



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:56 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

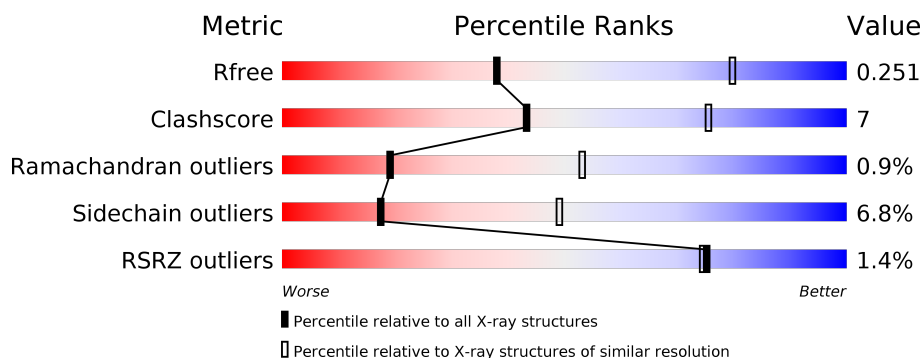
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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	665	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 18%, yellow 86%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 86% 13% </div> </div>
1	B	665	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 19%, yellow 79%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 79% 19% </div> </div>
1	C	665	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 17%, yellow 80%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 80% 17% </div> </div>
2	G	4	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 50%, orange 100%, yellow 50%, green 0%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 50% 100% 50% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1665[A]	-	-	-	X
3	MG	A	1665[B]	-	-	-	X
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	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16048 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 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		

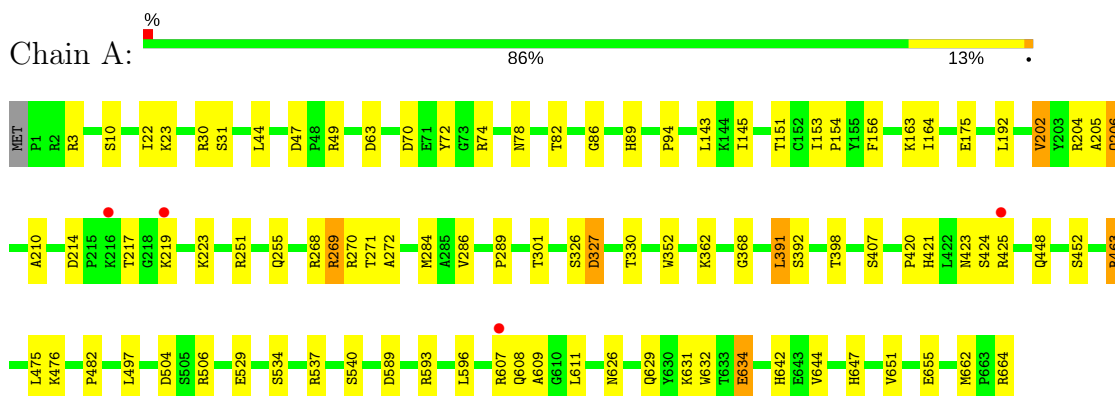
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



