



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:05 am BST

PDB ID : 4A8S  
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 : 2.90 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

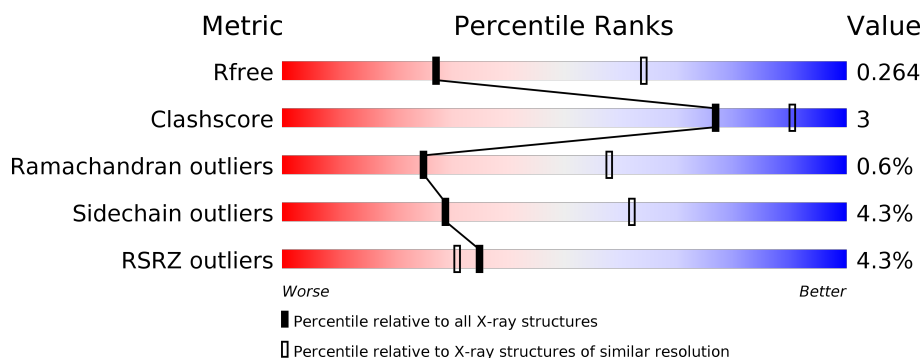
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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  $\leq 5\%$ . 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></div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	665	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	665	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	F	13	<div> <div>8%</div> <div>15%</div> <div>77%</div> </div>
2	G	13	<div> <div>15%</div> <div>23%</div> <div>8%</div> <div>69%</div> </div>
2	H	13	<div> <div>8%</div> <div>38%</div> <div>54%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15955 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	915	976	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	C	646	Total	C	N	O	S	0	0	0
			5123	3255	887	949	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
A	634	GLN	GLU	engineered mutation	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
B	634	GLN	GLU	engineered mutation	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
C	634	GLN	GLU	engineered mutation	UNP P11124

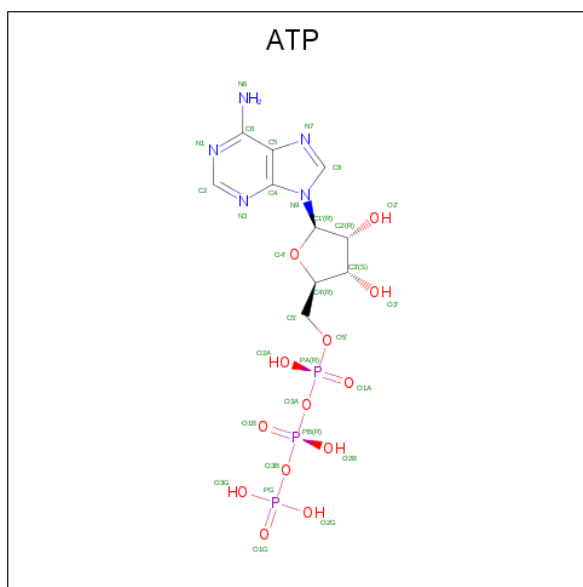
- Molecule 2 is a DNA chain called 5'-D(\*TP\*TP\*TP\*TP\*CP\*GP\*CP\*GP\*TP\*AP\*GP\*C P\*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	P	0	0	0
			60	29	13	16	2			
2	G	4	Total	C	N	O	P	0	0	0
			81	39	18	21	3			
2	H	6	Total	C	N	O	P	0	0	0
			118	59	16	38	5			

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

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

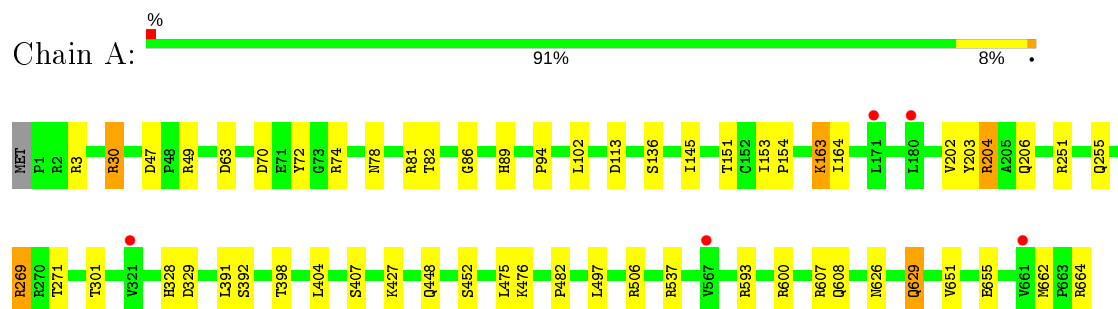
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



