Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:21 am 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 X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

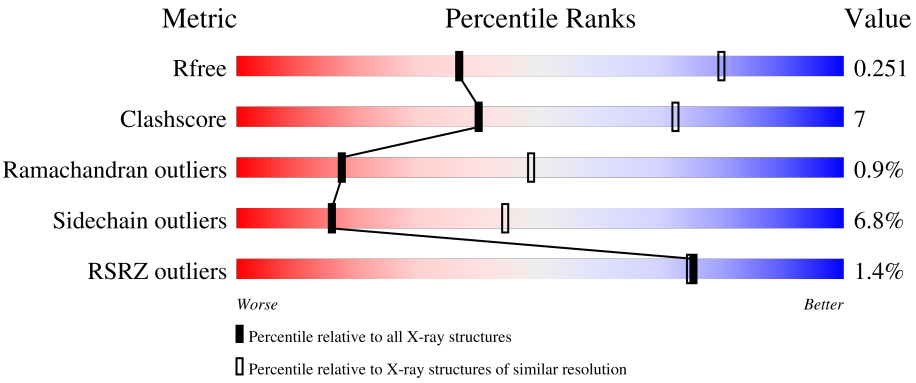
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	665	86% 13%
1	B	665	79% 19%
1	C	665	80% 17%
2	G	4	100% 50% 50%

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
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 (i)

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

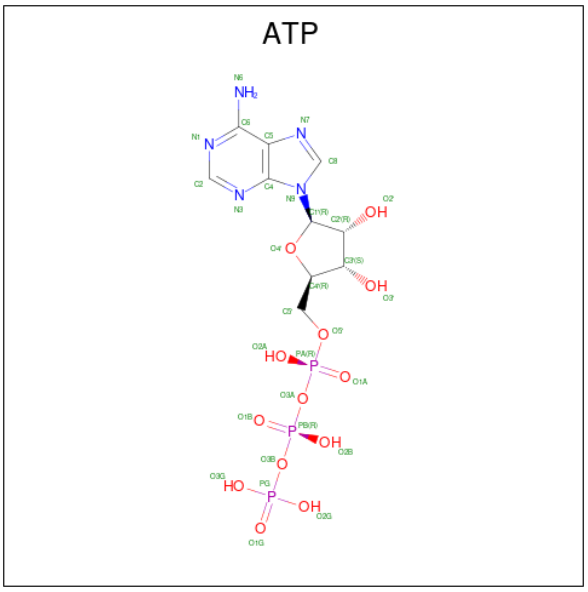
- Molecule 2 is a DNA chain called 5'-D(*DAP*GP*CP*GP)-3'.

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	A	1	Total	Mg	0	1
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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



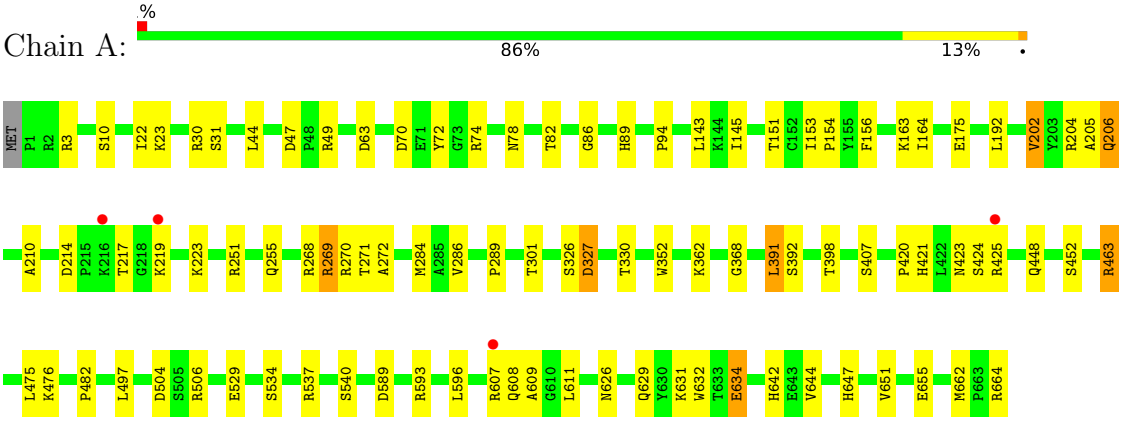
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	A	1	Total	O	P			0	0
			13	10	3				
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots (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.

