Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 06:17 pm GMT

PDB ID	:	6QCX
Title	:	Crystal structure of influenza B polymerase initiation state with capped 15-mer RNA primer
Authors	:	Cusack, S.; Drncova, P.
Deposited on	:	2018-12-31
Resolution	:	3.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

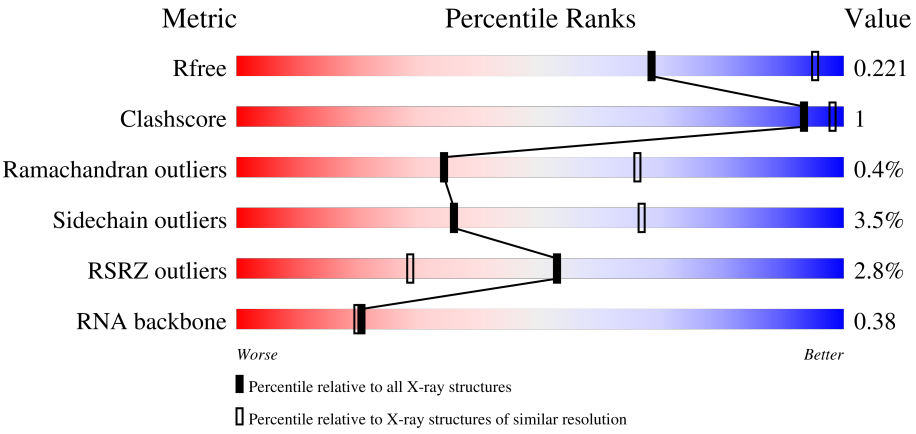
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)
RNA backbone	3102	1063 (3.36-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	751	4% 90% 5% •
2	B	772	2% 90% 6% • •
3	C	798	2% 84% 7% • 8%
4	M	16	6% 56% 44%

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Mol	Chain	Length	Quality of chain
5	R	21	71% 29%
6	V	14	36% 64%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18582 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	718	5760	3660	964	1096	40	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 Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	747	Total	C	N	O	S	0	0	0
			5860	3698	1017	1093	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	733	Total	C	N	O	S	0	0	0
			5863	3726	1026	1071	40			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	GLY	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	16	Total	C	N	O	P	0	0	0
			350	155	64	114	17			

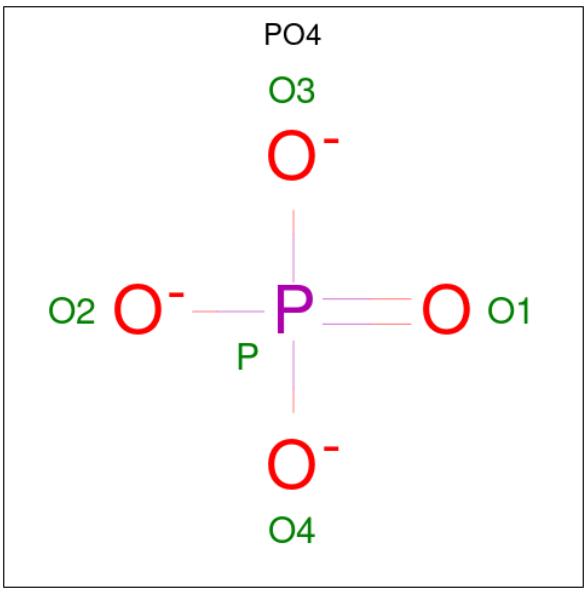
- Molecule 5 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP* CP*UP*UP*CP*UP*GP*CP*UP*AP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	21	Total	C	N	O	P	0	0	0
			427	193	63	151	20			

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP *AP*GP*AP*G)-3').

