



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:22 am BST

PDB ID : 4WSB
Title : Bat Influenza A polymerase with bound vRNA promoter
Authors : Cusack, S.; Pflug, A.; Guilligay, D.; Reich, S.
Deposited on : 2014-10-26
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

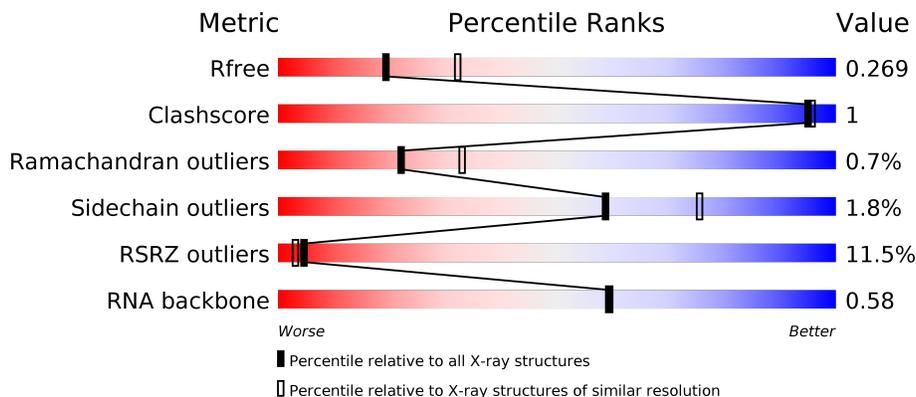
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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 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	
2	B	776	
3	C	787	
4	R	18	

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Mol	Chain	Length	Quality of chain
5	V	16	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '6%', a large green segment in the middle labeled '69%', and a yellow segment on the right labeled '31%'.</p>

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 18185 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 PA.

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 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
			Total	C	N	O	S			
2	B	745	5940	3737	1052	1111	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
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 PB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	734	5839	3680	1037	1090	32	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP H6QM90
C	-6	SER	-	expression tag	UNP H6QM90
C	-5	GLY	-	expression tag	UNP H6QM90
C	-4	SER	-	expression tag	UNP H6QM90
C	-3	GLY	-	expression tag	UNP H6QM90
C	-2	SER	-	expression tag	UNP H6QM90
C	-1	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	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	SER	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLU	-	expression tag	UNP H6QM90
C	775	ASN	-	expression tag	UNP H6QM90
C	776	LEU	-	expression tag	UNP H6QM90
C	777	TYR	-	expression tag	UNP H6QM90
C	778	PHE	-	expression tag	UNP H6QM90
C	779	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called Influenza A polymerase vRNA promoter 3' end.

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

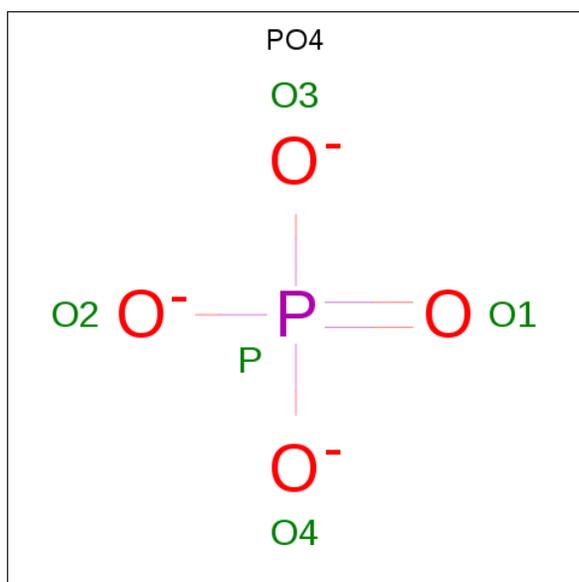
- Molecule 5 is a RNA chain called Influenza A polymerase vRNA promoter 5' end.

