Full wwPDB X-ray Structure Validation 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 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 following versions of software and data (see references ⓘ) were used in the production of this report:

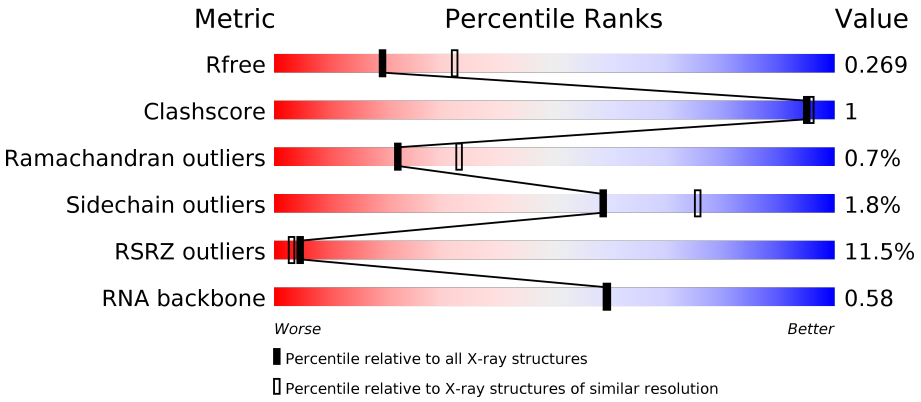
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=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	20% 89% 5% 5%
2	B	776	5% 91% 5% .
3	C	787	9% 87% 6% 7%
4	R	18	61% 11% 28%

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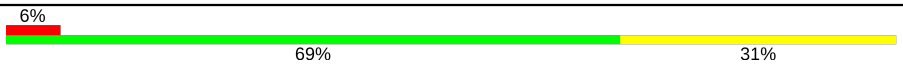
Mol	Chain	Length	Quality of chain
5	V	16	

2 Entry composition

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
1	A	699	Total	C	N	O	S	0	0	0
			5692	3617	959	1079	37			

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	745	Total	C	N	O	S	0	0	0
			5940	3737	1052	1111	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 PB2.

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

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
4	R	13	Total	C	N	O	P	0	0	0
			247	111	37	87	12			

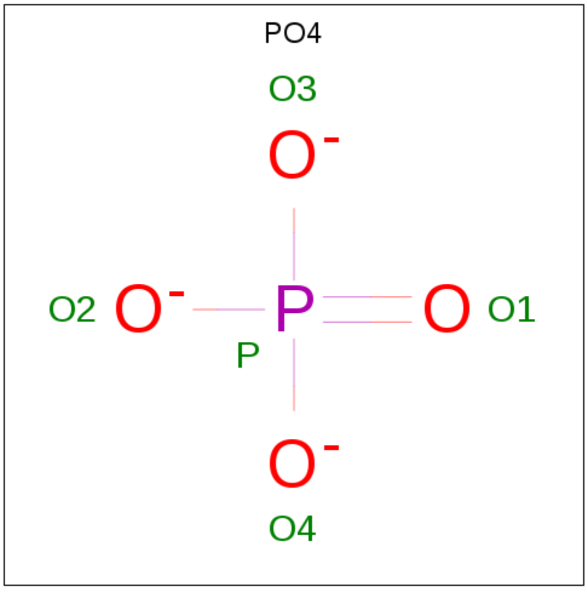
- Molecule 5 is a RNA chain called Influenza A polymerase vRNA promoter 5' end.

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 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: O_4P).