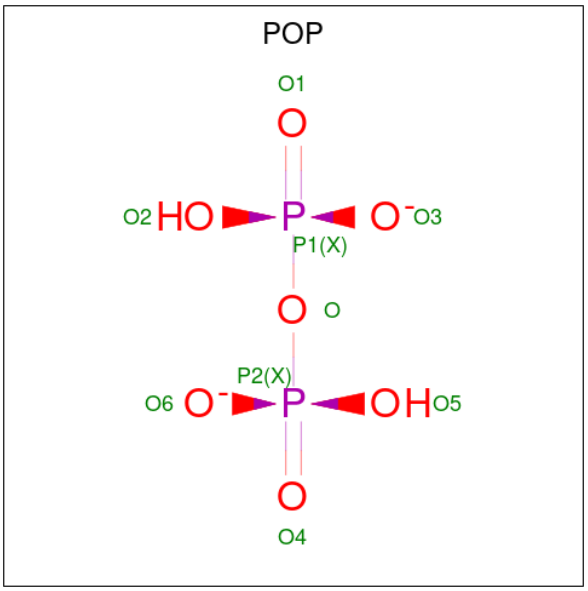
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	V	14	Total	C	N	O	P	0	0	0
			307	137	62	94	14			

- 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

- Molecule 8 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O P 9 7 2	0	0

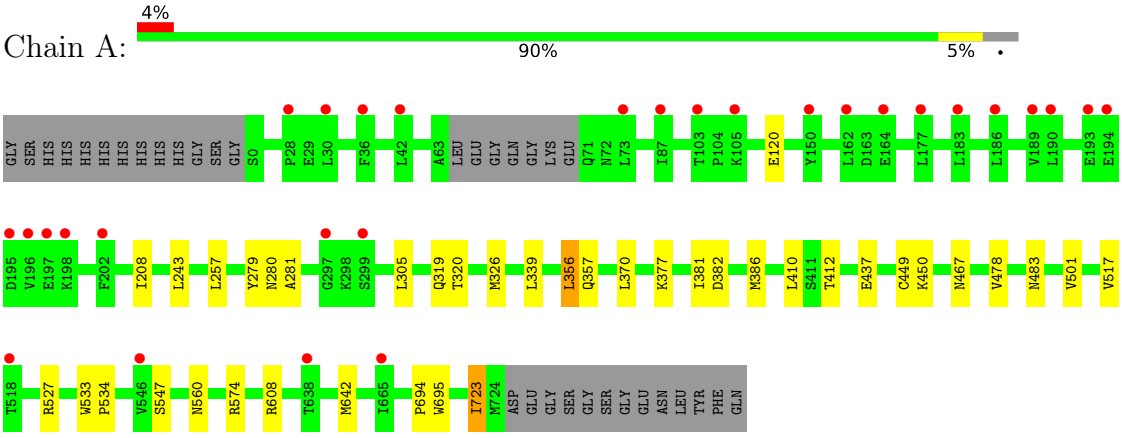
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0

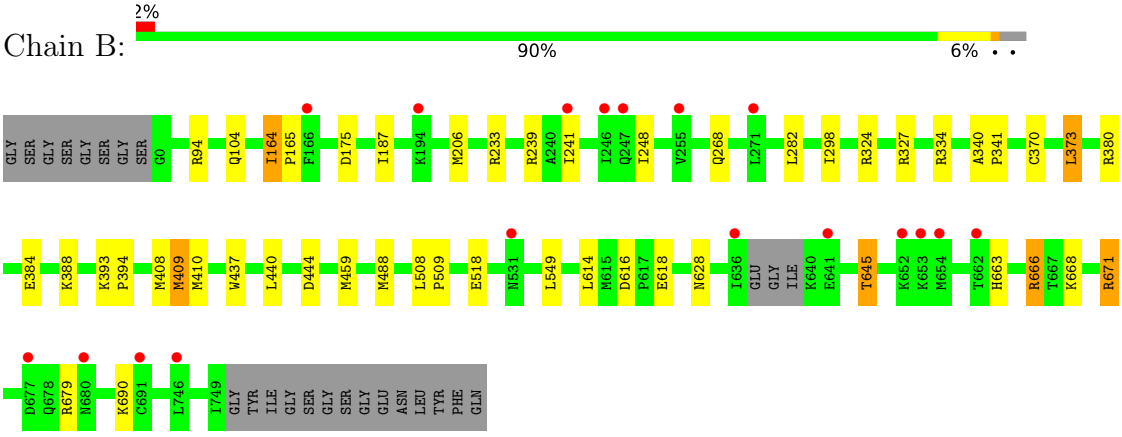
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

