WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2017 – 02:29 PM EST

PDB ID : 5M3H
Title : Bat influenza A/H17N10 polymerase bound to four heptad repeats of serine 5 phosphorylated Pol II CTD
Authors : Lukarska, M.; Pflug, A.; Cusack, S.
Deposited on : 2016-10-14
Resolution : 2.50 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

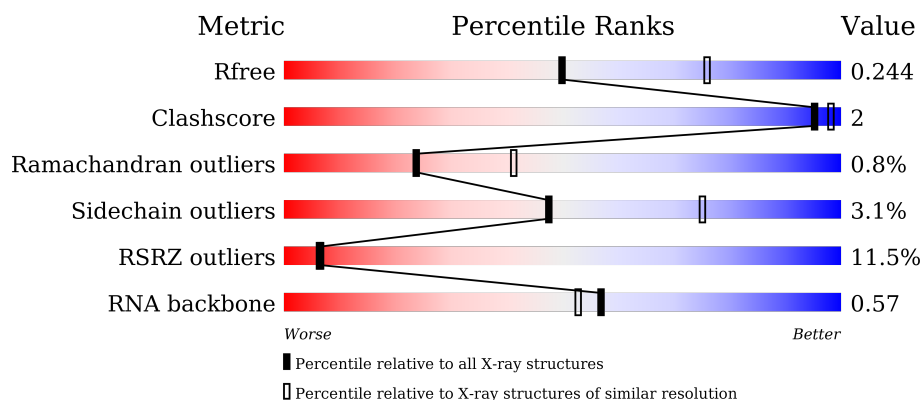|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.50 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.
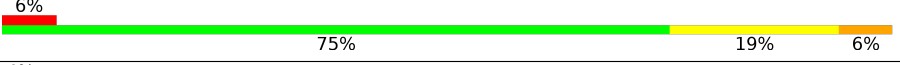
Metric	Percentile Ranks	Value
Rfree		0.244
Clashscore		2
Ramachandran outliers		0.8%
Sidechain outliers		3.1%
RSRZ outliers		11.5%
RNA backbone		0.57

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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 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 <=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	728	20% / 88% 7% · ·
2	B	776	5% / 91% 5% ·
3	C	797	9% / 86% 5% 8%
4	R	18	61% 11% 28%

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Mol	Chain	Length	Quality of chain
5	V	16	6% 75% 19% 6%
6	X	28	4% 18% • 79%
6	Y	28	36% 64%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PO4	A	802	-	-	-	X
8	PO4	A	803	-	-	-	X
8	PO4	A	804	-	-	-	X
8	PO4	B	807	-	-	-	X
8	PO4	C	804	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18529 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	699	5692	3617	959	1079	37	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
			Total	C	N	O	S			
2	B	750	5986	3766	1062	1118	40	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91

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Chain	Residue	Modelled	Actual	Comment	Reference
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
			Total	C	N	O	S			
3	C	730	5796	3657	1025	1082	32	0	0	0

There are 37 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	TRP	-	expression tag	UNP H6QM90
C	772	SER	-	expression tag	UNP H6QM90
C	773	HIS	-	expression tag	UNP H6QM90
C	774	PRO	-	expression tag	UNP H6QM90
C	775	GLN	-	expression tag	UNP H6QM90
C	776	PHE	-	expression tag	UNP H6QM90
C	777	GLU	-	expression tag	UNP H6QM90
C	778	LYS	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	GLY	-	expression tag	UNP H6QM90
C	782	SER	-	expression tag	UNP H6QM90
C	783	GLU	-	expression tag	UNP H6QM90
C	784	ASN	-	expression tag	UNP H6QM90
C	785	LEU	-	expression tag	UNP H6QM90
C	786	TYR	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	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'-pAGUAGUAACAAGAGGG.

