



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:50 AM UTC

PDB ID : 5FMZ / pdb_00005fmz
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

<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

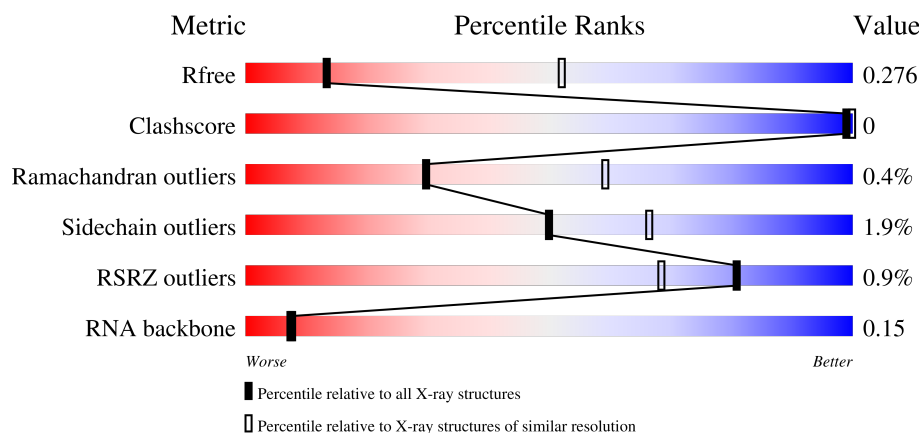
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

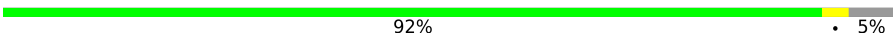
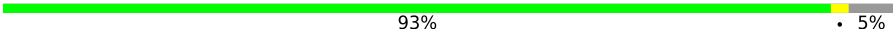
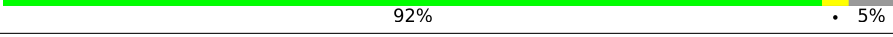
The reported resolution of this entry is 3.40 Å.

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	751	 92% • 5%
1	D	751	 93% • 5%
2	B	772	 88% • 8%
2	E	772	 92% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	798	% 86% 11%
3	F	798	2% 85% 12%
4	H	12	58% 42%
4	V	12	58% 42%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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*G P)-3'.

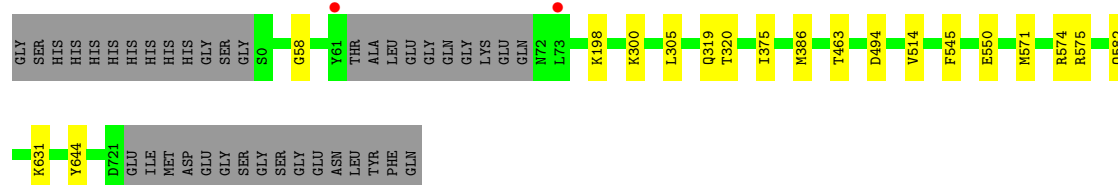
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			
4	V	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			

3 Residue-property plots

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.

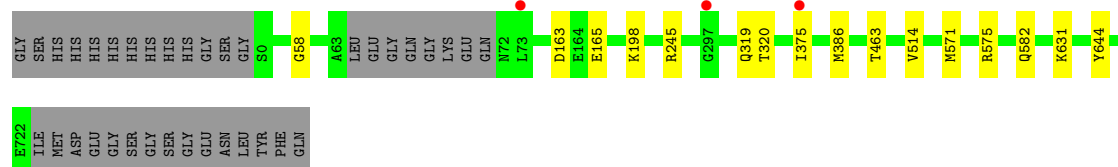
- Molecule 1: POLYMERASE ACIDIC PROTEIN

Chain A: 



