



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:07 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

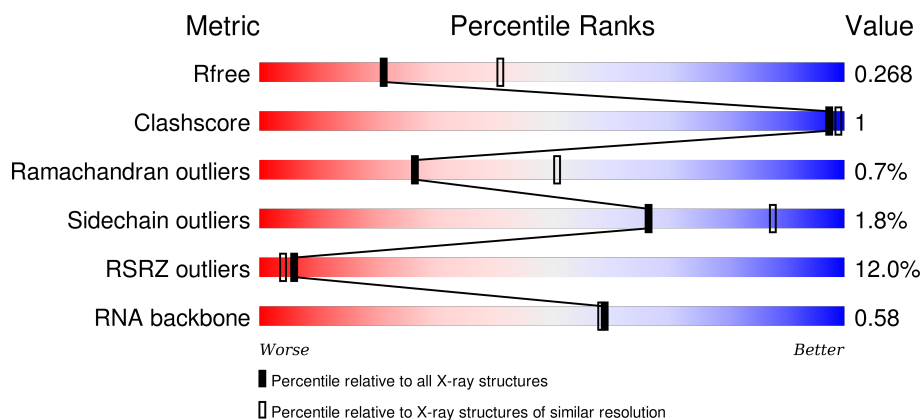
1 Overall quality at a glance

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)
RNA backbone	2183	1001 (3.08-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	<div> <div>21%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
2	B	776	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
3	C	787	<div> <div>9%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
4	R	18	<div> <div></div> <div> <div></div> <div>61%</div> <div>11%</div> <div>28%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	V	16	

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
7	PO4	B	805	-	-	-	X

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: O₄P).



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	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		

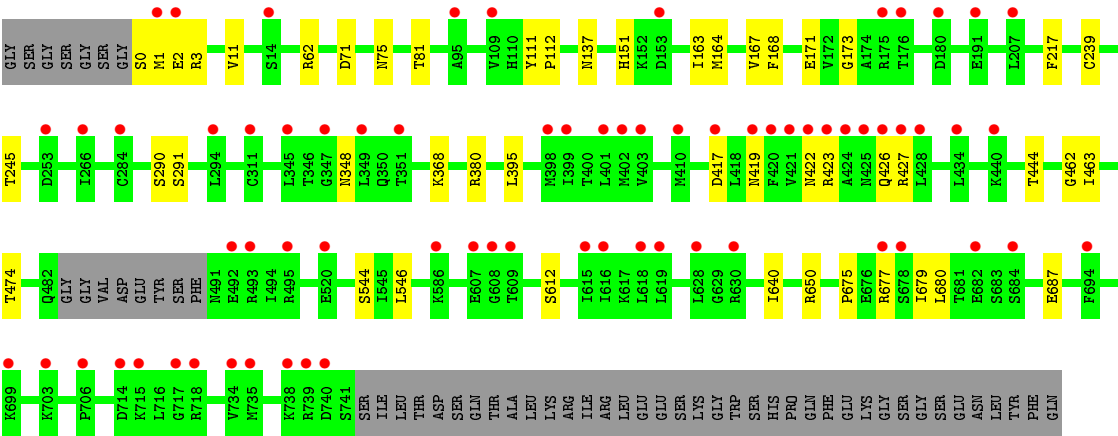
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

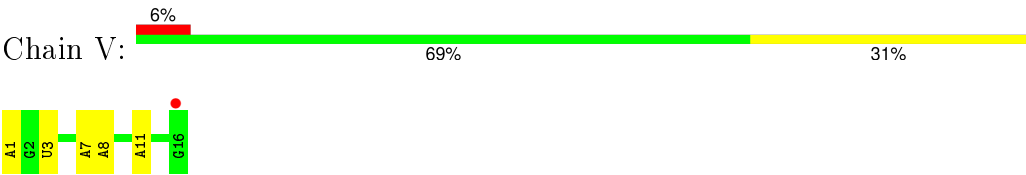
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	11	Total	O	0	0
			11	11		
8	C	9	Total	O	0	0
			9	9		
8	R	1	Total	O	0	0
			1	1		
8	V	3	Total	O	0	0
			3	3		



- 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)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.215 , 0.267 0.219 , 0.268	Depositor DCC
R_{free} test set	4750 reflections (4.78%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 99454 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [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.

