



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:39 PM UTC

PDB ID : 6QNW / pdb_00006qnw
Title : Influenza A Polymerase Heterotrimer Human H3N2 Northern Territory 1968
Authors : Keown, J.R.; Fan, H.; Grimes, J.M.
Deposited on : 2019-02-12
Resolution : 3.31 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

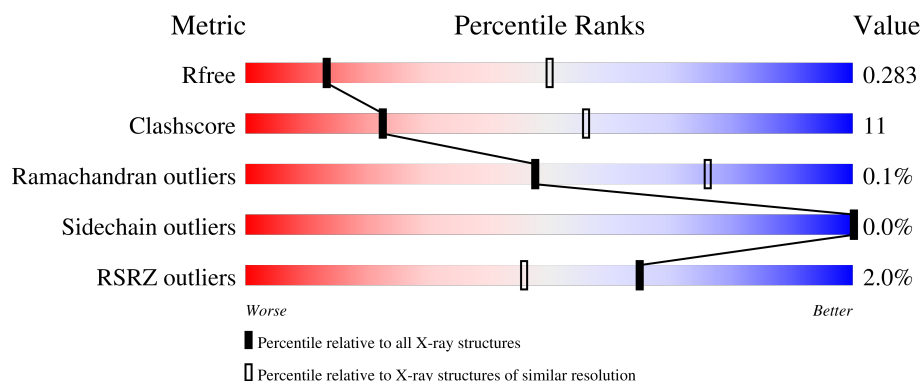
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	716	0.1% 72% 26% 0.1%
1	D	716	2% 73% 23% 0.1%
1	G	716	0.1% 72% 26% 0.1%
1	J	716	2% 75% 23% 0.1%
2	B	757	0.1% 70% 20% 10%

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Mol	Chain	Length	Quality of chain
2	E	757	4% 66% 22% 12%
2	H	757	% 67% 22% 11%
2	K	757	% 64% 24% 11%
3	C	765	% 67% 27% 5%
3	F	765	2% 69% 25% 6%
3	I	765	2% 68% 27% 5%
3	L	765	3% 71% 21% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67232 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	704	Total	C	N	O	S	0	0	0
			5733	3638	969	1084	42			
1	D	686	Total	C	N	O	S	0	0	0
			5604	3556	949	1058	41			
1	G	701	Total	C	N	O	S	0	0	0
			5707	3617	967	1081	42			
1	J	702	Total	C	N	O	S	0	0	0
			5713	3622	966	1083	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	679	Total	C	N	O	S	0	0	0
			5426	3417	932	1034	43			
2	E	665	Total	C	N	O	S	0	0	0
			5315	3351	910	1011	43			
2	H	676	Total	C	N	O	S	0	0	0
			5410	3410	929	1028	43			
2	K	673	Total	C	N	O	S	0	0	0
			5382	3390	925	1024	43			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	LYS	GLU	conflict	UNP P03432
E	577	LYS	GLU	conflict	UNP P03432
H	577	LYS	GLU	conflict	UNP P03432
K	577	LYS	GLU	conflict	UNP P03432

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	724	Total	C	N	O	S	0	0	0
			5772	3627	1044	1060	41			
3	F	720	Total	C	N	O	S	0	0	0
			5734	3604	1034	1056	40			
3	I	726	Total	C	N	O	S	0	0	0
			5789	3638	1047	1063	41			
3	L	709	Total	C	N	O	S	0	0	0
			5647	3552	1015	1039	41			

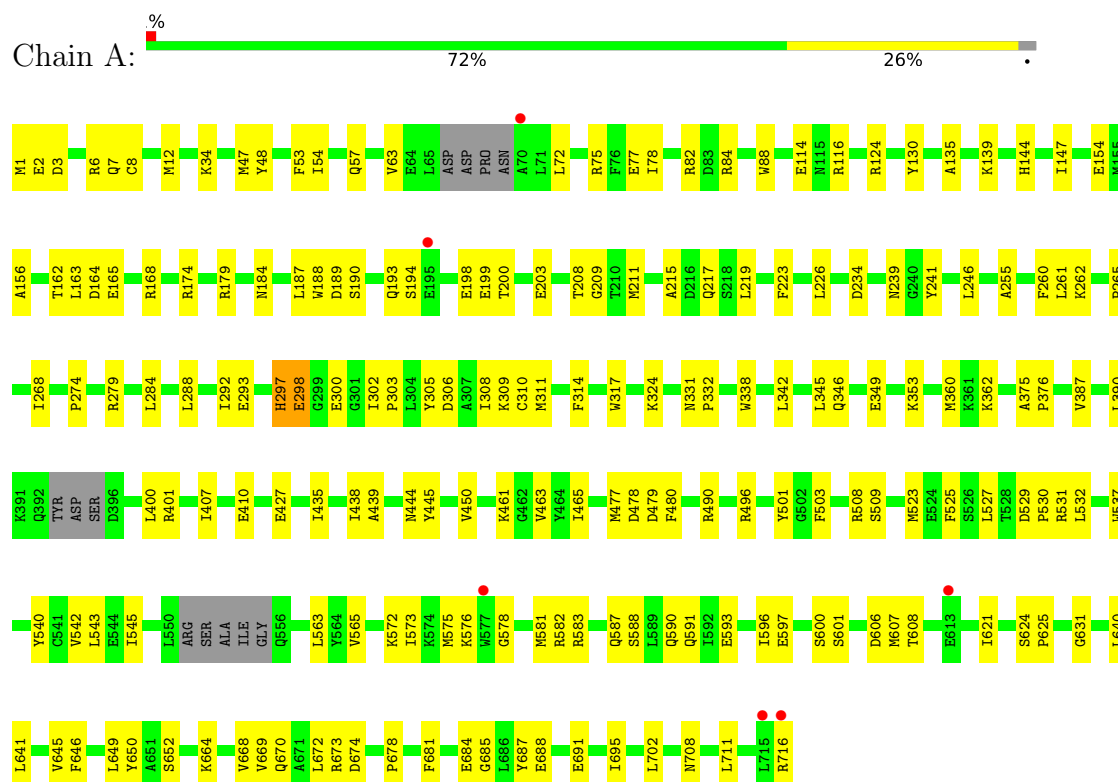
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP P03429
C	761	ASN	-	expression tag	UNP P03429
C	762	LEU	-	expression tag	UNP P03429
C	763	TYR	-	expression tag	UNP P03429
C	764	PHE	-	expression tag	UNP P03429
C	765	GLN	-	expression tag	UNP P03429
F	760	GLU	-	expression tag	UNP P03429
F	761	ASN	-	expression tag	UNP P03429
F	762	LEU	-	expression tag	UNP P03429
F	763	TYR	-	expression tag	UNP P03429
F	764	PHE	-	expression tag	UNP P03429
F	765	GLN	-	expression tag	UNP P03429
I	760	GLU	-	expression tag	UNP P03429
I	761	ASN	-	expression tag	UNP P03429
I	762	LEU	-	expression tag	UNP P03429
I	763	TYR	-	expression tag	UNP P03429
I	764	PHE	-	expression tag	UNP P03429
I	765	GLN	-	expression tag	UNP P03429
L	760	GLU	-	expression tag	UNP P03429
L	761	ASN	-	expression tag	UNP P03429
L	762	LEU	-	expression tag	UNP P03429
L	763	TYR	-	expression tag	UNP P03429
L	764	PHE	-	expression tag	UNP P03429
L	765	GLN	-	expression tag	UNP P03429

