



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:09 PM UTC

PDB ID : 6FHH / pdb_00006fhh
Title : Crystal structure of bat influenza A/H17N10 polymerase with viral RNA promoter bound to a 22-mer modified Pol II CTD peptide with serine 5 thiophosphorylated.
Authors : Lukarska, M.; Cusack, S.
Deposited on : 2018-01-14
Resolution : 2.70 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
Mogul : 2022.3.0, CSD as543be (2022)
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

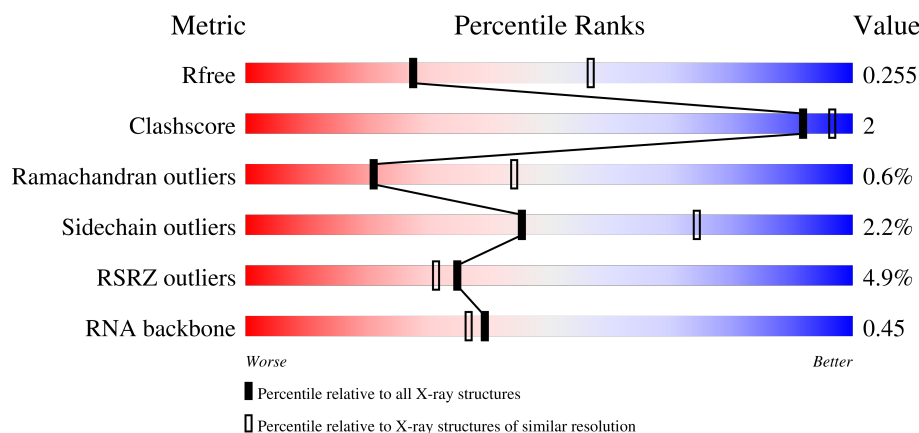
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	738	9% 89% 7% • •
2	B	776	2% 90% 6% •
3	C	809	2% 86% • 10%
4	R	18	67% 6% 28%

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Mol	Chain	Length	Quality of chain
5	V	16	69% 31%
6	X	22	5% 27% 5% 68%
6	Y	22	5% 41% 5% 55%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18457 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
			Total	C	N	O	S			
1	A	709	5770	3665	971	1097	37	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	750	Total	C	N	O	S	0	0	0
			5986	3766	1062	1118	40			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	725	Total	C	N	O	S	0	0	0
			5753	3631	1015	1075	32			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	13	Total	C	N	O	P	0	0	0
			247	111	37	87	12			

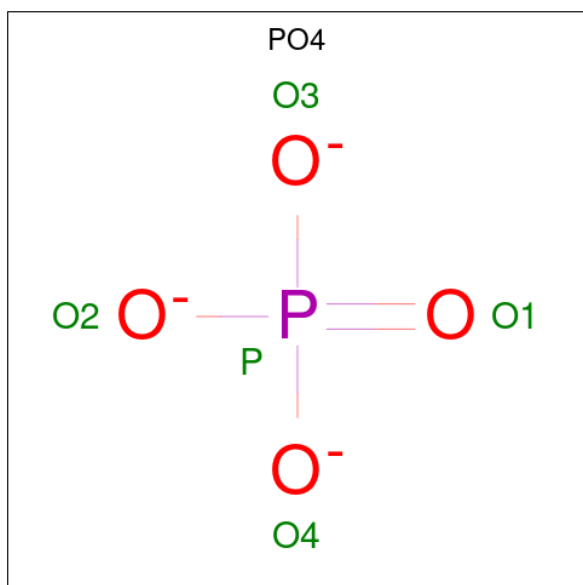
- Molecule 5 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	16	Total	C	N	O	P	0	0	0
			353	157	72	108	16			

- Molecule 6 is a protein called TYR-SER-PRO-THR-TPS-PRO-SER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	7	Total	C	N	O	P	0	0	0
			55	32	7	14	1			
6	Y	10	Total	C	N	O	P	0	0	0
			80	49	10	19	1			