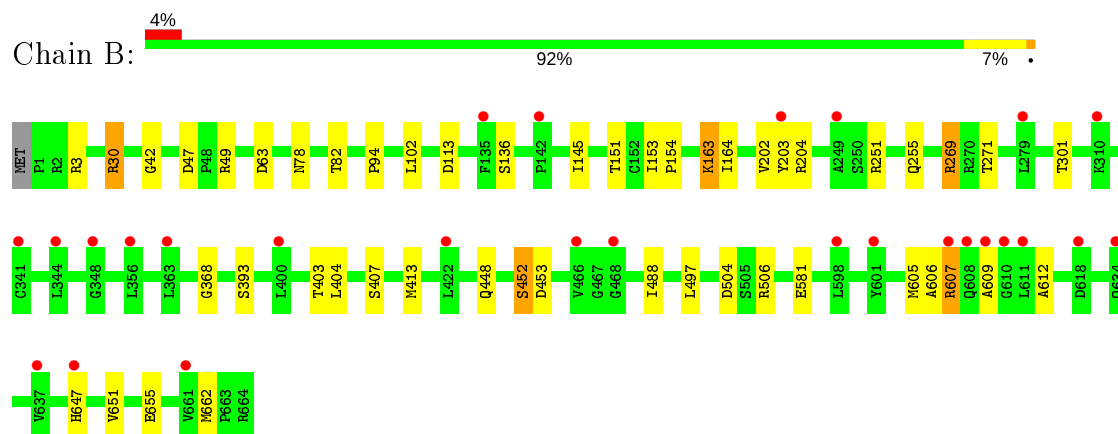
### 3 Residue-property plots [i](#)

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.

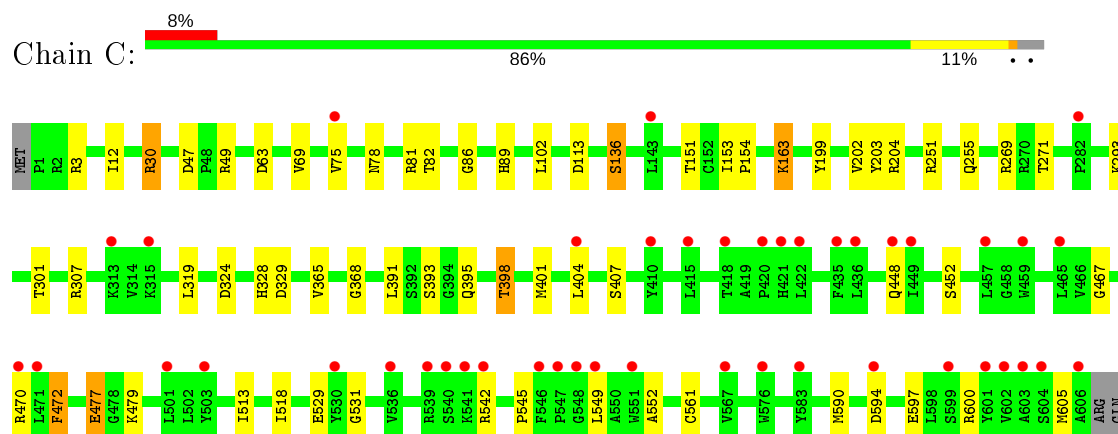
#### • Molecule 1: RNA-DIRECTED RNA POLYMERASE

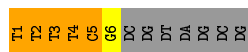


#### • Molecule 1: RNA-DIRECTED RNA POLYMERASE



#### • Molecule 1: RNA-DIRECTED RNA POLYMERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.51Å 91.71Å 142.08Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	33.49 – 2.90 65.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.49-2.90) 90.1 (65.57-2.90)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.216 , 0.250 0.232 , 0.264	Depositor DCC
$R_{free}$ test set	2743 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.45	0/5396	0.64	1/7297 (0.0%)
1	B	0.46	0/5396	0.67	0/7297
1	C	0.46	0/5249	0.68	0/7094
2	F	1.39	0/67	2.48	6/102 (5.9%)
2	G	1.35	0/91	2.24	7/139 (5.0%)
2	H	1.63	1/130 (0.8%)	2.89	16/199 (8.0%)
All	All	0.49	1/16329 (0.0%)	0.75	30/22128 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	5	DC	C1'-N1	5.32	1.56	1.49