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-SEP-PRO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	6	Total 49	C 29	N 6	O 13	P 1	0	0	0
6	Y	10	Total 80	C 49	N 10	O 20	P 1	0	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Zn 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
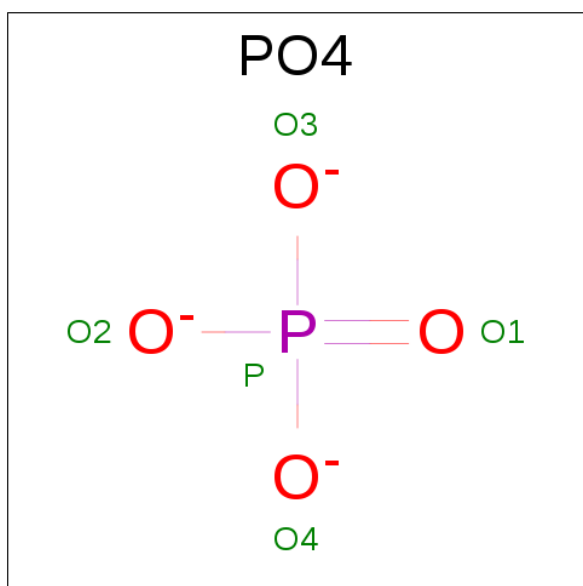
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 5	O 4	P 1	0	0
8	A	1	Total 5	O 4	P 1	0	0
8	A	1	Total 5	O 4	P 1	0	0
8	B	1	Total 5	O 4	P 1	0	0
8	B	1	Total 5	O 4	P 1	0	0
8	B	1	Total 5	O 4	P 1	0	0
8	B	1	Total 5	O 4	P 1	0	0

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

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	78	Total 78	O 78	0	0
9	B	105	Total 105	O 105	0	0
9	C	56	Total 56	O 56	0	0
9	R	3	Total 3	O 3	0	0
9	V	7	Total 7	O 7	0	0
9	X	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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 (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.
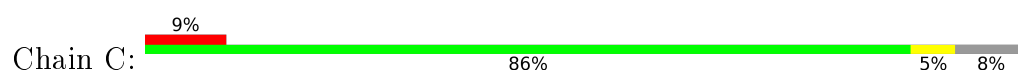
• Molecule 1: Polymerase acidic protein
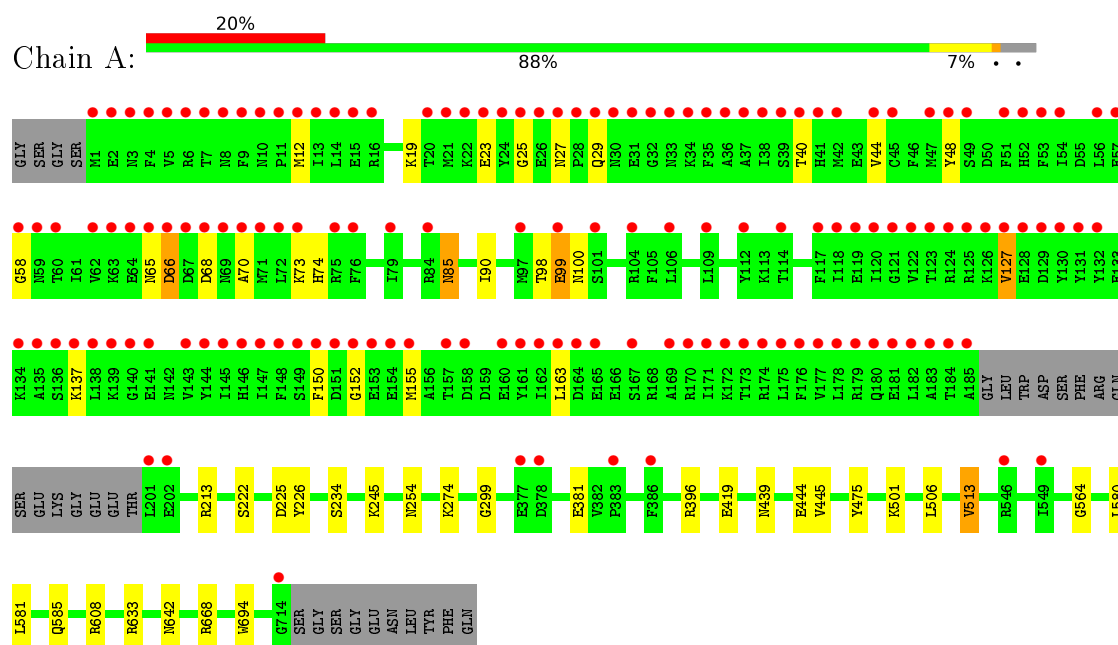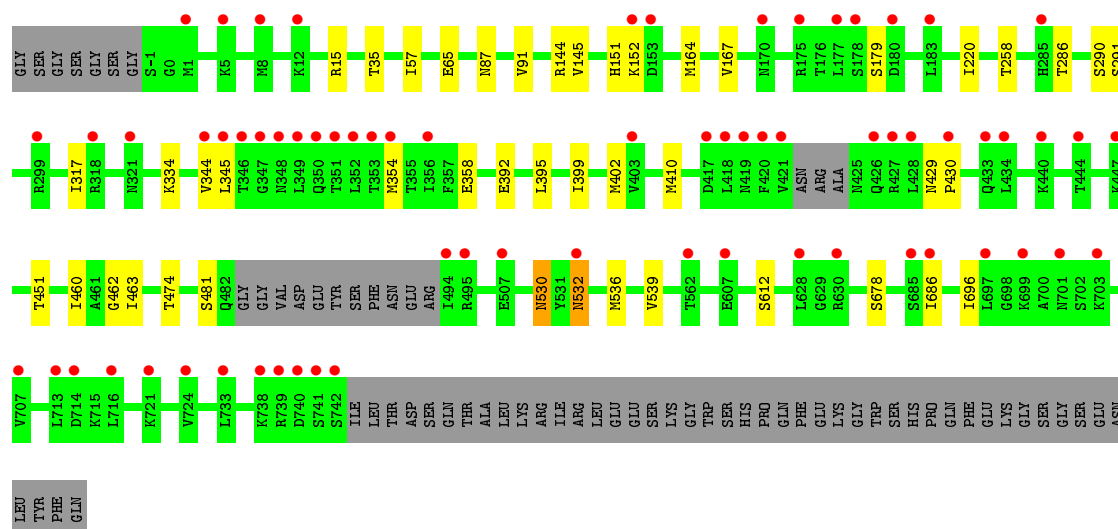