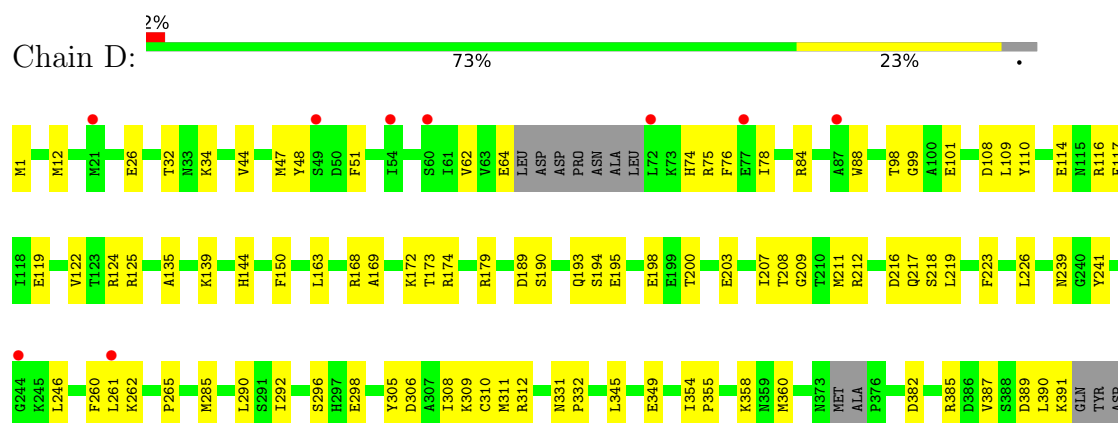
3 Residue-property plots

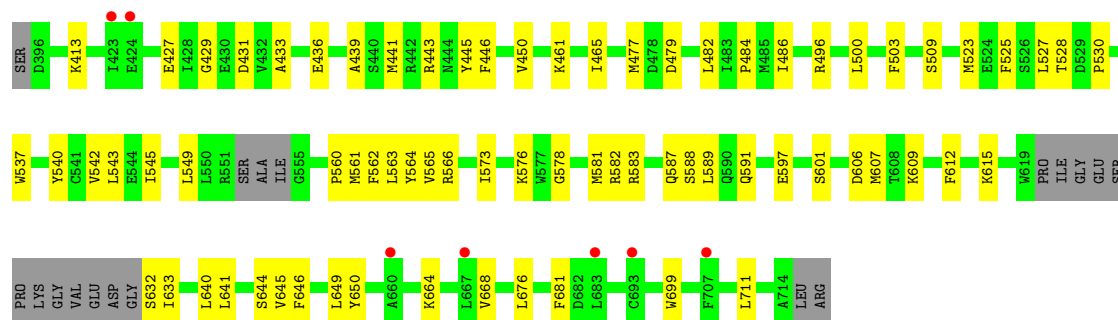
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