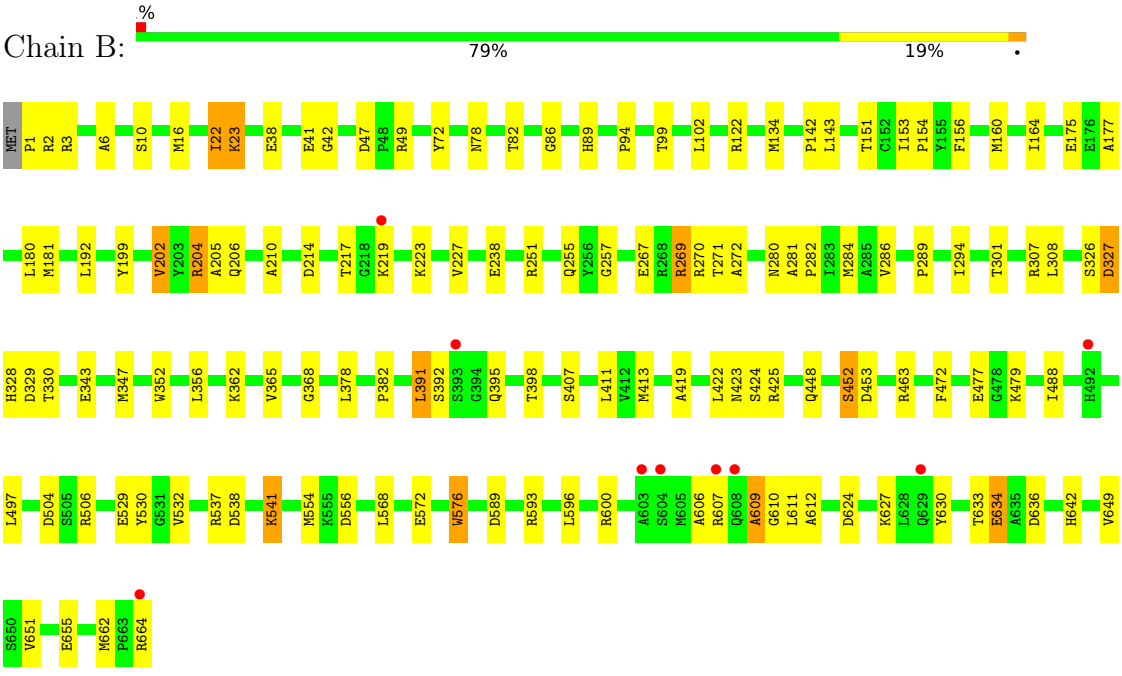
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain A:



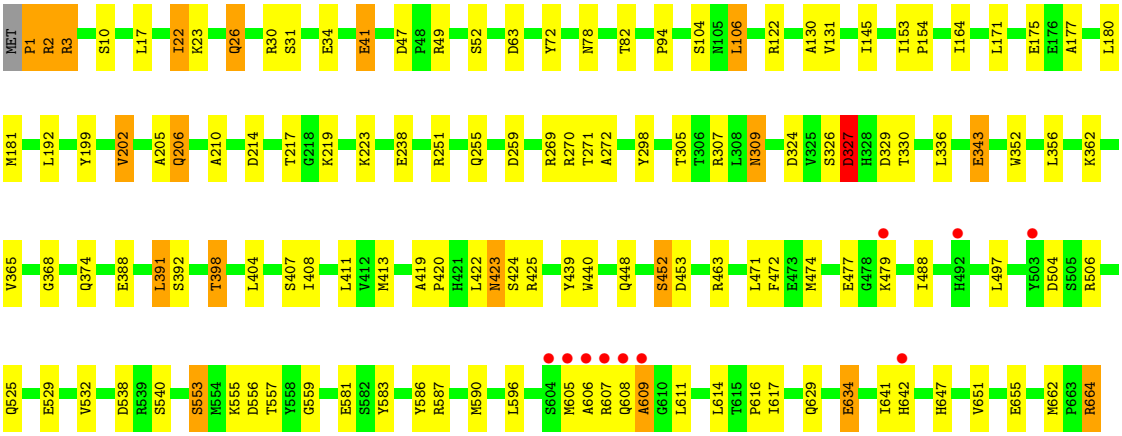
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain B:



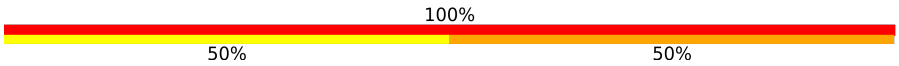
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain C:



• Molecule 2: 5’-D(*DAP*GP*CP*GP)-3’

Chain G:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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: ATP, MG

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(^{o})	Ideal(^{o})
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 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	5165	54	0
1	B	5265	0	5165	78	0
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.