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	DT	O4'-C1'-N1	14.61	118.22	108.00
2	H	1	DT	P-O3'-C3'	11.02	132.92	119.70
2	H	3	DT	P-O3'-C3'	11.01	132.91	119.70
2	H	5	DC	O4'-C1'-N1	9.12	114.38	108.00
2	H	3	DT	N3-C2-O2	-8.58	117.15	122.30
2	G	12	DC	O4'-C1'-N1	8.23	113.76	108.00
2	F	6	DG	O4'-C1'-N9	8.19	113.73	108.00
2	H	3	DT	O4'-C1'-N1	8.08	113.66	108.00
2	G	12	DC	P-O3'-C3'	7.57	128.78	119.70
2	H	5	DC	N1-C2-O2	6.73	122.94	118.90
2	F	6	DG	C8-N9-C4	-6.30	103.88	106.40
2	H	5	DC	C2-N1-C1'	6.15	125.56	118.80
2	H	4	DT	C1'-O4'-C4'	-6.13	103.97	110.10
2	H	4	DT	O4'-C1'-N1	5.60	111.92	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	DG	N7-C8-N9	5.50	115.85	113.10
2	H	2	DT	O4'-C1'-N1	5.40	111.78	108.00
2	G	11	DG	C8-N9-C4	-5.36	104.26	106.40
2	G	12	DC	C6-N1-C2	-5.34	118.16	120.30
2	G	11	DG	N7-C8-N9	5.34	115.77	113.10
2	F	7	DC	O4'-C1'-N1	5.30	111.71	108.00
2	G	13	DG	C2-N3-C4	5.25	114.53	111.90
2	H	5	DC	C6-N1-C2	-5.23	118.21	120.30
2	H	6	DG	O4'-C1'-N9	5.18	111.63	108.00
2	F	7	DC	P-O3'-C3'	5.17	125.91	119.70
2	F	7	DC	N1-C2-O2	5.13	121.98	118.90
2	G	11	DG	N3-C4-C5	-5.09	126.06	128.60
1	A	206	GLN	N-CA-C	-5.07	97.31	111.00
2	H	2	DT	N3-C2-O2	-5.05	119.27	122.30
2	H	5	DC	N3-C2-O2	-5.03	118.38	121.90
2	H	5	DC	O4'-C4'-C3'	-5.03	102.49	104.50

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	5265	0	5167	33	0
1	B	5265	0	5167	28	0
1	C	5123	0	5029	33	0
2	F	60	0	35	7	0
2	G	81	0	46	4	0
2	H	118	0	72	5	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
4	B	13	0	0	0	0
4	C	13	0	0	0	0
5	C	1	0	0	0	0
All	All	15955	0	15516	93	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 3.

All (93) 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:B:393:SER:HB2	2:G:11:DG:H21	1.36	0.91
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.22	0.75
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.40	0.70
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.39	0.69
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.37	0.69
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.62	0.64
1:C:467:GLY:HA2	1:C:470:ARG:HE	1.62	0.64
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.32	0.64
1:A:392:SER:O	1:A:398:THR:HG21	1.98	0.64
1:C:30:ARG:HD2	2:H:1:DT:H5"	1.82	0.62
1:C:391:LEU:HG	1:C:398:THR:HG22	1.84	0.60
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.84	0.59
1:A:30:ARG:HD2	2:F:6:DG:N2	2.17	0.59
1:B:151:THR:HG22	1:B:163:LYS:HG3	1.84	0.59
1:A:151:THR:HG22	1:A:163:LYS:HG3	1.84	0.58
1:B:393:SER:HB2	2:G:11:DG:N2	2.14	0.56
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.06	0.56
1:C:151:THR:HG22	1:C:163:LYS:HG3	1.87	0.56
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.42	0.55
1:B:393:SER:CB	2:G:11:DG:H21	2.16	0.54
2:H:3:DT:H2"	2:H:4:DT:H5'	1.88	0.54
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.08	0.52
1:C:477:GLU:CD	1:C:477:GLU:H	2.13	0.52
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.91	0.52
1:B:145:ILE:HD12	1:B:164:ILE:HD13	1.92	0.52
1:A:392:SER:O	1:A:398:THR:CG2	2.58	0.51
1:A:651:VAL:O	1:A:655:GLU:HB2	2.12	0.50
1:C:651:VAL:O	1:C:655:GLU:HB2	2.11	0.50
1:B:651:VAL:O	1:B:655:GLU:HB2	2.11	0.50
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.11	0.50
1:B:413:MET:CE	1:B:488:ILE:HG13	2.42	0.49
1:B:203:TYR:HB3	1:B:269:ARG:HD2	1.94	0.49
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.72	0.49
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.94	0.49
1:C:86:GLY:O	1:C:89:HIS:CD2	2.66	0.49
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.48	0.48
1:A:629:GLN:HG2	2:F:8:DG:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:SER:HA	1:B:448:GLN:HE22	1.79	0.48
1:C:136:SER:OG	1:C:293:LYS:NZ	2.47	0.48
1:C:407:SER:HA	1:C:448:GLN:HE22	1.79	0.48
1:B:504:ASP:OD2	1:B:506:ARG:NH1	2.47	0.47
1:A:407:SER:HA	1:A:448:GLN:HE22	1.79	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.45	0.47
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.97	0.47
1:C:549:LEU:HD22	1:C:619:LEU:HD22	1.96	0.47
1:A:30:ARG:HD2	2:F:6:DG:H21	1.78	0.46
1:C:621:VAL:HG22	1:C:627:LYS:HB2	1.97	0.46
1:C:629:GLN:NE2	2:H:4:DT:C4	2.84	0.46
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.96	0.46
1:C:395:GLN:HB3	1:C:398:THR:HG23	1.98	0.46
2:H:4:DT:H2'	2:H:5:DC:O4'	2.16	0.46
1:B:413:MET:HE2	1:B:488:ILE:HG13	1.98	0.45
1:A:204:ARG:CZ	2:F:7:DC:H41	2.27	0.45
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.13	0.45
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.17	0.44
1:C:301:THR:HG23	1:C:448:GLN:HG3	1.98	0.44
1:A:204:ARG:HD3	2:F:7:DC:N4	2.33	0.43
1:C:199:TYR:HB2	1:C:365:VAL:HG12	2.00	0.43
1:A:475:LEU:HD21	1:A:482:PRO:HG3	2.00	0.43
1:C:319:LEU:HD11	1:C:472:PHE:CD2	2.53	0.43
1:A:593:ARG:HG2	1:B:42:GLY:HA2	2.00	0.43
1:A:301:THR:HG23	1:A:448:GLN:HG3	2.01	0.43
1:A:600:ARG:HH12	1:B:581:GLU:CG	2.32	0.43
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.02	0.43
1:B:30:ARG:HD2	2:G:10:DA:H2	1.84	0.43
1:B:251:ARG:HH11	1:B:255:GLN:NE2	2.12	0.43
1:C:518:ILE:HB	1:C:561:CYS:SG	2.58	0.43
1:C:626:ASN:O	1:C:629:GLN:HB3	2.19	0.43
1:B:151:THR:CG2	1:B:163:LYS:HG3	2.49	0.43
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.02	0.43
2:H:1:DT:H1'	2:H:2:DT:OP2	2.19	0.43
1:A:427:LYS:HE3	1:C:12:ILE:HG21	2.01	0.42
1:A:204:ARG:HH12	1:A:626:ASN:HD21	1.66	0.42
1:C:151:THR:CG2	1:C:163:LYS:HG3	2.50	0.42
1:C:251:ARG:HH11	1:C:255:GLN:NE2	2.13	0.42
1:B:163:LYS:HE3	1:B:163:LYS:HB2	1.81	0.42
1:C:69:VAL:HG22	1:C:75:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLY:O	1:A:89:HIS:HD2	2.03	0.41
1:C:549:LEU:HD13	1:C:622:LEU:HD23	2.03	0.41
1:A:204:ARG:NE	2:F:7:DC:H41	2.17	0.41
1:A:153:ILE:HA	1:A:154:PRO:HA	1.89	0.41
1:B:452:SER:HB3	1:B:453:ASP:H	1.67	0.41
1:C:391:LEU:HD11	1:C:401:MET:HB2	2.02	0.41
1:A:151:THR:CG2	1:A:163:LYS:HG3	2.49	0.41
1:B:153:ILE:HA	1:B:154:PRO:HA	1.88	0.41
1:C:477:GLU:N	1:C:477:GLU:CD	2.73	0.40
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.87	0.40
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.85	0.40
1:C:153:ILE:HA	1:C:154:PRO:HA	1.88	0.40
1:C:204:ARG:HD2	1:C:529:GLU:OE2	2.21	0.40
1:B:94:PRO:HB3	1:B:269:ARG:HG3	2.02	0.40
1:A:204:ARG:HD3	2:F:7:DC:C5	2.56	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	662/665 (100%)	642 (97%)	18 (3%)	2 (0%)	41 71
1	B	662/665 (100%)	633 (96%)	25 (4%)	4 (1%)	25 58
1	C	640/665 (96%)	606 (95%)	28 (4%)	6 (1%)	17 48
All	All	1964/1995 (98%)	1881 (96%)	71 (4%)	12 (1%)	25 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	136	SER
1	A	607	ARG

