



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 12:14 AM GMT

PDB ID : 5D9A
Title : Influenza C Virus RNA-dependent RNA Polymerase - Space group P212121
Authors : Hengrung, N.; El Omari, K.; Serna Martin, I.; Vreede, F.T.; Cusack, S.;
Rambo, R.P.; Vonrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor,
E.
Deposited on : 2015-08-18
Resolution : 4.30 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
<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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

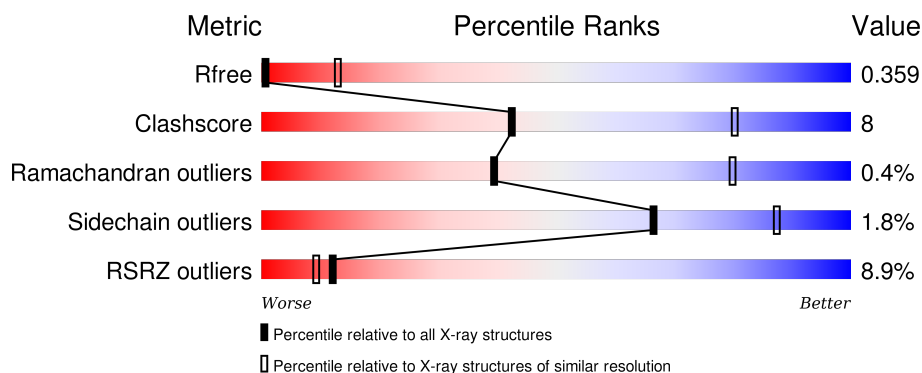
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	709	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	709	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	G	709	<div> <div>10%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	J	709	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	754	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	754	<div><div></div><div>4%</div><div>81%</div><div>13%</div><div>6%</div></div>
2	H	754	<div><div></div><div>6%</div><div>80%</div><div>14%</div><div>6%</div></div>
2	K	754	<div><div></div><div>8%</div><div>83%</div><div>11%</div><div>6%</div></div>
3	C	782	<div><div></div><div>21%</div><div>86%</div><div>10%</div><div></div></div>
3	F	782	<div><div></div><div>6%</div><div>82%</div><div>15%</div><div></div></div>
3	I	782	<div><div></div><div>12%</div><div>84%</div><div>13%</div><div></div></div>
3	L	782	<div><div></div><div>17%</div><div>87%</div><div>10%</div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69371 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	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	D	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	G	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	J	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	E	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	H	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	K	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	754	Total	C	N	O	S	0	0	0
			6015	3806	1056	1117	36			
3	F	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	I	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	L	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			

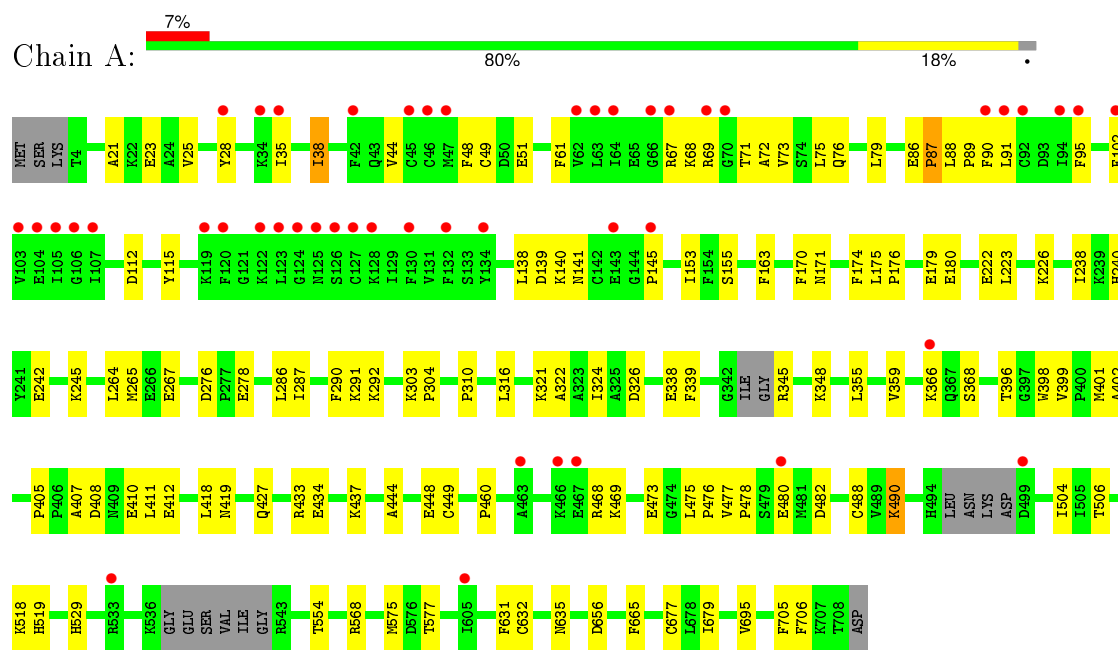
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	ALA	-	expression tag	UNP Q9IMP3
C	776	ARG	-	expression tag	UNP Q9IMP3
C	777	GLU	-	expression tag	UNP Q9IMP3
C	778	ASN	-	expression tag	UNP Q9IMP3
C	779	LEU	-	expression tag	UNP Q9IMP3
C	780	TYR	-	expression tag	UNP Q9IMP3
C	781	PHE	-	expression tag	UNP Q9IMP3
C	782	GLN	-	expression tag	UNP Q9IMP3
F	775	ALA	-	expression tag	UNP Q9IMP3
F	776	ARG	-	expression tag	UNP Q9IMP3
F	777	GLU	-	expression tag	UNP Q9IMP3
F	778	ASN	-	expression tag	UNP Q9IMP3
F	779	LEU	-	expression tag	UNP Q9IMP3
F	780	TYR	-	expression tag	UNP Q9IMP3
F	781	PHE	-	expression tag	UNP Q9IMP3
F	782	GLN	-	expression tag	UNP Q9IMP3
I	775	ALA	-	expression tag	UNP Q9IMP3
I	776	ARG	-	expression tag	UNP Q9IMP3
I	777	GLU	-	expression tag	UNP Q9IMP3
I	778	ASN	-	expression tag	UNP Q9IMP3
I	779	LEU	-	expression tag	UNP Q9IMP3
I	780	TYR	-	expression tag	UNP Q9IMP3
I	781	PHE	-	expression tag	UNP Q9IMP3
I	782	GLN	-	expression tag	UNP Q9IMP3
L	775	ALA	-	expression tag	UNP Q9IMP3
L	776	ARG	-	expression tag	UNP Q9IMP3
L	777	GLU	-	expression tag	UNP Q9IMP3
L	778	ASN	-	expression tag	UNP Q9IMP3
L	779	LEU	-	expression tag	UNP Q9IMP3
L	780	TYR	-	expression tag	UNP Q9IMP3
L	781	PHE	-	expression tag	UNP Q9IMP3
L	782	GLN	-	expression tag	UNP Q9IMP3