• Molecule 2: RNA-directed RNA polymerase catalytic subunit
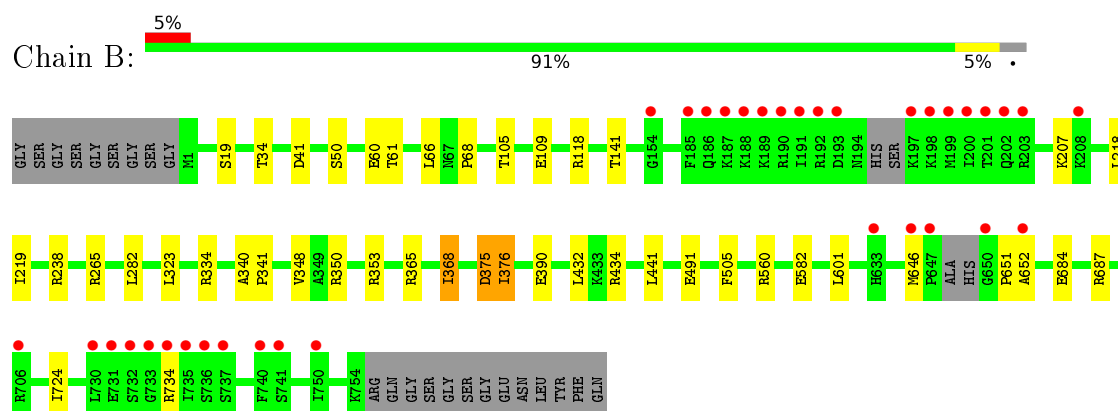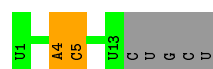

• Molecule 3: Polymerase basic protein 2

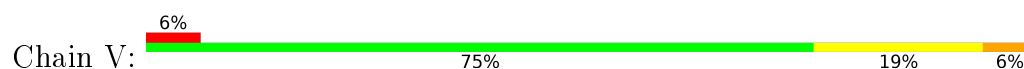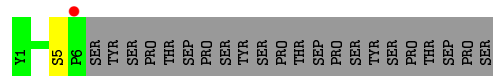- Molecule 4: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*U)-3')

Chain R:

- Molecule 5: RNA 5'-pAGUAGUAACAAGAGGG

Chain V:

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

Chain X:

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

Chain Y:
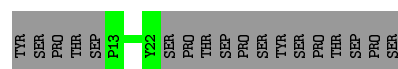
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	269.49Å 147.52Å 88.48Å 90.00° 97.22° 90.00°	Depositor
Resolution (Å)	49.53 – 2.50 49.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.53-2.50) 99.6 (49.53-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.58 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.210 , 0.245 0.209 , 0.244	Depositor DCC
R_{free} test set	5758 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18529	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, SEP