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Mol	Chain	Res	Type
1	B	607	ARG
1	B	136	SER
1	C	368	GLY
1	A	136	SER
1	B	368	GLY
1	C	393	SER
1	C	552	ALA
1	B	612	ALA
1	C	545	PRO
1	C	531	GLY

### 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	557/558 (100%)	536 (96%)	21 (4%)	33	67
1	B	557/558 (100%)	538 (97%)	19 (3%)	37	71
1	C	543/558 (97%)	512 (94%)	31 (6%)	20	51
All	All	1657/1674 (99%)	1586 (96%)	71 (4%)	29	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	63	ASP
1	A	78	ASN
1	A	81	ARG
1	A	82	THR
1	A	102	LEU
1	A	113	ASP
1	A	163	LYS
1	A	202	VAL
1	A	204	ARG
1	A	269	ARG

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Mol	Chain	Res	Type
1	A	391	LEU
1	A	404	LEU
1	A	452	SER
1	A	497	LEU
1	A	506	ARG
1	A	608	GLN
1	A	629	GLN
1	A	662	MET
1	A	664	ARG
1	B	3	ARG
1	B	30	ARG
1	B	63	ASP
1	B	78	ASN
1	B	82	THR
1	B	102	LEU
1	B	113	ASP
1	B	163	LYS
1	B	202	VAL
1	B	204	ARG
1	B	269	ARG
1	B	403	THR
1	B	404	LEU
1	B	452	SER
1	B	497	LEU
1	B	605	MET
1	B	607	ARG
1	B	647	HIS
1	B	662	MET
1	C	3	ARG
1	C	30	ARG
1	C	63	ASP
1	C	78	ASN
1	C	81	ARG
1	C	82	THR
1	C	102	LEU
1	C	113	ASP
1	C	163	LYS
1	C	202	VAL
1	C	269	ARG
1	C	307	ARG
1	C	324	ASP
1	C	398	THR