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 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

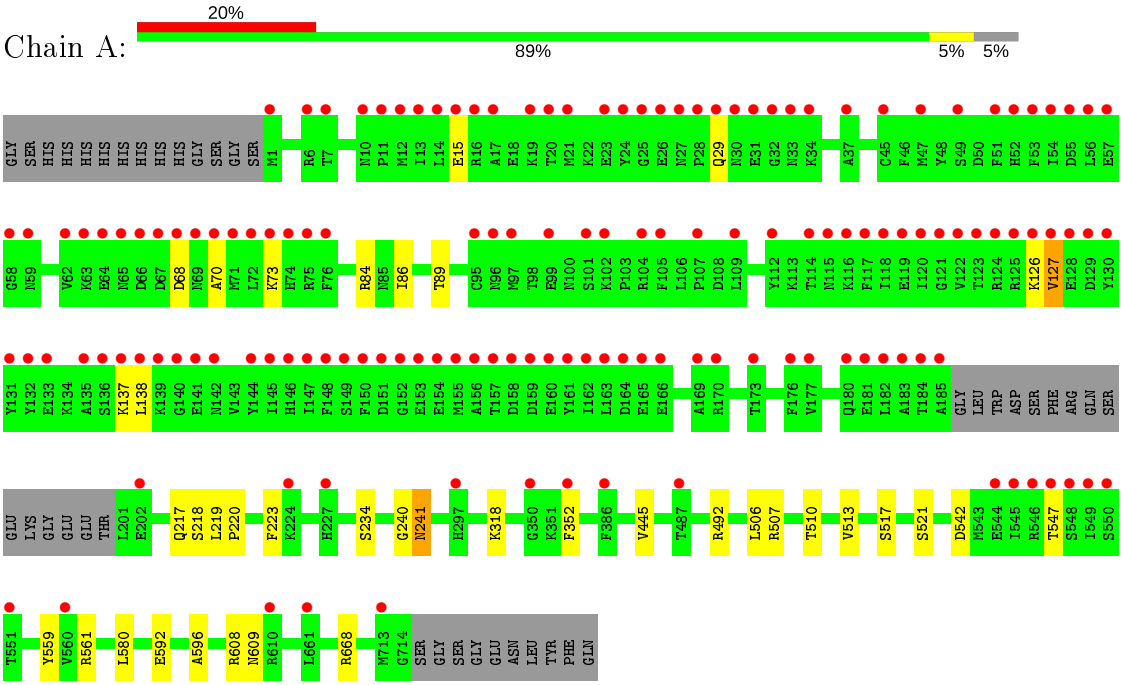
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	9	Total O 9 9	0	0
8	B	11	Total O 11 11	0	0
8	C	9	Total O 9 9	0	0
8	R	1	Total O 1 1	0	0
8	V	3	Total O 3 3	0	0

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 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.

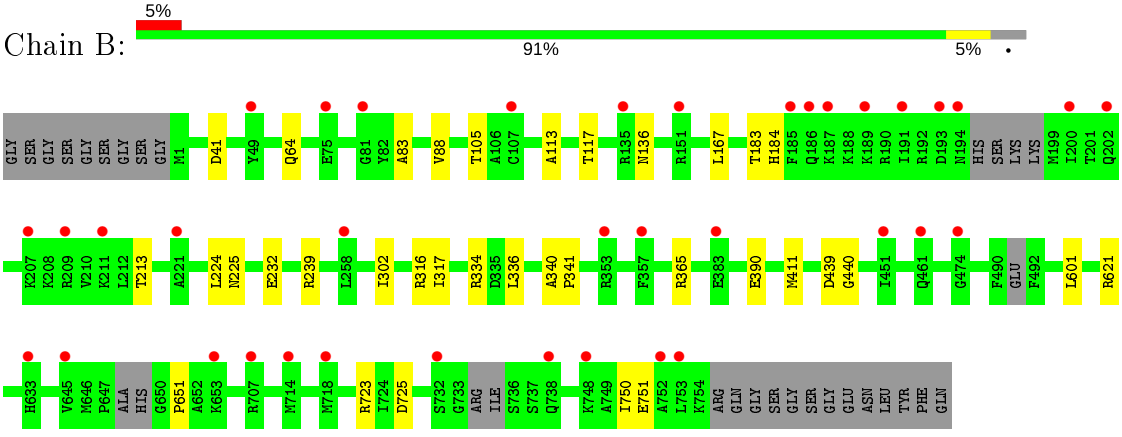
- Molecule 1: Polymerase PA

Chain A:

