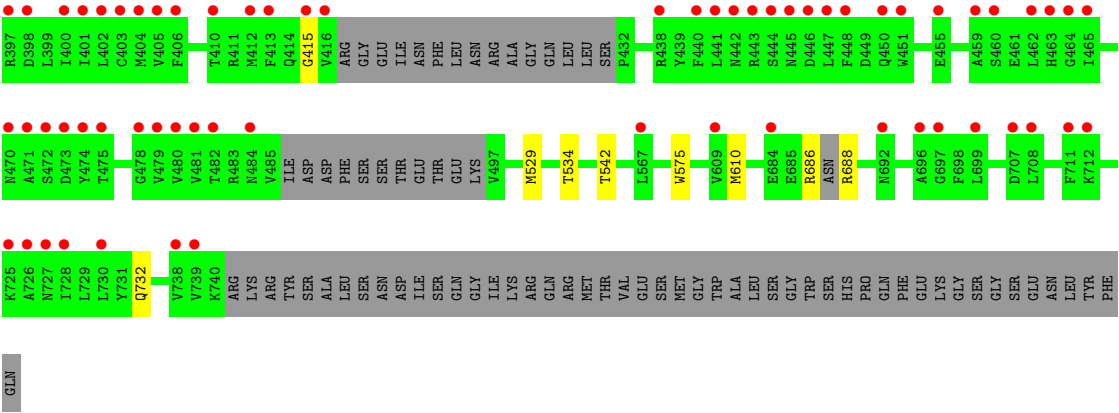


• Molecule 3: POLYMERASE BASIC PROTEIN 2



• Molecule 3: POLYMERASE BASIC PROTEIN 2

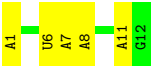




● Molecule 4: 5'-R(*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP)-3'



● Molecule 4: 5'-R(*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.57Å 200.54Å 133.13Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	126.83 – 3.40 48.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (126.83-3.40) 99.8 (48.98-3.40)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.255 , 0.277 0.254 , 0.276	Depositor DCC
R_{free} test set	2595 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34636	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/5833	0.50	0/7866
1	D	0.35	0/5853	0.51	0/7893
2	B	0.36	0/5655	0.53	0/7623
2	E	0.36	0/5867	0.53	0/7908
3	C	0.36	0/5816	0.54	0/7813
3	F	0.36	0/5733	0.54	0/7701
4	H	0.62	1/294 (0.3%)	0.65	0/455
4	V	0.62	1/294 (0.3%)	0.66	0/455
All	All	0.36	2/35345 (0.0%)	0.53	0/47714

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	A	OP3-P	-10.15	1.49	1.61
4	V	1	A	OP3-P	-10.12	1.49	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5717	0	5693	6	0
1	D	5737	0	5707	4	0
2	B	5547	0	5531	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5755	0	5772	4	0
3	C	5719	0	5893	2	0
3	F	5637	0	5807	3	0
4	H	262	0	131	0	0
4	V	262	0	131	0	0
All	All	34636	0	34665	18	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 0.

All (18) 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:631:VAL:HG12	2:B:634:LEU:HD11	1.82	0.60
1:A:644:TYR:HA	2:B:26:GLY:HA2	1.94	0.50
2:E:681:MET:HG3	3:F:38:THR:HG21	1.96	0.47
1:A:545:PHE:CD1	1:D:245:ARG:HB2	2.49	0.47
3:F:253:LEU:HD23	3:F:255:GLU:HB3	1.97	0.47
1:A:545:PHE:CE1	1:A:550:GLU:HG2	2.51	0.45
2:E:340:ALA:HB3	2:E:341:PRO:HD3	1.99	0.44
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.99	0.43
1:D:644:TYR:HA	2:E:26:GLY:HA2	2.01	0.42
1:D:582:GLN:HB2	2:E:542:THR:HG21	2.00	0.42
1:A:574:ARG:HB3	2:B:549:LEU:HD22	2.02	0.41
3:C:346:ILE:HD11	3:C:358:ILE:HD11	2.03	0.41
1:A:305:LEU:HD11	1:A:494:ASP:HB3	2.03	0.41
1:A:582:GLN:HB2	2:B:542:THR:HG21	2.02	0.41
3:C:695:LEU:HD11	3:C:717:LEU:HD13	2.03	0.40
3:F:686:ARG:O	3:F:688:ARG:N	2.53	0.40
2:B:244:ALA:HB3	2:B:412:MET:CE	2.52	0.40
1:D:163:ASP:OD2	1:D:165:GLU:HG2	2.21	0.40