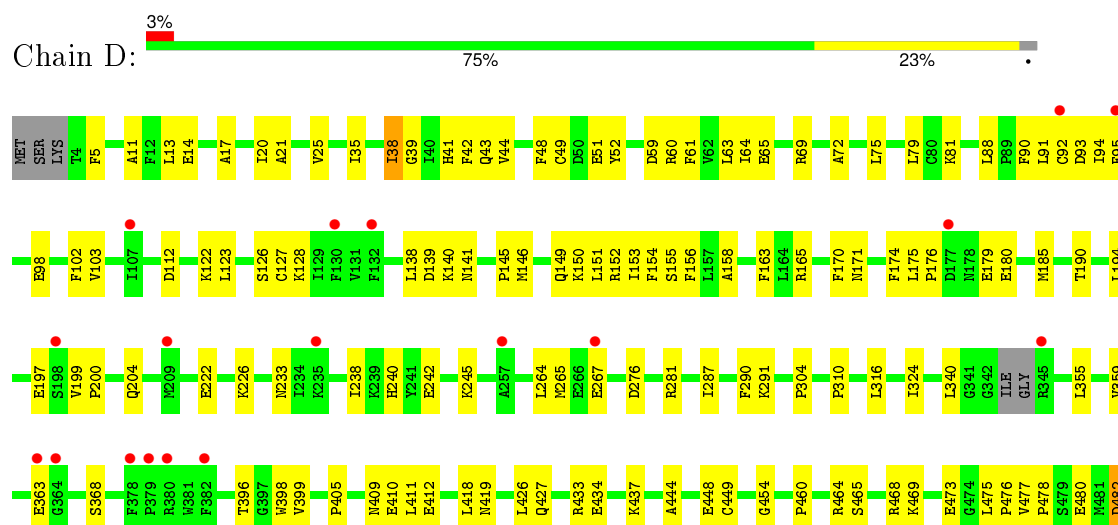
3 Residue-property plots [i](#)

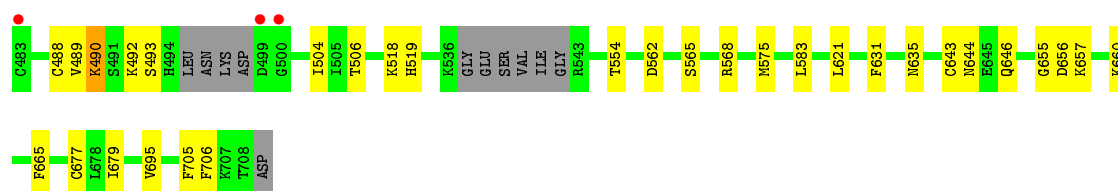
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