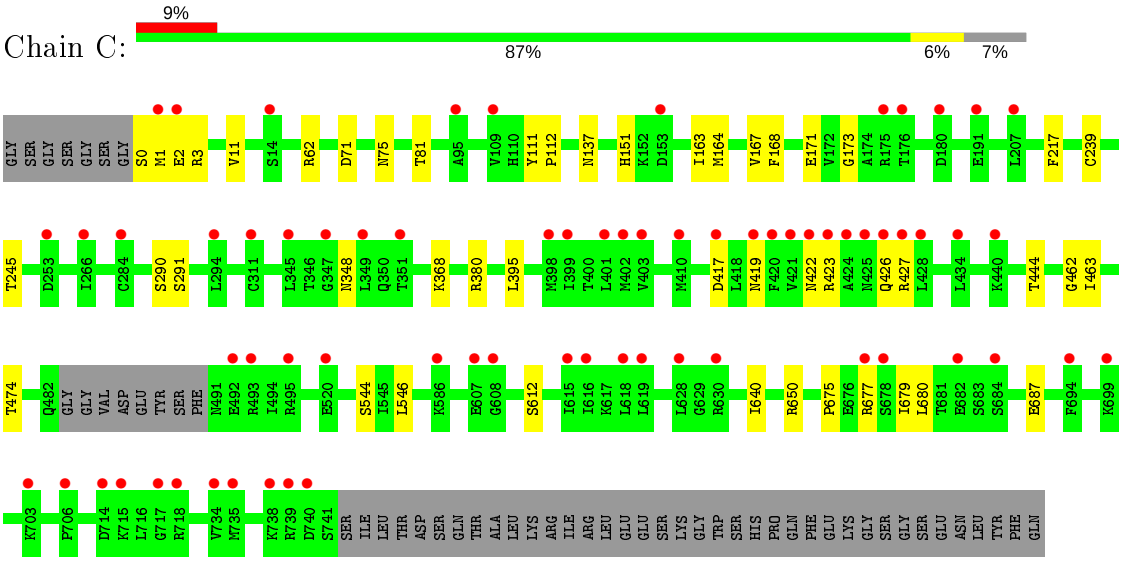


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain B:

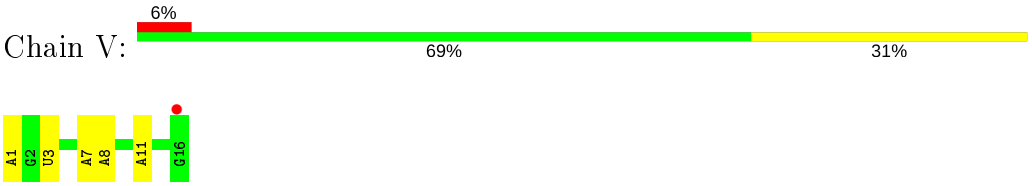


- Molecule 3: Polymerase PB2



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

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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.35 (at 2.67Å)	Xtriage
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	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.9	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	18185	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage'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.*

[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

5.1 Standard geometry

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

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.