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 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	708/751 (94%)	677 (96%)	30 (4%)	1 (0%)	55	87
1	D	711/751 (95%)	679 (96%)	31 (4%)	1 (0%)	55	87
2	B	700/772 (91%)	667 (95%)	30 (4%)	3 (0%)	38	75
2	E	729/772 (94%)	686 (94%)	37 (5%)	6 (1%)	22	62
3	C	706/798 (88%)	666 (94%)	37 (5%)	3 (0%)	38	75
3	F	693/798 (87%)	656 (95%)	33 (5%)	4 (1%)	28	68
All	All	4247/4642 (92%)	4031 (95%)	198 (5%)	18 (0%)	38	75

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	674	LEU
2	B	409	MET
3	C	732	GLN
2	E	409	MET
3	F	39	SER
3	F	732	GLN
3	C	292	ASP
2	E	100	PRO
3	F	292	ASP
1	A	58	GLY
1	D	58	GLY
2	E	196	ARG
3	C	415	GLY
3	F	415	GLY
2	B	208	VAL
2	E	208	VAL
2	B	376	ILE
2	E	376	ILE

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	634/664 (96%)	627 (99%)	7 (1%)	78	90
1	D	635/664 (96%)	629 (99%)	6 (1%)	82	92
2	B	607/657 (92%)	593 (98%)	14 (2%)	56	82
2	E	630/657 (96%)	616 (98%)	14 (2%)	57	83
3	C	625/694 (90%)	609 (97%)	16 (3%)	51	80
3	F	617/694 (89%)	604 (98%)	13 (2%)	59	83
All	All	3748/4030 (93%)	3678 (98%)	70 (2%)	62	84

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	198	LYS
1	A	300	LYS
1	A	317	ARG
1	A	320	THR
1	A	449	CYS
1	A	575	ARG
2	B	141	THR
2	B	159	ASP
2	B	179	MET
2	B	230	ASP
2	B	267	GLU
2	B	268	GLN
2	B	273	VAL
2	B	293	CYS
2	B	324	ARG
2	B	399	GLU
2	B	437	TRP
2	B	488	MET
2	B	666	ARG
2	B	681	MET
3	C	20	THR
3	C	34	ARG
3	C	125	MET
3	C	146	ARG
3	C	171	PRO
3	C	238	GLN
3	C	252	LYS
3	C	289	THR
3	C	294	GLU

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Mol	Chain	Res	Type
3	C	360	ASP
3	C	378	LYS
3	C	529	MET
3	C	534	THR
3	C	542	THR
3	C	575	TRP
3	C	610	MET
1	D	81	GLU
1	D	198	LYS
1	D	317	ARG
1	D	320	THR
1	D	449	CYS
1	D	575	ARG
2	E	20	THR
2	E	141	THR
2	E	159	ASP
2	E	179	MET
2	E	230	ASP
2	E	268	GLN
2	E	273	VAL
2	E	293	CYS
2	E	324	ARG
2	E	399	GLU
2	E	437	TRP
2	E	488	MET
2	E	666	ARG
2	E	681	MET
3	F	34	ARG
3	F	125	MET
3	F	146	ARG
3	F	171	PRO
3	F	238	GLN
3	F	289	THR
3	F	360	ASP
3	F	378	LYS
3	F	529	MET
3	F	534	THR
3	F	542	THR
3	F	575	TRP
3	F	610	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	11/12 (91%)	4 (36%)	0
4	V	11/12 (91%)	4 (36%)	0
All	All	22/24 (91%)	8 (36%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	6	U
4	H	7	A
4	H	8	A
4	H	11	A
4	V	6	U
4	V	7	A
4	V	8	A
4	V	11	A

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	712/751 (94%)	0.42	45 (6%) 21 20	62, 93, 175, 202	0
1	D	715/751 (95%)	0.72	113 (15%) 2 2	57, 90, 218, 239	0
2	B	708/772 (91%)	0.29	22 (3%) 49 46	57, 99, 133, 155	0
2	E	733/772 (94%)	0.39	19 (2%) 56 52	61, 104, 153, 189	0
3	C	714/798 (89%)	0.67	91 (12%) 4 4	67, 113, 187, 223	0
3	F	703/798 (88%)	0.88	111 (15%) 2 2	70, 124, 197, 229	0
4	H	12/12 (100%)	-0.11	0 100 100	69, 72, 81, 87	0
4	V	12/12 (100%)	-0.10	0 100 100	70, 78, 92, 105	0
All	All	4309/4666 (92%)	0.56	401 (9%) 9 10	57, 102, 190, 239	0