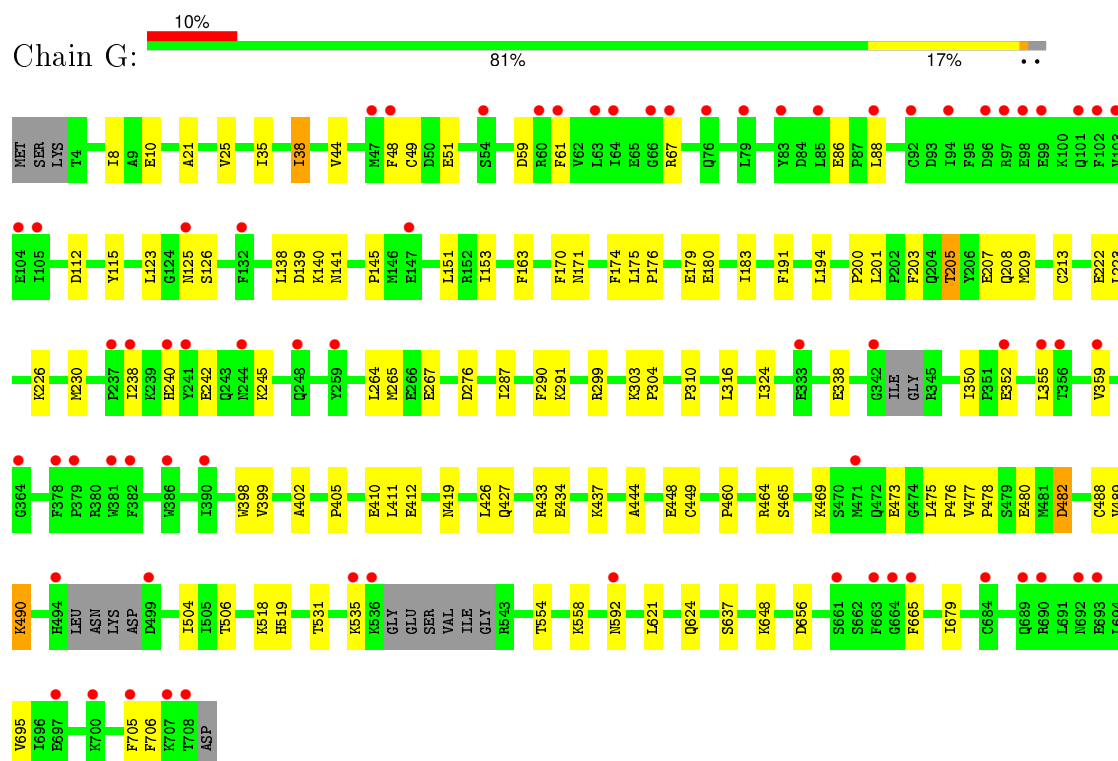


• Molecule 1: Polymerase acidic protein

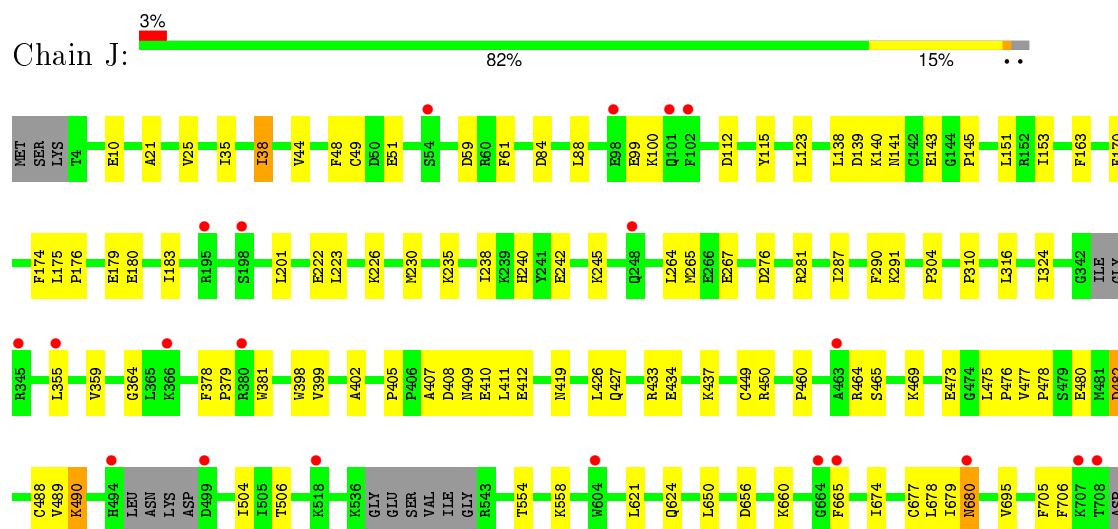




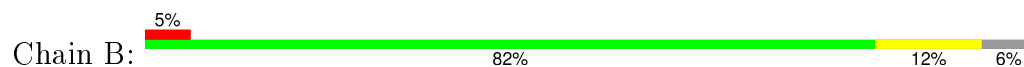
• Molecule 1: Polymerase acidic protein