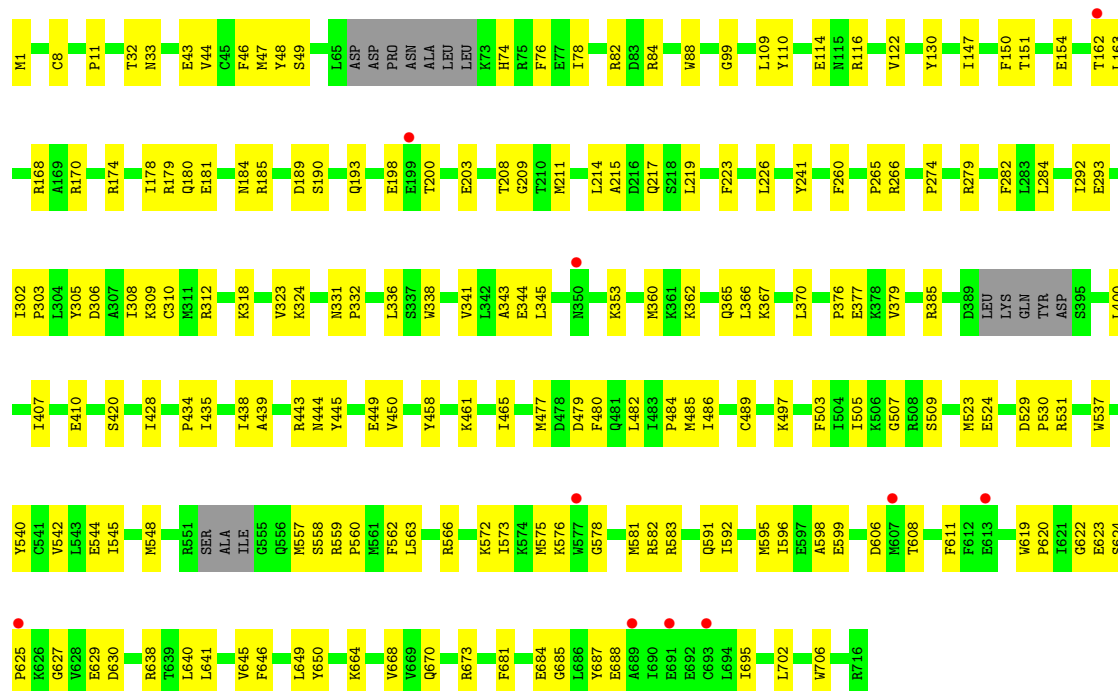
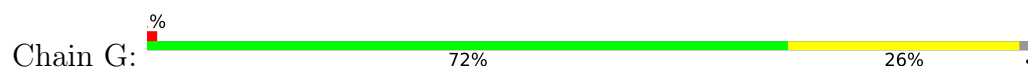


• Molecule 1: Polymerase acidic protein

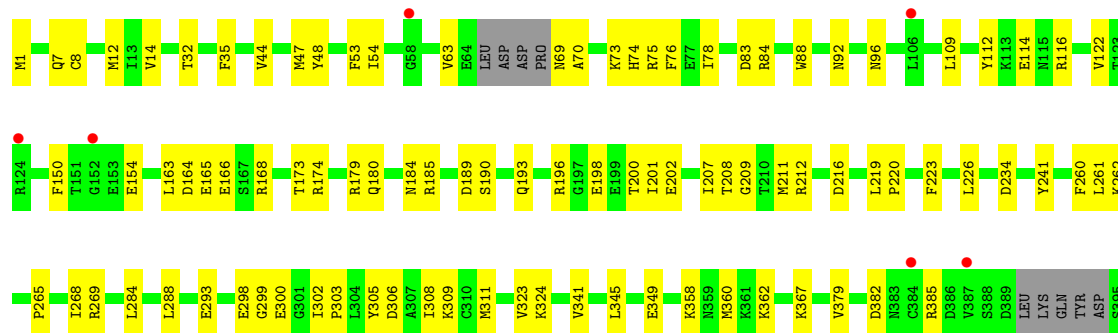
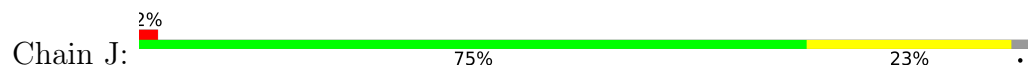