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O P	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	41	Total	O	0	0
			41	41		
9	B	54	Total	O	0	0
			54	54		

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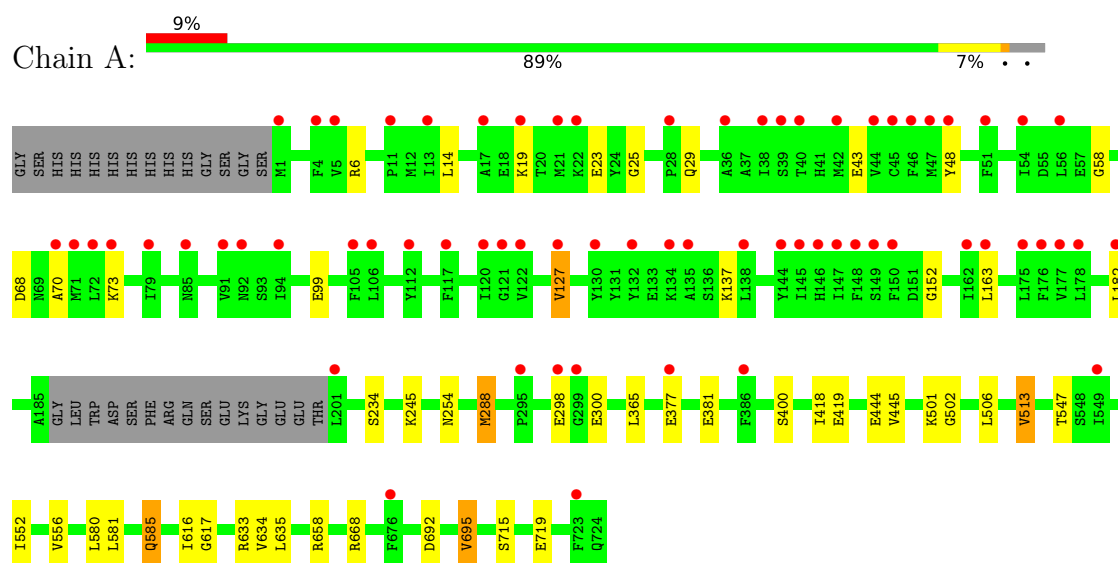
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	35	Total 35	O 35	0	0
9	R	1	Total 1	O 1	0	0
9	V	6	Total 6	O 6	0	0

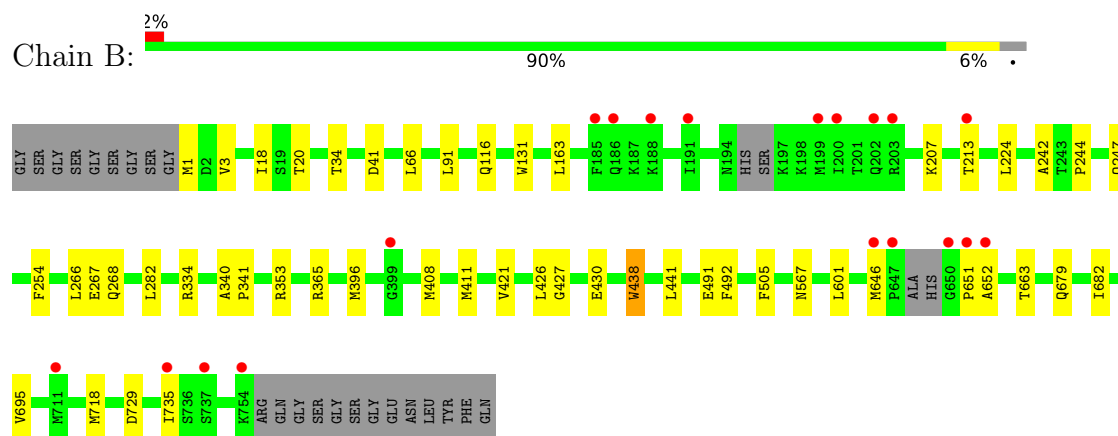
3 Residue-property plots [i](#)

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.