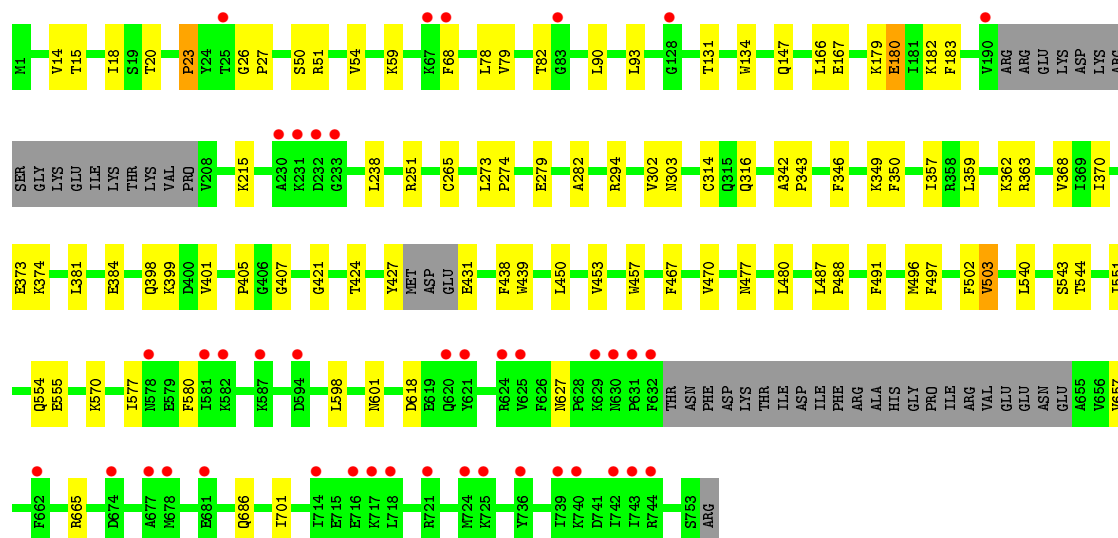


• Molecule 1: Polymerase acidic protein

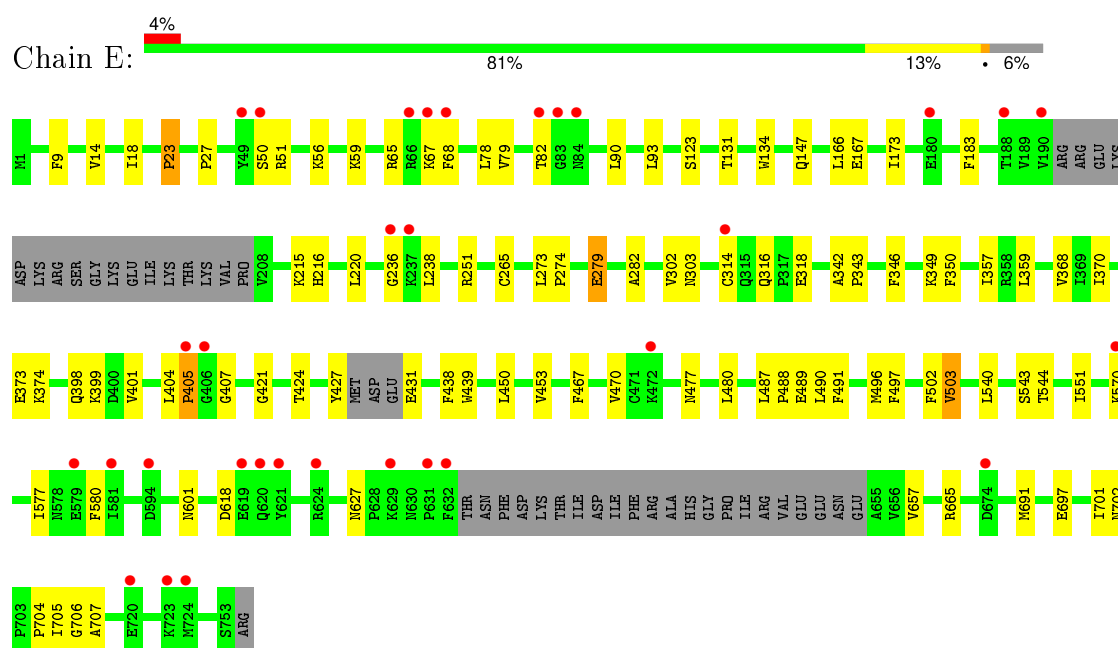


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

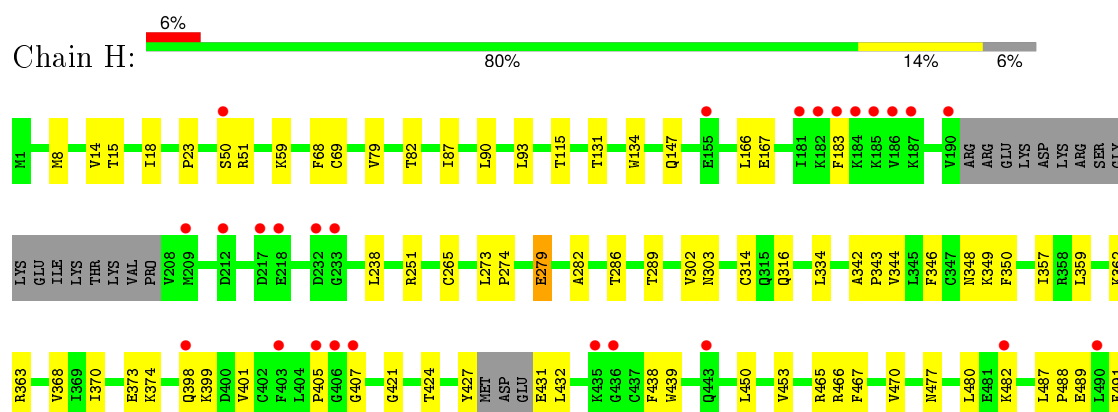