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Mol	Chain	Res	Type
1	C	404	LEU
1	C	452	SER
1	C	472	PHE
1	C	477	GLU
1	C	479	LYS
1	C	513	ILE
1	C	542	ARG
1	C	590	MET
1	C	594	ASP
1	C	597	GLU
1	C	600	ARG
1	C	605	MET
1	C	617	ILE
1	C	622	LEU
1	C	646	MET
1	C	662	MET
1	C	664	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	255	GLN
1	A	309	ASN
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	626	ASN
1	A	634	GLN
1	A	642	HIS
1	B	15	GLN
1	B	78	ASN
1	B	91	ASN
1	B	255	GLN
1	B	309	ASN
1	B	448	GLN
1	B	492	HIS
1	B	525	GLN

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Mol	Chain	Res	Type
1	B	642	HIS
1	C	15	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	255	GLN
1	C	303	HIS
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	492	HIS
1	C	525	GLN
1	C	647	HIS

### 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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	C	1665	-	8,12,33	1.00	0	15,20,52	1.04	1 (6%)
4	ATP	B	1666	-	8,12,33	1.16	0	15,20,52	1.05	1 (6%)
4	ATP	A	1666	3	8,12,33	1.08	0	15,20,52	0.96	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
4	ATP	C	1665	-	-	0/12/12/38	-
4	ATP	B	1666	-	-	1/12/12/38	-
4	ATP	A	1666	3	-	0/12/12/38	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1666	ATP	O2A-PA-O3A	3.26	115.55	104.64
4	C	1665	ATP	O2G-PG-O3B	2.34	112.49	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

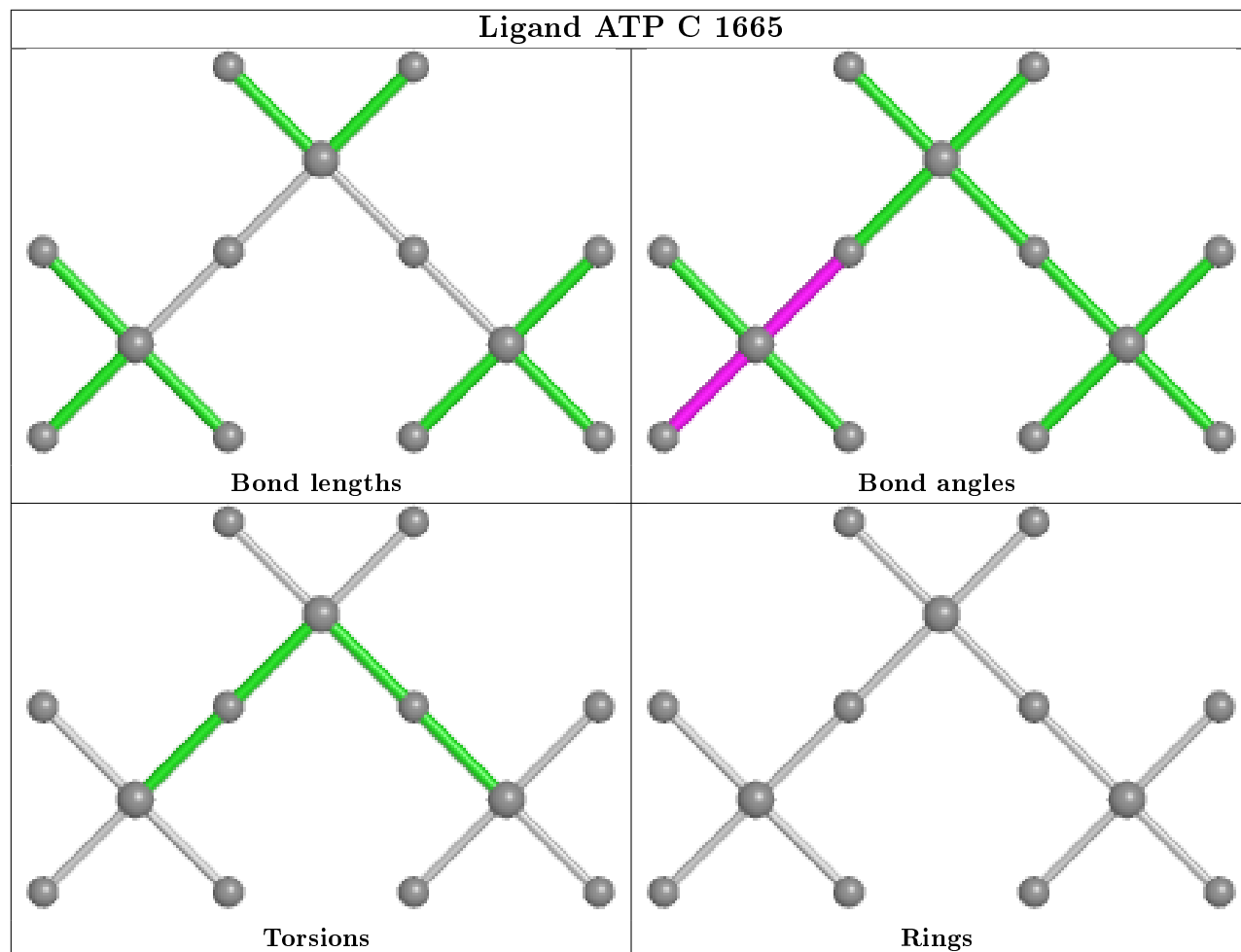
Mol	Chain	Res	Type	Atoms
4	B	1666	ATP	PA-O3A-PB-O2B