All (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
2:B:88:VAL:HG21	2:B:317:ILE:HD13	1.89	0.55
3:C:650:ARG:NH1	3:C:687:GLU:OE2	2.42	0.52
2:B:113:ALA:O	2:B:117:THR:OG1	2.26	0.51
3:C:151:HIS:ND1	3:C:151:HIS:O	2.44	0.51
3:C:290:SER:O	3:C:291:SER:OG	2.28	0.50
1:A:561:ARG:NH2	5:V:3:U:OP1	2.44	0.49
3:C:422:ASN:N	3:C:426:GLN:O	2.39	0.49
2:B:232:GLU:OE2	2:B:239:ARG:NH1	2.45	0.49
3:C:419:ASN:OD1	3:C:427:ARG:NH1	2.45	0.49
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.95	0.48
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.45	0.47
1:A:86:ILE:O	1:A:89:THR:N	2.48	0.47
1:A:241:ASN:N	1:A:241:ASN:OD1	2.47	0.47
3:C:675:PRO:CB	3:C:680:LEU:HD12	2.46	0.46
2:B:83:ALA:HB3	2:B:317:ILE:HD11	1.98	0.46
1:A:219:LEU:HB2	1:A:220:PRO:CD	2.45	0.45
1:A:445:VAL:HG11	1:A:580:LEU:HD22	1.98	0.45
3:C:395:LEU:HD21	3:C:463:ILE:HD11	1.99	0.45
1:A:219:LEU:HD13	1:A:223:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ARG:NH2	4:R:9:U:O2'	2.51	0.44
3:C:1:MET:O	3:C:3:ARG:N	2.51	0.44
2:B:224:LEU:HD13	2:B:411:MET:HE2	2.00	0.43
3:C:163:ILE:O	3:C:167:VAL:HG22	2.18	0.43
3:C:168:PHE:HB3	3:C:171:GLU:HG2	2.01	0.42
3:C:612:SER:OG	3:C:680:LEU:HD22	2.18	0.42
2:B:750:ILE:HG23	3:C:11:VAL:HG11	2.01	0.42
1:A:318:LYS:NZ	1:A:542:ASP:OD2	2.44	0.42
3:C:546:LEU:HD11	3:C:640:ILE:CD1	2.49	0.42
1:A:219:LEU:C	1:A:219:LEU:HD12	2.41	0.41
1:A:596:ALA:HB2	3:C:239:CYS:HB2	2.02	0.41
2:B:167:LEU:HD23	2:B:336:LEU:HD11	2.02	0.41
2:B:723:ARG:NH1	2:B:751:GLU:OE1	2.53	0.41
3:C:71:ASP:OD1	3:C:75:ASN:N	2.54	0.41
1:A:521:SER:HB3	1:A:559:TYR:CE1	2.56	0.41
2:B:183:THR:HG22	2:B:184:HIS:N	2.36	0.41
3:C:462:GLY:HA3	3:C:474:THR:HB	2.03	0.41
3:C:111:TYR:N	3:C:112:PRO:CD	2.84	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	695/738 (94%)	646 (93%)	42 (6%)	7 (1%)	15	23
2	B	735/776 (95%)	700 (95%)	34 (5%)	1 (0%)	51	69
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

All (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
1	A	68	ASP
1	A	127	VAL
1	A	240	GLY
2	B	651	PRO
3	C	368	LYS
3	C	423	ARG
1	A	70	ALA
1	A	609	ASN
3	C	2	GLU
3	C	137	ASN

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

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	29	GLN
1	A	73	LYS
1	A	84	ARG
1	A	127	VAL
1	A	138	LEU
1	A	217	GLN
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	352	PHE
1	A	492	ARG
1	A	510	THR
1	A	517	SER
1	A	547	THR
1	A	592	GLU
1	A	608	ARG
1	A	668	ARG
2	B	41	ASP
2	B	64	GLN
2	B	105	THR
2	B	213	THR
2	B	302	ILE
2	B	365	ARG
2	B	390	GLU
2	B	601	LEU
2	B	621	ARG
2	B	725	ASP
3	C	0	SER
3	C	62	ARG
3	C	81	THR
3	C	164	MET
3	C	217	PHE
3	C	245	THR
3	C	380	ARG
3	C	444	THR
3	C	544	SER

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

5.3.3 RNA

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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