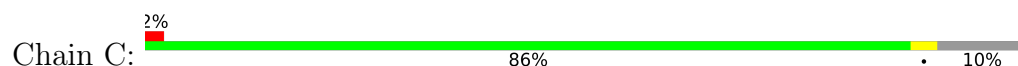
- Molecule 1: Polymerase acidic protein

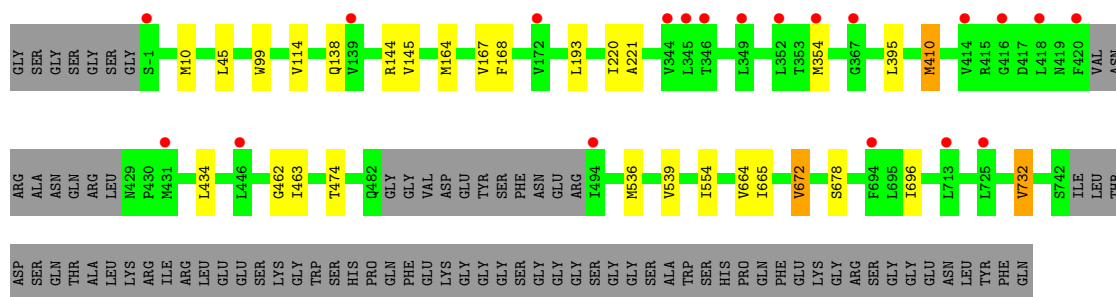


- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 3: Polymerase basic protein 2

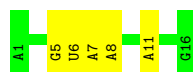




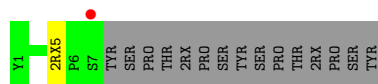
- Molecule 4: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3')



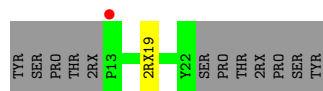
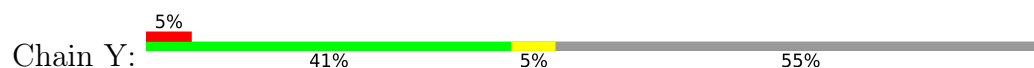
- Molecule 5: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*GP*GP*G)-3')



- Molecule 6: TYR-SER-PRO-THR-TPS-PRO-SER



- Molecule 6: TYR-SER-PRO-THR-TPS-PRO-SER



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	267.77Å 147.81Å 88.41Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.70) 98.6 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.258 0.218 , 0.255	Depositor DCC
R_{free} test set	4534 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18457	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, 2RX

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	0.54	0/5892	0.77	0/7934
2	B	0.54	0/6100	0.81	1/8229 (0.0%)
3	C	0.53	0/5851	0.78	0/7897
4	R	0.36	0/273	0.71	0/421
5	V	0.36	0/397	0.72	0/617
6	X	0.52	0/46	0.48	0/61
6	Y	0.43	0/73	0.61	0/98
All	All	0.53	0/18632	0.78	1/25257 (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	438	TRP	N-CA-C	5.15	117.02	109.24

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	5770	0	5678	22	0
2	B	5986	0	6006	30	0
3	C	5753	0	5876	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	247	0	128	0	0
5	V	353	0	175	0	0
6	X	55	0	48	0	0
6	Y	80	0	66	0	0
7	A	15	0	0	0	0
7	B	35	0	0	0	0
7	C	25	0	0	1	0
8	B	1	0	0	0	0
9	A	41	0	0	0	0
9	B	54	0	0	0	0
9	C	35	0	0	0	0
9	R	1	0	0	0	0
9	V	6	0	0	0	0
All	All	18457	0	17977	59	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 2.