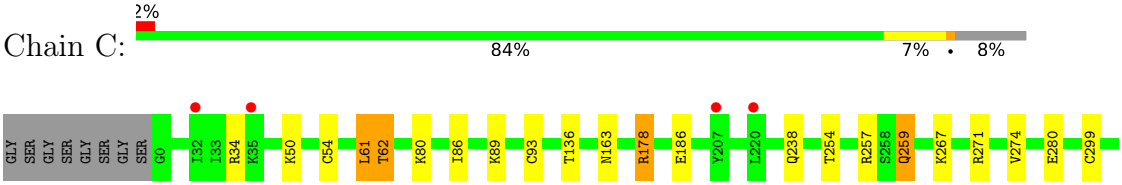
• Molecule 1: Polymerase acidic protein

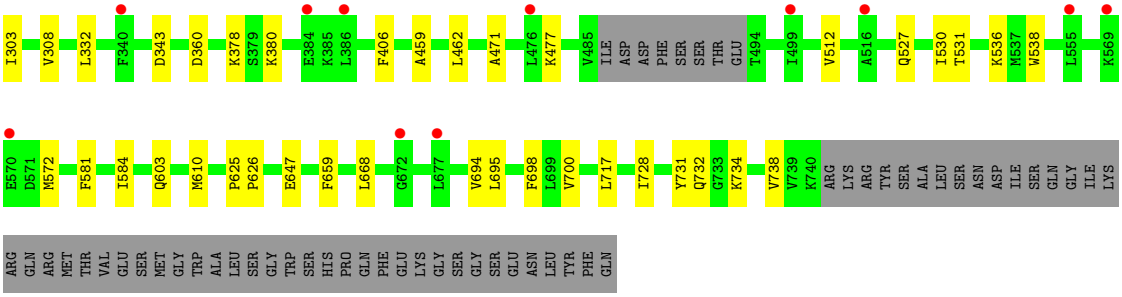


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

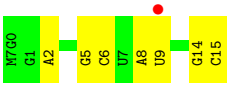


• Molecule 3: Polymerase basic protein 2

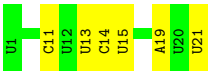




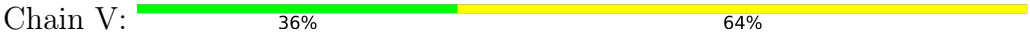
• Molecule 4: RNA (5'-D(*(GDM))-R(P*GP*AP*AP*UP*GP*CP*UP*AP*UP*AP*AP*UP*AP*GP*C)-3')

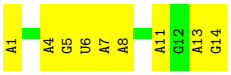


• Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP*CP*UP*AP*UP*U)-3')



• Molecule 6: RNA (5'-R(P*AP*GP*UP*AP*GP*UP*AP*AP*CP*AP*AP*GP*AP*G)-3')





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.41Å 200.41Å 256.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	173.56 – 3.08 173.56 – 3.08	Depositor EDS
% Data completeness (in resolution range)	75.2 (173.56-3.08) 75.2 (173.56-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.202 , 0.226 0.201 , 0.221	Depositor DCC
R_{free} test set	4024 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	97.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18582	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: MG, M7G, POP, PO4