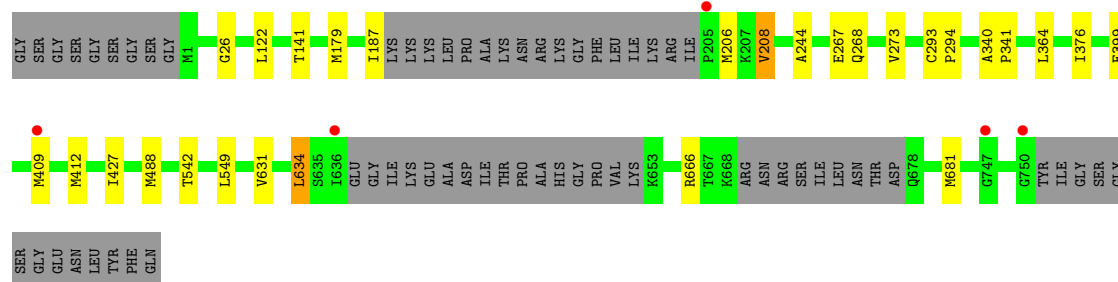
- Molecule 1: POLYMERASE ACIDIC PROTEIN

Chain D: 

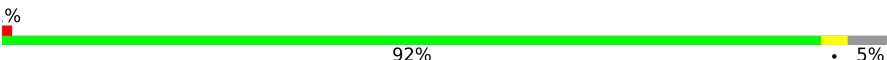


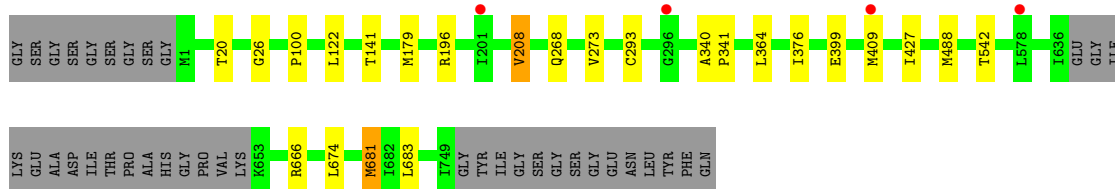
- Molecule 2: RNA-DIRECTED RNA POLYMERASE CATALYTIC SUBUNIT

Chain B: 

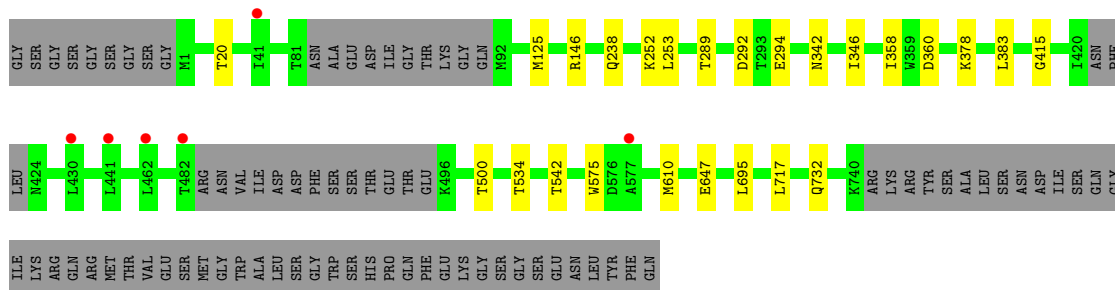
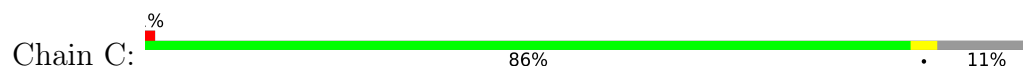


- Molecule 2: RNA-DIRECTED RNA POLYMERASE CATALYTIC SUBUNIT

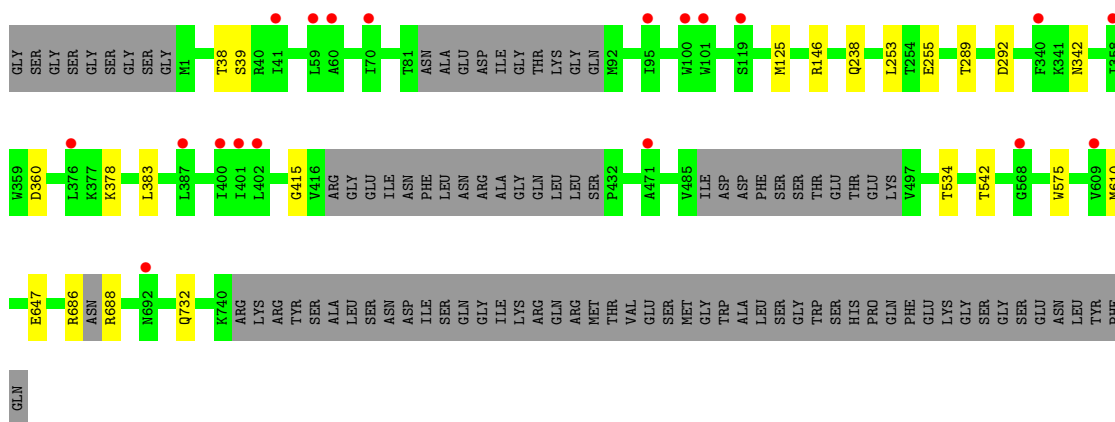
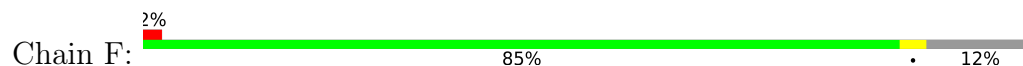
Chain E: 