All (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
1	A	66	ASP	12.5
1	A	28	PRO	11.6
1	A	24	TYR	11.3
1	A	13	ILE	11.3
1	A	58	GLY	11.0
1	A	121	GLY	11.0
1	A	12	MET	11.0
1	A	33	ASN	10.6
1	A	549	ILE	10.5
1	A	183	ALA	10.4
1	A	126	LYS	10.1
1	A	151	ASP	10.0
1	A	51	PHE	9.8
1	A	162	ILE	9.4
1	A	123	THR	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	21	MET	8.8
1	A	157	THR	8.8
1	A	32	GLY	8.6
1	A	72	LEU	8.5
1	A	155	MET	8.5
1	A	147	ILE	8.4
1	A	140	GLY	8.3
1	A	37	ALA	8.1
1	A	67	ASP	7.9
1	A	114	THR	7.8
1	A	7	THR	7.5
1	A	115	ASN	7.5
1	A	1	MET	6.8
1	A	70	ALA	6.8
1	A	176	PHE	6.6
1	A	548	SER	6.6
1	A	125	ARG	6.5
1	A	10	ASN	6.3
1	A	49	SER	6.3
1	A	550	SER	6.2
1	A	30	ASN	6.1
1	A	185	ALA	6.0
1	A	27	ASN	6.0
1	A	99	GLU	6.0
1	A	184	THR	6.0
1	A	181	GLU	5.9
1	A	159	ASP	5.9
3	C	424	ALA	5.9
3	C	347	GLY	5.9
1	A	144	TYR	5.8
1	A	53	PHE	5.8
1	A	132	TYR	5.7
1	A	65	ASN	5.7
1	A	547	THR	5.7
1	A	25	GLY	5.7
1	A	166	GLU	5.7
1	A	63	LYS	5.6
1	A	145	ILE	5.6
1	A	129	ASP	5.5
1	A	177	VAL	5.5
1	A	120	ILE	5.5
2	B	191	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	104	ARG	5.4
1	A	545	ILE	5.4
1	A	153	GLU	5.4
1	A	64	GLU	5.3
3	C	349	LEU	5.3
1	A	141	GLU	5.3
1	A	17	ALA	5.2
1	A	62	VAL	5.2
3	C	628	LEU	5.2
3	C	423	ARG	5.1
1	A	164	ASP	5.1
1	A	142	ASN	5.0
1	A	54	ILE	5.0
1	A	75	ARG	4.9
1	A	130	TYR	4.9
2	B	200	ILE	4.9
1	A	55	ASP	4.9
1	A	74	HIS	4.9
1	A	297	HIS	4.9
3	C	715	LYS	4.9
1	A	112	TYR	4.8
1	A	152	GLY	4.7
1	A	56	LEU	4.7
3	C	684	SER	4.7
1	A	158	ASP	4.7
3	C	495	ARG	4.7
1	A	59	ASN	4.6
1	A	124	ARG	4.6
1	A	117	PHE	4.5
3	C	425	ASN	4.5
3	C	703	LYS	4.4
1	A	136	SER	4.4
1	A	118	ILE	4.4
1	A	160	GLU	4.4
1	A	180	GLN	4.4
1	A	161	TYR	4.4
3	C	176	THR	4.3
2	B	194	ASN	4.3
1	A	165	GLU	4.3
3	C	734	VAL	4.3
3	C	740	ASP	4.3
1	A	47	MET	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	153	ASP	4.2
1	A	135	ALA	4.2
1	A	57	GLU	4.2
5	V	16	G	4.2
3	C	739	ARG	4.2
3	C	175	ARG	4.2
1	A	128	GLU	4.1
1	A	386	PHE	4.1
2	B	645	VAL	4.0
1	A	127	VAL	4.0
3	C	682	GLU	4.0
3	C	706	PRO	3.9
1	A	19	LYS	3.9
1	A	97	MET	3.9
2	B	732	SER	3.9
3	C	493	ARG	3.8
1	A	45	CYS	3.8
1	A	14	LEU	3.8
1	A	23	GLU	3.8
1	A	150	PHE	3.8
1	A	154	GLU	3.7
3	C	630	ARG	3.7
1	A	133	GLU	3.7
3	C	440	LYS	3.7
1	A	69	ASN	3.7
3	C	422	ASN	3.7
3	C	426	GLN	3.6