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	0.25	0/5812	0.42	0/7828
2	B	0.24	0/6100	0.48	3/8229 (0.0%)
3	C	0.24	0/5894	0.43	0/7955
4	R	0.23	0/273	0.74	0/421
5	V	0.56	1/397 (0.3%)	0.73	0/617
6	X	0.33	0/40	0.38	0/53
6	Y	0.22	0/73	0.37	0/98
All	All	0.25	1/18589 (0.0%)	0.46	3/25201 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	A	OP3-P	-10.53	1.48	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	376	ILE	N-CA-C	11.62	142.38	111.00
2	B	375	ASP	CB-CA-C	9.40	129.20	110.40
2	B	376	ILE	N-CA-CB	-6.42	96.04	110.80

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	5692	0	5613	17	0
2	B	5986	0	6006	22	0
3	C	5796	0	5923	21	0
4	R	247	0	128	4	0
5	V	353	0	175	1	0
6	X	49	0	40	1	0
6	Y	80	0	64	0	0
7	A	1	0	0	0	0
8	A	15	0	0	0	0
8	B	35	0	0	0	0
8	C	25	0	0	1	0
9	A	78	0	0	0	0
9	B	105	0	0	0	0
9	C	56	0	0	1	0
9	R	3	0	0	0	0
9	V	7	0	0	0	0
9	X	1	0	0	0	0
All	All	18529	0	17949	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.

The worst 5 of 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)
2:B:61:THR:HG22	2:B:218:LEU:HD23	1.36	1.05
4:R:4:A:H5"	4:R:4:A:H8	1.36	0.88
2:B:61:THR:CG2	2:B:218:LEU:HD23	2.06	0.84
4:R:4:A:H5"	4:R:4:A:C8	2.19	0.77
3:C:286:THR:HB	3:C:532:ASN:O	1.86	0.74

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	695/728 (96%)	638 (92%)	45 (6%)	12 (2%)	11	19
2	B	744/776 (96%)	712 (96%)	28 (4%)	4 (0%)	34	55
3	C	724/797 (91%)	702 (97%)	21 (3%)	1 (0%)	56	78
6	X	3/28 (11%)	3 (100%)	0	0	100	100
6	Y	7/28 (25%)	7 (100%)	0	0	100	100
All	All	2173/2357 (92%)	2062 (95%)	94 (4%)	17 (1%)	24	41

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	376	ILE
1	A	66	ASP
1	A	68	ASP
1	A	99	GLU
1	A	19	LYS

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	625/648 (96%)	603 (96%)	22 (4%)	43	70
2	B	659/676 (98%)	641 (97%)	18 (3%)	52	79
3	C	647/703 (92%)	627 (97%)	20 (3%)	47	75
6	X	5/24 (21%)	5 (100%)	0	100	100
6	Y	9/24 (38%)	9 (100%)	0	100	100
All	All	1945/2075 (94%)	1885 (97%)	60 (3%)	47	75

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	207	LYS

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Mol	Chain	Res	Type
2	B	390	GLU
3	C	532	ASN
2	B	350	ARG
2	B	560	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	530	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	11/18 (61%)	2 (18%)	1 (9%)
5	V	15/16 (93%)	3 (20%)	0
All	All	26/34 (76%)	5 (19%)	1 (3%)

All (5) RNA backbone outliers are listed below:

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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	R	4	A

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

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	SEP	X	5	6	7,9,10	1.70	1 (14%)	8,12,14	1.31	2 (25%)
6	SEP	Y	19	6	7,9,10	1.73	1 (14%)	8,12,14	1.49	2 (25%)

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	SEP	X	5	6	-	0/5/8/10	0/0/0/0
6	SEP	Y	19	6	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	5	SEP	P-O1P	3.37	1.61	1.50
6	Y	19	SEP	P-O1P	3.42	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	5	SEP	O-C-CA	-2.04	120.24	125.72
6	Y	19	SEP	O-C-CA	-2.00	120.35	125.72
6	X	5	SEP	OG-CB-CA	2.65	110.57	108.26
6	Y	19	SEP	OG-CB-CA	2.96	110.84	108.26