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	0.67	0/5876	0.70	0/7925
2	B	0.66	0/5975	0.70	0/8054
3	C	0.66	0/5963	0.70	0/8014
4	M	0.20	0/359	0.65	0/557
5	R	0.27	0/473	0.69	0/732
6	V	0.59	1/345 (0.3%)	0.63	0/535
All	All	0.65	1/18991 (0.0%)	0.70	0/25817

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	A	OP3-P	-9.88	1.49	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	5760	0	5732	13	0
2	B	5860	0	5883	21	0
3	C	5863	0	6031	23	0
4	M	350	0	178	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	427	0	219	1	0
6	V	307	0	153	1	0
7	A	5	0	0	0	0
8	B	9	0	0	0	0
9	B	1	0	0	0	0
All	All	18582	0	18196	52	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 (52) 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:340:ALA:HB3	2:B:341:PRO:HD3	1.83	0.61
2:B:666:ARG:HH22	3:C:62:THR:HG23	1.66	0.60
1:A:386:MET:O	2:B:380:ARG:NH1	2.38	0.57
1:A:574:ARG:HB3	2:B:549:LEU:HD22	1.87	0.57
1:A:356:LEU:HD13	1:A:478:VAL:HG23	1.88	0.56
3:C:581:PHE:O	3:C:584:ILE:HG13	2.08	0.53
3:C:659:PHE:CZ	3:C:668:LEU:HD11	2.43	0.53
1:A:467:ASN:HA	3:C:54:CYS:SG	2.48	0.53
2:B:370:CYS:HA	2:B:373:LEU:HD13	1.94	0.50
1:A:642:MET:HG3	1:A:695:TRP:CZ3	2.47	0.49
3:C:163:ASN:HD22	3:C:178:ARG:HG3	1.78	0.49
2:B:645:THR:HG21	2:B:690:LYS:HA	1.95	0.48
2:B:645:THR:CG2	2:B:690:LYS:HA	2.44	0.48
2:B:282:LEU:HD22	2:B:440:LEU:HD13	1.96	0.48
3:C:80:LYS:HA	3:C:93:CYS:HA	1.96	0.48
3:C:459:ALA:HB3	3:C:462:LEU:HB2	1.96	0.48
1:A:279:TYR:CE1	1:A:281:ALA:HB3	2.50	0.47
1:A:280:ASN:HD21	1:A:694:PRO:HD3	1.80	0.45
2:B:241:ILE:HG22	2:B:410:MET:HG2	1.98	0.45
3:C:731:TYR:CE2	3:C:734:LYS:HG3	2.52	0.45
2:B:298:ILE:HD12	3:C:732:GLN:HG3	1.99	0.44
2:B:187:ILE:HD12	2:B:206:MET:HG3	1.99	0.44
2:B:671:ARG:HB3	3:C:86:ILE:HD11	2.00	0.44
3:C:728:ILE:HD13	3:C:738:VAL:HB	2.00	0.44
3:C:267:LYS:HE2	3:C:267:LYS:HA	1.99	0.44
1:A:723:ILE:HD12	3:C:700:VAL:HG11	2.00	0.44
3:C:717:LEU:HD21	3:C:728:ILE:HD11	1.99	0.44
3:C:61:LEU:HD21	3:C:93:CYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ARG:HA	2:B:334:ARG:NH1	2.33	0.43
3:C:254:THR:HG22	3:C:257:ARG:HH21	1.83	0.43
3:C:259:GLN:NE2	4:M:2:A:OP2	2.51	0.43
1:A:501:VAL:CG2	1:A:517:VAL:HB	2.49	0.43
2:B:393:LYS:HB3	2:B:394:PRO:HD3	2.00	0.43
2:B:164:ILE:N	2:B:165:PRO:HD2	2.34	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.82	0.42
3:C:625:PRO:HA	3:C:626:PRO:HD3	1.93	0.42
1:A:410:LEU:HA	1:A:450:LYS:HB3	2.02	0.42
3:C:694:VAL:HG12	3:C:695:LEU:HG	2.01	0.42
3:C:536:LYS:HA	3:C:538:TRP:CD1	2.55	0.42
3:C:603:GLN:NE2	3:C:698:PHE:O	2.52	0.42
2:B:384:GLU:HG2	2:B:388:LYS:HE3	2.01	0.42
3:C:332:LEU:HD22	3:C:406:PHE:CZ	2.55	0.41
1:A:381:ILE:O	2:B:380:ARG:NH2	2.54	0.41
2:B:518:GLU:OE1	2:B:663:HIS:ND1	2.49	0.41
5:R:21:U:O2	5:R:21:U:O4'	2.37	0.41
6:V:7:A:C2	6:V:8:A:C4	3.09	0.41
2:B:408:MET:O	2:B:409:MET:HB2	2.21	0.41
4:M:14:G:H2'	4:M:15:C:O4'	2.20	0.41
1:A:642:MET:HG3	1:A:695:TRP:CH2	2.56	0.40
1:A:533:TRP:N	1:A:534:PRO:CD	2.84	0.40
2:B:508:LEU:HB3	2:B:509:PRO:HD3	2.04	0.40
3:C:257:ARG:HB3	3:C:303:ILE:HD11	2.03	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	714/751 (95%)	651 (91%)	60 (8%)	3 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	743/772 (96%)	690 (93%)	52 (7%)	1 (0%)	51 82
3	C	729/798 (91%)	673 (92%)	52 (7%)	4 (0%)	29 61
All	All	2186/2321 (94%)	2014 (92%)	164 (8%)	8 (0%)	34 66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	SER
1	A	483	ASN
1	A	723	ILE
3	C	380	LYS
3	C	471	ALA
3	C	477	LYS
2	B	679	ARG
3	C	308	VAL