All (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: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:CD1	1:B:22:ILE:CG1	1.84	1.54
4:C:1666:ATP:O4'	4:C:1666:ATP:C1'	1.64	1.45
1:B:16:MET:SD	1:B:16:MET:CE	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
1:A:608:GLN:HE22	1:B:593:ARG:HD3	1.12	1.09
1:C:270:ARG:HH22	4:C:1666:ATP:C3'	1.73	1.02
4:C:1665:ATP:N9	4:C:1666:ATP:O2'	1.94	1.01
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.42	0.98
1:B:1:PRO:HD3	1:B:238:GLU:HG3	1.48	0.95
1:C:664:ARG:N	1:C:664:ARG:HD3	1.83	0.94
4:C:1665:ATP:C8	4:C:1666:ATP:C2'	2.52	0.91
1:A:608:GLN:NE2	1:B:593:ARG:HD3	1.86	0.89
1:C:270:ARG:HH22	4:C:1666:ATP:C2'	1.89	0.84
1:B:541:LYS:HE2	2:G:4:DA:H3'	1.59	0.84
1:B:204:ARG:HE	2:G:7:DG:H21	1.27	0.81
1:B:651:VAL:O	1:B:655:GLU:HB2	1.81	0.80
1:C:270:ARG:HH22	4:C:1666:ATP:H2'	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1665:ATP:H5'1	4:C:1666:ATP:O3'	1.87	0.75
1:A:270:ARG:HH22	4:A:1667:ATP:PA	2.09	0.74
1:B:391:LEU:HD22	1:B:398:THR:HG22	1.67	0.74
1:A:608:GLN:HE22	1:B:593:ARG:CD	1.97	0.74
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.37	0.72
1:C:343:GLU:OE1	1:C:343:GLU:HA	1.87	0.72
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.69	0.72
4:C:1665:ATP:O4'	4:C:1666:ATP:O3'	2.07	0.71
1:B:328:HIS:HB3	4:B:1666:ATP:O2'	1.90	0.71
1:C:1:PRO:HG2	1:C:238:GLU:HG3	1.73	0.71
1:C:391:LEU:HD22	1:C:398:THR:HG22	1.73	0.70
1:A:593:ARG:HG2	1:B:42:GLY:HA2	1.73	0.70
1:B:160:MET:HB3	2:G:4:DA:N1	2.07	0.70
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.24	0.70
1:C:664:ARG:HD3	1:C:664:ARG:H	1.57	0.69
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.40	0.67
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.76	0.67
1:C:177:ALA:HA	1:C:180:LEU:HD12	1.75	0.67
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:22:ILE:CD1	1:C:22:ILE:HA	2.26	0.66
1:C:34:GLU:HG2	1:C:94:PRO:HD2	1.77	0.66
1:C:651:VAL:O	1:C:655:GLU:HB2	1.97	0.65
1:C:305:THR:H	1:C:309:ASN:ND2	1.94	0.65
1:C:106:LEU:HD21	1:C:388:GLU:HG3	1.80	0.64
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.45	0.64
1:C:617:ILE:H	1:C:617:ILE:HD12	1.63	0.63
1:B:22:ILE:CD1	1:B:22:ILE:HA	2.28	0.63
1:C:664:ARG:N	1:C:664:ARG:CD	2.60	0.63
1:A:22:ILE:CD1	1:A:22:ILE:HA	2.30	0.61
1:A:392:SER:O	1:A:398:THR:HG21	2.00	0.61
1:C:130:ALA:HB2	1:C:408:ILE:HD11	1.84	0.59
1:C:202:VAL:HG22	1:C:272:ALA:HB3	1.84	0.59
1:C:664:ARG:H	1:C:664:ARG:CD	2.16	0.59
4:C:1666:ATP:C4	4:C:1666:ATP:H5'2	2.38	0.59
1:C:538:ASP:OD1	1:C:540:SER:HB3	2.02	0.59
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.68	0.59
1:C:22:ILE:HG23	1:C:26:GLN:OE1	2.02	0.58
1:C:420:PRO:HA	1:C:423:ASN:HD21	1.68	0.58
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.04	0.58
1:C:1:PRO:HG2	1:C:238:GLU:CG	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG22	1:B:272:ALA:HB3	1.86	0.58
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.86	0.57
1:A:651:VAL:O	1:A:655:GLU:HB2	2.05	0.57
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.05	0.56
1:C:164:ILE:HD11	1:C:647:HIS:HD2	1.71	0.56
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.71	0.56
1:B:214:ASP:OD2	1:B:217:THR:HG22	2.06	0.55
1:B:453:ASP:OD2	4:B:1666:ATP:H1'	2.07	0.55
1:C:605:MET:HG2	1:C:609:ALA:HB3	1.87	0.55
1:B:554:MET:CE	1:B:568:LEU:HD11	2.36	0.55
1:A:206:GLN:HE21	1:A:268:ARG:HH11	1.55	0.55
1:C:270:ARG:HH21	4:C:1666:ATP:H3'	1.64	0.55
1:C:270:ARG:HH12	4:C:1666:ATP:H5'2	1.72	0.55
1:B:47:ASP:OD1	1:B:49:ARG:HD3	2.06	0.55
1:C:419:ALA:CB	1:C:422:LEU:HD12	2.27	0.55
1:C:22:ILE:HA	1:C:22:ILE:HD13	1.87	0.54
1:B:160:MET:HB3	2:G:4:DA:C2	2.42	0.54
1:C:270:ARG:NH2	4:C:1666:ATP:C2'	2.68	0.54
1:C:214:ASP:OD2	1:C:217:THR:HG22	2.07	0.54
1:A:202:VAL:HG22	1:A:272:ALA:HB3	1.88	0.54
1:C:270:ARG:NH2	4:C:1666:ATP:C3'	2.39	0.54
1:B:22:ILE:HA	1:B:22:ILE:HD13	1.89	0.53
1:B:1:PRO:CD	1:B:238:GLU:HG3	2.32	0.53
1:A:407:SER:HA	1:A:448:GLN:HE22	1.74	0.53
1:B:392:SER:O	1:B:398:THR:HG21	2.07	0.53
1:B:634:GLU:HG3	1:B:642:HIS:NE2	2.24	0.53
1:C:270:ARG:NH2	4:C:1666:ATP:H2'	2.21	0.53
1:A:164:ILE:HD11	1:A:647:HIS:HD2	1.74	0.52
1:B:181:MET:CE	1:B:356:LEU:HD23	2.39	0.52
1:B:452:SER:OG	4:B:1666:ATP:H2	1.92	0.52
1:A:420:PRO:HA	1:A:423:ASN:ND2	2.24	0.52
1:C:634:GLU:HG3	1:C:642:HIS:NE2	2.24	0.52
1:C:34:GLU:CG	1:C:94:PRO:HD2	2.39	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:214:ASP:OD2	1:A:217:THR:HG22	2.10	0.51
1:B:210:ALA:HB3	1:B:223:LYS:HB2	1.91	0.51
1:A:151:THR:CG2	1:A:163:LYS:HG2	2.41	0.51
1:B:205:ALA:O	1:B:529:GLU:HG3	2.10	0.51
1:B:554:MET:HE3	1:B:568:LEU:HD11	1.92	0.51
1:C:407:SER:HA	1:C:448:GLN:HE22	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:O	1:B:289:PRO:HD2	2.11	0.51
1:A:537:ARG:HD2	1:B:49:ARG:HG3	1.93	0.50
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.94	0.50
1:C:106:LEU:CD2	1:C:388:GLU:HG3	2.41	0.50
1:C:210:ALA:HB3	1:C:223:LYS:HB2	1.93	0.50
1:A:151:THR:HG22	1:A:163:LYS:HG2	1.94	0.50
4:C:1665:ATP:C5'	4:C:1666:ATP:O3'	2.58	0.50
1:A:210:ALA:HB3	1:A:223:LYS:HB2	1.94	0.49
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.76	0.49
1:C:131:VAL:HG11	1:C:343:GLU:HB3	1.93	0.49
1:B:395:GLN:HB3	1:B:398:THR:HG23	1.93	0.49
1:C:206:GLN:HB2	1:C:270:ARG:HD2	1.93	0.49
1:A:44:LEU:HD21	1:B:257:GLY:HA3	1.95	0.49
1:C:104:SER:OG	1:C:106:LEU:HD22	2.13	0.48
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.95	0.48
