



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:11 PM GMT

PDB ID : 4A8F  
Title : Non-Catalytic Ions Direct the RNA-Dependent RNA Polymerase of Bacterial dsRNA virus phi6 from De Novo Initiation to Elongation  
Authors : Wright, S.; Poranen, M.M.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.  
Deposited on : 2011-11-21  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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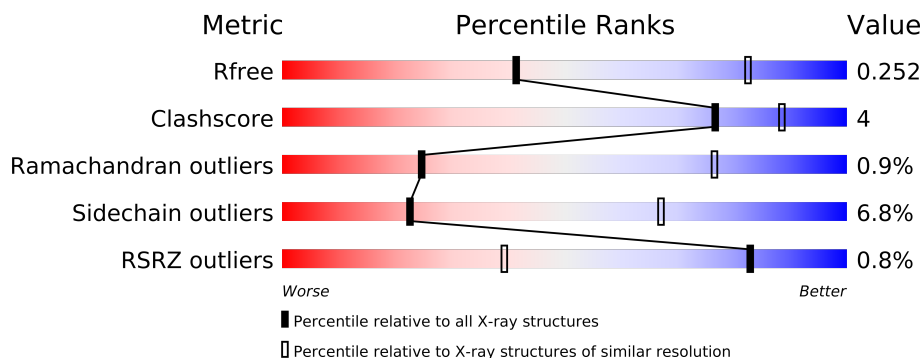
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	665	
1	B	665	
1	C	665	
2	G	4	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	1665[A]	-	X
3	MG	A	1665[B]	-	X
3	MG	B	1667	-	X
4	ATP	A	1666	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	ATP	A	1667	-	X
4	ATP	B	1665	-	X
4	ATP	B	1666	-	X
4	ATP	C	1665	-	X
4	ATP	C	1666	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16048 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	CONFLICT	UNP P11124
B	456	MET	ILE	CONFLICT	UNP P11124
C	456	MET	ILE	CONFLICT	UNP P11124

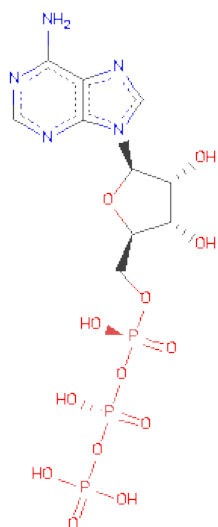
- Molecule 2 is a DNA chain called 5'-D(\*DAP\*GP\*CP\*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	1
			2	2		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



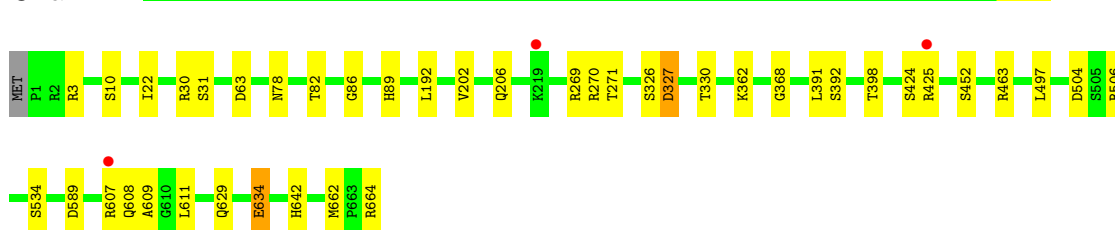
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	A	1	Total	O	P			0	0
			13	10	3				
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RNA-DIRECTED RNA POLYMERASE

Chain A:



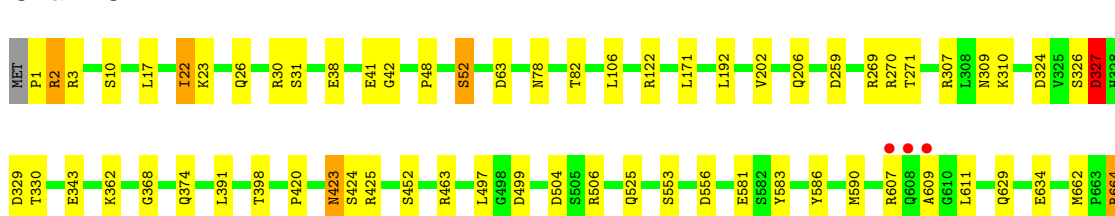
- Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain B:



- Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain C:



- Molecule 2: 5'-D(\*DAP\*GP\*CP\*GP)-3'

Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.92Å 91.77Å 140.46Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	46.01 – 3.30 46.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.01-3.30) 99.8 (46.01-3.30)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.243 , 0.290 0.203 , 0.252	Depositor DCC
$R_{free}$ test set	2000 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39842 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.69	0/5396	0.78	0/7297
1	B	0.75	0/5396	0.86	0/7297
1	C	0.78	0/5396	0.87	4/7297 (0.1%)
2	G	1.48	0/91	2.45	7/139 (5.0%)
All	All	0.74	0/16279	0.86	11/22030 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	DG	P-O3'-C3'	10.03	131.74	119.70
2	G	6	DC	P-O3'-C3'	8.31	129.67	119.70
2	G	6	DC	O4'-C1'-N1	7.23	113.06	108.00
2	G	4	DA	O4'-C1'-N9	6.99	112.89	108.00
1	C	327	ASP	C-N-CA	5.76	136.10	121.70
2	G	6	DC	N1-C1'-C2'	5.46	122.97	112.60
2	G	5	DG	N3-C4-C5	-5.44	125.88	128.60
1	C	1	PRO	C-N-CA	5.39	135.16	121.70
2	G	5	DG	C2-N3-C4	5.14	114.47	111.90
1	C	581	GLU	CB-CG-CD	5.10	127.97	114.20
1	C	327	ASP	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens