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:612:SER:OG	3:C:680:LEU:HD22	2.18	0.42
3:C:168:PHE:HB3	3:C:171:GLU:HG2	2.01	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
2:B:167:LEU:HD23	2:B:336:LEU:HD11	2.02	0.41
1:A:596:ALA:HB2	3:C:239:CYS:HB2	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 [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%)	19	41
2	B	735/776 (95%)	700 (95%)	34 (5%)	1 (0%)	56	81
3	C	730/787 (93%)	689 (94%)	34 (5%)	7 (1%)	19	41
All	All	2160/2301 (94%)	2035 (94%)	110 (5%)	15 (1%)	26	51

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 ⓘ

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%)	54	81
2	B	654/676 (97%)	644 (98%)	10 (2%)	72	90
3	C	652/695 (94%)	643 (99%)	9 (1%)	74	91
All	All	1931/2028 (95%)	1896 (98%)	35 (2%)	66	88

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	A	802	-	4,4,4	0.47	0	6,6,6	0.27	0
7	PO4	A	803	-	4,4,4	0.47	0	6,6,6	0.27	0
7	PO4	A	804	-	4,4,4	0.46	0	6,6,6	0.27	0
7	PO4	A	805	-	4,4,4	0.48	0	6,6,6	0.28	0
7	PO4	B	801	-	4,4,4	0.47	0	6,6,6	0.28	0
7	PO4	B	802	-	4,4,4	0.46	0	6,6,6	0.28	0
7	PO4	B	803	-	4,4,4	0.45	0	6,6,6	0.27	0
7	PO4	B	804	-	4,4,4	0.45	0	6,6,6	0.27	0
7	PO4	B	805	-	4,4,4	0.48	0	6,6,6	0.27	0
7	PO4	B	806	-	4,4,4	0.49	0	6,6,6	0.27	0
7	PO4	B	807	-	4,4,4	0.46	0	6,6,6	0.27	0
7	PO4	B	808	-	4,4,4	0.46	0	6,6,6	0.27	0
7	PO4	B	809	-	4,4,4	0.47	0	6,6,6	0.27	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	0.47	0	6,6,6	0.27	0
7	PO4	C	802	-	4,4,4	0.43	0	6,6,6	0.27	0
7	PO4	C	803	-	4,4,4	0.47	0	6,6,6	0.27	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
7	PO4	A	802	-	-	0/0/0/0	0/0/0/0
7	PO4	A	803	-	-	0/0/0/0	0/0/0/0
7	PO4	A	804	-	-	0/0/0/0	0/0/0/0
7	PO4	A	805	-	-	0/0/0/0	0/0/0/0
7	PO4	B	801	-	-	0/0/0/0	0/0/0/0
7	PO4	B	802	-	-	0/0/0/0	0/0/0/0
7	PO4	B	803	-	-	0/0/0/0	0/0/0/0
7	PO4	B	804	-	-	0/0/0/0	0/0/0/0
7	PO4	B	805	-	-	0/0/0/0	0/0/0/0
7	PO4	B	806	-	-	0/0/0/0	0/0/0/0
7	PO4	B	807	-	-	0/0/0/0	0/0/0/0
7	PO4	B	808	-	-	0/0/0/0	0/0/0/0
7	PO4	B	809	-	-	0/0/0/0	0/0/0/0
7	PO4	C	801	-	-	0/0/0/0	0/0/0/0
7	PO4	C	802	-	-	0/0/0/0	0/0/0/0
7	PO4	C	803	-	-	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.