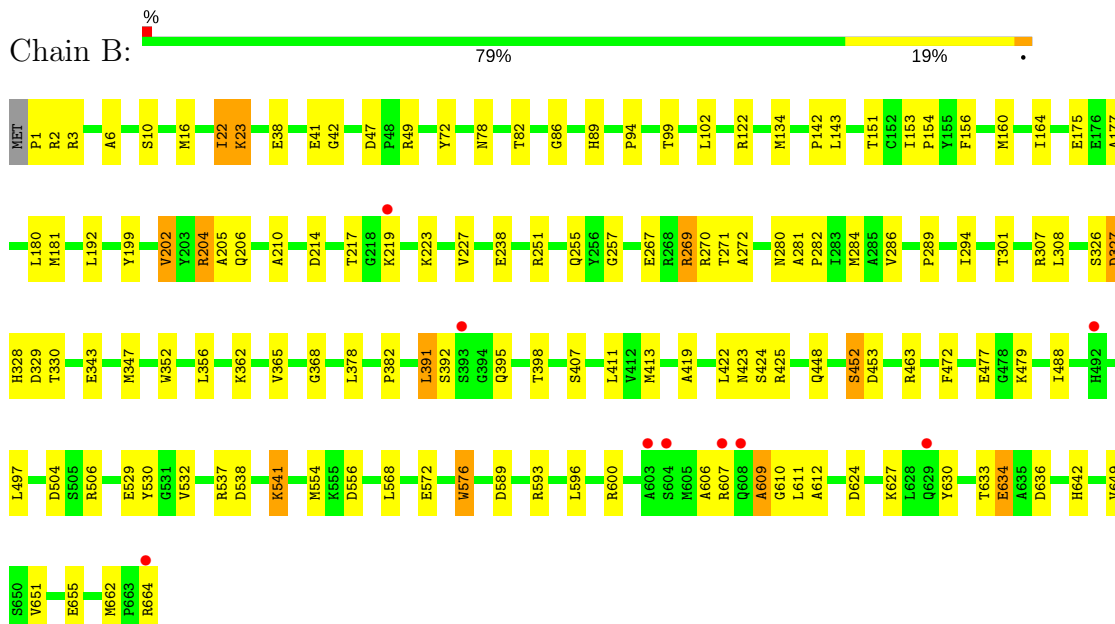
3 Residue-property plots [i](#)

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

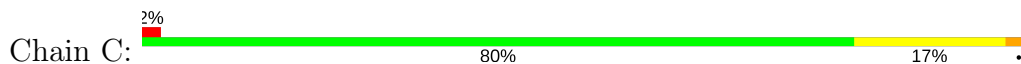
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

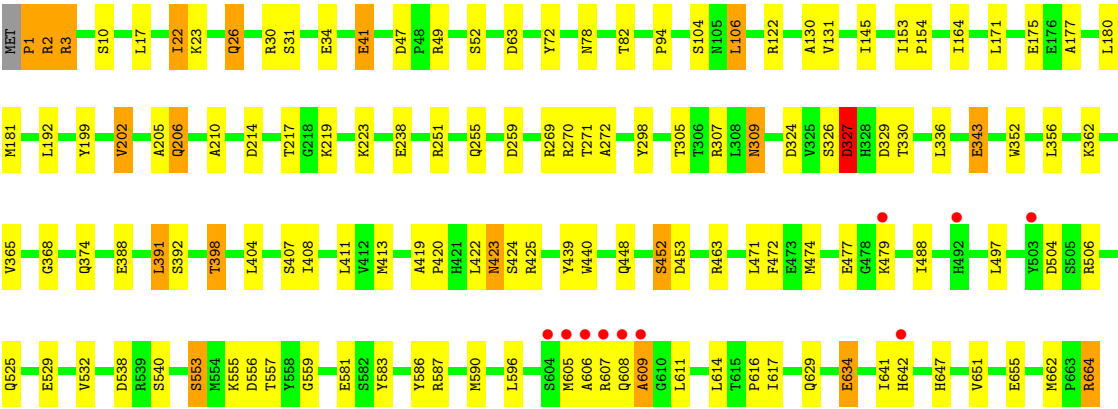


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE





● Molecule 2: 5'-D(*DAP*GP*CP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.243 , 0.290 0.202 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16048	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

The worst 5 of 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

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	5265	0	5165	54	0
1	B	5265	0	5165	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5265	0	5165	88	0
2	G	81	0	46	8	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	8	0
4	C	62	0	24	24	0
All	All	16048	0	15600	231	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 7.

The worst 5 of 231 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)
1:C:22:ILE:CG1	1:C:22:ILE:CD1	1.75	1.62
1:A:22:ILE:CD1	1:A:22:ILE:CG1	1.79	1.59
1:B:22:ILE:CD1	1:B:22:ILE:CG1	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

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	662/665 (100%)	634 (96%)	23 (4%)	5 (1%)	21	55
1	B	662/665 (100%)	628 (95%)	28 (4%)	6 (1%)	19	53
1	C	662/665 (100%)	616 (93%)	40 (6%)	6 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1986/1995 (100%)	1878 (95%)	91 (5%)	17 (1%)	19	53