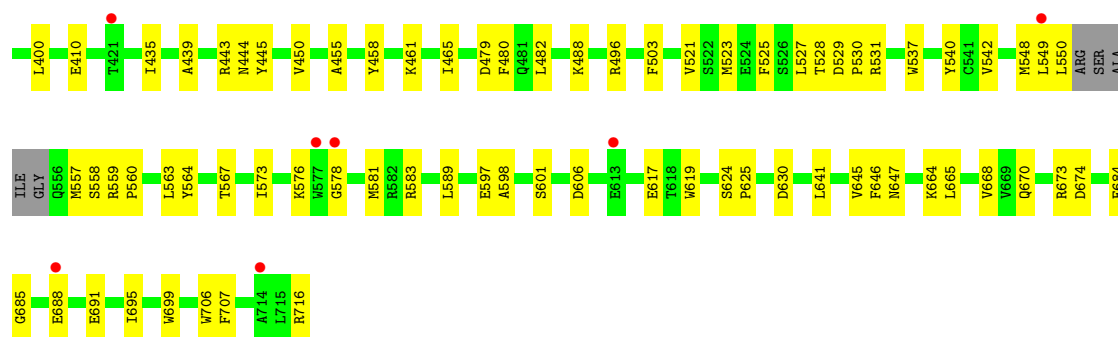


● Molecule 1: Polymerase acidic protein

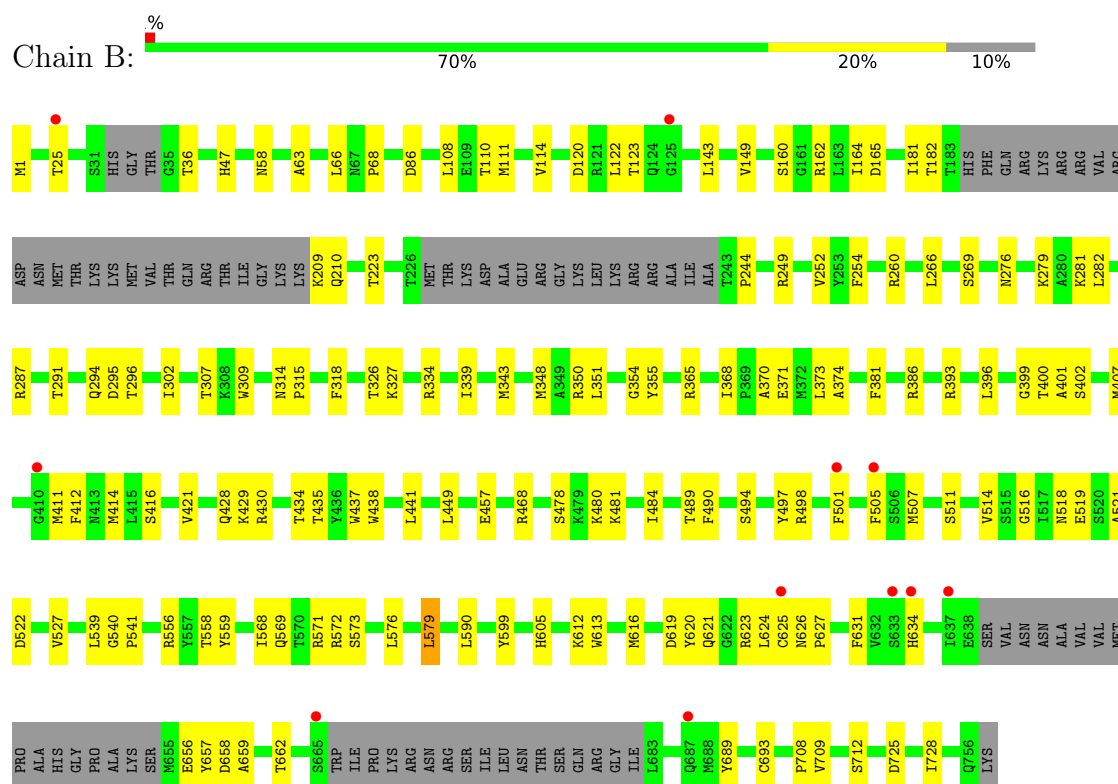


● Molecule 1: Polymerase acidic protein

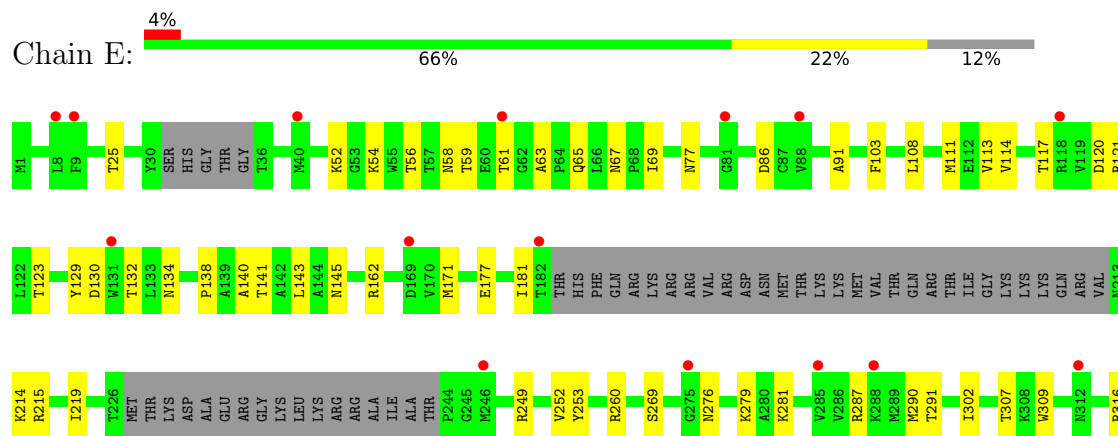


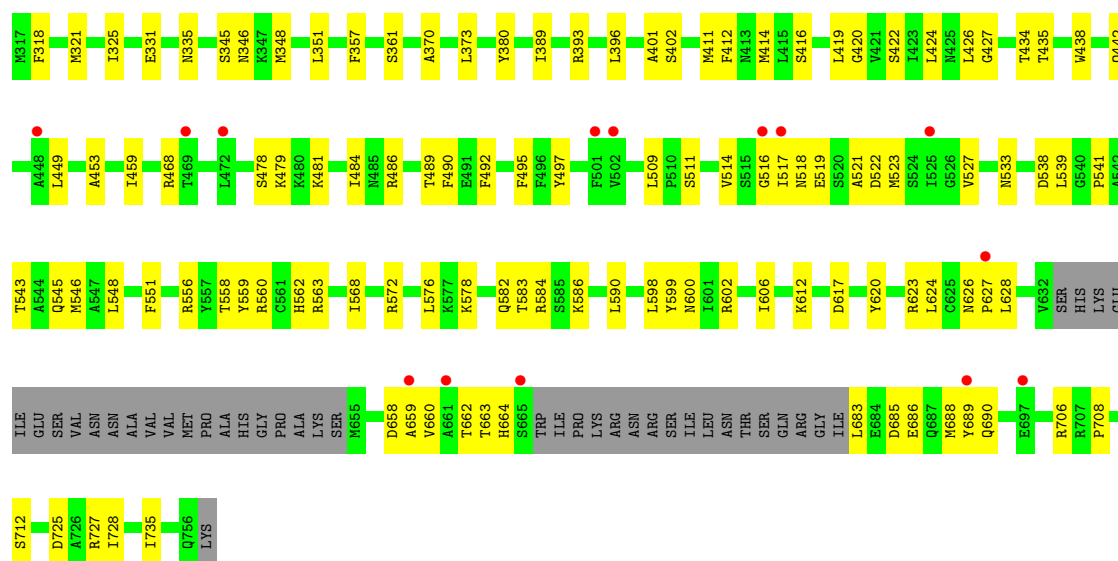


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

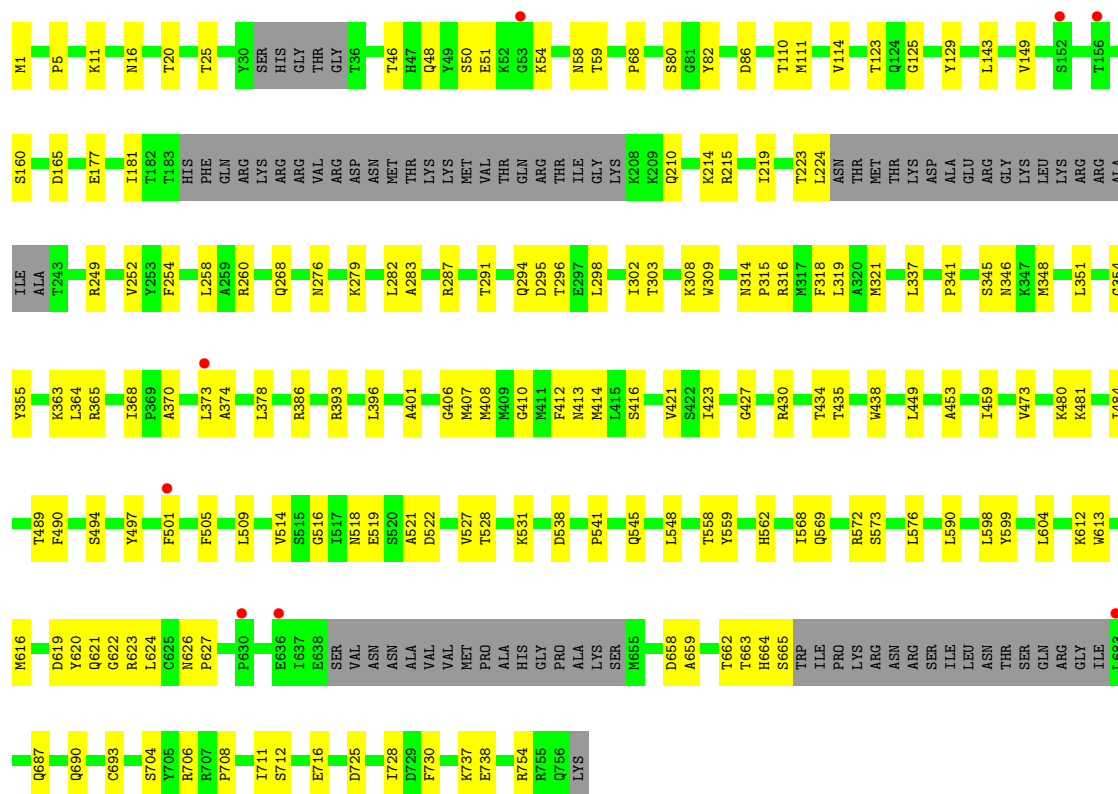


- Molecule 2: RNA-directed RNA polymerase catalytic subunit