1:A:634:GLU:HG3	1:A:642:HIS:NE2	2.28	0.48
1:B:407:SER:HA	1:B:448:GLN:HE22	1.78	0.48
1:B:392:SER:O	1:B:398:THR:CG2	2.62	0.48
1:B:72:TYR:HB3	1:B:472:PHE:CZ	2.48	0.48
1:C:41:GLU:HG2	1:C:532:VAL:HG11	1.96	0.48
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.95	0.48
1:B:217:THR:HG23	1:B:219:LYS:HB2	1.96	0.48
1:C:1:PRO:CG	1:C:238:GLU:HG3	2.43	0.48
1:B:270:ARG:NH1	4:B:1666:ATP:H5'1	2.29	0.48
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.44	0.47
1:A:22:ILE:CD1	1:A:22:ILE:CB	2.82	0.47
1:A:72:TYR:CE2	1:A:476:LYS:HD3	2.49	0.47
1:A:23:LYS:HE2	1:A:156:PHE:O	2.13	0.47
1:A:540:SER:HB2	1:A:644:VAL:O	2.14	0.47
1:B:204:ARG:HD2	1:B:530:TYR:OH	2.14	0.47
1:B:630:TYR:CE2	4:B:1665:ATP:H2'	2.50	0.47
1:A:504:ASP:OD2	1:A:506:ARG:NH1	2.47	0.47
1:C:420:PRO:O	1:C:423:ASN:ND2	2.48	0.47
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.97	0.47
1:B:477:GLU:HB3	1:B:479:LYS:HG3	1.97	0.46
1:C:72:TYR:HD2	1:C:472:PHE:CZ	2.33	0.46
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.97	0.46
4:C:1665:ATP:H5'1	4:C:1666:ATP:C3'	2.46	0.46
1:C:471:LEU:HD12	1:C:474:MET:HE3	1.97	0.46
1:B:301:THR:HG23	1:B:448:GLN:HG3	1.98	0.46
1:B:38:GLU:HB3	1:B:532:VAL:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:ASP:HB3	1:B:627:LYS:HD2	1.97	0.46
1:B:160:MET:O	1:B:164:ILE:HD12	2.16	0.46
1:C:72:TYR:HD2	1:C:472:PHE:CE2	2.34	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.97	0.46
1:C:452:SER:HB3	1:C:453:ASP:H	1.61	0.45
1:A:251:ARG:HH11	1:A:255:GLN:NE2	2.12	0.45
1:A:270:ARG:NH1	4:A:1666:ATP:H3'	2.32	0.45
1:A:301:THR:HG23	1:A:448:GLN:HG3	1.99	0.45
1:B:164:ILE:HG23	1:B:649:VAL:HG22	1.98	0.45
1:C:34:GLU:HG2	1:C:94:PRO:CD	2.46	0.45
1:B:572:GLU:O	1:B:576:TRP:HB2	2.16	0.45
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.51	0.45
1:C:586:TYR:CE2	1:C:590:MET:CE	2.99	0.45
1:C:26:GLN:HE21	1:C:26:GLN:HB2	1.58	0.45
1:B:504:ASP:OD2	1:B:506:ARG:NH1	2.49	0.45
1:C:411:LEU:HD22	1:C:439:TYR:CD2	2.51	0.45
1:C:477:GLU:HB3	1:C:479:LYS:HE3	1.97	0.45
1:A:204:ARG:NH2	1:A:626:ASN:HD21	2.15	0.45
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.52	0.45
1:A:270:ARG:NH2	4:A:1667:ATP:O1A	2.44	0.45
1:B:633:THR:HG22	1:B:636:ASP:OD2	2.17	0.45
1:C:217:THR:HG23	1:C:219:LYS:HB2	1.99	0.45
1:C:251:ARG:HH11	1:C:255:GLN:NE2	2.08	0.45
1:A:143:LEU:HD21	1:A:284:MET:HE2	1.98	0.44
1:B:538:ASP:OD2	2:G:4:DA:H8	2.00	0.44
1:A:70:ASP:OD2	1:A:74:ARG:HD2	2.17	0.44
4:B:1665:ATP:O5'	4:B:1665:ATP:H8	2.00	0.44
1:A:205:ALA:O	1:A:529:GLU:HG3	2.17	0.44
4:C:1665:ATP:C4'	4:C:1666:ATP:O3'	2.65	0.44
1:B:413:MET:HE1	1:B:488:ILE:HG21	2.00	0.44
1:B:143:LEU:HD21	1:B:284:MET:HE2	2.00	0.43
1:A:217:THR:HG23	1:A:219:LYS:HB2	2.00	0.43
1:C:336:LEU:HD21	1:C:404:LEU:HD12	1.98	0.43
1:C:122:ARG:NH1	1:C:423:ASN:OD1	2.49	0.43
1:B:23:LYS:HE2	1:B:156:PHE:O	2.19	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	2.01	0.43
1:C:3:ARG:O	1:C:3:ARG:HG3	2.13	0.43
1:C:205:ALA:O	1:C:529:GLU:HG3	2.19	0.43
1:A:421:HIS:CE1	1:A:463:ARG:HB2	2.54	0.42
1:B:329:ASP:OD2	4:B:1666:ATP:H2'	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HA	1:A:154:PRO:HA	1.81	0.42
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.81	0.42
1:C:22:ILE:CD1	1:C:22:ILE:CB	2.81	0.42
1:C:181:MET:SD	1:C:356:LEU:HD23	2.60	0.42
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.54	0.42
1:B:99:THR:HB	1:B:227:VAL:HG12	2.00	0.42
1:A:286:VAL:O	1:A:289:PRO:HD2	2.20	0.42
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.55	0.42
1:B:199:TYR:HB2	1:B:365:VAL:HG12	2.02	0.42
1:A:391:LEU:HD22	1:A:398:THR:HG22	2.02	0.42
1:B:122:ARG:NH1	1:B:423:ASN:HD21	2.17	0.42
1:B:153:ILE:HA	1:B:154:PRO:HA	1.80	0.42
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.50	0.42
1:B:6:ALA:HA	1:B:378:LEU:O	2.20	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
1:C:22:ILE:CD1	1:C:22:ILE:CA	2.97	0.42
1:C:413:MET:HE1	1:C:488:ILE:HG21	2.01	0.42
1:B:160:MET:HG3	1:B:164:ILE:HD11	2.02	0.41
1:C:130:ALA:HB1	1:C:404:LEU:HD22	2.02	0.41
1:C:553:SER:HB3	1:C:616:PRO:HA	2.01	0.41
1:C:555:LYS:O	1:C:559:GLY:HA3	2.20	0.41
1:C:298:TYR:CD1	1:C:440:TRP:HB3	2.56	0.41
1:B:134:MET:HG2	1:B:294:ILE:HG21	2.01	0.41
1:B:343:GLU:O	1:B:347:MET:N	2.47	0.41
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.56	0.41
4:C:1666:ATP:C4	4:C:1666:ATP:C5'	3.04	0.41
1:B:142:PRO:HD3	1:B:651:VAL:HB	2.01	0.41
2:G:6:DC:H1'	2:G:7:DG:OP1	2.20	0.41
1:A:217:THR:HG23	1:A:219:LYS:H	1.86	0.41
1:B:177:ALA:HA	1:B:180:LEU:HD12	2.02	0.41
1:C:555:LYS:C	1:C:557:THR:H	2.23	0.41
2:G:7:DG:OP1	2:G:7:DG:H3'	2.20	0.41
1:B:86:GLY:O	1:B:89:HIS:CD2	2.73	0.41
1:B:181:MET:HE1	1:B:356:LEU:HD23	2.03	0.41
1:B:378:LEU:HD21	1:B:382:PRO:HD3	2.03	0.41
1:C:305:THR:H	1:C:309:ASN:HD21	1.68	0.41
1:C:392:SER:O	1:C:398:THR:HG21	2.20	0.41
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.41
1:C:614:LEU:HD21	1:C:641:ILE:HD11	2.03	0.41
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLU:CB	1:A:642:HIS:NE2	2.84	0.40
1:A:206:GLN:HE21	1:A:268:ARG:NH1	2.18	0.40
1:C:153:ILE:HA	1:C:154:PRO:HA	1.80	0.40
1:C:270:ARG:NH2	4:C:1666:ATP:H5'1	2.37	0.40
1:B:610:GLY:C	1:B:612:ALA:H	2.25	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%)	634 (96%)	23 (4%)	5 (1%)	19	51
1	B	662/665 (100%)	628 (95%)	28 (4%)	6 (1%)	17	48
1	C	662/665 (100%)	616 (93%)	40 (6%)	6 (1%)	17	48
All	All	1986/1995 (100%)	1878 (95%)	91 (5%)	17 (1%)	17	48