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	404	MET	8.3
3	F	481	VAL	8.2
1	D	73	LEU	7.9
1	A	191	ILE	7.7
3	F	401	ILE	7.4
3	F	376	LEU	7.2
3	C	482	THR	7.1
1	D	187	TRP	7.0
1	D	36	PHE	7.0
3	F	370	GLY	6.8
3	F	374	GLY	6.5
1	D	183	LEU	6.1
1	D	190	LEU	5.8
3	C	462	LEU	5.8
3	C	395	ASP	5.7
1	D	125	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	186	LEU	5.7
3	C	457	PRO	5.6
3	F	440	PHE	5.5
1	A	73	LEU	5.5
1	D	62	THR	5.5
3	C	463	HIS	5.5
3	C	394	GLU	5.4
1	D	174	LEU	5.4
1	D	152	GLN	5.4
1	D	123	ILE	5.4
3	F	100	TRP	5.2
3	C	447	LEU	5.1
1	A	150	TYR	5.1
1	D	72	ASN	5.1
3	C	446	ASP	5.1
1	D	4	PHE	5.0
1	D	9	PHE	5.0
1	D	161	SER	4.9
3	F	92	MET	4.9
3	F	465	ILE	4.9
1	D	8	ASN	4.9
1	D	162	LEU	4.8
1	D	122	GLY	4.8
3	C	481	VAL	4.8
1	D	150	TYR	4.7
1	D	51	MET	4.7
3	F	480	VAL	4.7
1	A	7	ARG	4.6
1	D	189	VAL	4.6
1	D	99	HIS	4.6
1	D	191	ILE	4.6
1	D	196	VAL	4.5
3	F	354	GLN	4.5
1	D	32	PRO	4.5
2	B	653	LYS	4.4
1	D	63	ALA	4.4
1	D	170	VAL	4.4
3	F	70	ILE	4.4
3	F	403	CYS	4.3
3	F	395	ASP	4.3
3	F	394	GLU	4.3
3	C	392	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	37	ASN	4.3
3	F	373	ARG	4.2
3	C	479	VAL	4.2
1	D	7	ARG	4.2
3	F	447	LEU	4.2
3	C	461	GLU	4.2
3	C	460	SER	4.2
3	F	442	ASN	4.2
3	C	476	LEU	4.2
3	F	451	TRP	4.2
1	D	193	GLU	4.1
1	D	195	ASP	4.1
1	D	143	MET	4.1
3	F	725	LYS	4.1
1	A	195	ASP	4.0
1	A	186	LEU	4.0
1	D	58	GLY	4.0
3	F	371	GLU	4.0
3	F	443	ARG	4.0
3	F	482	THR	4.0
1	D	77	TYR	4.0
3	F	726	ALA	4.0
3	F	328	GLY	3.9
3	F	707	ASP	3.9
1	D	61	TYR	3.9
1	D	33	ALA	3.9
3	F	398	ASP	3.8
3	C	440	PHE	3.8
1	D	160	SER	3.8
3	C	430	LEU	3.8
3	C	469	MET	3.8
3	F	415	GLY	3.8
3	F	101	TRP	3.8
2	E	180	THR	3.8
1	A	381	ILE	3.8
1	D	43	GLU	3.8
1	D	149	SER	3.8
3	C	477	LYS	3.8
1	D	138	LYS	3.7
1	A	122	GLY	3.7
3	F	72	LEU	3.7
1	D	1	MET	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	63	LYS	3.7
3	C	450	GLN	3.7
3	F	473	ASP	3.7
1	A	192	GLY	3.6
1	D	13	ILE	3.6
3	C	390	SER	3.6
1	D	48	ILE	3.6
1	D	11	THR	3.6
3	F	479	VAL	3.5
3	C	78	GLN	3.5
3	F	327	PHE	3.5
3	F	478	GLY	3.5
3	C	567	LEU	3.5
1	A	193	GLU	3.5
1	D	5	ILE	3.5
1	A	164	GLU	3.5
1	D	177	LEU	3.5
3	F	67	ALA	3.5
1	A	188	GLN	3.4
3	F	81	THR	3.4
3	F	692	ASN	3.4
3	C	480	VAL	3.4
1	A	187	TRP	3.4
1	D	57	GLU	3.4
1	D	156	LEU	3.4
3	F	386	LEU	3.4
3	F	446	ASP	3.4
1	D	151	ASN	3.4
3	F	405	VAL	3.4
3	F	385	LYS	3.4
3	C	374	GLY	3.4
3	F	350	ASN	3.4
3	F	110	THR	3.3
3	C	376	LEU	3.3