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
6	X	5	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	#$|Z| > 2$
8	PO4	A	802	-	4,4,4	0.66	0	6,6,6	0.23	0
8	PO4	A	803	-	4,4,4	0.66	0	6,6,6	0.23	0
8	PO4	A	804	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	B	801	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	B	802	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	B	803	-	4,4,4	0.66	0	6,6,6	0.23	0
8	PO4	B	804	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	B	805	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	B	806	-	4,4,4	0.68	0	6,6,6	0.23	0
8	PO4	B	807	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	C	801	-	4,4,4	0.66	0	6,6,6	0.23	0
8	PO4	C	802	-	4,4,4	0.68	0	6,6,6	0.23	0
8	PO4	C	803	-	4,4,4	0.66	0	6,6,6	0.23	0
8	PO4	C	804	-	4,4,4	0.67	0	6,6,6	0.23	0
8	PO4	C	805	-	4,4,4	0.68	0	6,6,6	0.23	0

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
8	PO4	A	802	-	-	0/0/0/0	0/0/0/0
8	PO4	A	803	-	-	0/0/0/0	0/0/0/0
8	PO4	A	804	-	-	0/0/0/0	0/0/0/0
8	PO4	B	801	-	-	0/0/0/0	0/0/0/0
8	PO4	B	802	-	-	0/0/0/0	0/0/0/0
8	PO4	B	803	-	-	0/0/0/0	0/0/0/0
8	PO4	B	804	-	-	0/0/0/0	0/0/0/0
8	PO4	B	805	-	-	0/0/0/0	0/0/0/0
8	PO4	B	806	-	-	0/0/0/0	0/0/0/0
8	PO4	B	807	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PO4	C	801	-	-	0/0/0/0	0/0/0/0
8	PO4	C	802	-	-	0/0/0/0	0/0/0/0
8	PO4	C	803	-	-	0/0/0/0	0/0/0/0
8	PO4	C	804	-	-	0/0/0/0	0/0/0/0
8	PO4	C	805	-	-	0/0/0/0	0/0/0/0

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
8	C	801	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 (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	699/728 (96%)	1.37	149 (21%)	1	1	37, 63, 208, 256	0
2	B	750/776 (96%)	0.35	35 (4%)	35	40	36, 61, 114, 153	0
3	C	730/797 (91%)	0.48	69 (9%)	10	11	40, 70, 118, 157	0
4	R	13/18 (72%)	-0.02	0	100	100	52, 62, 88, 90	0
5	V	16/16 (100%)	-0.29	1 (6%)	23	26	51, 54, 80, 141	0
6	X	5/28 (17%)	1.61	1 (20%)	1	1	66, 68, 77, 91	0
6	Y	9/28 (32%)	0.13	0	100	100	58, 66, 107, 119	0
All	All	2222/2391 (92%)	0.71	255 (11%)	6	6	36, 65, 175, 256	0

The worst 5 of 255 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	GLY	28.7
1	A	122	VAL	16.3
1	A	24	TYR	15.2
1	A	132	TYR	15.1
1	A	70	ALA	14.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	SEP	X	5	10/11	0.93	0.16	-	65,74,89,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
6	SEP	Y	19	10/11	0.97	0.14	-	52,57,63,63	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
8	PO4	C	804	5/5	0.81	0.33	9.81	75,83,94,98	0
8	PO4	B	807	5/5	0.86	0.33	8.89	78,81,84,105	0
8	PO4	A	802	5/5	0.82	0.25	3.13	93,93,110,110	0
8	PO4	A	803	5/5	0.89	0.23	2.43	67,74,91,92	0
8	PO4	A	804	5/5	0.90	0.23	2.15	94,101,119,125	0
8	PO4	C	805	5/5	0.88	0.20	0.27	88,93,95,98	0
8	PO4	B	802	5/5	0.93	0.17	-0.50	68,69,85,92	0
8	PO4	C	801	5/5	0.88	0.15	-0.91	72,83,90,100	0
8	PO4	B	804	5/5	0.88	0.19	-1.08	47,59,67,89	0
8	PO4	C	802	5/5	0.95	0.11	-1.25	75,77,93,93	0
8	PO4	B	806	5/5	0.92	0.14	-1.73	95,105,116,120	0
8	PO4	B	801	5/5	0.97	0.11	-2.24	64,67,93,94	0
8	PO4	B	805	5/5	0.99	0.11	-2.75	63,66,67,72	0
8	PO4	B	803	5/5	0.94	0.12	-4.21	65,68,80,83	0
7	ZN	A	801	1/1	0.97	0.22	-	74,74,74,74	0
8	PO4	C	803	5/5	0.93	0.14	-	62,67,81,86	0

6.5 Other polymers (i)

There are no such residues in this entry.