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

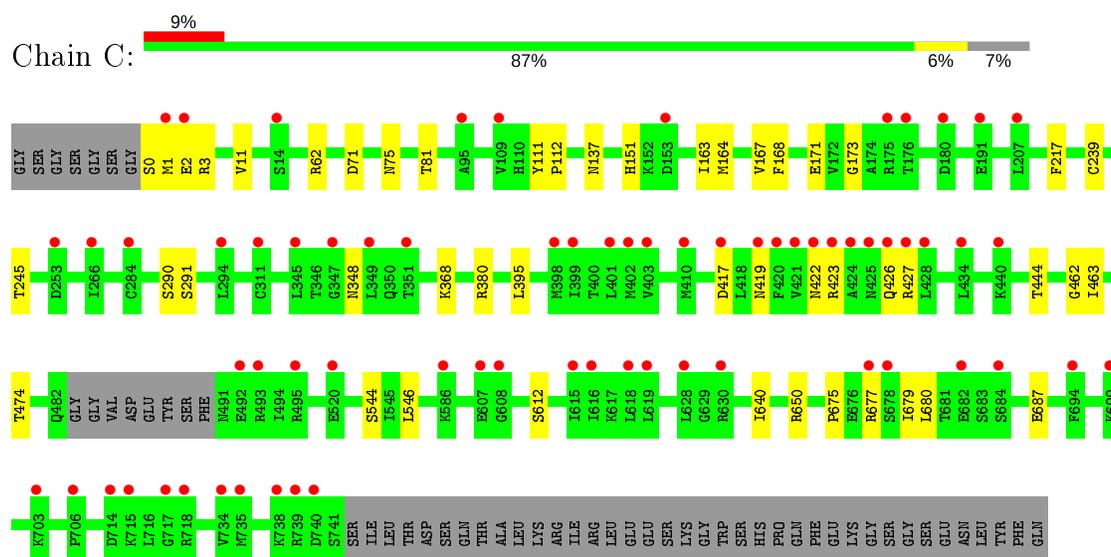
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

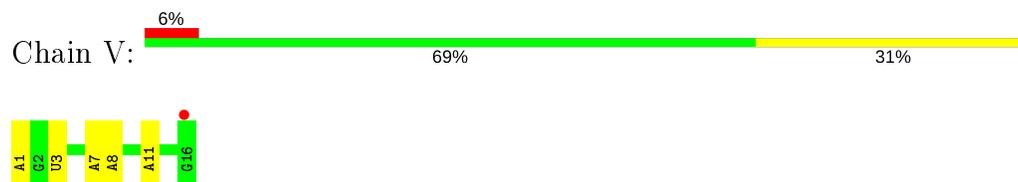
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	11	Total	O	0	0
			11	11		
8	C	9	Total	O	0	0
			9	9		
8	R	1	Total	O	0	0
			1	1		
8	V	3	Total	O	0	0
			3	3		



- Molecule 4: Influenza A polymerase vRNA promoter 3' end



- Molecule 5: Influenza A polymerase vRNA promoter 5' end



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.19Å 149.32Å 88.62Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.65) 99.5 (20.00-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.67Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.215 , 0.267 0.224 , 0.269	Depositor DCC
R_{free} test set	4756 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18185	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

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	0.25	0/6052	0.43	0/8164
3	C	0.24	0/5938	0.43	0/8015
4	R	0.21	0/273	0.75	0/421
5	V	0.58	1/397 (0.3%)	0.72	0/617
All	All	0.26	1/18472 (0.0%)	0.44	0/25045

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	A	OP3-P	-10.35	1.48	1.61

There are no bond angle outliers.

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	14	0
2	B	5940	0	5948	14	0
3	C	5839	0	5968	18	0
4	R	247	0	128	1	0
5	V	353	0	175	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	20	0	0	0	0
7	B	45	0	0	0	0
7	C	15	0	0	0	0
8	A	9	0	0	0	0
8	B	11	0	0	0	0
8	C	9	0	0	0	0
8	R	1	0	0	0	0
8	V	3	0	0	0	0
All	All	18185	0	17832	42	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 1.