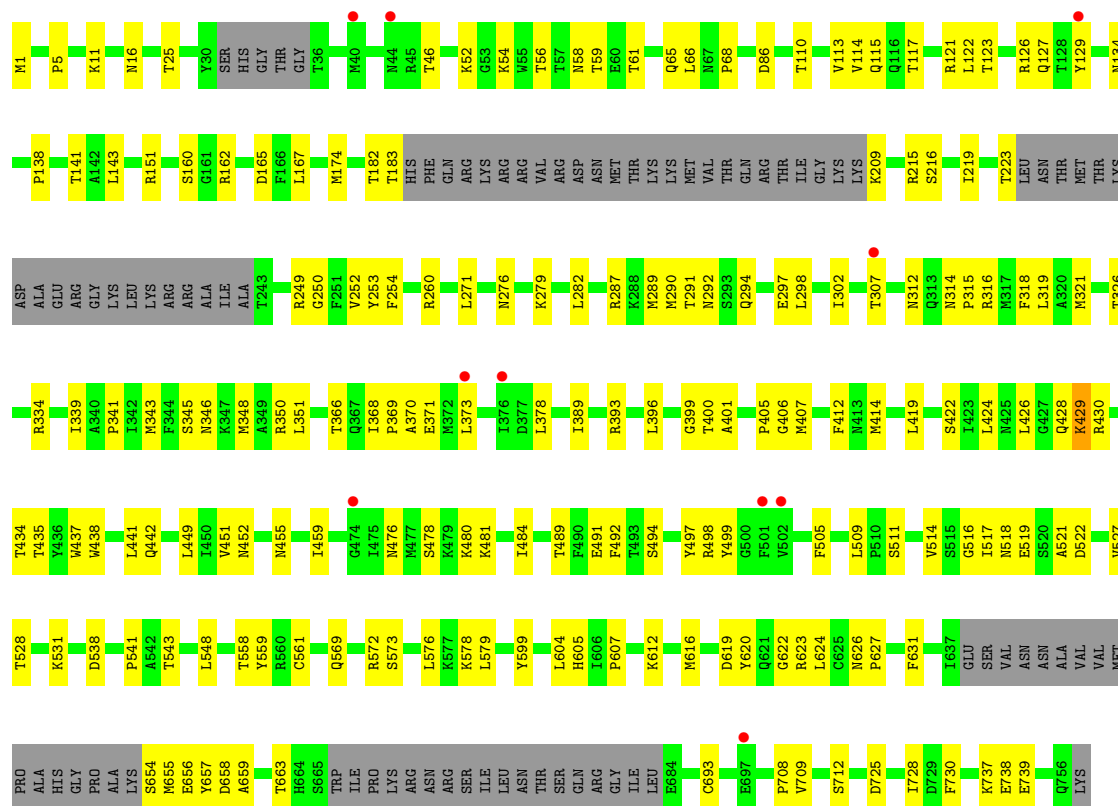


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

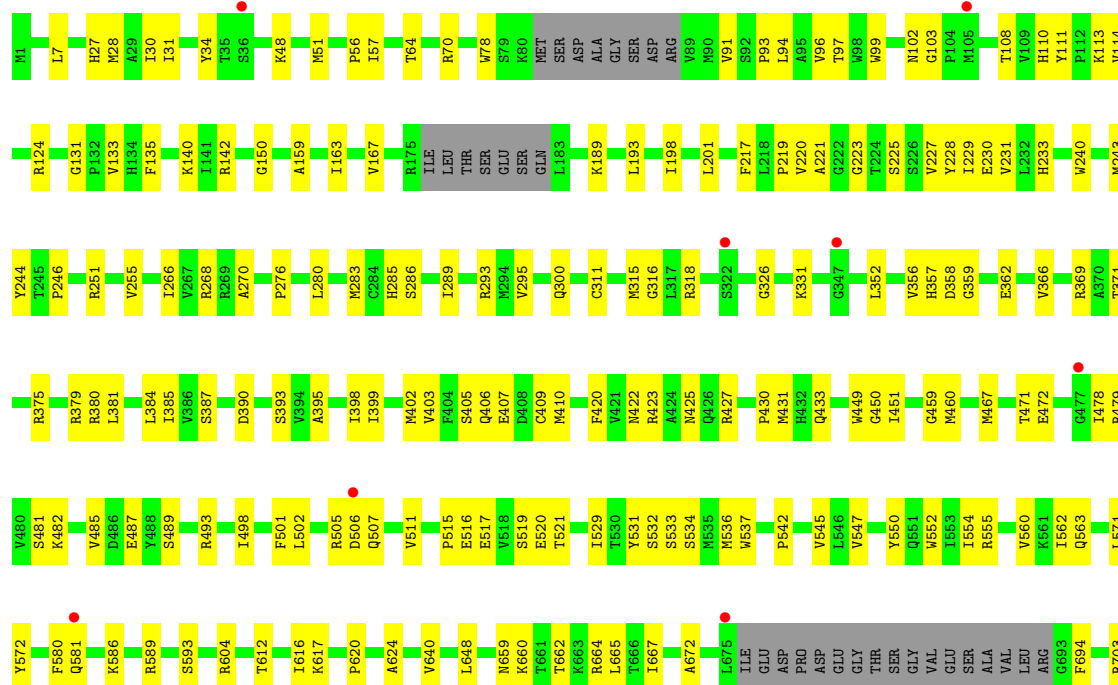


• Molecule 2: RNA-directed RNA polymerase catalytic subunit



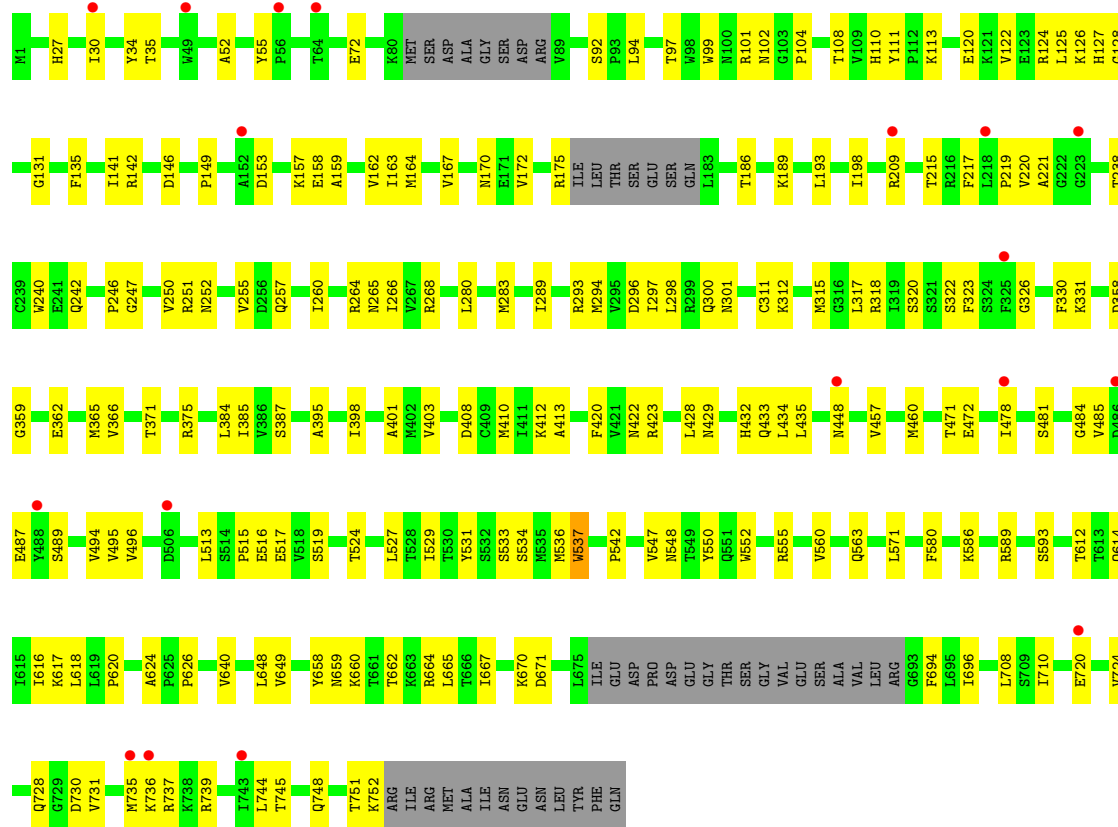


• Molecule 3: Polymerase basic protein 2

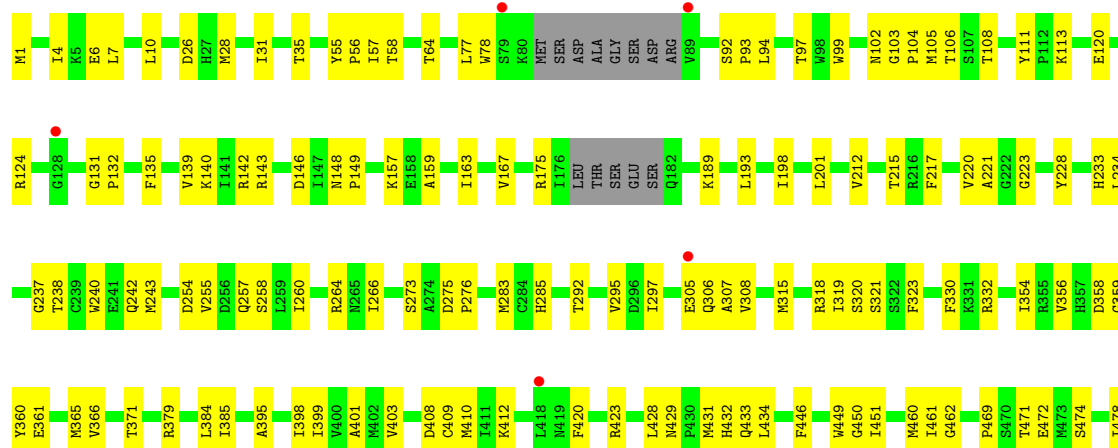


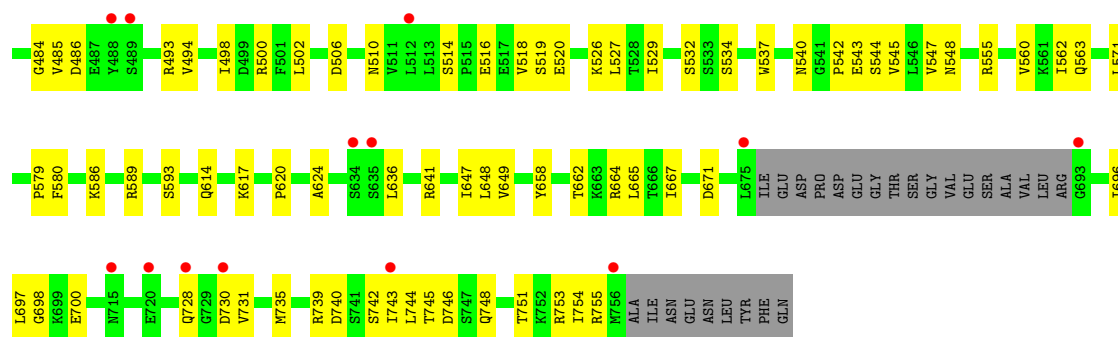


• Molecule 3: Polymerase basic protein 2

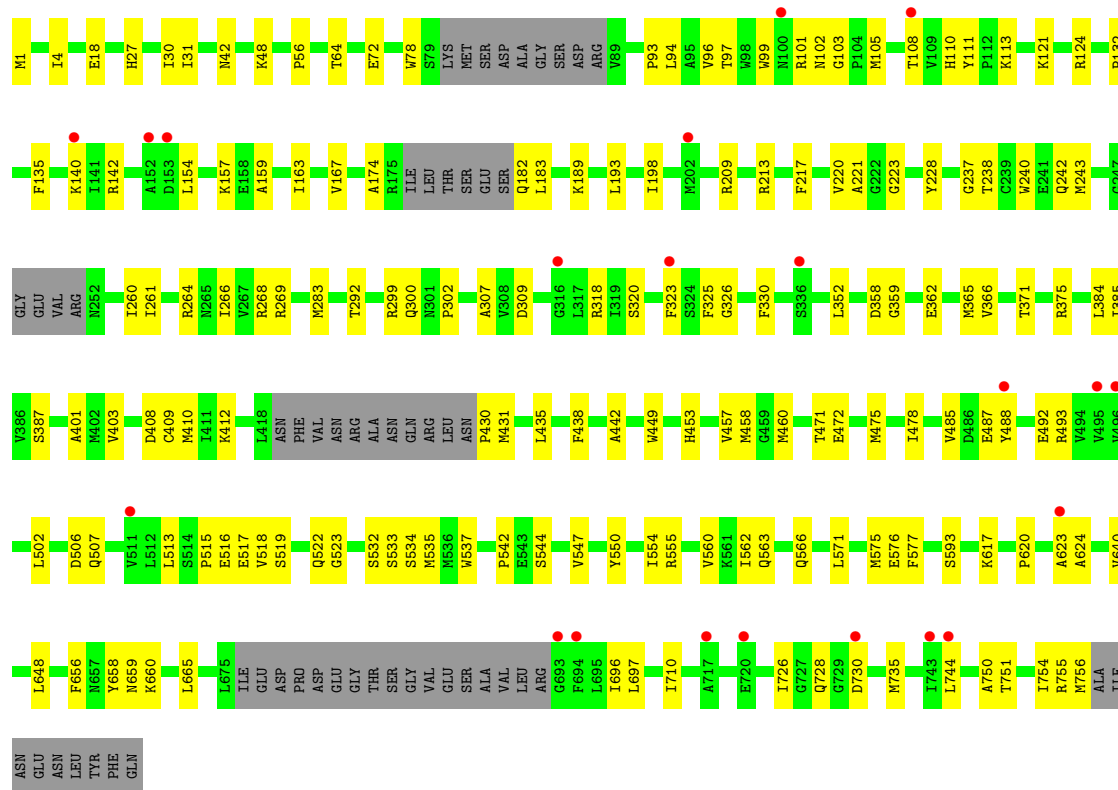


• Molecule 3: Polymerase basic protein 2





● Molecule 3: Polymerase basic protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	336.48Å 191.90Å 235.74Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	138.62 – 3.31 138.62 – 3.31	Depositor EDS
% Data completeness (in resolution range)	55.1 (138.62-3.31) 55.3 (138.62-3.31)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.235 , 0.279 0.240 , 0.283	Depositor DCC
R_{free} test set	6174 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 109.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.025 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.027 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.024 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	67232	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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