added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5265	0	0	10	0
1	B	5265	0	0	18	0
1	C	5265	0	0	17	0
2	G	81	0	46	6	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	44	0	11	3	0
4	B	62	0	24	7	0
4	C	62	0	24	19	0
All	All	16048	0	105	61	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:ILE:CD1	1:C:22:ILE:CG1	1.75	1.62
1:A:22:ILE:CD1	1:A:22:ILE:CG1	1.79	1.59
1:B:22:ILE:CG1	1:B:22:ILE:CD1	1.84	1.54
4:C:1666:ATP:C1'	4:C:1666:ATP:O4'	1.64	1.45
1:B:16:MET:CE	1:B:16:MET:SD	2.03	1.45
4:C:1666:ATP:O4'	4:C:1666:ATP:C4'	1.63	1.44
4:C:1665:ATP:C8	4:C:1666:ATP:O2'	1.86	1.27
1:C:270:ARG:NH2	4:C:1666:ATP:H3'	1.60	1.15
4:C:1665:ATP:N9	4:C:1666:ATP:O2'	1.94	1.01
4:C:1665:ATP:C8	4:C:1666:ATP:C2'	2.52	0.91
1:C:270:ARG:NH2	4:C:1666:ATP:C3'	2.39	0.84
4:C:1665:ATP:H5'1	4:C:1666:ATP:O3'	1.87	0.75
4:C:1665:ATP:O4'	4:C:1666:ATP:O3'	2.07	0.71
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.24	0.70
4:C:1666:ATP:O4'	4:C:1666:ATP:C2'	2.42	0.67
4:C:1666:ATP:O4'	4:C:1666:ATP:C3'	2.42	0.66
1:C:664:ARG:CD	1:C:664:ARG:N	2.60	0.64
4:C:1666:ATP:C4	4:C:1666:ATP:H5'2	2.38	0.59
1:C:270:ARG:NH2	4:C:1666:ATP:C2'	2.68	0.57
1:A:608:GLN:NE2	1:B:593:ARG:CD	2.69	0.56
1:C:270:ARG:NH2	4:C:1666:ATP:H2'	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:ASP:OD2	4:B:1666:ATP:H1'	2.07	0.55
1:B:452:SER:OG	4:B:1666:ATP:H2	1.92	0.52
1:C:504:ASP:OD2	1:C:506:ARG:NH1	2.42	0.52
1:A:392:SER:O	1:A:398:THR:CG2	2.57	0.52
1:A:270:ARG:NH2	4:A:1667:ATP:O1A	2.44	0.50
4:C:1665:ATP:C5'	4:C:1666:ATP:O3'	2.58	0.50
1:B:204:ARG:NE	2:G:7:DG:H21	2.11	0.48
1:B:392:SER:O	1:B:398:THR:CG2	2.62	0.48
1:B:270:ARG:NH1	4:B:1666:ATP:H5'1	2.29	0.48
1:B:343:GLU:O	1:B:347:MET:N	2.47	0.47
1:A:504:ASP:OD2	1:A:506:ARG:NH1	2.47	0.47
1:A:22:ILE:CD1	1:A:22:ILE:CB	2.82	0.47
1:B:630:TYR:CE2	4:B:1665:ATP:H2'	2.50	0.47
1:C:420:PRO:O	1:C:423:ASN:ND2	2.48	0.47
4:C:1665:ATP:H5'1	4:C:1666:ATP:C3'	2.46	0.46
1:B:504:ASP:OD2	1:B:506:ARG:NH1	2.49	0.46
1:B:132:ARG:NH1	1:B:343:GLU:OE2	2.49	0.46
1:C:122:ARG:NH1	1:C:423:ASN:OD1	2.49	0.46
1:A:270:ARG:NH1	4:A:1666:ATP:H3'	2.32	0.45
1:A:270:ARG:NH2	4:A:1667:ATP:PA	2.90	0.45
1:C:586:TYR:CE2	1:C:590:MET:CE	2.99	0.45
1:B:538:ASP:OD2	2:G:4:DA:H8	2.00	0.44
4:B:1665:ATP:O5'	4:B:1665:ATP:H8	2.00	0.44
4:C:1665:ATP:C4'	4:C:1666:ATP:O3'	2.65	0.44
1:C:310:LYS:NZ	1:C:499:ASP:OD2	2.51	0.43
1:C:38:GLU:OE2	1:C:42:GLY:N	2.52	0.43
1:B:329:ASP:OD2	4:B:1666:ATP:H2'	2.18	0.42
1:C:22:ILE:CD1	1:C:22:ILE:CB	2.81	0.42
1:C:22:ILE:CD1	1:C:22:ILE:CA	2.97	0.42
1:B:452:SER:OG	4:B:1666:ATP:C2	2.73	0.42
1:B:538:ASP:OD2	2:G:4:DA:C8	2.73	0.42
4:C:1666:ATP:C5'	4:C:1666:ATP:C4	3.04	0.41
2:G:6:DC:H1'	2:G:7:DG:OP1	2.20	0.41
1:B:541:LYS:CE	2:G:4:DA:H3'	2.51	0.41
2:G:7:DG:H3'	2:G:7:DG:OP1	2.20	0.41
1:C:48:PRO:O	1:C:52:SER:N	2.54	0.41
1:B:86:GLY:O	1:B:89:HIS:CD2	2.73	0.41
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.41
1:A:634:GLU:CB	1:A:642:HIS:NE2	2.84	0.40
1:C:270:ARG:NH2	4:C:1666:ATP:H5'1	2.37	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	662/665 (100%)	634 (96%)	23 (4%)	5 (1%)	27	78
1	B	662/665 (100%)	628 (95%)	28 (4%)	6 (1%)	25	76
1	C	662/665 (100%)	616 (93%)	40 (6%)	6 (1%)	25	76
All	All	1986/1995 (100%)	1878 (95%)	91 (5%)	17 (1%)	25	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ARG
1	B	2	ARG
1	B	607	ARG
1	C	2	ARG
1	B	327	ASP
1	B	611	LEU
1	C	327	ASP
1	C	607	ARG
1	C	609	ALA
1	C	611	LEU
1	A	327	ASP
1	A	609	ALA
1	A	611	LEU
1	B	609	ALA
1	C	368	GLY
1	B	368	GLY
1	A	368	GLY