The worst 5 of 42 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:C:348:ASN:ND2	3:C:417:ASP:OD1	2.28	0.65
1:A:506:LEU:HD11	1:A:513:VAL:CG2	2.33	0.58
1:A:234:SER:OG	2:B:334:ARG:NH2	2.37	0.57
1:A:218:SER:O	2:B:316:ARG:NE	2.39	0.56
2:B:439:ASP:OD1	2:B:440:GLY:N	2.37	0.56

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	695/738 (94%)	646 (93%)	42 (6%)	7 (1%)	15 23
2	B	735/776 (95%)	700 (95%)	34 (5%)	1 (0%)	51 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	730/787 (93%)	689 (94%)	34 (5%)	7 (1%)	15 23
All	All	2160/2301 (94%)	2035 (94%)	110 (5%)	15 (1%)	22 33

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
3	C	677	ARG
3	C	679	ILE
1	A	137	LYS
3	C	173	GLY

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	625/657 (95%)	609 (97%)	16 (3%)	46 64
2	B	654/676 (97%)	644 (98%)	10 (2%)	65 80
3	C	652/695 (94%)	643 (99%)	9 (1%)	67 81
All	All	1931/2028 (95%)	1896 (98%)	35 (2%)	59 75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	668	ARG
2	B	213	THR
3	C	380	ARG
2	B	41	ASP
2	B	64	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

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

All (4) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	804	-	4,4,4	0.90	0	6,6,6	0.45	0
7	PO4	A	804	-	4,4,4	0.90	0	6,6,6	0.40	0
7	PO4	B	808	-	4,4,4	0.90	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	A	803	-	4,4,4	0.92	0	6,6,6	0.41	0
7	PO4	B	809	-	4,4,4	0.91	0	6,6,6	0.42	0
7	PO4	B	806	-	4,4,4	0.92	0	6,6,6	0.46	0
7	PO4	B	801	-	4,4,4	0.90	0	6,6,6	0.51	0
7	PO4	C	803	-	4,4,4	0.90	0	6,6,6	0.45	0
7	PO4	B	805	-	4,4,4	0.93	0	6,6,6	0.40	0
7	PO4	C	802	-	4,4,4	0.87	0	6,6,6	0.44	0
7	PO4	A	805	-	4,4,4	0.91	0	6,6,6	0.50	0
7	PO4	A	802	-	4,4,4	0.91	0	6,6,6	0.41	0
7	PO4	B	802	-	4,4,4	0.89	0	6,6,6	0.49	0
7	PO4	C	801	-	4,4,4	0.91	0	6,6,6	0.46	0
7	PO4	B	803	-	4,4,4	0.89	0	6,6,6	0.43	0
7	PO4	B	807	-	4,4,4	0.89	0	6,6,6	0.46	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.

No monomer is involved in short contacts.

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	699/738 (94%)	1.25	147 (21%) 1 1	52, 91, 246, 298	0
2	B	745/776 (96%)	0.22	37 (4%) 28 25	50, 92, 139, 169	0
3	C	734/787 (93%)	0.40	69 (9%) 8 6	56, 93, 146, 171	0
4	R	13/18 (72%)	0.11	0 100 100	72, 88, 103, 111	0
5	V	16/16 (100%)	-0.15	1 (6%) 20 17	74, 80, 97, 159	0
All	All	2207/2335 (94%)	0.60	254 (11%) 4 3	50, 92, 217, 298	0

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ARG	14.9
1	A	146	HIS	13.1
1	A	20	THR	13.1
1	A	26	GLU	12.7
1	A	71	MET	12.7

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](#)

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	B	808	5/5	0.80	0.24	144,145,151,154	0
7	PO4	B	805	5/5	0.84	0.22	101,103,115,121	0
7	PO4	B	807	5/5	0.86	0.20	105,112,123,126	0
7	PO4	A	803	5/5	0.88	0.14	96,107,110,117	0
7	PO4	B	801	5/5	0.89	0.12	92,94,110,121	0
7	PO4	C	803	5/5	0.90	0.22	108,116,117,119	0
7	PO4	B	804	5/5	0.91	0.21	78,84,103,112	0
7	PO4	C	802	5/5	0.92	0.17	97,101,119,120	0
7	PO4	B	809	5/5	0.93	0.19	115,120,126,130	0
7	PO4	A	805	5/5	0.93	0.18	100,109,113,116	0
7	PO4	B	803	5/5	0.93	0.11	91,92,100,106	0
7	PO4	B	802	5/5	0.93	0.20	91,94,98,98	0
7	PO4	A	804	5/5	0.93	0.20	101,107,111,112	0
7	PO4	A	802	5/5	0.94	0.20	82,89,100,101	0
7	PO4	C	801	5/5	0.96	0.10	87,87,93,94	0
7	PO4	B	806	5/5	0.97	0.18	88,91,105,113	0
6	ZN	A	801	1/1	0.99	0.11	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.