3	C	471	ALA	3.3
3	C	727	ASN	3.3
3	C	7	GLU	3.3
1	A	183	LEU	3.3
3	C	398	ASP	3.3
3	C	386	LEU	3.3
1	A	162	LEU	3.3
3	F	463	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	VAL	3.3
2	B	678	GLN	3.3
3	F	739	VAL	3.3
1	A	133	TRP	3.2
3	C	459	ALA	3.2
3	F	475	THR	3.2
2	E	630	PHE	3.2
1	D	146	MET	3.2
1	D	126	GLY	3.2
2	B	633	HIS	3.2
3	C	449	ASP	3.2
3	C	369	CYS	3.2
3	C	451	TRP	3.2
1	D	197	GLU	3.2
3	C	342	ASN	3.2
1	A	137	GLU	3.2
3	F	474	TYR	3.2
1	D	181	LEU	3.1
1	D	29	GLU	3.1
3	C	397	ARG	3.1
3	F	460	SER	3.1
1	D	163	ASP	3.1
3	F	375	ILE	3.1
3	F	387	LEU	3.1
1	D	375	ILE	3.1
1	D	120	GLU	3.1
3	F	462	LEU	3.1
1	D	172	SER	3.1
3	C	474	TYR	3.1
1	D	182	SER	3.1
3	F	402	LEU	3.1
1	D	374	LYS	3.0
3	C	391	ALA	3.0
1	D	28	PRO	3.0
1	D	175	THR	3.0
1	A	114	LYS	3.0
3	C	448	PHE	3.0
3	C	353	ILE	3.0
3	F	59	LEU	3.0
1	D	76	GLN	3.0
1	D	180	GLU	3.0
3	F	372	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	708	LEU	3.0
1	A	138	LYS	3.0
2	E	734	MET	3.0
1	A	61	TYR	2.9
2	E	615	MET	2.9
3	F	381	MET	2.9
1	D	26	GLU	2.9
3	C	458	LYS	2.9
1	D	0	SER	2.9
3	F	445	ASN	2.9
1	D	110	LEU	2.9
3	C	465	ILE	2.9
1	D	35	LEU	2.9
3	F	609	VAL	2.9
3	C	375	ILE	2.8
1	D	31	GLN	2.8
2	E	625	HIS	2.8
2	B	187	ILE	2.8
3	C	199	MET	2.8
3	F	464	GLY	2.8
3	C	464	GLY	2.8
1	D	178	GLN	2.8
1	D	2	ASP	2.8
3	C	384	GLU	2.8
2	E	588	LEU	2.8
3	F	438	ARG	2.8
3	F	352	THR	2.8
1	D	39	CYS	2.8
3	F	727	ASN	2.8
3	F	400	ILE	2.7
1	D	145	LEU	2.7
1	D	147	ILE	2.7
3	F	388	ILE	2.7
3	F	336	SER	2.7
3	C	352	THR	2.7
1	D	45	CYS	2.7
1	D	30	LEU	2.7
1	A	118	PHE	2.7
3	F	406	PHE	2.7
3	F	471	ALA	2.7
3	F	728	ILE	2.7
1	A	148	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	412	MET	2.7
3	F	369	CYS	2.7
1	A	171	LEU	2.7
3	F	78	GLN	2.6
1	D	129	ASP	2.6
1	D	21	MET	2.6
1	D	297	GLY	2.6
3	C	467	GLU	2.6
3	F	696	ALA	2.6
1	A	159	GLU	2.6
3	F	416	VAL	2.6
3	F	348	ILE	2.6
2	B	680	ASN	2.6
1	A	121	VAL	2.6
3	F	76	GLY	2.6
3	F	341	LYS	2.6
3	C	728	ILE	2.6
3	C	468	SER	2.6
1	D	185	ASN	2.6
3	F	195	LEU	2.6
3	F	10	LYS	2.5
1	D	18	LYS	2.5
1	A	181	LEU	2.5
1	A	386	MET	2.5
2	E	166	PHE	2.5
1	A	123	ILE	2.5
3	C	420	ILE	2.5
3	C	61	LEU	2.5
3	C	195	LEU	2.5
3	C	413	PHE	2.5
3	C	454	GLU	2.5
3	F	738	VAL	2.5
3	F	3	LEU	2.5
1	D	188	GLN	2.5
1	D	118	PHE	2.5
2	B	736	LYS	2.5
2	E	653	LYS	2.5
1	D	164	GLU	2.5
3	C	399	LEU	2.5
3	F	377	LYS	2.4
1	A	175	THR	2.4
3	F	410	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	354	GLN	2.4