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, 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%)	1.29	152 (21%) 1 1	52, 91, 246, 298	0
2	B	745/776 (96%)	0.26	41 (5%) 29 26	50, 92, 139, 169	0
3	C	734/787 (93%)	0.44	70 (9%) 10 8	56, 93, 146, 171	0
4	R	13/18 (72%)	0.21	0 100 100	72, 88, 103, 111	0
5	V	16/16 (100%)	-0.05	1 (6%) 23 21	74, 80, 97, 159	0
All	All	2207/2335 (94%)	0.64	264 (11%) 6 4	50, 92, 217, 298	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ARG	14.8
1	A	146	HIS	13.4
1	A	20	THR	13.3
1	A	71	MET	13.0
1	A	26	GLU	12.8
1	A	66	ASP	12.8
1	A	28	PRO	11.7
1	A	12	MET	11.5
1	A	24	TYR	11.4
1	A	13	ILE	11.4
1	A	58	GLY	11.2
1	A	121	GLY	11.0
1	A	33	ASN	10.8
1	A	183	ALA	10.8
1	A	549	ILE	10.7
1	A	126	LYS	10.4
1	A	151	ASP	10.2
1	A	51	PHE	9.7
1	A	162	ILE	9.4
1	A	21	MET	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	123	THR	9.1
1	A	32	GLY	9.1
1	A	157	THR	8.7
1	A	155	MET	8.6
1	A	147	ILE	8.6
1	A	72	LEU	8.5
1	A	140	GLY	8.4
1	A	37	ALA	8.2
1	A	67	ASP	8.1
1	A	114	THR	8.0
1	A	115	ASN	7.6
1	A	7	THR	7.4
1	A	70	ALA	6.9
1	A	1	MET	6.9
1	A	176	PHE	6.8
1	A	548	SER	6.7
1	A	10	ASN	6.6
1	A	125	ARG	6.5
1	A	49	SER	6.2
1	A	550	SER	6.2
1	A	30	ASN	6.2
1	A	185	ALA	6.2
1	A	159	ASP	6.2
1	A	99	GLU	6.1
1	A	184	THR	6.1
1	A	27	ASN	6.1
3	C	424	ALA	6.0
3	C	347	GLY	5.9
1	A	65	ASN	5.9
1	A	144	TYR	5.9
1	A	181	GLU	5.9
1	A	129	ASP	5.8
1	A	53	PHE	5.8
1	A	166	GLU	5.8
1	A	547	THR	5.8
1	A	63	LYS	5.7
1	A	177	VAL	5.7
1	A	25	GLY	5.7
1	A	132	TYR	5.6
1	A	145	ILE	5.6
1	A	153	GLU	5.5
2	B	191	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	GLU	5.5
1	A	120	ILE	5.5
1	A	141	GLU	5.5
1	A	17	ALA	5.5
1	A	104	ARG	5.4
1	A	545	ILE	5.4
3	C	349	LEU	5.3
3	C	628	LEU	5.3
1	A	164	ASP	5.3
3	C	423	ARG	5.2
1	A	142	ASN	5.2
1	A	55	ASP	5.1
1	A	62	VAL	5.1
1	A	130	TYR	5.0
2	B	200	ILE	5.0
1	A	54	ILE	5.0
1	A	74	HIS	4.9
3	C	715	LYS	4.9
1	A	297	HIS	4.9
1	A	75	ARG	4.9
3	C	684	SER	4.8
1	A	158	ASP	4.8
1	A	112	TYR	4.8
1	A	152	GLY	4.8
3	C	495	ARG	4.7
1	A	56	LEU	4.7
1	A	124	ARG	4.7
1	A	59	ASN	4.6
1	A	117	PHE	4.6
3	C	425	ASN	4.6
3	C	703	LYS	4.6
1	A	161	TYR	4.5
1	A	160	GLU	4.5
1	A	165	GLU	4.5
1	A	180	GLN	4.5
3	C	153	ASP	4.5
1	A	118	ILE	4.4
2	B	194	ASN	4.4
1	A	136	SER	4.4
1	A	47	MET	4.3
5	V	16	G	4.3
3	C	734	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	135	ALA	4.3
3	C	740	ASP	4.3
3	C	739	ARG	4.3
1	A	57	GLU	4.3
3	C	176	THR	4.3
3	C	175	ARG	4.3
1	A	128	GLU	4.2
1	A	127	VAL	4.2
3	C	682	GLU	4.2
2	B	645	VAL	4.1
1	A	386	PHE	4.1
1	A	97	MET	4.1
1	A	19	LYS	4.1
3	C	706	PRO	3.9
2	B	732	SER	3.9
1	A	45	CYS	3.9
3	C	493	ARG	3.9
1	A	154	GLU	3.9
1	A	14	LEU	3.9
1	A	173	THR	3.8
1	A	150	PHE	3.8
3	C	630	ARG	3.8
1	A	23	GLU	3.8
1	A	133	GLU	3.8
3	C	440	LYS	3.8
3	C	422	ASN	3.7
2	B	752	ALA	3.7
3	C	426	GLN	3.7
1	A	69	ASN	3.7
1	A	202	GLU	3.7
1	A	29	GLN	3.6
3	C	1	MET	3.6
3	C	420	PHE	3.6
3	C	738	LYS	3.5
1	A	11	PRO	3.4
3	C	492	GLU	3.4
1	A	551	THR	3.4
1	A	156	ALA	3.4
3	C	284	CYS	3.4
2	B	135	ARG	3.4
1	A	119	GLU	3.4
