Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2024 – 06:20 pm GMT

PDB ID	:	6QCW
Title	:	Crystal structure of influenza B polymerase initiation state with capped 14-mer RNA primer
Authors	:	Cusack, S.; Drncova, P.
Deposited on	:	2018-12-31
Resolution	:	2.88 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 (i) 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 (i)) were used in the production of this report:

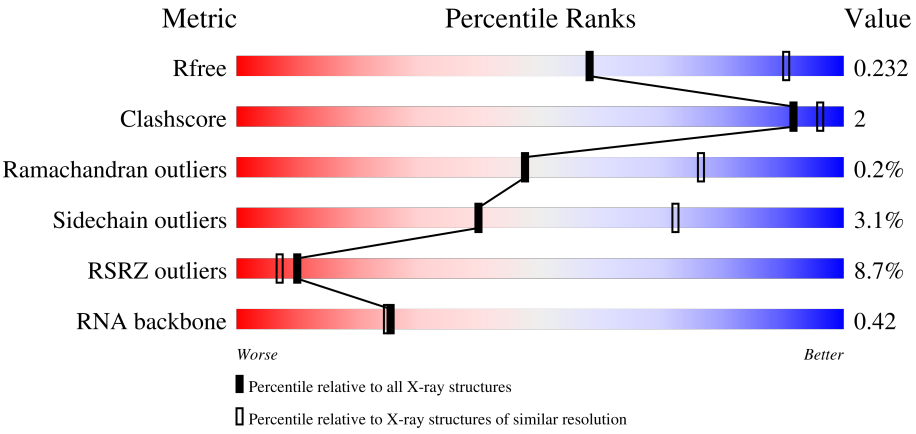
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)
RNA backbone	3102	1121 (3.16-2.60)

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	12% 91% · 5%
2	B	772	9% 91% 6% ·
3	C	798	5% 83% 9% 8%
4	M	15	13% 47% 47% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	R	21	71% 24% 5%
6	V	14	43% 50% 7%

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	802	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18540 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	717	5755	3657	963	1095	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	745	Total	C	N	O	S	0	0	0
			5843	3686	1014	1091	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

Continued on next page...

Continued from previous page...

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*CP *AP*UP*AP*AP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	15	Total	C	N	O	P	0	0	0
			330	146	61	107	16			

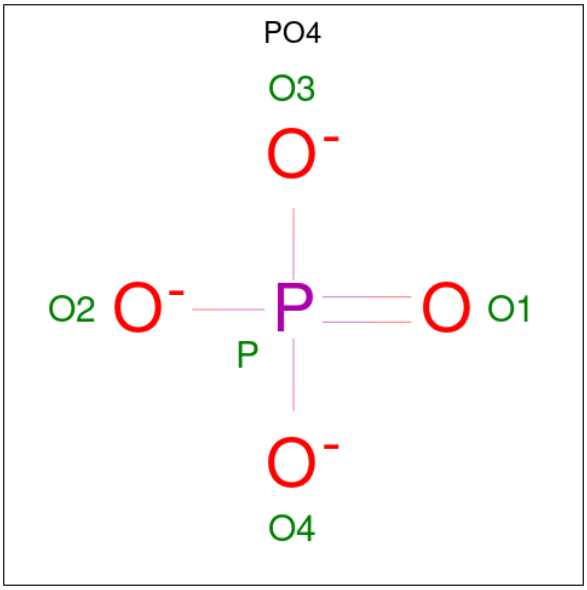
- Molecule 5 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP* CP*UP*UP*CP*UP*GP*CP*UP*AP*UP*U)-3').

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).