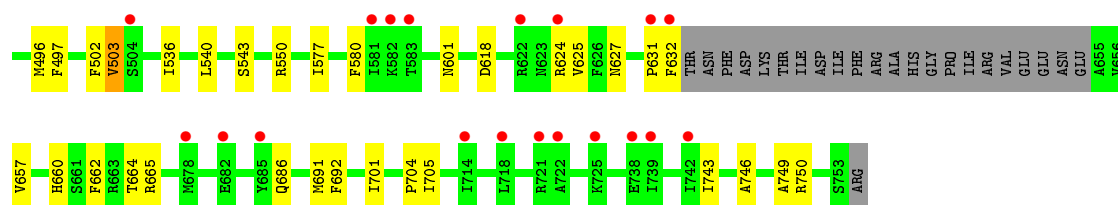


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

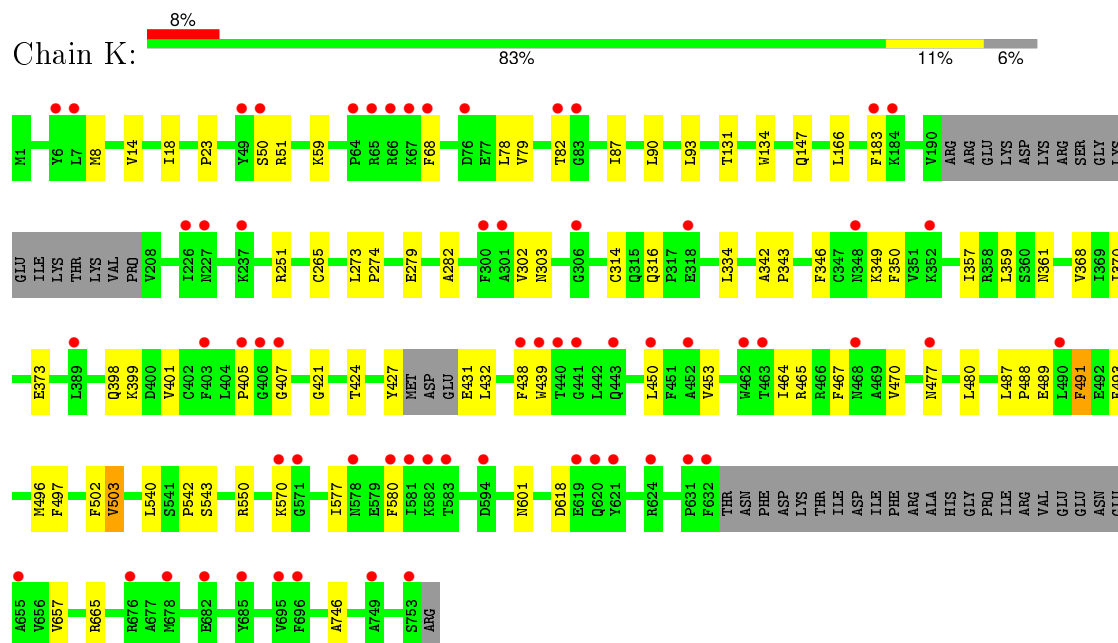


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

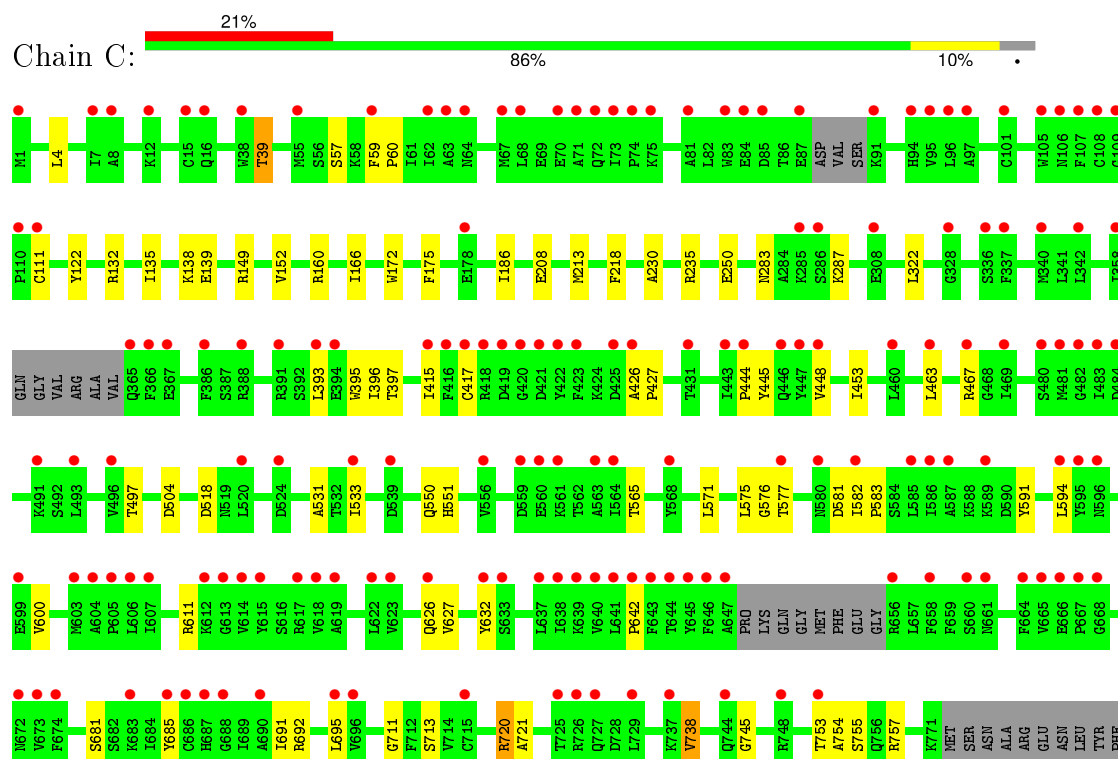