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	0.14	0/5853	0.39	1/7886 (0.0%)
1	D	0.12	0/5720	0.36	0/7701
1	G	0.13	0/5827	0.37	0/7850
1	J	0.12	0/5833	0.37	0/7860
2	B	0.12	0/5529	0.37	1/7456 (0.0%)
2	E	0.12	0/5417	0.34	0/7306
2	H	0.12	0/5513	0.37	0/7433
2	K	0.12	0/5485	0.36	0/7396
3	C	0.13	0/5866	0.42	2/7900 (0.0%)
3	F	0.13	0/5828	0.41	0/7851
3	I	0.13	0/5883	0.40	0/7923
3	L	0.12	0/5738	0.39	0/7725
All	All	0.13	0/68492	0.38	4/92287 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	N-CA-C	5.42	121.79	113.28
3	C	532	SER	CA-C-N	-5.28	111.45	121.54
3	C	532	SER	C-N-CA	-5.28	111.45	121.54
2	B	579	LEU	CB-CG-CD2	-5.17	95.18	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	HIS	Peptide
3	C	739	ARG	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	5733	0	5662	131	0
1	D	5604	0	5527	129	0
1	G	5707	0	5624	140	0
1	J	5713	0	5630	122	0
2	B	5426	0	5374	114	0
2	E	5315	0	5262	134	0
2	H	5410	0	5366	142	0
2	K	5382	0	5330	143	0
3	C	5772	0	5915	158	0
3	F	5734	0	5869	150	0
3	I	5789	0	5934	161	0
3	L	5647	0	5786	127	0
All	All	67232	0	67279	1417	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 11.

The worst 5 of 1417 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)
3:F:317:LEU:HD12	3:F:496:VAL:H	1.41	0.86
3:F:289:ILE:HG22	3:F:529:ILE:HG13	1.63	0.81
2:E:708:PRO:HA	3:F:728:GLN:HE21	1.46	0.79
3:F:149:PRO:HD2	3:F:209:ARG:HH12	1.49	0.77
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.49	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	696/716 (97%)	646 (93%)	49 (7%)	1 (0%)	48	76
1	D	674/716 (94%)	632 (94%)	42 (6%)	0	100	100
1	G	693/716 (97%)	644 (93%)	49 (7%)	0	100	100
1	J	694/716 (97%)	646 (93%)	48 (7%)	0	100	100
2	B	667/757 (88%)	628 (94%)	38 (6%)	1 (0%)	48	76
2	E	653/757 (86%)	621 (95%)	32 (5%)	0	100	100
2	H	664/757 (88%)	629 (95%)	34 (5%)	1 (0%)	43	72
2	K	661/757 (87%)	623 (94%)	37 (6%)	1 (0%)	43	72
3	C	716/765 (94%)	658 (92%)	56 (8%)	2 (0%)	36	66
3	F	712/765 (93%)	660 (93%)	52 (7%)	0	100	100
3	I	718/765 (94%)	658 (92%)	59 (8%)	1 (0%)	48	76
3	L	697/765 (91%)	647 (93%)	49 (7%)	1 (0%)	48	76
All	All	8245/8952 (92%)	7692 (93%)	545 (7%)	8 (0%)	48	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
2	B	295	ASP
2	K	429	LYS
3	I	745	THR
3	L	516	GLU

5.3.2 Protein sidechains [i](#)

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	634/644 (98%)	634 (100%)	0	100	100
1	D	620/644 (96%)	620 (100%)	0	100	100
1	G	631/644 (98%)	631 (100%)	0	100	100
1	J	632/644 (98%)	632 (100%)	0	100	100
2	B	602/669 (90%)	602 (100%)	0	100	100
2	E	589/669 (88%)	589 (100%)	0	100	100
2	H	600/669 (90%)	600 (100%)	0	100	100
2	K	597/669 (89%)	597 (100%)	0	100	100
3	C	641/676 (95%)	641 (100%)	0	100	100
3	F	637/676 (94%)	636 (100%)	1 (0%)	87	87
3	I	643/676 (95%)	643 (100%)	0	100	100
3	L	628/676 (93%)	628 (100%)	0	100	100
All	All	7454/7956 (94%)	7453 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	537	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	48	GLN
2	K	276	ASN
3	L	728	GLN
3	F	100	ASN
2	E	605	HIS

5.3.3 RNA ⓘ

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	704/716 (98%)	-0.03	6 (0%) 81 66	36, 86, 152, 183	0
1	D	686/716 (95%)	0.31	16 (2%) 61 42	89, 142, 214, 261	0
1	G	701/716 (97%)	0.00	10 (1%) 73 55	39, 86, 147, 214	0
1	J	702/716 (98%)	0.24	13 (1%) 66 47	67, 121, 184, 240	0
2	B	679/757 (89%)	0.04	11 (1%) 70 52	35, 82, 137, 210	0
2	E	665/757 (87%)	0.52	29 (4%) 39 25	93, 164, 215, 239	0
2	H	676/757 (89%)	0.08	8 (1%) 76 58	35, 89, 157, 214	0
2	K	673/757 (88%)	0.23	10 (1%) 72 53	65, 124, 184, 221	0
3	C	724/765 (94%)	0.19	9 (1%) 76 58	46, 110, 167, 217	0
3	F	720/765 (94%)	0.30	18 (2%) 58 39	55, 134, 185, 220	0
3	I	726/765 (94%)	0.29	18 (2%) 58 39	42, 107, 163, 200	0
3	L	709/765 (92%)	0.26	21 (2%) 52 35	70, 123, 173, 215	0
All	All	8365/8952 (93%)	0.20	169 (2%) 65 46	35, 114, 186, 261	0

The worst 5 of 169 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	384	CYS	4.8
2	E	448	ALA	4.1
2	B	410	GLY	4.1
2	H	683	LEU	4.0
2	K	373	LEU	3.8

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.