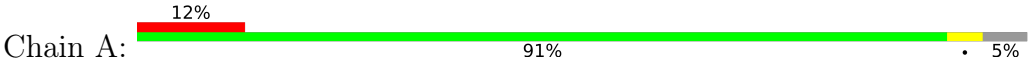
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0

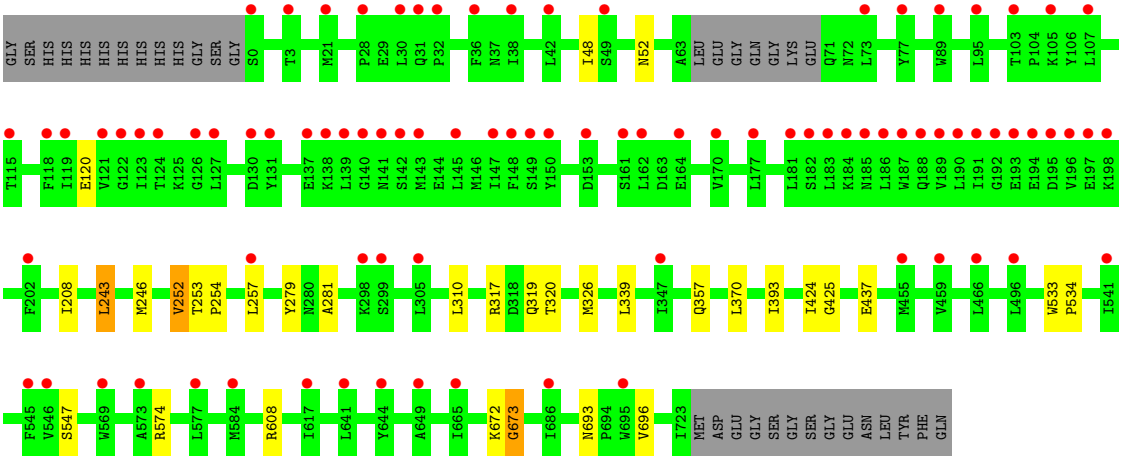
3 Residue-property plots (i)

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

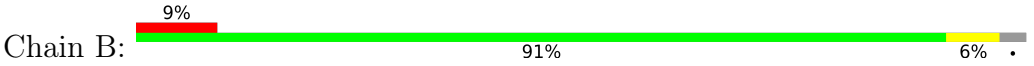
Chain A:

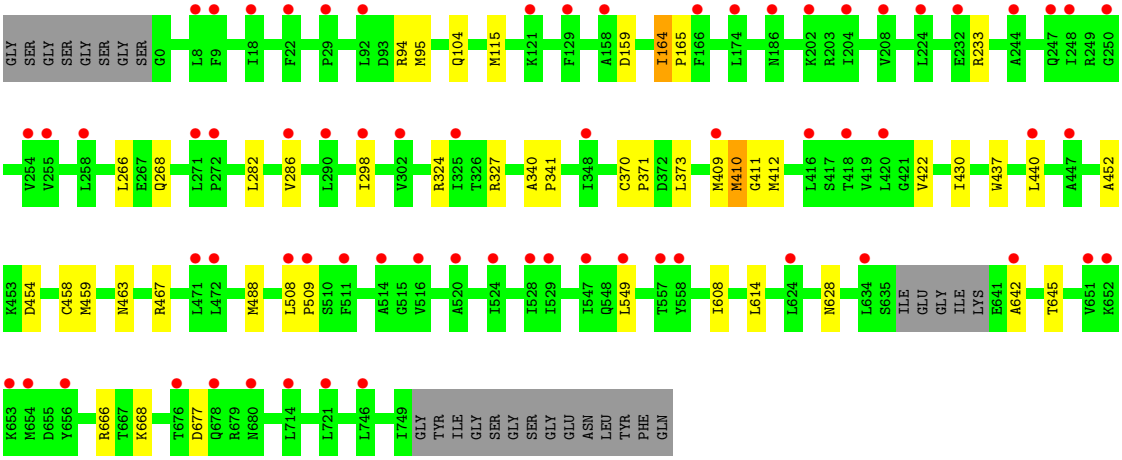




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

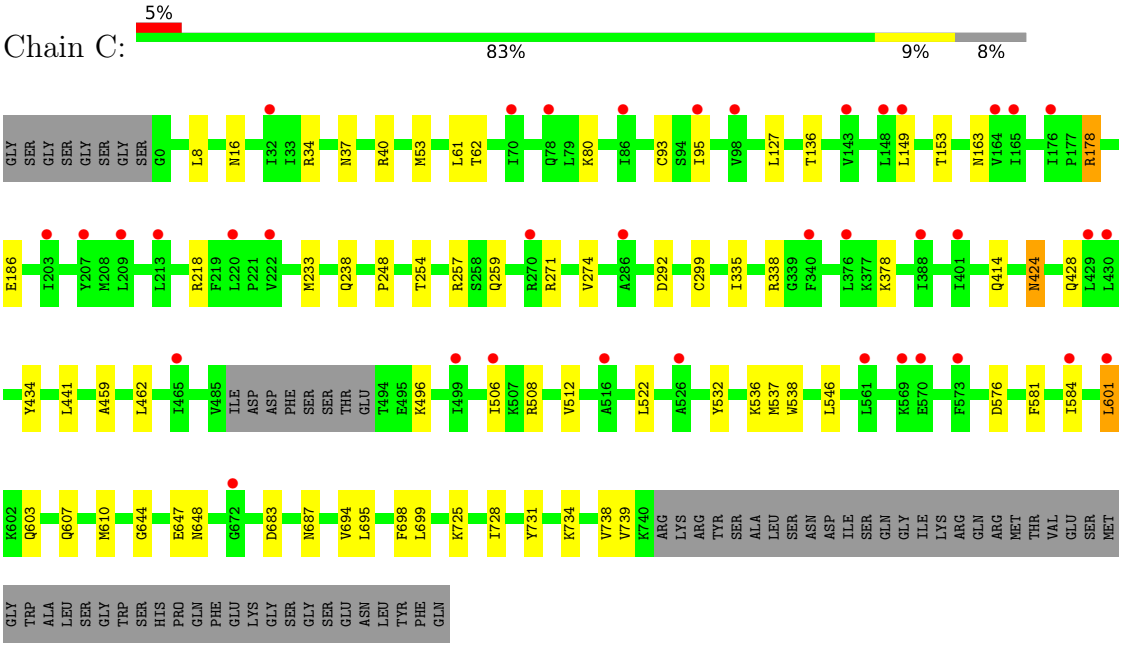
Chain B:





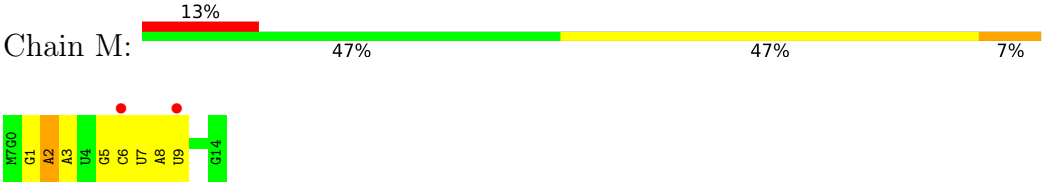
• Molecule 3: Polymerase basic protein 2

Chain C:



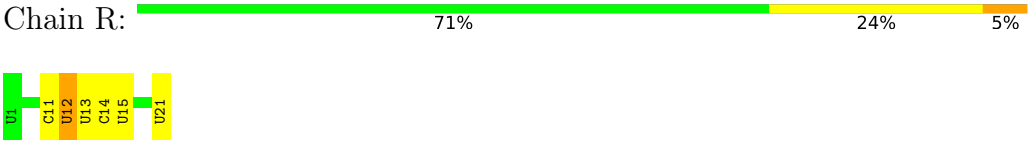
• Molecule 4: RNA (5'-D(*(GDM))-R(P*GP*AP*AP*UP*GP*CP*CP*AP*UP*AP*AP*UP*AP*G)-3')

Chain M:



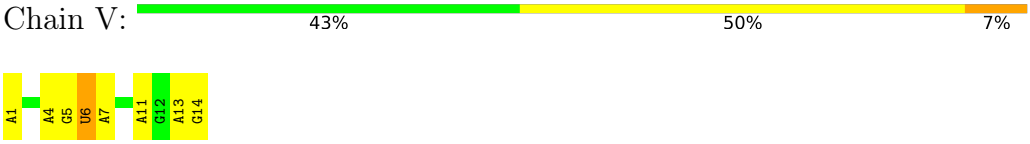
• Molecule 5: RNA (5'-R(*UP*AP*UP*AP*CP*CP*UP*CP*UP*GP*CP*UP*UP*CP*UP*GP*CP*UP*AP*UP*U)-3')

Chain R:



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

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.35Å 200.35Å 256.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.88 173.51 – 2.88	Depositor EDS
% Data completeness (in resolution range)	60.7 (50.00-2.88) 60.7 (173.51-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.215 , 0.234 0.213 , 0.232	Depositor DCC
R_{free} test set	3942 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	18540	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: M7G, 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	0.30	0/5871	0.46	0/7918
2	B	0.29	0/5958	0.46	0/8032
3	C	0.29	0/5963	0.47	0/8014
4	M	0.19	0/337	0.65	0/523
5	R	0.24	0/473	0.66	0/732
6	V	0.58	1/345 (0.3%)	0.63	0/535
All	All	0.30	1/18947 (0.0%)	0.48	0/25754

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	A	OP3-P	-10.04	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	5755	0	5730	13	0
2	B	5843	0	5859	18	0
3	C	5863	0	6031	30	0
4	M	330	0	167	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	427	0	219	2	0
6	V	307	0	153	1	0
7	A	5	0	0	0	0
7	B	10	0	0	0	0
All	All	18540	0	18159	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:LEU:HD13	3:C:233:MET:CE	2.21	0.70
3:C:127:LEU:HD13	3:C:233:MET:HE1	1.75	0.67
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.87	0.55
3:C:506:ILE:HG22	3:C:512:VAL:HG12	1.88	0.54
5:R:21:U:O4'	5:R:21:U:O2	2.24	0.54
3:C:603:GLN:NE2	3:C:698:PHE:O	2.40	0.54
3:C:163:ASN:HD22	3:C:178:ARG:HG3	1.74	0.53
1:A:574:ARG:HB3	2:B:549:LEU:HD22	1.89	0.53
4:M:7:U:H6	4:M:7:U:O5'	1.92	0.52
3:C:424:ASN:ND2	3:C:428:GLN:HB2	2.24	0.51
2:B:282:LEU:HD22	2:B:440:LEU:HD13	1.92	0.51
2:B:266:LEU:HD13	2:B:422:VAL:HG11	1.93	0.50
3:C:127:LEU:HD13	3:C:233:MET:HE3	1.92	0.50
3:C:80:LYS:HA	3:C:93:CYS:HA	1.93	0.50
2:B:642:ALA:O	3:C:8:LEU:HD21	2.11	0.50
1:A:310:LEU:HB3	1:A:317:ARG:HG3	1.93	0.50
1:A:693:ASN:HB3	1:A:696:VAL:HB	1.95	0.49
3:C:338:ARG:HH21	3:C:512:VAL:HG23	1.77	0.49
3:C:644:GLY:HA3	3:C:648:ASN:HD22	1.78	0.48
3:C:728:ILE:HD13	3:C:738:VAL:HB	1.95	0.48
2:B:370:CYS:O	2:B:373:LEU:HB2	2.13	0.48
3:C:546:LEU:HD13	3:C:584:ILE:CG2	2.44	0.48
2:B:95:MET:HE1	2:B:266:LEU:HD11	1.96	0.46
2:B:452:ALA:HB3	2:B:458:CYS:SG	2.56	0.46
1:A:246:MET:HB3	2:B:467:ARG:HH12	1.81	0.46
2:B:508:LEU:N	2:B:509:PRO:CD	2.79	0.46
1:A:48:ILE:O	1:A:52:ASN:ND2	2.48	0.46
3:C:731:TYR:CE2	3:C:734:LYS:HG3	2.51	0.45
3:C:496:LYS:HB2	3:C:508:ARG:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ILE:N	2:B:165:PRO:HD2	2.32	0.45
3:C:254:THR:HG22	3:C:257:ARG:HH21	1.82	0.44
1:A:252:VAL:HG22	2:B:463:ASN:HA	1.99	0.44
3:C:694:VAL:HG12	3:C:695:LEU:HG	2.00	0.44
2:B:298:ILE:HD12	2:B:454:ASP:HA	1.99	0.43
3:C:536:LYS:HA	3:C:538:TRP:CD1	2.53	0.43
3:C:725:LYS:HG2	3:C:739:VAL:HG22	2.00	0.43
3:C:581:PHE:O	3:C:584:ILE:HG13	2.18	0.43
1:A:243:LEU:HD13	2:B:430:ILE:HD13	1.99	0.43
3:C:149:LEU:HD11	3:C:218:ARG:HD2	2.01	0.43
4:M:7:U:O5'	4:M:7:U:C6	2.71	0.42
3:C:53:MET:SD	3:C:95:ILE:HG21	2.59	0.42
2:B:370:CYS:N	2:B:371:PRO:CD	2.83	0.42
3:C:532:TYR:HB2	3:C:537:MET:HB2	2.01	0.42
1:A:533:TRP:N	1:A:534:PRO:CD	2.83	0.41
1:A:672:LYS:O	1:A:673:GLY:C	2.59	0.41
3:C:607:GLN:HG2	3:C:699:LEU:HD11	2.02	0.41
1:A:393:ILE:HD11	6:V:6:U:C2	2.56	0.41
3:C:459:ALA:HB3	3:C:462:LEU:HB2	2.01	0.41
1:A:253:THR:N	1:A:254:PRO:HD3	2.36	0.41
1:A:279:TYR:CE1	1:A:281:ALA:HB3	2.56	0.41
1:A:424:ILE:HG23	1:A:425:GLY:O	2.21	0.41
3:C:695:LEU:HB2	3:C:698:PHE:HB2	2.02	0.41
2:B:608:ILE:HD12	2:B:608:ILE:H	1.85	0.40
2:B:410:MET:SD	2:B:410:MET:N	2.89	0.40
3:C:434:TYR:HB3	4:M:2:A:N3	2.37	0.40
3:C:538:TRP:CZ3	3:C:546:LEU:HD23	2.57	0.40
2:B:282:LEU:O	2:B:286:VAL:HG23	2.21	0.40
3:C:40:ARG:NH1	5:R:12:U:O4'	2.55	0.40
3:C:601:LEU:HD22	3:C:601:LEU:HA	1.94	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	713/751 (95%)	669 (94%)	42 (6%)	2 (0%)	41	70
2	B	741/772 (96%)	702 (95%)	38 (5%)	1 (0%)	51	80
3	C	729/798 (91%)	689 (94%)	38 (5%)	2 (0%)	41	70
All	All	2183/2321 (94%)	2060 (94%)	118 (5%)	5 (0%)	47	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	GLY
1	A	547	SER
2	B	411	GLY
3	C	292	ASP
3	C	248	PRO