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

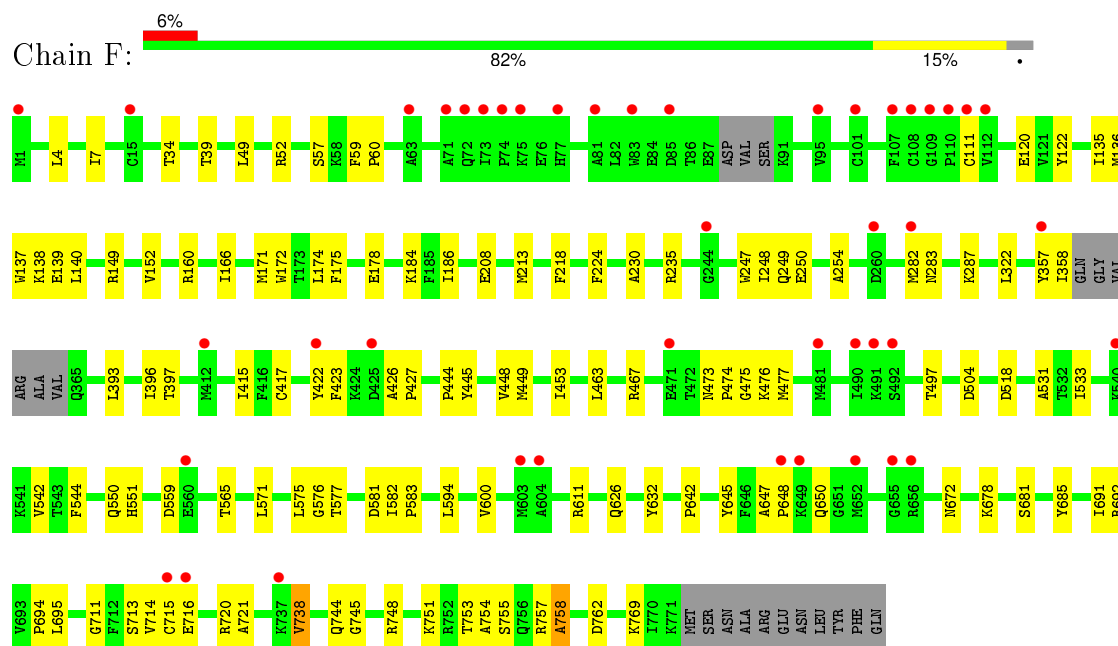


• Molecule 3: Polymerase basic protein 2



GLN

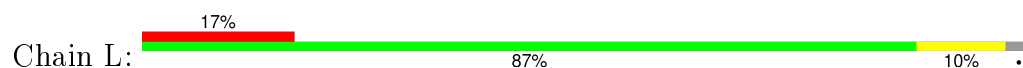
- Molecule 3: Polymerase basic protein 2