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	638/664 (96%)	618 (97%)	20 (3%)	40 69
2	B	641/657 (98%)	618 (96%)	23 (4%)	35 66
3	C	640/694 (92%)	616 (96%)	24 (4%)	33 64
All	All	1919/2015 (95%)	1852 (96%)	67 (4%)	36 67

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	208	ILE
1	A	243	LEU
1	A	257	LEU
1	A	305	LEU
1	A	319	GLN

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Mol	Chain	Res	Type
1	A	320	THR
1	A	326	MET
1	A	339	LEU
1	A	356	LEU
1	A	357	GLN
1	A	370	LEU
1	A	377	LYS
1	A	382	ASP
1	A	412	THR
1	A	437	GLU
1	A	449	CYS
1	A	527	ARG
1	A	560	ASN
1	A	608	ARG
2	B	94	ARG
2	B	104	GLN
2	B	164	ILE
2	B	175	ASP
2	B	233	ARG
2	B	239	ARG
2	B	248	ILE
2	B	268	GLN
2	B	324	ARG
2	B	373	LEU
2	B	409	MET
2	B	437	TRP
2	B	444	ASP
2	B	459	MET
2	B	488	MET
2	B	614	LEU
2	B	616	ASP
2	B	618	GLU
2	B	628	ASN
2	B	645	THR
2	B	666	ARG
2	B	668	LYS
2	B	671	ARG
3	C	34	ARG
3	C	50	LYS
3	C	61	LEU
3	C	62	THR
3	C	89	LYS

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Mol	Chain	Res	Type
3	C	136	THR
3	C	178	ARG
3	C	186	GLU
3	C	238	GLN
3	C	259	GLN
3	C	271	ARG
3	C	274	VAL
3	C	280	GLU
3	C	299	CYS
3	C	343	ASP
3	C	360	ASP
3	C	378	LYS
3	C	512	VAL
3	C	527	GLN
3	C	530	ILE
3	C	531	THR
3	C	572	MET
3	C	610	MET
3	C	647	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	129	ASN
3	C	235	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	14/16 (87%)	4 (28%)	1 (7%)
5	R	19/21 (90%)	4 (21%)	1 (5%)
6	V	13/14 (92%)	6 (46%)	1 (7%)
All	All	46/51 (90%)	14 (30%)	3 (6%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	5	G
4	M	6	C
4	M	8	A