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%)	625 (98%)	13 (2%)	55	81
2	B	639/657 (97%)	618 (97%)	21 (3%)	38	70
3	C	640/694 (92%)	614 (96%)	26 (4%)	30	62
All	All	1917/2015 (95%)	1857 (97%)	60 (3%)	40	72

All (60) 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	252	VAL
1	A	257	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	GLN
1	A	320	THR
1	A	326	MET
1	A	339	LEU
1	A	357	GLN
1	A	370	LEU
1	A	437	GLU
1	A	608	ARG
2	B	94	ARG
2	B	104	GLN
2	B	115	MET
2	B	159	ASP
2	B	164	ILE
2	B	233	ARG
2	B	268	GLN
2	B	324	ARG
2	B	327	ARG
2	B	409	MET
2	B	410	MET
2	B	412	MET
2	B	437	TRP
2	B	459	MET
2	B	488	MET
2	B	614	LEU
2	B	628	ASN
2	B	645	THR
2	B	666	ARG
2	B	668	LYS
2	B	677	ASP
3	C	16	ASN
3	C	34	ARG
3	C	37	ASN
3	C	61	LEU
3	C	62	THR
3	C	136	THR
3	C	153	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	299	CYS
3	C	335	ILE
3	C	378	LYS
3	C	414	GLN
3	C	424	ASN
3	C	441	LEU
3	C	522	LEU
3	C	576	ASP
3	C	601	LEU
3	C	610	MET
3	C	647	GLU
3	C	683	ASP
3	C	687	ASN