5 of 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

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%)	27	60
1	B	557/558 (100%)	517 (93%)	40 (7%)	16	46
1	C	557/558 (100%)	511 (92%)	46 (8%)	12	40
All	All	1671/1674 (100%)	1557 (93%)	114 (7%)	17	49

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	391	LEU
1	B	596	LEU
1	C	452	SER
1	B	424	SER
1	B	497	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	ASN
1	B	309	ASN

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Mol	Chain	Res	Type
1	C	448	GLN
1	B	91	ASN
1	A	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 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	-	27,33,33	4.56	19 (70%)	27,52,52	2.24	10 (37%)
4	ATP	A	1667	-	10,12,33	1.68	2 (20%)	11,20,52	1.63	3 (27%)
4	ATP	B	1665	-	27,33,33	2.22	5 (18%)	27,52,52	1.56	5 (18%)
4	ATP	B	1666	-	27,33,33	1.54	2 (7%)	27,52,52	1.88	7 (25%)
4	ATP	C	1665	-	27,33,33	3.40	8 (29%)	27,52,52	2.29	11 (40%)
4	ATP	C	1666	-	27,33,33	5.77	22 (81%)	27,52,52	4.17	15 (55%)

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	-	-	0/18/38/38	0/3/3/3
4	ATP	A	1667	-	-	0/12/12/38	0/0/0/3
4	ATP	B	1665	-	-	0/18/38/38	0/3/3/3
4	ATP	B	1666	-	-	0/18/38/38	0/3/3/3
4	ATP	C	1665	-	-	0/18/38/38	0/3/3/3
4	ATP	C	1666	-	-	0/18/38/38	0/3/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1666	ATP	C3'-C4'	-3.19	1.44	1.53
4	B	1665	ATP	C8-N7	-2.88	1.29	1.34
4	A	1666	ATP	C6-N6	2.12	1.42	1.34
4	A	1666	ATP	PB-O2B	2.13	1.65	1.55
4	B	1665	ATP	PB-O1B	2.27	1.59	1.50

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1666	ATP	C4'-O4'-C1'	-8.37	101.11	109.83
4	C	1666	ATP	N3-C2-N1	-7.70	122.27	128.86
4	C	1666	ATP	C1'-N9-C4	-7.67	113.39	126.64
4	C	1666	ATP	O3'-C3'-C4'	-7.53	89.25	111.06
4	C	1666	ATP	O5'-PA-O1A	-6.48	83.74	109.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1666	ATP	1	0
4	A	1667	ATP	2	0
4	B	1665	ATP	2	0
4	B	1666	ATP	6	0
4	C	1665	ATP	8	0
4	C	1666	ATP	24	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	664/665 (99%)	-0.03	4 (0%) 89 89	41, 73, 109, 140	0
1	B	664/665 (99%)	0.08	9 (1%) 75 74	43, 69, 101, 149	0
1	C	664/665 (99%)	-0.03	10 (1%) 73 71	38, 69, 104, 180	1 (0%)
2	G	4/4 (100%)	3.62	4 (100%) 0 0	171, 187, 187, 192	0
All	All	1996/1999 (99%)	0.02	27 (1%) 75 74	38, 70, 106, 192	1 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	608	GLN	9.0
1	C	607	ARG	7.2
2	G	7	DG	5.7
1	B	607	ARG	4.7
1	B	603	ALA	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(\AA^2)	Q<0.9
4	ATP	C	1665	31/31	0.57	0.48	176,178,179,181	0
4	ATP	B	1665	31/31	0.64	0.70	172,174,191,193	0
4	ATP	B	1666	31/31	0.68	0.57	170,172,179,180	0
4	ATP	C	1666	31/31	0.68	0.32	94,106,122,125	0
4	ATP	A	1666	31/31	0.69	0.37	89,104,131,133	0
3	MG	B	1667	1/1	0.70	0.35	49,49,49,49	0
3	MG	A	1665[A]	1/1	0.76	0.60	29,29,29,29	1
3	MG	A	1665[B]	1/1	0.76	0.60	57,57,57,57	1
4	ATP	A	1667	13/31	0.76	0.44	167,171,179,180	0
3	MG	C	1667	1/1	0.93	0.27	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.