All (59) 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:A:719:GLU:OE1	1:A:719:GLU:N	2.20	0.72
1:A:719:GLU:H	1:A:719:GLU:CD	1.99	0.70
1:A:506:LEU:HD11	1:A:513:VAL:HG22	1.73	0.69
1:A:445:VAL:CG1	1:A:580:LEU:HD22	2.26	0.65
2:B:224:LEU:HD12	2:B:411:MET:HE2	1.78	0.64
1:A:288:MET:HE1	1:A:556:VAL:HG13	1.78	0.64
2:B:1:MET:HE2	2:B:3:VAL:HG22	1.81	0.62
1:A:585:GLN:HG2	2:B:505:PHE:CD2	2.37	0.59
3:C:145:VAL:HG21	3:C:220:ILE:HD11	1.85	0.59
2:B:242:ALA:HB2	2:B:408:MET:HE3	1.84	0.58
1:A:445:VAL:HG13	1:A:580:LEU:HD22	1.85	0.57
2:B:224:LEU:HD22	2:B:244:PRO:HA	1.85	0.57
1:A:547:THR:HG21	1:A:552:ILE:HD12	1.89	0.54
1:A:617:GLY:HA3	2:B:1:MET:HE3	1.90	0.54
2:B:34:THR:HG22	2:B:353:ARG:HB2	1.90	0.52
2:B:224:LEU:CD1	2:B:411:MET:HE2	2.40	0.52
3:C:395:LEU:HD21	3:C:463:ILE:HD11	1.92	0.51
3:C:554:ILE:HD12	3:C:672:VAL:HG13	1.92	0.51
2:B:282:LEU:HG	2:B:441:LEU:HD22	1.92	0.51
3:C:144:ARG:NH2	7:C:901:PO4:O2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:VAL:HG11	3:C:220:ILE:CD1	2.42	0.50
3:C:554:ILE:HD11	3:C:665:ILE:HD12	1.94	0.49
3:C:462:GLY:HA3	3:C:474:THR:HB	1.93	0.49
2:B:427:GLY:HA3	2:B:438:TRP:CD1	2.48	0.48
1:A:506:LEU:HD11	1:A:513:VAL:CG2	2.43	0.48
2:B:679:GLN:HB3	2:B:682:ILE:HD12	1.96	0.48
1:A:635:LEU:HD22	2:B:20:THR:HG22	1.96	0.47
3:C:114:VAL:HG22	3:C:193:LEU:HD22	1.96	0.47
2:B:163:LEU:HD23	2:B:254:PHE:CZ	2.50	0.46
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.97	0.46
3:C:696:ILE:HG23	3:C:732:VAL:HG13	1.98	0.46
2:B:34:THR:HG22	2:B:353:ARG:CB	2.46	0.45
3:C:395:LEU:HD21	3:C:463:ILE:CD1	2.47	0.45
2:B:91:LEU:HD23	2:B:426:LEU:HD13	1.98	0.44
2:B:441:LEU:HD23	2:B:492:PHE:CZ	2.52	0.44
1:A:444:GLU:OE2	1:A:633:ARG:NH1	2.51	0.44
2:B:242:ALA:HB2	2:B:408:MET:CE	2.48	0.43
1:A:300:GLU:HG3	2:B:567:ASN:HB2	2.01	0.43
1:A:418:ILE:HD13	1:A:580:LEU:HD11	2.01	0.43
2:B:268:GLN:HB2	2:B:421:VAL:HG13	2.01	0.43
3:C:138:GLN:HE21	3:C:221:ALA:HB1	1.84	0.43
1:A:6:ARG:HA	1:A:14:LEU:HD21	2.01	0.42
1:A:658:ARG:HD3	2:B:18:ILE:HD11	2.01	0.42
2:B:695:VAL:HG13	2:B:718:MET:HE1	2.01	0.42
2:B:266:LEU:HD13	2:B:421:VAL:HG11	2.02	0.42
3:C:410:MET:HE1	3:C:434:LEU:HD13	2.02	0.42
1:A:616:ILE:HD13	2:B:1:MET:HE1	2.01	0.42
2:B:663:THR:HG21	3:C:99:TRP:CD1	2.55	0.41
2:B:729:ASP:HB3	2:B:735:ILE:HD12	2.02	0.41
1:A:445:VAL:HG11	1:A:580:LEU:HD22	2.00	0.41
3:C:696:ILE:HG23	3:C:732:VAL:CG1	2.51	0.41
3:C:45:LEU:C	3:C:45:LEU:HD23	2.46	0.41
1:A:365:LEU:HD13	1:A:502:GLY:HA2	2.02	0.41
3:C:167:VAL:HG23	3:C:168:PHE:CD2	2.55	0.41
1:A:634:VAL:HG22	2:B:3:VAL:HG11	2.03	0.41
2:B:131:TRP:CD1	2:B:247:GLN:HE22	2.39	0.41
2:B:695:VAL:HG11	3:C:10:MET:HE1	2.02	0.41
1:A:692:ASP:HB3	1:A:695:VAL:HG12	2.03	0.41
1:A:234:SER:OG	2:B:334:ARG:NH2	2.50	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	705/738 (96%)	652 (92%)	43 (6%)	10 (1%)	9	23
2	B	744/776 (96%)	718 (96%)	24 (3%)	2 (0%)	36	60
3	C	719/809 (89%)	692 (96%)	27 (4%)	0	100	100
6	X	4/22 (18%)	3 (75%)	1 (25%)	0	100	100
6	Y	7/22 (32%)	7 (100%)	0	0	100	100
All	All	2179/2367 (92%)	2072 (95%)	95 (4%)	12 (1%)	21	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	68	ASP
1	A	127	VAL
1	A	137	LYS
2	B	651	PRO
1	A	58	GLY
1	A	23	GLU
1	A	70	ALA
1	A	25	GLY
1	A	99	GLU
2	B	652	ALA
1	A	152	GLY