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Mol	Chain	Res	Type
4	M	9	U
5	R	11	C
5	R	14	C
5	R	15	U
5	R	19	A
6	V	4	A
6	V	5	G
6	V	6	U
6	V	11	A
6	V	13	A
6	V	14	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	M	8	A
5	R	13	U
6	V	5	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	POP	B	801	9	6,8,8	0.75	0	13,13,13	1.17	1 (7%)
7	PO4	A	801	-	4,4,4	0.63	0	6,6,6	0.45	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	POP	B	801	9	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	801	POP	P2-O-P1	-2.60	123.92	132.83

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	718/751 (95%)	0.51	29 (4%) 38 19	81, 114, 222, 252	0
2	B	747/772 (96%)	0.65	18 (2%) 59 35	77, 109, 145, 187	0
3	C	733/798 (91%)	0.48	15 (2%) 65 43	83, 119, 189, 248	0
4	M	15/16 (93%)	0.66	1 (6%) 17 7	109, 135, 187, 200	0
5	R	21/21 (100%)	0.71	0 100 100	81, 101, 132, 135	0
6	V	14/14 (100%)	0.70	0 100 100	86, 92, 99, 103	0
All	All	2248/2372 (94%)	0.55	63 (2%) 53 28	77, 113, 202, 252	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	653	LYS	6.7
1	A	150	TYR	6.3
3	C	570	GLU	5.2
1	A	194	GLU	5.0
1	A	195	ASP	4.2
1	A	73	LEU	4.1
1	A	30	LEU	3.8
2	B	652	LYS	3.8
2	B	636	ILE	3.7
3	C	569	LYS	3.5
1	A	196	VAL	3.5
3	C	476	LEU	3.1
1	A	186	LEU	3.1
3	C	340	PHE	3.0
2	B	691	CYS	3.0
1	A	28	PRO	2.9
1	A	299	SER	2.9
1	A	42	LEU	2.8
1	A	546	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	LYS	2.6
3	C	35	LYS	2.5
2	B	271	LEU	2.5
1	A	202	PHE	2.5
3	C	220	LEU	2.4
1	A	190	LEU	2.4
4	M	9	U	2.4
2	B	746	LEU	2.3
1	A	198	LYS	2.3
3	C	207	TYR	2.3
1	A	297	GLY	2.3
3	C	386	LEU	2.3
2	B	166	PHE	2.2
2	B	247	GLN	2.2
2	B	662	THR	2.2
2	B	654	MET	2.2
1	A	518	THR	2.2
1	A	162	LEU	2.2
2	B	246	ILE	2.2
3	C	516	ALA	2.1
1	A	164	GLU	2.1
2	B	241	ILE	2.1
1	A	87	ILE	2.1
1	A	193	GLU	2.1
2	B	255	VAL	2.1
3	C	499	ILE	2.1
1	A	197	GLU	2.1
1	A	665	ILE	2.1
3	C	384	GLU	2.1
1	A	638	THR	2.1
2	B	531	ASN	2.1
3	C	555	LEU	2.1
2	B	641	GLU	2.1
1	A	103	THR	2.1
1	A	189	VAL	2.1
3	C	672	GLY	2.1
3	C	677	LEU	2.1
3	C	32	ILE	2.0
2	B	677	ASP	2.0
1	A	177	LEU	2.0
1	A	36	PHE	2.0
2	B	194	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	680	ASN	2.0
1	A	183	LEU	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 monosaccharides 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
8	POP	B	801	9/9	0.88	0.14	151,153,164,166	0
7	PO4	A	801	5/5	0.91	0.21	131,132,133,135	0
9	MG	B	802	1/1	0.93	0.15	122,122,122,122	0

6.5 Other polymers (i)

There are no such residues in this entry.