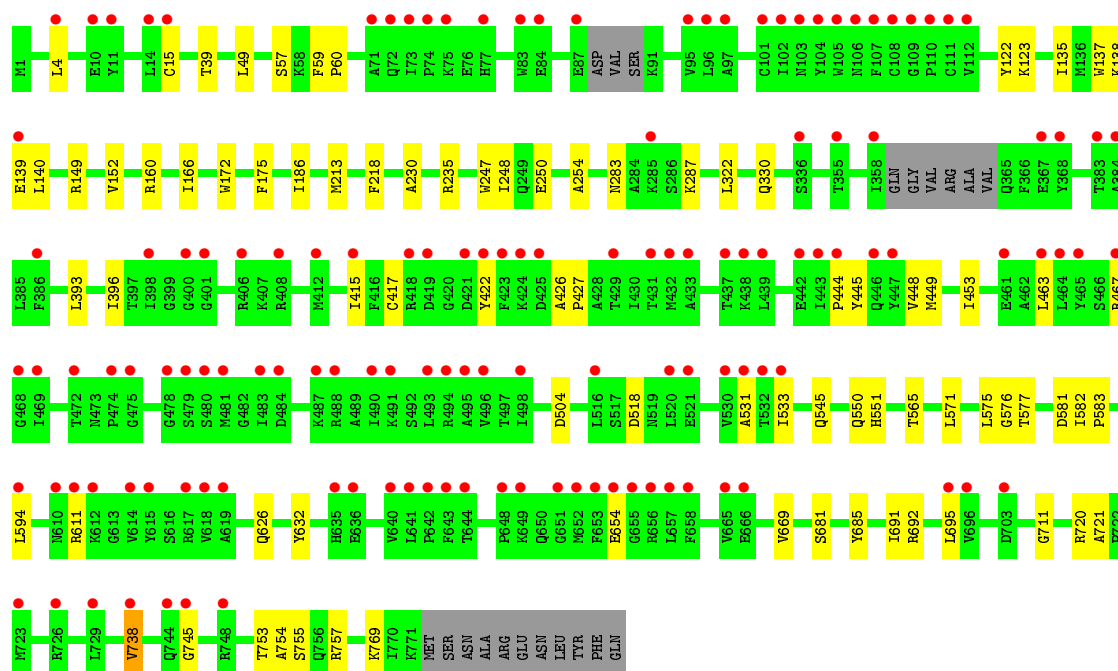


- Molecule 3: Polymerase basic protein 2



- Molecule 3: Polymerase basic protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.28Å 217.50Å 597.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 4.30 80.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-4.30) 98.9 (80.90-4.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.30Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.316 , 0.368 0.311 , 0.359	Depositor DCC
R_{free} test set	4744 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	146.0	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 108.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 95180 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	69371	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/5746	0.65	0/7717
1	D	0.47	0/5746	0.66	0/7717
1	G	0.46	0/5746	0.64	0/7717
1	J	0.46	0/5746	0.64	0/7717
2	B	0.45	0/5749	0.65	1/7723 (0.0%)
2	E	0.44	0/5749	0.65	0/7723
2	H	0.44	0/5749	0.64	0/7723
2	K	0.43	0/5749	0.64	0/7723
3	C	0.45	0/6121	0.69	1/8236 (0.0%)
3	F	0.46	0/6185	0.69	0/8322
3	I	0.45	0/6185	0.68	1/8322 (0.0%)
3	L	0.44	0/6185	0.68	0/8322
All	All	0.45	0/70656	0.66	3/94962 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	720	ARG	NE-CZ-NH1	6.60	123.60	120.30
3	C	720	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	B	180	GLU	OE1-CD-OE2	-6.36	115.67	123.30

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	5630	0	5632	144	1
1	D	5630	0	5632	192	5
1	G	5630	0	5632	167	2
1	J	5630	0	5632	116	6
2	B	5652	0	5749	122	6
2	E	5652	0	5749	104	3
2	H	5652	0	5749	129	0
2	K	5652	0	5749	77	0
3	C	6015	0	6124	54	0
3	F	6076	0	6183	171	8
3	I	6076	0	6183	119	3
3	L	6076	0	6183	80	0
All	All	69371	0	70197	1164	17

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 8.