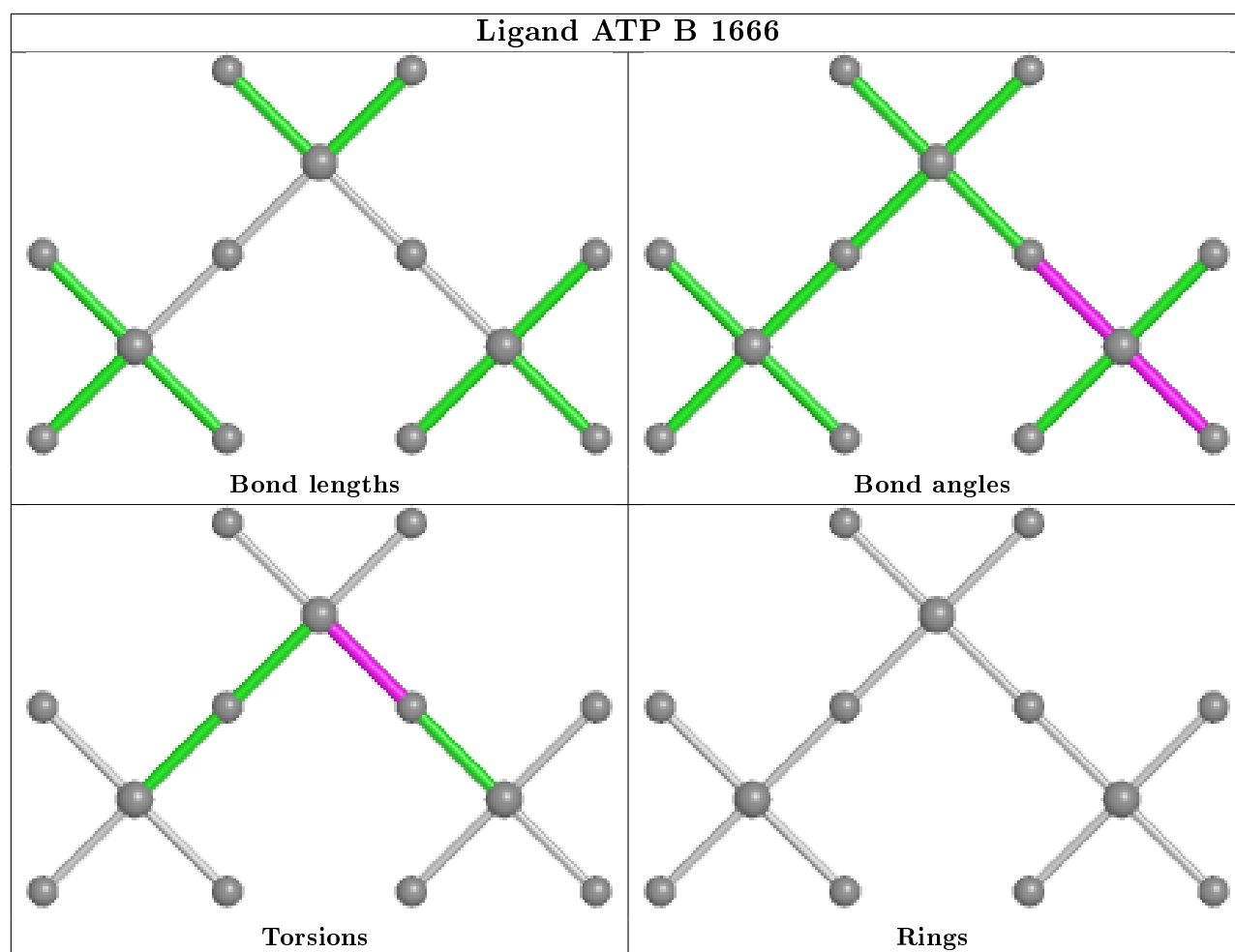
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