### 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	557/558 (100%)	529 (95%)	28 (5%)	34	78
1	B	557/558 (100%)	517 (93%)	40 (7%)	21	64
1	C	557/558 (100%)	511 (92%)	46 (8%)	16	56
All	All	1671/1674 (100%)	1557 (93%)	114 (7%)	22	67

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	SER
1	A	30	ARG
1	A	31	SER
1	A	63	ASP
1	A	78	ASN
1	A	82	THR
1	A	192	LEU
1	A	202	VAL
1	A	206	GLN
1	A	269	ARG
1	A	271	THR
1	A	326	SER
1	A	327	ASP
1	A	330	THR
1	A	362	LYS
1	A	391	LEU
1	A	424	SER
1	A	425	ARG
1	A	452	SER
1	A	463	ARG
1	A	497	LEU
1	A	534	SER
1	A	589	ASP
1	A	629	GLN
1	A	634	GLU
1	A	662	MET
1	A	664	ARG
1	B	3	ARG
1	B	10	SER
1	B	22	ILE
1	B	23	LYS
1	B	41	GLU
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	82	THR
1	B	102	LEU
1	B	151	THR
1	B	192	LEU
1	B	202	VAL
1	B	204	ARG
1	B	206	GLN
1	B	267	GLU
1	B	269	ARG
1	B	271	THR
1	B	280	ASN
1	B	307	ARG
1	B	308	LEU
1	B	326	SER
1	B	327	ASP
1	B	330	THR
1	B	362	LYS
1	B	391	LEU
1	B	411	LEU
1	B	424	SER
1	B	425	ARG
1	B	452	SER
1	B	463	ARG
1	B	497	LEU
1	B	537	ARG
1	B	541	LYS
1	B	556	ASP
1	B	576	TRP
1	B	589	ASP
1	B	596	LEU
1	B	600	ARG
1	B	634	GLU
1	B	662	MET
1	B	664	ARG
1	C	2	ARG
1	C	3	ARG
1	C	10	SER
1	C	17	LEU
1	C	22	ILE
1	C	23	LYS
1	C	26	GLN
1	C	30	ARG

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Mol	Chain	Res	Type
1	C	31	SER
1	C	41	GLU
1	C	52	SER
1	C	63	ASP
1	C	78	ASN
1	C	82	THR
1	C	106	LEU
1	C	171	LEU
1	C	192	LEU
1	C	202	VAL
1	C	206	GLN
1	C	259	ASP
1	C	269	ARG
1	C	271	THR
1	C	307	ARG
1	C	309	ASN
1	C	324	ASP
1	C	326	SER
1	C	327	ASP
1	C	329	ASP
1	C	330	THR
1	C	343	GLU
1	C	362	LYS
1	C	374	GLN
1	C	391	LEU
1	C	398	THR
1	C	423	ASN
1	C	424	SER
1	C	425	ARG
1	C	452	SER
1	C	463	ARG
1	C	497	LEU
1	C	553	SER
1	C	556	ASP
1	C	629	GLN
1	C	634	GLU
1	C	662	MET
1	C	664	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
4	ATP	A	1666	3	33,33,33	4.99	26 (78%)	52,52,52	2.34	20 (38%)
4	ATP	A	1667	-	12,12,33	1.97	3 (25%)	20,20,52	2.17	6 (30%)
4	ATP	B	1665	-	33,33,33	2.14	7 (21%)	52,52,52	1.72	11 (21%)
4	ATP	B	1666	-	33,33,33	1.96	4 (12%)	52,52,52	2.22	15 (28%)
4	ATP	C	1665	-	33,33,33	2.95	11 (33%)	52,52,52	4.21	19 (36%)
4	ATP	C	1666	3	33,33,33	5.75	26 (78%)	52,52,52	4.52	31 (59%)