Sometimes 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	M	14/15 (93%)	6 (42%)	3 (21%)
5	R	19/21 (90%)	5 (26%)	1 (5%)
6	V	13/14 (92%)	7 (53%)	1 (7%)
All	All	46/50 (92%)	18 (39%)	5 (10%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	2	A
4	M	3	A
4	M	5	G
4	M	6	C
4	M	8	A
4	M	9	U
5	R	11	C
5	R	12	U
5	R	13	U
5	R	14	C
5	R	15	U
6	V	4	A
6	V	5	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	V	6	U
6	V	7	A
6	V	11	A
6	V	13	A
6	V	14	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	M	1	G
4	M	5	G
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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PO4	A	801	-	4,4,4	0.91	0	6,6,6	0.48	0
7	PO4	B	802	-	4,4,4	0.93	0	6,6,6	0.43	0
7	PO4	B	801	-	4,4,4	0.92	0	6,6,6	0.44	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

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	717/751 (95%)	0.96	89 (12%) 4 2	67, 99, 210, 233	0
2	B	745/772 (96%)	0.91	67 (8%) 9 6	69, 96, 130, 174	0
3	C	733/798 (91%)	0.66	38 (5%) 27 23	73, 105, 167, 213	0
4	M	14/15 (93%)	1.26	2 (14%) 2 2	96, 123, 180, 185	0
5	R	21/21 (100%)	0.78	0 100 100	72, 87, 106, 112	0
6	V	14/14 (100%)	0.76	0 100 100	72, 79, 85, 87	0
All	All	2244/2371 (94%)	0.84	196 (8%) 10 7	67, 99, 192, 233	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	TYR	13.3
1	A	183	LEU	8.1
1	A	189	VAL	8.1
2	B	653	LYS	8.0
1	A	30	LEU	6.9
1	A	195	ASP	5.6
1	A	138	LYS	5.4
3	C	570	GLU	5.3
1	A	184	LYS	4.9
1	A	193	GLU	4.8
1	A	186	LEU	4.8
1	A	546	VAL	4.7
1	A	21	MET	4.6
1	A	147	ILE	4.6
1	A	73	LEU	4.5
1	A	148	PHE	4.5
1	A	123	ILE	4.4
1	A	181	LEU	4.4
1	A	194	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	149	SER	4.3
1	A	196	VAL	4.3
1	A	191	ILE	4.2
1	A	182	SER	4.1
3	C	569	LYS	4.1
2	B	652	LYS	4.1
2	B	651	VAL	4.1
2	B	271	LEU	4.0
3	C	207	TYR	3.9
1	A	162	LEU	3.9
1	A	140	GLY	3.9
1	A	0	SER	3.9
1	A	142	SER	3.9
2	B	654	MET	3.9
1	A	107	LEU	3.8
1	A	161	SER	3.8
1	A	28	PRO	3.8
3	C	340	PHE	3.7
1	A	127	LEU	3.6
1	A	145	LEU	3.6
1	A	139	LEU	3.6
1	A	141	ASN	3.5
1	A	190	LEU	3.5
4	M	9	U	3.5
1	A	130	ASP	3.5
2	B	529	ILE	3.5
2	B	642	ALA	3.4
1	A	197	GLU	3.4
1	A	185	ASN	3.3
1	A	38	ILE	3.3
1	A	143	MET	3.3
1	A	105	LYS	3.2
1	A	192	GLY	3.2
1	A	131	TYR	3.2
1	A	126	GLY	3.1
1	A	177	LEU	3.1
1	A	3	THR	3.1
1	A	77	TYR	3.1
1	A	118	PHE	3.1
1	A	122	GLY	3.0
3	C	465	ILE	3.0
1	A	188	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	PHE	2.9
3	C	176	ILE	2.9
2	B	447	ALA	2.9
1	A	187	TRP	2.9
3	C	209	LEU	2.9
1	A	32	PRO	2.8