## 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<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%)	0.29	5 (0%) 86 86	59, 83, 107, 136	0
1	B	664/665 (99%)	0.40	27 (4%) 37 32	69, 92, 124, 157	0
1	C	646/665 (97%)	0.65	52 (8%) 12 9	61, 105, 159, 217	0
2	F	3/13 (23%)	0.89	0 100 100	108, 108, 112, 118	0
2	G	4/13 (30%)	1.73	2 (50%) 0 0	160, 166, 170, 181	0
2	H	6/13 (46%)	0.80	0 100 100	121, 131, 141, 142	0
All	All	1987/2034 (97%)	0.45	86 (4%) 35 31	59, 90, 141, 217	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	601	TYR	8.3
1	C	612	ALA	8.3
1	C	541	LYS	7.8
1	C	540	SER	6.1
1	C	606	ALA	6.1
1	B	611	LEU	5.4
1	C	546	PHE	5.2
1	C	594	ASP	5.1
1	C	457	LEU	4.9
1	C	614	LEU	4.7
1	C	602	VAL	4.0
1	B	661	VAL	3.9
1	C	315	LYS	3.9
1	C	630	TYR	3.8
1	C	539	ARG	3.8
1	C	603	ALA	3.7
1	C	415	LEU	3.6
1	C	646	MET	3.6
1	C	503	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	604	SER	3.4
1	C	547	PRO	3.4
1	C	542	ARG	3.3
1	C	410	TYR	3.2
1	C	567	VAL	3.2
1	C	619	LEU	3.1
1	C	576	TRP	3.1
1	C	583	TYR	3.1
1	C	551	TRP	3.1
1	B	135	PHE	3.0
1	B	607	ARG	3.0
1	C	422	LEU	3.0
1	C	404	LEU	2.9
1	C	420	PRO	2.8
1	B	142	PRO	2.8
1	B	356	LEU	2.7
1	C	613	GLU	2.7
1	B	610	GLY	2.7
1	B	647	HIS	2.7
1	C	548	GLY	2.7
1	B	363	LEU	2.6
1	B	203	TYR	2.6
1	B	249	ALA	2.6
1	C	435	PHE	2.6
1	B	466	VAL	2.5
1	C	624	ASP	2.5
1	C	501	LEU	2.5
1	B	609	ALA	2.5
1	B	608	GLN	2.5
1	C	448	GLN	2.5
1	C	75	VAL	2.5
2	G	10	DA	2.5
1	C	282	PRO	2.5
1	B	310	LYS	2.5
1	B	341	CYS	2.5
1	C	421	HIS	2.4
1	C	471	LEU	2.4
1	A	661	VAL	2.4
1	B	422	LEU	2.4
1	C	459	TRP	2.4
1	A	180	LEU	2.4
1	C	418	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	598	LEU	2.4
1	C	449	ILE	2.3
1	C	465	LEU	2.3
1	B	400	LEU	2.3
1	B	348	GLY	2.3
1	C	436	LEU	2.3
1	B	618	ASP	2.2
1	B	279	LEU	2.2
1	C	143	LEU	2.2
1	A	567	VAL	2.2
1	C	549	LEU	2.1
1	C	313	LYS	2.1
2	G	11	DG	2.1
1	B	468	GLY	2.1
1	A	171	LEU	2.1
1	C	599	SER	2.1
1	B	344	LEU	2.1
1	C	470	ARG	2.1
1	B	634	GLN	2.1
1	C	530	TYR	2.1
1	B	637	VAL	2.1
1	C	536	VAL	2.0
1	C	645	LEU	2.0
1	B	601	TYR	2.0
1	A	321	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