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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%)	529 (95%)	28 (5%)	24	55
1	B	557/558 (100%)	517 (93%)	40 (7%)	14	41
1	C	557/558 (100%)	511 (92%)	46 (8%)	11	36
All	All	1671/1674 (100%)	1557 (93%)	114 (7%)	16	44

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	206	GLN
1	A	255	GLN
1	A	309	ASN
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	A	626	ASN
1	A	647	HIS
1	B	15	GLN
1	B	26	GLN
1	B	78	ASN
1	B	89	HIS
1	B	91	ASN
1	B	255	GLN
1	B	309	ASN
1	B	423	ASN
1	B	448	GLN
1	B	492	HIS
1	B	608	GLN
1	B	647	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
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 monosaccharides 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	B	1665	-	26,33,33	2.26	5 (19%)	31,52,52	1.90	8 (25%)
4	ATP	C	1666	-	26,33,33	5.71	21 (80%)	31,52,52	4.10	19 (61%)
4	ATP	A	1666	-	26,33,33	4.92	20 (76%)	31,52,52	2.33	9 (29%)
4	ATP	B	1666	-	26,33,33	1.73	3 (11%)	31,52,52	1.77	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	A	1667	-	8,12,33	1.42	1 (12%)	15,20,52	2.14	5 (33%)
4	ATP	C	1665	-	26,33,33	2.61	6 (23%)	31,52,52	2.41	11 (35%)