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	633/657 (96%)	611 (96%)	22 (4%)	32	61
2	B	659/676 (98%)	647 (98%)	12 (2%)	51	78
3	C	642/706 (91%)	633 (99%)	9 (1%)	59	82
6	X	6/19 (32%)	6 (100%)	0	100	100
6	Y	9/19 (47%)	9 (100%)	0	100	100
All	All	1949/2077 (94%)	1906 (98%)	43 (2%)	45	74

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	43	GLU
1	A	48	TYR
1	A	73	LYS
1	A	127	VAL
1	A	163	LEU
1	A	182	LEU
1	A	245	LYS
1	A	254	ASN
1	A	288	MET
1	A	298	GLU
1	A	377	GLU
1	A	381	GLU
1	A	400	SER
1	A	419	GLU
1	A	501	LYS
1	A	513	VAL
1	A	581	LEU
1	A	585	GLN
1	A	668	ARG
1	A	695	VAL
1	A	715	SER
2	B	41	ASP
2	B	66	LEU
2	B	116	GLN
2	B	207	LYS
2	B	213	THR
2	B	267	GLU
2	B	365	ARG
2	B	396	MET
2	B	430	GLU

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Mol	Chain	Res	Type
2	B	491	GLU
2	B	601	LEU
2	B	646	MET
3	C	164	MET
3	C	354	MET
3	C	410	MET
3	C	536	MET
3	C	539	VAL
3	C	664	VAL
3	C	672	VAL
3	C	678	SER
3	C	732	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	30	ASN
1	A	59	ASN
1	A	69	ASN
1	A	582	GLN
1	A	720	ASN
2	B	84	GLN
2	B	158	ASN
2	B	186	GLN
2	B	202	GLN
2	B	367	GLN
2	B	549	GLN
2	B	628	ASN
2	B	679	GLN
3	C	138	GLN
3	C	306	GLN
3	C	429	ASN
3	C	473	GLN
3	C	548	ASN
3	C	624	HIS
3	C	660	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	11/18 (61%)	1 (9%)	0
5	V	15/16 (93%)	5 (33%)	1 (6%)
All	All	26/34 (76%)	6 (23%)	1 (3%)

All (6) RNA backbone outliers are listed below:

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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	5	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	2RX	Y	19	6	6,9,10	1.52	2 (33%)	3,12,14	1.29	0
6	2RX	X	5	6	6,9,10	1.30	2 (33%)	3,12,14	1.91	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2RX	Y	19	6	-	0/5/8/10	-
6	2RX	X	5	6	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	19	2RX	P40-O43	2.55	1.52	1.46
6	Y	19	2RX	P40-O42	-2.39	1.50	1.56
6	X	5	2RX	P40-O43	2.09	1.51	1.46
6	X	5	2RX	P40-O42	-2.09	1.51	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	5	2RX	OG-CB-CA	3.03	111.09	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	5	2RX	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PO4	B	808	-	4,4,4	0.94	0	6,6,6	0.46	0
7	PO4	A	803	-	4,4,4	0.94	0	6,6,6	0.42	0
7	PO4	C	902	-	4,4,4	1.01	0	6,6,6	0.49	0
7	PO4	B	802	-	4,4,4	0.87	0	6,6,6	0.54	0
7	PO4	B	806	-	4,4,4	1.02	0	6,6,6	0.58	0
7	PO4	A	801	-	4,4,4	0.93	0	6,6,6	0.53	0
7	PO4	B	803	-	4,4,4	0.89	0	6,6,6	0.54	0
7	PO4	B	805	-	4,4,4	0.86	0	6,6,6	0.55	0
7	PO4	B	807	-	4,4,4	0.97	0	6,6,6	0.55	0
7	PO4	C	904	-	4,4,4	1.06	0	6,6,6	0.43	0
7	PO4	A	802	-	4,4,4	0.96	0	6,6,6	0.59	0
7	PO4	C	901	-	4,4,4	0.99	0	6,6,6	0.39	0
7	PO4	B	804	-	4,4,4	0.87	0	6,6,6	0.51	0
7	PO4	C	903	-	4,4,4	0.91	0	6,6,6	0.45	0
7	PO4	C	905	-	4,4,4	1.00	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	901	PO4	1	0