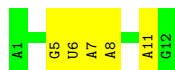
• Molecule 3: POLYMERASE BASIC PROTEIN 2



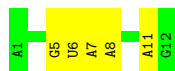
• Molecule 3: POLYMERASE BASIC PROTEIN 2



• 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 – 3.40 126.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (126.83-3.40) 99.7 (126.83-3.40)	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 (3.00%)	wwPDB-VP
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 , 46.2	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	0.51	0/5833	0.76	0/7866
1	D	0.51	0/5853	0.77	0/7893
2	B	0.54	0/5655	0.78	1/7623 (0.0%)
2	E	0.54	0/5867	0.77	0/7908
3	C	0.53	0/5816	0.75	0/7813
3	F	0.53	0/5733	0.75	0/7701
4	H	0.35	0/294	0.65	0/455
4	V	0.34	0/294	0.65	0/455
All	All	0.52	0/35345	0.76	1/47714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	PRO	N-CA-C	8.28	120.81	110.70

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	9	0
1	D	5737	0	5707	7	0
2	B	5547	0	5531	8	0
2	E	5755	0	5772	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	25	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 (25) 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:187:ILE:HD11	2:B:206:MET:HE3	1.83	0.61
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:463:THR:HG23	1:A:571:MET:HE3	1.97	0.47
1:D:463:THR:HG23	1:D:571:MET:HE3	1.97	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
1:A:386:MET:HE2	2:B:364:LEU:HB2	2.00	0.43
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.99	0.43
1:D:375:ILE:CD1	1:D:386:MET:HE1	2.49	0.43
1:A:375:ILE:CD1	1:A:386:MET:HE1	2.49	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:D:386:MET:HE2	2:E:364:LEU:HB2	2.01	0.41
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%)	48	78
1	D	711/751 (95%)	679 (96%)	31 (4%)	1 (0%)	48	78
2	B	700/772 (91%)	667 (95%)	30 (4%)	3 (0%)	30	59
2	E	729/772 (94%)	686 (94%)	37 (5%)	6 (1%)	16	44
3	C	706/798 (88%)	666 (94%)	37 (5%)	3 (0%)	30	59
3	F	693/798 (87%)	656 (95%)	33 (5%)	4 (1%)	21	50
All	All	4247/4642 (92%)	4031 (95%)	198 (5%)	18 (0%)	30	59

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%)	65	74
1	D	635/664 (96%)	629 (99%)	6 (1%)	70	76
2	B	607/657 (92%)	593 (98%)	14 (2%)	44	63
2	E	630/657 (96%)	616 (98%)	14 (2%)	45	63
3	C	625/694 (90%)	607 (97%)	18 (3%)	37	60
3	F	617/694 (89%)	604 (98%)	13 (2%)	47	64
All	All	3748/4030 (93%)	3676 (98%)	72 (2%)	50	66