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	B	1665	-	-	3/18/38/38	0/3/3/3
4	ATP	C	1666	-	-	4/18/38/38	0/3/3/3
4	ATP	A	1666	-	-	6/18/38/38	0/3/3/3
4	ATP	B	1666	-	-	5/18/38/38	0/3/3/3
4	ATP	A	1667	-	-	1/12/12/38	-
4	ATP	C	1665	-	-	6/18/38/38	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1666	ATP	O4'-C1'	16.71	1.64	1.41
4	C	1666	ATP	C4-N3	10.54	1.50	1.35
4	A	1666	ATP	O4'-C1'	10.47	1.55	1.41
4	C	1665	ATP	O4'-C1'	10.18	1.55	1.41
4	A	1666	ATP	C2-N3	9.72	1.47	1.32
4	A	1666	ATP	PA-O1A	8.44	1.80	1.50
4	C	1666	ATP	O4'-C4'	8.31	1.63	1.45
4	B	1665	ATP	O4'-C1'	8.08	1.52	1.41
4	A	1666	ATP	C4-N3	7.84	1.46	1.35
4	A	1666	ATP	C2'-C1'	7.84	1.65	1.53
4	C	1666	ATP	C5'-C4'	7.24	1.74	1.51
4	C	1666	ATP	C2-N1	6.99	1.46	1.33
4	C	1666	ATP	PB-O1B	6.51	1.74	1.50
4	C	1666	ATP	PG-O2G	6.10	1.78	1.54
4	C	1666	ATP	PG-O1G	5.76	1.69	1.50
4	A	1666	ATP	O4'-C4'	5.58	1.57	1.45
4	C	1666	ATP	PA-O1A	5.58	1.70	1.50
4	B	1666	ATP	O4'-C1'	5.55	1.48	1.41
4	A	1666	ATP	PG-O1G	5.41	1.68	1.50
4	C	1666	ATP	O3'-C3'	5.24	1.55	1.43
4	A	1666	ATP	PB-O1B	5.12	1.69	1.50
4	A	1666	ATP	C2'-C3'	4.82	1.66	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1666	ATP	C2'-C3'	4.74	1.66	1.53
4	A	1666	ATP	PA-O5'	4.67	1.78	1.59
4	B	1665	ATP	C2-N3	4.12	1.38	1.32
4	A	1666	ATP	O3'-C3'	4.06	1.52	1.43
4	C	1665	ATP	C2-N1	4.02	1.41	1.33
4	B	1665	ATP	C2'-C1'	3.95	1.59	1.53
4	B	1666	ATP	C2-N3	3.90	1.38	1.32
4	C	1665	ATP	C5-C4	3.70	1.50	1.40
4	B	1666	ATP	C2'-C1'	3.61	1.59	1.53
4	A	1666	ATP	C2-N1	3.56	1.40	1.33
4	C	1666	ATP	PA-O2A	3.53	1.71	1.55
4	C	1666	ATP	C6-C5	3.39	1.55	1.43
4	C	1666	ATP	C3'-C4'	-3.22	1.44	1.53
4	C	1665	ATP	C2-N3	3.18	1.37	1.32
4	C	1666	ATP	C2'-C1'	3.11	1.58	1.53
4	A	1666	ATP	PG-O2G	3.10	1.66	1.54
4	C	1666	ATP	PA-O5'	3.07	1.71	1.59
4	C	1665	ATP	O4'-C4'	3.01	1.51	1.45
4	A	1667	ATP	PA-O5'	3.01	1.66	1.54
4	B	1665	ATP	C8-N7	-2.98	1.29	1.34
4	A	1666	ATP	C6-N1	2.98	1.50	1.37
4	A	1666	ATP	O2'-C2'	2.91	1.49	1.43
4	C	1666	ATP	C6-N6	2.89	1.44	1.34
4	C	1666	ATP	C8-N7	2.88	1.39	1.34
4	A	1666	ATP	C3'-C4'	2.72	1.59	1.53
4	C	1665	ATP	C5'-C4'	2.68	1.59	1.51
4	C	1666	ATP	C6-N1	2.64	1.48	1.37
4	C	1666	ATP	C5-N7	2.56	1.49	1.39
4	C	1666	ATP	C2-N3	2.49	1.36	1.32
4	A	1666	ATP	C6-N6	2.38	1.42	1.34
4	A	1666	ATP	C6-C5	2.35	1.52	1.43
4	B	1665	ATP	PB-O1B	2.32	1.59	1.50
4	A	1666	ATP	PB-O2B	2.19	1.65	1.55
4	A	1666	ATP	C5-C4	2.12	1.46	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1666	ATP	C1'-N9-C4	-7.54	113.39	126.64
4	C	1666	ATP	O3'-C3'-C4'	-7.54	89.25	111.05
4	C	1666	ATP	C3'-C2'-C1'	7.50	112.28	100.98
4	C	1666	ATP	O4'-C4'-C5'	7.12	132.79	109.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1666	ATP	O4'-C1'-C2'	-6.52	97.39	106.93
4	C	1666	ATP	O5'-PA-O1A	-6.48	83.74	109.07
4	A	1666	ATP	C3'-C2'-C1'	6.42	110.64	100.98
4	C	1665	ATP	C3'-C2'-C1'	6.13	110.20	100.98
4	C	1665	ATP	O4'-C1'-C2'	-5.81	98.43	106.93
4	C	1666	ATP	O2'-C2'-C1'	-5.75	89.63	110.85
4	C	1665	ATP	C4-C5-N7	5.55	115.19	109.40
4	C	1666	ATP	O3'-C3'-C2'	5.41	129.31	111.82
4	A	1666	ATP	O4'-C4'-C3'	4.93	114.88	105.11
4	B	1666	ATP	C1'-N9-C4	4.92	135.28	126.64
4	A	1667	ATP	O2A-PA-O3A	4.81	120.77	104.64
4	C	1666	ATP	C5'-C4'-C3'	-4.53	98.20	115.18
4	B	1665	ATP	O2'-C2'-C1'	4.38	127.03	110.85
4	C	1666	ATP	N3-C2-N1	-4.10	122.27	128.68
4	C	1666	ATP	O2'-C2'-C3'	-4.05	98.73	111.82
4	C	1666	ATP	O2G-PG-O3B	-4.05	91.07	104.64
4	B	1665	ATP	C3'-C2'-C1'	3.97	106.95	100.98
4	A	1666	ATP	C4-C5-N7	-3.94	105.29	109.40
4	A	1667	ATP	O2G-PG-O3B	3.80	117.37	104.64
4	B	1665	ATP	O3'-C3'-C4'	3.63	121.55	111.05
4	C	1665	ATP	O4'-C4'-C5'	3.61	121.24	109.37
4	A	1666	ATP	O4'-C4'-C5'	3.45	120.71	109.37
4	A	1666	ATP	N6-C6-N1	3.43	125.69	118.57
4	C	1666	ATP	C5-C6-N6	3.42	125.55	120.35
4	C	1666	ATP	O3G-PG-O3B	3.41	116.06	104.64
4	B	1666	ATP	O2'-C2'-C3'	-3.34	101.01	111.82
4	C	1666	ATP	O3G-PG-O2G	3.30	120.23	107.64
4	A	1666	ATP	PB-O3B-PG	-3.22	121.77	132.83
4	B	1666	ATP	O3G-PG-O3B	3.18	115.31	104.64
4	C	1666	ATP	C2'-C3'-C4'	-3.16	96.49	102.64
4	B	1665	ATP	C4-C5-N7	3.13	112.66	109.40
4	B	1666	ATP	C2'-C3'-C4'	-3.12	96.58	102.64
4	B	1665	ATP	O2G-PG-O3B	3.08	114.97	104.64
4	C	1665	ATP	O2G-PG-O3B	3.05	114.87	104.64
4	A	1667	ATP	O2G-PG-O1G	-3.05	98.74	110.68
4	C	1666	ATP	PA-O3A-PB	-3.02	122.45	132.83
4	C	1666	ATP	PB-O3B-PG	-3.00	122.53	132.83
4	C	1665	ATP	O5'-C5'-C4'	2.94	119.09	108.99
4	B	1665	ATP	O3G-PG-O3B	2.88	114.29	104.64
4	B	1665	ATP	C1'-N9-C4	2.79	131.54	126.64
4	A	1667	ATP	O2A-PA-O1A	-2.79	99.77	110.68
4	B	1666	ATP	C5-C6-N6	2.79	124.59	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1665	ATP	C2'-C3'-C4'	2.77	108.03	102.64
4	A	1666	ATP	C5-C6-N6	-2.75	116.17	120.35
4	A	1666	ATP	O2A-PA-O1A	2.71	125.63	112.24
4	B	1666	ATP	O4'-C1'-C2'	-2.38	103.44	106.93
4	A	1667	ATP	O5'-PA-O1A	2.33	119.82	110.68
4	C	1665	ATP	O5'-PA-O1A	2.28	117.98	109.07
4	C	1665	ATP	O4'-C4'-C3'	-2.26	100.64	105.11
4	A	1666	ATP	O2'-C2'-C3'	2.24	119.07	111.82
4	C	1665	ATP	O2A-PA-O1A	-2.17	101.52	112.24
4	C	1665	ATP	C2'-C3'-C4'	2.16	106.83	102.64
4	B	1666	ATP	C4-C5-N7	-2.09	107.22	109.40
4	C	1666	ATP	O2A-PA-O1A	2.06	122.43	112.24
4	C	1665	ATP	PB-O3B-PG	2.02	139.75	132.83