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
4	ATP	A	1666	3	-	0/22/38/38	0/1/3/3
4	ATP	A	1667	-	-	0/12/12/38	0/0/0/3
4	ATP	B	1665	-	-	0/22/38/38	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	1666	-	-	0/22/38/38	0/1/3/3
4	ATP	C	1665	-	-	0/22/38/38	0/1/3/3
4	ATP	C	1666	3	-	0/22/38/38	0/1/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1666	ATP	O4'-C1'	14.98	1.64	1.41
4	A	1666	ATP	PA-O3A	13.01	1.83	1.59
4	C	1666	ATP	PA-O3A	11.41	1.80	1.59
4	C	1666	ATP	PB-O3B	10.10	1.78	1.59
4	C	1666	ATP	C4-N3	9.54	1.50	1.35
4	A	1666	ATP	O4'-C1'	9.33	1.55	1.41
4	C	1665	ATP	C8-N9	9.23	1.50	1.36
4	C	1665	ATP	O4'-C1'	9.06	1.55	1.41
4	A	1666	ATP	C2'-C1'	8.59	1.65	1.53
4	C	1666	ATP	O4'-C4'	7.91	1.63	1.45
4	A	1666	ATP	C2-N3	7.91	1.47	1.32
4	A	1666	ATP	PA-O1A	7.73	1.80	1.51
4	C	1666	ATP	PG-O3B	7.62	1.73	1.60
4	B	1666	ATP	C4-N9	7.43	1.48	1.37
4	A	1666	ATP	C4-N9	7.27	1.48	1.37
4	B	1665	ATP	O4'-C1'	7.16	1.52	1.41
4	A	1666	ATP	C4-N3	7.11	1.46	1.35
4	C	1666	ATP	C5'-C4'	6.93	1.74	1.51
4	C	1666	ATP	PB-O3A	6.93	1.72	1.59
4	C	1666	ATP	C2-N1	6.62	1.46	1.33
4	C	1666	ATP	PG-O2G	6.47	1.78	1.54
4	A	1666	ATP	PB-O3A	6.18	1.71	1.59
4	C	1666	ATP	PB-O1B	5.94	1.74	1.51
4	C	1666	ATP	PG-O1G	5.34	1.69	1.51
4	A	1666	ATP	O4'-C4'	5.31	1.57	1.45
4	C	1666	ATP	O3'-C3'	5.11	1.55	1.43
4	C	1666	ATP	PA-O1A	5.06	1.70	1.51
4	A	1666	ATP	PG-O1G	5.00	1.68	1.51
4	B	1666	ATP	O4'-C1'	4.86	1.48	1.41
4	C	1665	ATP	C1'-N9	4.74	1.63	1.48
4	A	1666	ATP	C2'-C3'	4.71	1.66	1.53
4	A	1667	ATP	PA-O5'	4.69	1.66	1.50
4	C	1666	ATP	C2'-C3'	4.64	1.66	1.53
4	A	1666	ATP	PB-O1B	4.64	1.69	1.51
4	C	1665	ATP	C5-C4	4.53	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1665	ATP	C2'-C1'	4.44	1.59	1.53
4	B	1665	ATP	PB-O3B	4.42	1.67	1.59
4	A	1666	ATP	PA-O5'	4.20	1.78	1.59
4	B	1666	ATP	C2'-C1'	4.08	1.59	1.53
4	A	1666	ATP	O3'-C3'	3.96	1.52	1.43
4	B	1665	ATP	PG-O3B	3.94	1.67	1.60
4	C	1665	ATP	C2-N1	3.80	1.41	1.33
4	C	1666	ATP	PA-O2A	3.77	1.71	1.55
4	C	1666	ATP	C8-N9	3.63	1.42	1.36
4	C	1666	ATP	C2'-C1'	3.54	1.58	1.53
4	A	1666	ATP	C2-N1	3.36	1.40	1.33
4	B	1665	ATP	C2-N3	3.32	1.38	1.32
4	A	1666	ATP	PG-O2G	3.31	1.66	1.54
4	A	1666	ATP	PG-O3B	3.23	1.65	1.60
4	C	1665	ATP	PB-O3B	3.17	1.65	1.59
4	B	1666	ATP	C2-N3	3.14	1.38	1.32
4	A	1667	ATP	PG-O3B	3.11	1.65	1.60
4	C	1666	ATP	C3'-C4'	-3.00	1.44	1.53
4	C	1666	ATP	C6-N6	2.96	1.44	1.35
4	C	1665	ATP	PG-O3B	2.86	1.65	1.60
4	C	1665	ATP	O4'-C4'	2.86	1.51	1.45
4	A	1666	ATP	O2'-C2'	2.84	1.49	1.43
4	A	1666	ATP	C6-N1	2.84	1.50	1.37
4	C	1666	ATP	PA-O5'	2.77	1.71	1.59
4	C	1665	ATP	C4-N9	2.74	1.41	1.37
4	A	1667	ATP	PB-O3B	2.72	1.64	1.59
4	A	1666	ATP	C5-C4	2.68	1.46	1.40
4	B	1665	ATP	C8-N7	-2.65	1.29	1.34
4	C	1666	ATP	C8-N7	2.65	1.39	1.34
4	C	1666	ATP	C4-N9	2.63	1.41	1.37
4	A	1666	ATP	PB-O3B	2.63	1.64	1.59
4	C	1665	ATP	C5'-C4'	2.56	1.59	1.51
4	C	1665	ATP	C2-N3	2.55	1.37	1.32
4	A	1666	ATP	C3'-C4'	2.52	1.59	1.53
4	C	1666	ATP	C6-N1	2.50	1.48	1.37
4	A	1666	ATP	C6-N6	2.38	1.42	1.35
4	A	1666	ATP	PB-O2B	2.36	1.65	1.55
4	C	1666	ATP	C6-C5	2.34	1.55	1.42
4	C	1666	ATP	C5-N7	2.22	1.49	1.40
4	A	1666	ATP	PA-O2A	2.11	1.64	1.55
4	B	1665	ATP	PB-O1B	2.03	1.59	1.51
4	A	1666	ATP	PG-O3G	2.03	1.62	1.54