2	B	204	ILE	2.8
1	A	49	SER	2.8
2	B	409	MET	2.8
2	B	511	PHE	2.8
1	A	42	LEU	2.8
1	A	577	LEU	2.7
1	A	153	ASP	2.7
2	B	440	LEU	2.7
1	A	299	SER	2.7
1	A	573	ALA	2.7
2	B	250	GLY	2.7
1	A	115	THR	2.7
1	A	164	GLU	2.7
1	A	298	LYS	2.6
2	B	514	ALA	2.6
2	B	558	TYR	2.6
1	A	665	ILE	2.6
3	C	149	LEU	2.6
2	B	471	LEU	2.5
3	C	561	LEU	2.5
2	B	208	VAL	2.5
2	B	721	LEU	2.5
2	B	420	LEU	2.5
3	C	98	VAL	2.5
3	C	220	LEU	2.5
3	C	95	ILE	2.5
2	B	92	LEU	2.5
3	C	516	ALA	2.5
1	A	31	GLN	2.5
2	B	121	LYS	2.5
1	A	137	GLU	2.5
2	B	416	LEU	2.5
3	C	86	ILE	2.5
3	C	213	LEU	2.5
3	C	164	VAL	2.4
2	B	634	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	290	LEU	2.4
3	C	203	ILE	2.4
2	B	29	PRO	2.4
1	A	617	ILE	2.4
1	A	198	LYS	2.4
1	A	569	TRP	2.4
2	B	472	LEU	2.4
3	C	286	ALA	2.4
1	A	170	VAL	2.4
2	B	8	LEU	2.4
4	M	6	C	2.4
1	A	545	PHE	2.3
2	B	254	VAL	2.3
1	A	119	ILE	2.3
2	B	714	LEU	2.3
3	C	388	ILE	2.3
3	C	148	LEU	2.3
2	B	129	PHE	2.3
3	C	270	ARG	2.3
3	C	499	ILE	2.3
1	A	649	ALA	2.3
2	B	528	ILE	2.3
3	C	376	LEU	2.3
2	B	224	LEU	2.3
2	B	656	TYR	2.3
2	B	746	LEU	2.3
1	A	644	TYR	2.3
2	B	255	VAL	2.3
3	C	430	LEU	2.3
2	B	547	ILE	2.3
2	B	22	PHE	2.3
1	A	695	TRP	2.2
2	B	348	ILE	2.2
2	B	524	ILE	2.2
2	B	186	ASN	2.2
2	B	557	THR	2.2
3	C	32	ILE	2.2
1	A	459	VAL	2.2
3	C	506	ILE	2.2
2	B	516	VAL	2.2
1	A	305	LEU	2.2
3	C	601	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	541	ILE	2.2
2	B	676	THR	2.2
1	A	202	PHE	2.2
1	A	121	VAL	2.2
2	B	302	VAL	2.2
1	A	496	LEU	2.1
2	B	258	LEU	2.1
1	A	89	TRP	2.1
3	C	78	GLN	2.1
3	C	584	ILE	2.1
2	B	244	ALA	2.1
2	B	520	ALA	2.1
3	C	401	ILE	2.1
2	B	286	VAL	2.1
3	C	672	GLY	2.1
1	A	686	ILE	2.1
2	B	298	ILE	2.1
2	B	325	ILE	2.1
2	B	418	THR	2.1
1	A	95	LEU	2.1
1	A	466	LEU	2.1
2	B	9	PHE	2.1
3	C	573	PHE	2.1
3	C	165	ILE	2.1
1	A	584	MET	2.1
1	A	124	THR	2.1
2	B	174	LEU	2.1
2	B	624	LEU	2.1
2	B	18	ILE	2.1
1	A	257	LEU	2.1
2	B	247	GLN	2.1
3	C	70	ILE	2.1
3	C	222	VAL	2.1
2	B	202	LYS	2.1
2	B	166	PHE	2.1
2	B	248	ILE	2.1
1	A	455	MET	2.1
2	B	509	PRO	2.1
2	B	508	LEU	2.0
1	A	347	ILE	2.0
3	C	526	ALA	2.0
2	B	678	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	429	LEU	2.0
2	B	158	ALA	2.0
1	A	103	THR	2.0
1	A	641	LEU	2.0
2	B	680	ASN	2.0
2	B	549	LEU	2.0
2	B	232	GLU	2.0
3	C	143	VAL	2.0
2	B	272	PRO	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
7	PO4	B	802	5/5	0.67	0.56	141,142,143,144	0
7	PO4	A	801	5/5	0.89	0.20	128,128,130,130	0
7	PO4	B	801	5/5	0.93	0.16	117,117,118,120	0

6.5 Other polymers (i)

There are no such residues in this entry.