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1666	ATP	C5'-O5'-PA-O1A
4	A	1666	ATP	C5'-O5'-PA-O2A
4	A	1666	ATP	C5'-O5'-PA-O3A
4	A	1666	ATP	C4'-C5'-O5'-PA
4	B	1666	ATP	C5'-O5'-PA-O2A
4	C	1665	ATP	PB-O3B-PG-O2G
4	C	1666	ATP	C4'-C5'-O5'-PA
4	A	1666	ATP	C3'-C4'-C5'-O5'
4	C	1665	ATP	O4'-C4'-C5'-O5'
4	C	1665	ATP	C3'-C4'-C5'-O5'
4	A	1666	ATP	O4'-C4'-C5'-O5'
4	C	1666	ATP	C3'-C4'-C5'-O5'
4	B	1665	ATP	PB-O3B-PG-O3G
4	B	1666	ATP	C5'-O5'-PA-O1A
4	B	1665	ATP	PA-O3A-PB-O2B
4	B	1666	ATP	C4'-C5'-O5'-PA
4	C	1665	ATP	PB-O3B-PG-O1G
4	B	1666	ATP	O4'-C4'-C5'-O5'
4	C	1666	ATP	O4'-C4'-C5'-O5'
4	A	1667	ATP	PB-O3A-PA-O2A
4	C	1665	ATP	PB-O3B-PG-O3G
4	B	1666	ATP	C5'-O5'-PA-O3A
4	B	1665	ATP	PA-O3A-PB-O1B
4	C	1665	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	1666	ATP	C5'-O5'-PA-O1A