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1665	ATP	O4'-C1'-N9	20.19	127.22	108.44
4	C	1666	ATP	O4'-C1'-N9	15.65	123.00	108.44
4	C	1665	ATP	C8-N9-C4	-13.91	96.28	106.90
4	C	1665	ATP	O3A-PB-O3B	8.16	118.26	101.66
4	C	1666	ATP	C4'-O4'-C1'	-7.96	101.11	109.75
4	C	1666	ATP	N3-C2-N1	-7.70	122.27	128.71
4	C	1666	ATP	C1'-N9-C4	-7.67	113.39	126.64
4	C	1666	ATP	C8-N9-C4	7.48	112.61	106.90
4	C	1666	ATP	O3'-C3'-C4'	-7.41	89.25	111.08
4	C	1666	ATP	C2'-C1'-N9	-7.40	94.28	113.27
4	C	1666	ATP	C3'-C2'-C1'	7.26	112.28	100.91
4	C	1666	ATP	O2'-C2'-C1'	-7.14	89.63	111.23
4	C	1665	ATP	C4-C5-N7	6.62	115.19	109.52
4	C	1666	ATP	O4'-C4'-C5'	6.56	132.79	109.36
4	C	1666	ATP	O5'-PA-O1A	-6.54	83.74	109.37
4	A	1666	ATP	C3'-C2'-C1'	6.22	110.64	100.91
4	C	1666	ATP	O4'-C1'-C2'	-6.12	97.39	106.77
4	B	1666	ATP	O3A-PB-O3B	6.00	113.86	101.66
4	C	1665	ATP	C3'-C2'-C1'	5.94	110.20	100.91
4	C	1665	ATP	C4'-O4'-C1'	5.88	116.14	109.75
4	B	1666	ATP	O4'-C1'-N9	5.70	113.74	108.44
4	C	1665	ATP	O4'-C1'-C2'	-5.44	98.43	106.77
4	C	1666	ATP	O3'-C3'-C2'	5.37	129.31	111.83
4	B	1665	ATP	O2'-C2'-C1'	5.22	127.03	111.23
4	A	1667	ATP	O3A-PB-O3B	5.19	112.23	101.66
4	A	1667	ATP	O2A-PA-O3A	5.17	120.77	104.29
4	A	1666	ATP	N3-C4-N9	5.11	134.66	125.43
4	B	1666	ATP	C1'-N9-C4	5.00	135.28	126.64
4	A	1666	ATP	C4-C5-N7	-4.94	105.29	109.52
4	A	1666	ATP	O4'-C4'-C3'	4.79	114.88	105.17
4	B	1666	ATP	N3-C4-N9	4.68	133.88	125.43
4	B	1666	ATP	C8-N9-C4	-4.32	103.60	106.90
4	C	1666	ATP	C5'-C4'-C3'	-4.25	98.20	115.21
4	A	1666	ATP	C2'-C1'-N9	-4.15	102.62	113.27
4	B	1666	ATP	C4'-O4'-C1'	-4.06	105.34	109.75
4	C	1666	ATP	O2'-C2'-C3'	-4.03	98.73	111.83
4	A	1666	ATP	C8-N9-C4	4.00	109.95	106.90
4	C	1666	ATP	O3A-PB-O3B	-3.91	93.71	101.66
4	B	1665	ATP	C3'-C2'-C1'	3.86	106.95	100.91
4	C	1666	ATP	O3A-PA-O5'	3.84	120.60	103.41
4	C	1666	ATP	C8-N9-C1'	3.83	133.93	126.38
4	B	1665	ATP	C4-C5-N7	3.66	112.66	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1666	ATP	O2B-PB-O3A	3.65	122.48	105.14