3	C	330	LEU	2.4
3	F	567	LEU	2.4
3	C	443	ARG	2.4
1	A	143	MET	2.4
1	A	160	SER	2.4
3	C	708	LEU	2.4
3	F	697	GLY	2.4
3	F	397	ARG	2.4
3	C	400	ILE	2.4
3	F	450	GLN	2.4
2	B	206	MET	2.4
3	F	340	PHE	2.4
1	A	167	LYS	2.4
2	E	577	GLU	2.4
1	D	115	THR	2.4
3	F	470	ASN	2.4
2	B	185	LYS	2.4
3	C	393	LYS	2.4
1	D	46	TYR	2.4
2	E	396	PHE	2.4
2	E	619	TYR	2.4
3	C	455	GLU	2.4
3	F	95	ILE	2.4
1	D	44	VAL	2.4
1	D	106	TYR	2.4
3	C	721	LYS	2.4
1	D	59	LYS	2.4
1	D	84	PRO	2.4
3	F	699	LEU	2.4
2	B	208	VAL	2.3
2	E	154	ASP	2.3
3	C	401	ILE	2.3
2	E	84	GLN	2.3
1	D	12	THR	2.3
1	D	159	GLU	2.3
1	D	54	LEU	2.3
2	B	620	LYS	2.3
1	D	3	THR	2.3
3	C	701	SER	2.3
3	F	441	LEU	2.3
1	D	154	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	739	VAL	2.3
3	F	711	PHE	2.3
1	D	15	GLN	2.3
1	D	119	ILE	2.3
3	C	101	TRP	2.3
3	F	484	ASN	2.3
1	A	57	GLU	2.3
1	D	116	LYS	2.3
3	F	366	HIS	2.3
3	C	92	MET	2.3
1	D	127	LEU	2.3
3	C	456	SER	2.3
3	C	403	CYS	2.3
2	E	618	GLU	2.3
1	A	385	THR	2.3
1	D	130	ASP	2.3
1	A	190	LEU	2.2
2	B	364	LEU	2.2
2	E	737	ASP	2.2
1	D	114	LYS	2.2
2	B	750	GLY	2.2
3	C	100	TRP	2.2
3	C	575	TRP	2.2
3	C	566	LEU	2.2
3	F	353	ILE	2.2
2	B	186	ASN	2.2
2	B	694	LEU	2.2
1	A	149	SER	2.2
1	A	147	ILE	2.2
2	B	409	MET	2.2
1	A	1	MET	2.2
2	B	376	ILE	2.2
1	A	8	ASN	2.2
1	D	616	SER	2.2
1	A	377	LYS	2.2
2	B	355	PHE	2.2
3	C	429	LEU	2.2
3	F	459	ALA	2.2
1	D	184	LYS	2.2
3	F	77	ILE	2.2
3	C	349	GLY	2.2
1	A	201	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	2.2
2	B	207	LYS	2.2
1	D	179	ALA	2.2
1	D	148	PHE	2.2
3	F	413	PHE	2.2
1	A	14	ILE	2.2
3	C	109	ASP	2.2
3	F	455	GLU	2.2
3	C	81	THR	2.2
3	C	11	GLN	2.1
2	B	632	GLY	2.1
3	F	330	LEU	2.1
3	C	712	LYS	2.1
3	F	730	LEU	2.1
3	C	470	ASN	2.1
3	F	448	PHE	2.1
3	C	572	MET	2.1
3	C	707	ASP	2.1
3	F	365	PHE	2.1
3	C	736	VAL	2.1
1	D	381	ILE	2.1
3	F	444	SER	2.1
1	A	504	GLN	2.1
3	C	110	THR	2.1
3	F	187	LEU	2.1
1	D	24	PHE	2.1
3	F	472	SER	2.1
1	A	151	ASN	2.1
3	F	392	LYS	2.1
2	E	587	GLY	2.1
3	C	496	LYS	2.1
3	C	346	ILE	2.1
2	E	59	ASP	2.1
3	F	684	GLU	2.1
2	B	205	PRO	2.1
1	D	171	LEU	2.1
2	B	615	MET	2.1
3	F	712	LYS	2.0
3	C	327	PHE	2.0
2	B	660	SER	2.0
3	C	60	ALA	2.0
3	C	389	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	351	LEU	2.0
1	D	386	MET	2.0
1	D	95	LEU	2.0
2	E	86	ASP	2.0
3	C	70	ILE	2.0
1	D	158	ASN	2.0
1	A	373	GLN	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.