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LYS
1	A	300	LYS
1	A	319	GLN
1	A	320	THR
1	A	514	VAL
1	A	575	ARG
1	A	631	LYS
2	B	122	LEU
2	B	141	THR
2	B	179	MET
2	B	208	VAL
2	B	267	GLU
2	B	268	GLN
2	B	273	VAL
2	B	293	CYS
2	B	399	GLU
2	B	427	ILE
2	B	488	MET
2	B	634	LEU
2	B	666	ARG
2	B	681	MET
3	C	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	125	MET
3	C	146	ARG
3	C	238	GLN
3	C	252	LYS
3	C	253	LEU
3	C	289	THR
3	C	294	GLU
3	C	342	ASN
3	C	360	ASP
3	C	378	LYS
3	C	383	LEU
3	C	500	THR
3	C	534	THR
3	C	542	THR
3	C	575	TRP
3	C	610	MET
3	C	647	GLU
1	D	198	LYS
1	D	319	GLN
1	D	320	THR
1	D	514	VAL
1	D	575	ARG
1	D	631	LYS
2	E	20	THR
2	E	122	LEU
2	E	141	THR
2	E	179	MET
2	E	208	VAL
2	E	268	GLN
2	E	273	VAL
2	E	293	CYS
2	E	399	GLU
2	E	427	ILE
2	E	488	MET
2	E	666	ARG
2	E	681	MET
2	E	683	LEU
3	F	125	MET
3	F	146	ARG
3	F	238	GLN
3	F	289	THR
3	F	342	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	360	ASP
3	F	378	LYS
3	F	383	LEU
3	F	534	THR
3	F	542	THR
3	F	575	TRP
3	F	610	MET
3	F	647	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	152	GLN
1	A	188	GLN
1	A	242	ASN
1	A	467	ASN
1	A	506	HIS
2	B	268	GLN
2	B	710	GLN
3	C	323	GLN
3	C	342	ASN
3	C	527	GLN
3	C	549	ASN
3	C	662	ASN
1	D	31	GLN
1	D	152	GLN
1	D	188	GLN
1	D	242	ASN
1	D	467	ASN
1	D	620	GLN
2	E	463	ASN
2	E	678	GLN
2	E	710	GLN
3	F	323	GLN
3	F	442	ASN
3	F	517	ASN
3	F	549	ASN
3	F	587	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	11/12 (91%)	5 (45%)	1 (9%)
4	V	11/12 (91%)	5 (45%)	1 (9%)
All	All	22/24 (91%)	10 (45%)	2 (9%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	5	G
4	H	6	U
4	H	7	A
4	H	8	A
4	H	11	A
4	V	5	G
4	V	6	U
4	V	7	A
4	V	8	A
4	V	11	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	5	G
4	V	5	G

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 ⓘ

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%)	0.09	2 (0%) 90 84	62, 93, 175, 202	0
1	D	715/751 (95%)	0.09	3 (0%) 88 81	57, 90, 218, 239	0
2	B	708/772 (91%)	0.04	5 (0%) 84 73	57, 99, 133, 155	0
2	E	733/772 (94%)	0.23	4 (0%) 87 78	61, 104, 153, 189	0
3	C	714/798 (89%)	0.22	6 (0%) 82 71	67, 113, 187, 223	0
3	F	703/798 (88%)	0.38	19 (2%) 56 42	70, 124, 197, 229	0
4	H	12/12 (100%)	-0.68	0 100 100	69, 72, 81, 87	0
4	V	12/12 (100%)	-0.56	0 100 100	70, 78, 92, 105	0
All	All	4309/4666 (92%)	0.17	39 (0%) 81 68	57, 102, 190, 239	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	6.5
2	B	750	GLY	3.9
3	F	70	ILE	3.7
3	C	430	LEU	3.4
3	F	95	ILE	3.3
3	F	41	ILE	3.2
2	B	205	PRO	3.1
3	F	401	ILE	3.0
2	B	747	GLY	3.0
3	F	340	PHE	2.9
1	D	73	LEU	2.8
1	A	61	TYR	2.8
3	F	60	ALA	2.7
3	F	358	ILE	2.6
3	F	400	ILE	2.6
3	F	402	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	41	ILE	2.6
3	F	471	ALA	2.5
3	F	59	LEU	2.4
3	C	482	THR	2.4
2	E	578	LEU	2.4
3	F	101	TRP	2.3
3	F	376	LEU	2.3
3	F	387	LEU	2.3
3	F	692	ASN	2.3
1	D	375	ILE	2.2
1	D	297	GLY	2.2
3	C	462	LEU	2.2
2	B	409	MET	2.1
2	E	409	MET	2.1
3	F	119	SER	2.1
3	C	441	LEU	2.1
2	E	201	ILE	2.1
3	F	568	GLY	2.1
3	F	100	TRP	2.0
3	C	577	ALA	2.0
2	E	296	GLY	2.0
3	F	609	VAL	2.0
2	B	636	ILE	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 oligosaccharides 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.