1	A	173	THR	3.6
2	B	752	ALA	3.6
1	A	29	GLN	3.6
1	A	202	GLU	3.5
3	C	1	MET	3.5
3	C	738	LYS	3.5
3	C	420	PHE	3.4
1	A	156	ALA	3.4
1	A	11	PRO	3.4
1	A	551	THR	3.4
2	B	135	ARG	3.4
3	C	492	GLU	3.3
1	A	73	LYS	3.3
3	C	284	CYS	3.3
1	A	119	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	345	LEU	3.3
1	A	610	ARG	3.2
1	A	182	LEU	3.2
2	B	353	ARG	3.2
2	B	383	GLU	3.2
2	B	189	LYS	3.2
3	C	311	CYS	3.1
1	A	131	TYR	3.1
1	A	560	VAL	3.1
3	C	616	ILE	3.0
1	A	15	GLU	3.0
3	C	428	LEU	3.0
2	B	707	ARG	3.0
1	A	122	VAL	3.0
1	A	105	PHE	3.0
3	C	618	LEU	3.0
1	A	139	LYS	2.9
1	A	76	PHE	2.9
1	A	6	ARG	2.9
1	A	137	LYS	2.9
1	A	148	PHE	2.9
3	C	677	ARG	2.9
3	C	417	ASP	2.8
1	A	149	SER	2.8
2	B	653	LYS	2.8
3	C	434	LEU	2.8
1	A	544	GLU	2.7
2	B	193	ASP	2.7
2	B	718	MET	2.7
2	B	753	LEU	2.7
1	A	170	ARG	2.7
2	B	185	PHE	2.7
3	C	109	VAL	2.7
1	A	96	ASN	2.7
1	A	109	LEU	2.6
2	B	209	ARG	2.6
1	A	95	CYS	2.6
1	A	169	ALA	2.6
3	C	608	GLY	2.6
2	B	151	ARG	2.6
2	B	357	PHE	2.6
1	A	52	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	2.6
3	C	678	SER	2.5
3	C	735	MET	2.5
1	A	34	LYS	2.5
3	C	2	GLU	2.5
3	C	402	MET	2.5
1	A	102	LYS	2.5
2	B	748	LYS	2.5
3	C	398	MET	2.5
3	C	401	LEU	2.4
3	C	410	MET	2.4
1	A	138	LEU	2.4
3	C	694	PHE	2.4
1	A	546	ARG	2.4
3	C	399	ILE	2.4
1	A	107	PRO	2.4
3	C	351	THR	2.4
3	C	419	ASN	2.3
2	B	451	ILE	2.3
2	B	107	CYS	2.3
3	C	421	VAL	2.3
1	A	487	THR	2.3
3	C	180	ASP	2.3
1	A	31	GLU	2.3
3	C	607	GLU	2.3
2	B	738	GLN	2.3
3	C	717	GLY	2.3
3	C	615	ILE	2.3
3	C	586	LYS	2.3
2	B	211	LYS	2.3
2	B	461	GLN	2.2
1	A	713	MET	2.2
2	B	207	LYS	2.2
3	C	294	LEU	2.2
3	C	207	LEU	2.2
3	C	699	LYS	2.2
2	B	474	GLY	2.2
1	A	224	LYS	2.2
2	B	258	LEU	2.2
1	A	350	GLY	2.2
2	B	81	GLY	2.2
1	A	163	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	253	ASP	2.2
1	A	227	HIS	2.2
2	B	187	LYS	2.2
2	B	714	MET	2.1
1	A	101	SER	2.1
3	C	619	LEU	2.1
3	C	95	ALA	2.1
3	C	266	ILE	2.1
1	A	352	PHE	2.1
3	C	403	VAL	2.1
3	C	191	GLU	2.1
3	C	714	ASP	2.1
2	B	633	HIS	2.1
2	B	75	GLU	2.0
2	B	186	GLN	2.0
3	C	427	ARG	2.0
2	B	202	GLN	2.0
3	C	718	ARG	2.0
2	B	49	TYR	2.0
2	B	221	ALA	2.0
3	C	14	SER	2.0
1	A	661	LEU	2.0
3	C	520	GLU	2.0
1	A	116	LYS	2.0

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, 95^{th} 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.