The worst 5 of 1164 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:D:69:ARG:CZ	1:D:91:LEU:HD11	1.14	1.55
2:B:180:GLU:HG2	1:G:203:PHE:CE1	1.47	1.50
3:I:577:THR:HG23	3:I:754:ALA:CB	1.43	1.49
2:H:363:ARG:HA	1:J:409:ASN:ND2	1.20	1.42
1:D:69:ARG:NE	1:D:91:LEU:HD11	1.33	1.41

The worst 5 of 17 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)
2:E:215:LYS:CE	3:I:628:THR:OG1[3_554]	0.85	1.35
2:E:215:LYS:NZ	3:I:628:THR:OG1[3_554]	0.92	1.28
2:B:457:TRP:N	1:J:84:ASP:OD2[1_565]	1.72	0.48
2:B:362:LYS:CE	1:D:81:LYS:NZ[1_655]	1.75	0.45
2:B:54:VAL:CG2	3:F:282:MET:CG[1_655]	1.75	0.45

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	685/709 (97%)	631 (92%)	51 (7%)	3 (0%)	39	80
1	D	685/709 (97%)	634 (93%)	49 (7%)	2 (0%)	46	83
1	G	685/709 (97%)	635 (93%)	48 (7%)	2 (0%)	46	83
1	J	685/709 (97%)	633 (92%)	50 (7%)	2 (0%)	46	83
2	B	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	39	80
2	E	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	39	80
2	H	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	39	80
2	K	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	39	80
3	C	746/782 (95%)	679 (91%)	64 (9%)	3 (0%)	39	80
3	F	756/782 (97%)	683 (90%)	69 (9%)	4 (0%)	34	77
3	I	756/782 (97%)	685 (91%)	68 (9%)	3 (0%)	39	80
3	L	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	39	80
All	All	8566/8980 (95%)	7944 (93%)	588 (7%)	34 (0%)	39	80

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	503	VAL
2	E	503	VAL
3	F	758	ALA
2	H	503	VAL
2	K	503	VAL

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	618/631 (98%)	610 (99%)	8 (1%)	76	89
1	D	618/631 (98%)	610 (99%)	8 (1%)	76	89
1	G	618/631 (98%)	608 (98%)	10 (2%)	70	88
1	J	618/631 (98%)	608 (98%)	10 (2%)	70	88
2	B	629/669 (94%)	617 (98%)	12 (2%)	65	86
2	E	629/669 (94%)	617 (98%)	12 (2%)	65	86
2	H	629/669 (94%)	617 (98%)	12 (2%)	65	86
2	K	629/669 (94%)	617 (98%)	12 (2%)	65	86
3	C	663/686 (97%)	649 (98%)	14 (2%)	61	85
3	F	669/686 (98%)	656 (98%)	13 (2%)	65	86
3	I	669/686 (98%)	656 (98%)	13 (2%)	65	86
3	L	669/686 (98%)	656 (98%)	13 (2%)	65	86
All	All	7658/7944 (96%)	7521 (98%)	137 (2%)	66	87

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	518	ASP
1	G	554	THR
3	L	135	ILE
3	F	611	ARG
1	G	163	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	550	GLN
1	G	519	HIS
2	K	477	ASN
1	G	31	HIS
1	G	208	GLN

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 carbohydrates 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	693/709 (97%)	0.36	47 (6%) 20 15	66, 164, 326, 490	0
1	D	693/709 (97%)	0.14	21 (3%) 54 42	72, 156, 252, 382	0
1	G	693/709 (97%)	0.42	68 (9%) 10 8	90, 180, 290, 407	0
1	J	693/709 (97%)	0.18	21 (3%) 54 42	105, 181, 273, 414	0
2	B	711/754 (94%)	0.20	41 (5%) 26 19	70, 147, 290, 437	0
2	E	711/754 (94%)	0.21	32 (4%) 37 29	71, 143, 270, 490	0
2	H	711/754 (94%)	0.33	45 (6%) 23 16	82, 170, 287, 498	0
2	K	711/754 (94%)	0.49	63 (8%) 12 9	83, 173, 284, 424	0
3	C	754/782 (96%)	1.00	164 (21%) 1 2	99, 240, 349, 416	0
3	F	762/782 (97%)	0.30	44 (5%) 26 19	87, 174, 295, 481	0
3	I	762/782 (97%)	0.67	90 (11%) 6 6	95, 224, 337, 500	0
3	L	762/782 (97%)	0.85	135 (17%) 2 3	108, 226, 332, 476	0
All	All	8656/8980 (96%)	0.44	771 (8%) 12 9	66, 181, 315, 500	0

The worst 5 of 771 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	95	VAL	16.6
3	C	665	VAL	10.7
3	L	656	ARG	10.6
3	I	96	LEU	9.9
3	L	655	GLY	9.6

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.