1	A	73	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	189	LYS	3.3
1	A	610	ARG	3.3
2	B	383	GLU	3.3
3	C	345	LEU	3.2
3	C	311	CYS	3.2
1	A	560	VAL	3.2
1	A	131	TYR	3.2
1	A	182	LEU	3.2
2	B	353	ARG	3.2
1	A	15	GLU	3.1
3	C	616	ILE	3.1
3	C	428	LEU	3.0
3	C	618	LEU	3.0
2	B	707	ARG	3.0
1	A	76	PHE	3.0
3	C	417	ASP	3.0
1	A	122	VAL	3.0
1	A	139	LYS	3.0
1	A	105	PHE	2.9
3	C	677	ARG	2.9
1	A	6	ARG	2.9
1	A	137	LYS	2.9
2	B	193	ASP	2.9
2	B	653	LYS	2.9
2	B	718	MET	2.9
1	A	544	GLU	2.8
1	A	148	PHE	2.8
1	A	149	SER	2.8
2	B	753	LEU	2.8
3	C	434	LEU	2.8
1	A	95	CYS	2.8
2	B	185	PHE	2.8
1	A	170	ARG	2.8
1	A	96	ASN	2.7
3	C	608	GLY	2.7
1	A	109	LEU	2.7
1	A	52	HIS	2.7
3	C	109	VAL	2.7
2	B	209	ARG	2.7
1	A	102	LYS	2.7
3	C	735	MET	2.7
2	B	151	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	402	MET	2.6
3	C	678	SER	2.6
1	A	68	ASP	2.6
2	B	357	PHE	2.6
3	C	398	MET	2.6
1	A	34	LYS	2.6
1	A	107	PRO	2.6
1	A	169	ALA	2.6
2	B	748	LYS	2.5
3	C	2	GLU	2.5
3	C	421	VAL	2.5
3	C	410	MET	2.5
1	A	138	LEU	2.5
3	C	401	LEU	2.5
2	B	107	CYS	2.4
3	C	694	PHE	2.4
1	A	546	ARG	2.4
3	C	351	THR	2.4
1	A	31	GLU	2.4
3	C	399	ILE	2.4
3	C	419	ASN	2.4
3	C	180	ASP	2.4
3	C	607	GLU	2.3
3	C	586	LYS	2.3
3	C	699	LYS	2.3
2	B	451	ILE	2.3
1	A	487	THR	2.3
2	B	738	GLN	2.3
3	C	615	ILE	2.3
2	B	211	LYS	2.3
3	C	717	GLY	2.3
2	B	461	GLN	2.3
1	A	713	MET	2.3
3	C	253	ASP	2.3
1	A	224	LYS	2.3
2	B	207	LYS	2.3
3	C	294	LEU	2.3
2	B	81	GLY	2.2
2	B	474	GLY	2.2
1	A	163	LEU	2.2
3	C	207	LEU	2.2
1	A	350	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	95	ALA	2.2
2	B	714	MET	2.2
2	B	187	LYS	2.2
2	B	258	LEU	2.2
3	C	714	ASP	2.2
3	C	619	LEU	2.2
1	A	101	SER	2.2
3	C	520	GLU	2.2
1	A	352	PHE	2.1
2	B	633	HIS	2.1
3	C	191	GLU	2.1
2	B	186	GLN	2.1
3	C	266	ILE	2.1
1	A	227	HIS	2.1
3	C	403	VAL	2.1
3	C	427	ARG	2.1
1	A	116	LYS	2.1
2	B	75	GLU	2.1
2	B	49	TYR	2.1
3	C	14	SER	2.1
2	B	221	ALA	2.1
1	A	4	PHE	2.1
3	C	718	ARG	2.1
1	A	204	GLU	2.1
2	B	78	GLU	2.1
2	B	202	GLN	2.0
1	A	82	GLN	2.0
1	A	661	LEU	2.0
3	C	609	THR	2.0
2	B	733	GLY	2.0
2	B	203	ARG	2.0
2	B	646	MET	2.0
1	A	106	LEU	2.0
1	A	9	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
7	PO4	B	805	5/5	0.85	0.22	2.56	101,103,115,121	0
7	PO4	A	804	5/5	0.93	0.21	1.85	101,107,111,112	0
7	PO4	B	804	5/5	0.91	0.21	1.24	78,84,103,112	0
7	PO4	C	803	5/5	0.91	0.22	1.17	108,116,117,119	0
7	PO4	B	807	5/5	0.86	0.20	0.71	105,112,123,126	0
7	PO4	B	806	5/5	0.97	0.18	0.32	88,91,105,113	0
7	PO4	A	805	5/5	0.93	0.19	0.16	100,109,113,116	0
7	PO4	A	803	5/5	0.88	0.14	-0.89	96,107,110,117	0
7	PO4	B	803	5/5	0.94	0.11	-1.25	91,92,100,106	0
7	PO4	B	801	5/5	0.89	0.12	-1.34	92,94,110,121	0
7	PO4	C	801	5/5	0.96	0.10	-1.50	87,87,93,94	0
7	PO4	A	802	5/5	0.94	0.20	-	82,89,100,101	0
6	ZN	A	801	1/1	0.99	0.11	-	84,84,84,84	0
7	PO4	B	809	5/5	0.93	0.20	-	115,120,126,130	0
7	PO4	C	802	5/5	0.92	0.17	-	97,101,119,120	0
7	PO4	B	802	5/5	0.93	0.20	-	91,94,98,98	0
7	PO4	B	808	5/5	0.80	0.24	-	144,145,151,154	0

6.5 Other polymers ⓘ

There are no such residues in this entry.