4	C	1665	ATP	C8-N9-C1'	3.60	133.47	126.38
4	A	1667	ATP	O2G-PG-O1G	-3.58	98.74	110.44
4	B	1665	ATP	O3'-C3'-C4'	3.55	121.55	111.08
4	B	1666	ATP	C2'-C1'-N9	3.48	122.20	113.27
4	A	1666	ATP	PB-O3B-PG	-3.38	121.77	131.68
4	B	1665	ATP	N3-C4-N9	3.36	131.49	125.43
4	B	1666	ATP	O2'-C2'-C3'	-3.33	101.01	111.83
4	C	1665	ATP	O4'-C4'-C5'	3.33	121.24	109.36
4	C	1665	ATP	N7-C8-N9	3.32	123.75	114.36
4	B	1665	ATP	C8-N9-C4	-3.29	104.39	106.90
4	C	1666	ATP	O3G-PG-O2G	3.24	120.23	107.61
4	A	1666	ATP	N6-C6-N1	3.22	125.69	119.36
4	A	1666	ATP	C4'-O4'-C1'	-3.22	106.25	109.75
4	A	1666	ATP	O4'-C4'-C5'	3.18	120.71	109.36
4	C	1666	ATP	PA-O3A-PB	-3.15	122.45	131.68
4	C	1666	ATP	PB-O3B-PG	-3.12	122.53	131.68
4	C	1666	ATP	C2'-C3'-C4'	-3.09	96.49	102.65
4	C	1666	ATP	C6-C5-C4	-3.07	111.61	117.25
4	A	1667	ATP	O2A-PA-O1A	-3.06	99.77	110.82
4	B	1666	ATP	C2'-C3'-C4'	-3.05	96.58	102.65
4	B	1666	ATP	C5-C4-N3	-2.98	119.21	125.70
4	C	1666	ATP	O2G-PG-O3B	-2.97	91.07	105.14
4	A	1666	ATP	C8-N9-C1'	-2.89	120.69	126.38
4	B	1665	ATP	C1'-N9-C4	2.84	131.54	126.64
4	A	1666	ATP	N3-C2-N1	-2.83	126.34	128.71
4	C	1666	ATP	C5-C4-N9	-2.81	103.11	107.16
4	C	1666	ATP	O2B-PB-O3B	2.80	118.42	105.14
4	C	1665	ATP	O5'-C5'-C4'	2.77	119.09	108.94
4	C	1665	ATP	PB-O3B-PG	2.75	139.75	131.68
4	B	1665	ATP	C2'-C3'-C4'	2.70	108.03	102.65
4	B	1666	ATP	C4-C5-N7	-2.69	107.22	109.52
4	B	1666	ATP	C8-N9-C1'	-2.68	121.11	126.38
4	A	1666	ATP	C8-N7-C5	2.66	111.82	103.58
4	A	1667	ATP	O2G-PG-O3B	2.58	117.37	105.14
4	C	1665	ATP	O2A-PA-O3A	2.49	116.93	105.14
4	A	1666	ATP	O2A-PA-O1A	2.40	125.63	112.21
4	A	1666	ATP	O2'-C2'-C1'	-2.33	104.17	111.23
4	C	1666	ATP	O3G-PG-O3B	2.30	116.06	105.14
4	B	1666	ATP	N3-C2-N1	2.29	130.62	128.71
4	C	1665	ATP	C8-N7-C5	-2.29	96.49	103.58
4	C	1665	ATP	O4'-C4'-C3'	-2.23	100.64	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1666	ATP	O2'-C2'-C3'	2.22	119.07	111.83