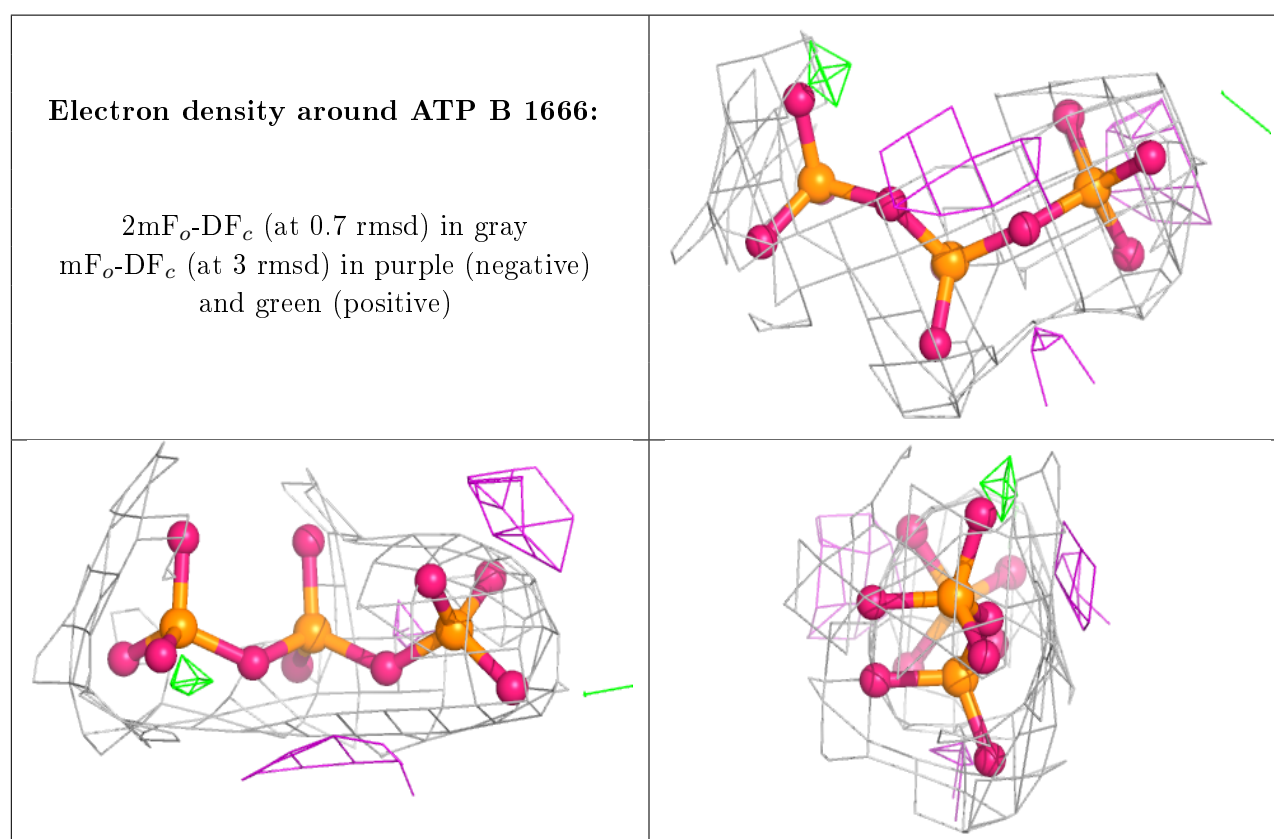
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

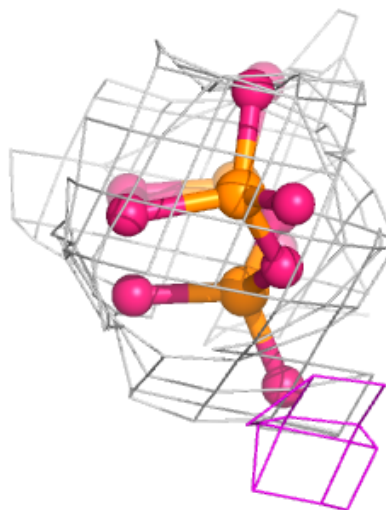
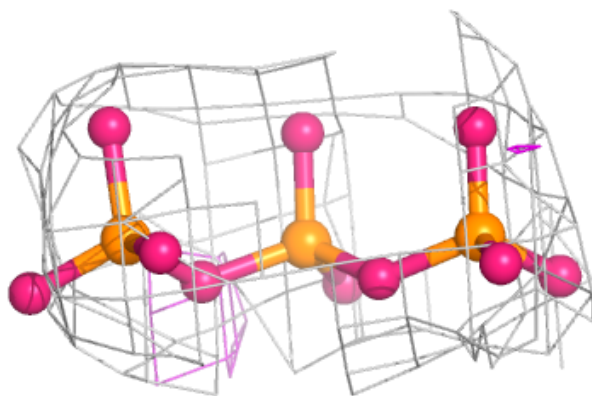
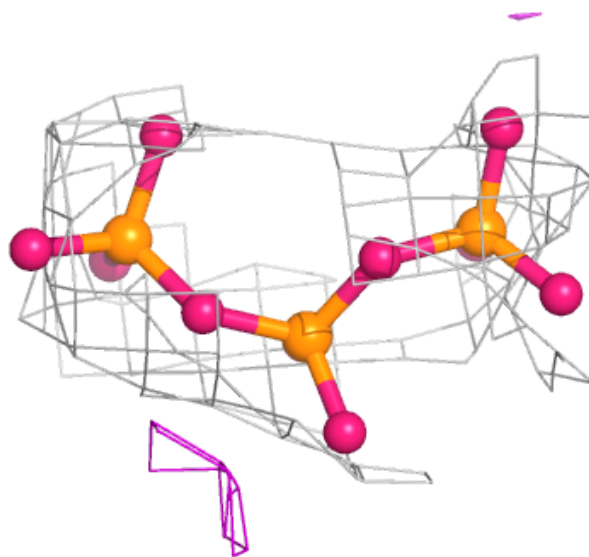
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	A	1666	13/31	0.72	0.19	180,184,185,186	0
4	ATP	B	1666	13/31	0.83	0.17	154,159,164,165	0
4	ATP	C	1665	13/31	0.83	0.16	201,206,211,212	0
3	MG	A	1667	1/1	0.89	0.11	69,69,69,69	0
3	MG	B	1665	1/1	0.93	0.12	71,71,71,71	0
3	MG	A	1665	1/1	0.97	0.17	72,72,72,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around ATP C 1665:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.