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

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	709/738 (96%)	0.53	68 (9%)	13	11	49, 80, 228, 288	0
2	B	750/776 (96%)	0.23	19 (2%)	58	55	45, 77, 136, 177	0
3	C	725/809 (89%)	0.30	20 (2%)	55	51	49, 83, 132, 162	0
4	R	13/18 (72%)	-0.00	0	100	100	62, 74, 111, 113	0
5	V	16/16 (100%)	-0.14	0	100	100	64, 70, 103, 167	0
6	X	6/22 (27%)	0.34	1 (16%)	4	3	70, 74, 98, 110	0
6	Y	9/22 (40%)	0.04	1 (11%)	10	8	61, 66, 108, 125	0
All	All	2228/2401 (92%)	0.35	109 (4%)	35	31	45, 80, 193, 288	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	TYR	4.8
1	A	138	LEU	4.3
1	A	175	LEU	4.2
1	A	148	PHE	4.0
1	A	70	ALA	4.0
1	A	40	THR	4.0
2	B	203	ARG	3.9
1	A	549	ILE	3.8
1	A	121	GLY	3.8
1	A	145	ILE	3.7
1	A	5	VAL	3.7
1	A	54	ILE	3.6
3	C	-1	SER	3.6
1	A	117	PHE	3.6
2	B	647	PRO	3.6
3	C	446	LEU	3.4
1	A	182	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	147	ILE	3.3
1	A	120	ILE	3.3
1	A	298	GLU	3.3
1	A	36	ALA	3.3
2	B	399	GLY	3.2
1	A	56	LEU	3.2
1	A	85	ASN	3.1
1	A	72	LEU	3.1
3	C	352	LEU	3.1
1	A	112	TYR	3.0
1	A	106	LEU	3.0
2	B	199	MET	3.0
1	A	162	ILE	2.9
1	A	73	LYS	2.9
1	A	178	LEU	2.9
3	C	345	LEU	2.9
1	A	723	PHE	2.9
1	A	4	PHE	2.8
1	A	71	MET	2.8
3	C	494	ILE	2.8
1	A	39	SER	2.8
1	A	149	SER	2.8
3	C	418	LEU	2.8
1	A	42	MET	2.8
1	A	91	VAL	2.8
6	Y	13	PRO	2.7
2	B	652	ALA	2.7
3	C	713	LEU	2.7
1	A	135	ALA	2.7
1	A	44	VAL	2.7
1	A	146	HIS	2.7
1	A	127	VAL	2.7
1	A	79	ILE	2.6
1	A	19	LYS	2.6
2	B	737	SER	2.6
1	A	177	VAL	2.6
1	A	201	LEU	2.6
3	C	346	THR	2.6
3	C	431	MET	2.6
2	B	185	PHE	2.6
3	C	694	PHE	2.6
3	C	367	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	38	ILE	2.5
2	B	188	LYS	2.5
2	B	191	ILE	2.5
3	C	420	PHE	2.5
1	A	28	PRO	2.5
1	A	105	PHE	2.5
2	B	186	GLN	2.4
1	A	92	ASN	2.4
1	A	45	CYS	2.4
3	C	349	LEU	2.4
3	C	414	VAL	2.4
1	A	17	ALA	2.4
1	A	386	PHE	2.4
1	A	676	PHE	2.4
1	A	132	TYR	2.3
1	A	163	LEU	2.3
2	B	735	ILE	2.3
1	A	130	TYR	2.2
2	B	651	PRO	2.2
3	C	139	VAL	2.2
1	A	22	LYS	2.2
1	A	150	PHE	2.2
2	B	754	LYS	2.2
2	B	711	MET	2.2
1	A	377	GLU	2.2
1	A	47	MET	2.2
2	B	646	MET	2.2
1	A	176	PHE	2.2
1	A	299	GLY	2.2
3	C	725	LEU	2.2
6	X	7	SER	2.2
1	A	94	ILE	2.2
1	A	46	PHE	2.2
1	A	1	MET	2.1
1	A	21	MET	2.1
1	A	122	VAL	2.1
2	B	213	THR	2.1
1	A	11	PRO	2.1
1	A	295	PRO	2.1
3	C	354	MET	2.1
2	B	650	GLY	2.1
1	A	51	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	200	ILE	2.1
3	C	416	GLY	2.0
1	A	134	LYS	2.0
2	B	202	GLN	2.0
1	A	13	ILE	2.0
3	C	172	VAL	2.0
3	C	344	VAL	2.0
1	A	144	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	2RX	X	5	10/11	0.96	0.07	68,78,89,94	0
6	2RX	Y	19	10/11	0.97	0.05	61,64,66,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PO4	A	801	5/5	0.81	0.13	140,144,146,148	0
7	PO4	A	803	5/5	0.82	0.09	126,129,133,133	0
7	PO4	A	802	5/5	0.84	0.20	88,92,98,102	0
7	PO4	B	802	5/5	0.85	0.11	90,90,101,101	0
7	PO4	B	804	5/5	0.85	0.11	98,100,105,109	0
7	PO4	C	904	5/5	0.85	0.14	108,110,113,113	0
7	PO4	C	903	5/5	0.86	0.15	98,101,108,109	0
7	PO4	B	805	5/5	0.86	0.14	101,106,113,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	B	807	5/5	0.89	0.10	89,90,93,93	0
7	PO4	C	901	5/5	0.89	0.11	99,99,105,107	0
7	PO4	C	905	5/5	0.89	0.09	123,126,128,132	0
7	PO4	B	808	5/5	0.90	0.14	110,111,116,119	0
7	PO4	B	806	5/5	0.92	0.20	95,101,111,114	0
7	PO4	B	803	5/5	0.92	0.13	98,100,101,107	0
7	PO4	C	902	5/5	0.92	0.11	95,97,98,99	0
8	ZN	B	801	1/1	0.96	0.06	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.