4	C	1665	ATP	O5'-PA-O1A	2.20	117.98	109.37
4	B	1665	ATP	N3-C2-N1	-2.19	126.88	128.71
4	B	1666	ATP	O4'-C1'-C2'	-2.17	103.44	106.77
4	A	1666	ATP	C5-C4-N3	-2.17	120.98	125.70
4	B	1666	ATP	O3G-PG-O3B	2.14	115.31	105.14
4	C	1666	ATP	C5-C6-N6	2.14	125.55	120.72
4	C	1666	ATP	O2A-PA-O3A	-2.10	95.17	105.14
4	C	1665	ATP	C2'-C3'-C4'	2.10	106.83	102.65
4	B	1665	ATP	C5-C4-N9	-2.08	104.16	107.16
4	B	1665	ATP	O2G-PG-O3B	2.07	114.97	105.14
4	A	1666	ATP	N7-C8-N9	-2.06	108.55	114.36
4	C	1665	ATP	O2G-PG-O3B	2.05	114.87	105.14
4	C	1666	ATP	N7-C8-N9	-2.04	108.58	114.36
4	C	1665	ATP	C1'-N9-C4	2.03	130.14	126.64
4	A	1667	ATP	O3A-PA-O1A	-2.03	101.54	107.57
4	A	1666	ATP	O4'-C1'-N9	2.02	110.31	108.44
4	A	1666	ATP	C5-C6-N6	-2.01	116.17	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	664/665 (99%)	-0.08	3 (0%)	88 51	41, 73, 109, 140	0
1	B	664/665 (99%)	-0.01	5 (0%)	83 39	43, 69, 101, 149	0
1	C	664/665 (99%)	-0.08	3 (0%)	88 51	38, 69, 104, 180	1 (0%)
2	G	4/4 (100%)	3.03	2 (50%)	0 0	171, 187, 187, 192	0
All	All	1996/1999 (99%)	-0.05	13 (0%)	83 42	38, 70, 106, 192	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	608	GLN	5.4
2	G	7	DG	4.7
1	C	607	ARG	4.5
1	B	607	ARG	3.9
2	G	6	DC	3.8
1	B	608	GLN	2.9
1	B	219	LYS	2.7
1	A	607	ARG	2.6
1	B	603	ALA	2.4
1	B	629	GLN	2.3
1	A	425	ARG	2.2
1	C	609	ALA	2.2
1	A	219	LYS	2.2

### 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	1665[B]	1/1	0.66	11.79	57,57,57,57	1
3	MG	A	1665[A]	1/1	0.66	7.75	29,29,29,29	1
4	ATP	C	1665	31/31	0.48	7.35	176,178,179,181	0
3	MG	B	1667	1/1	0.34	5.59	49,49,49,49	0
4	ATP	B	1665	31/31	0.73	3.98	172,174,191,193	0
4	ATP	A	1667	13/31	0.45	2.95	167,171,179,180	0
4	ATP	A	1666	31/31	0.37	2.70	89,104,131,133	0
4	ATP	B	1666	31/31	0.60	2.58	170,172,179,180	0
4	ATP	C	1666	31/31	0.32	2.17	94,106,122,125	0
3	MG	C	1667	1/1	0.27	1.35	56,56,56,56	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.