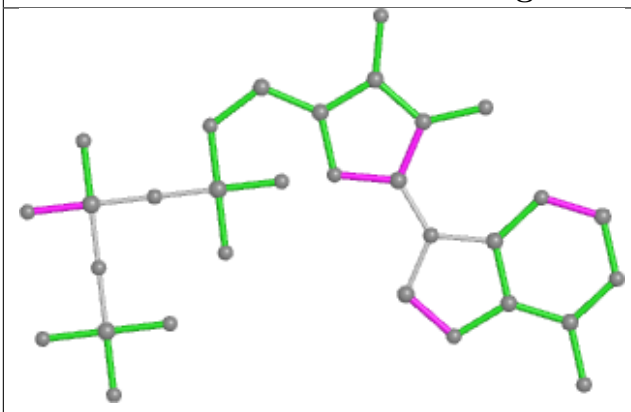
There are no ring outliers.

6 monomers are involved in 35 short contacts:

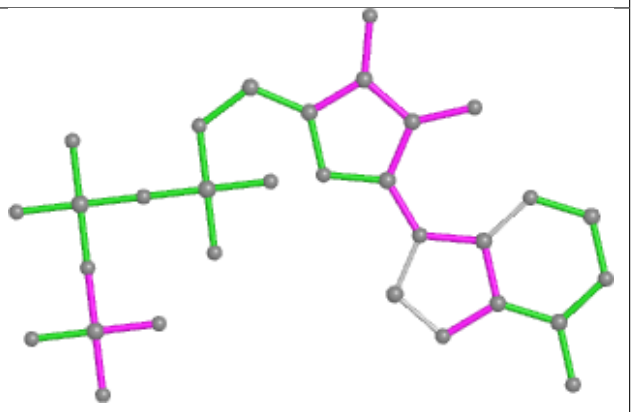
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1665	ATP	2	0
4	C	1666	ATP	24	0
4	A	1666	ATP	1	0
4	B	1666	ATP	6	0
4	A	1667	ATP	2	0
4	C	1665	ATP	8	0

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 then 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.

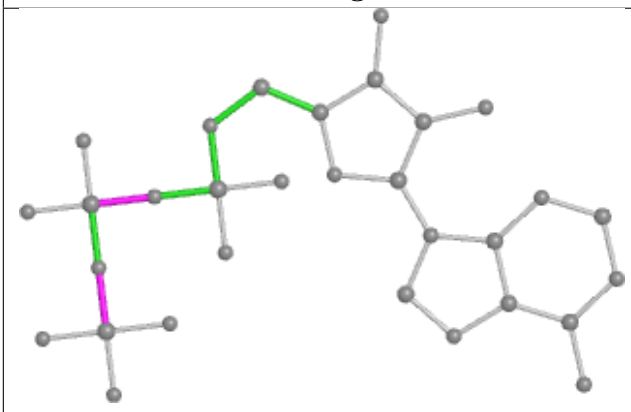
Ligand ATP B 1665



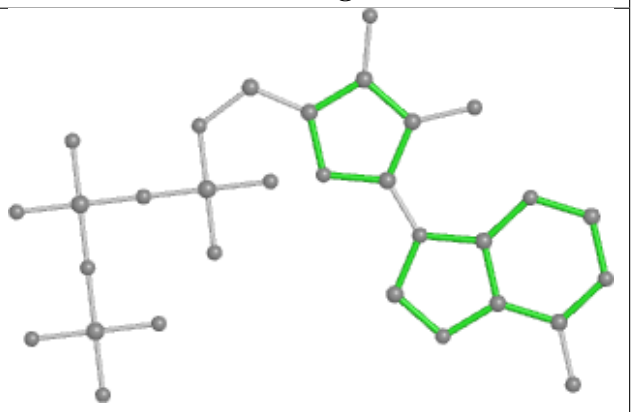
Bond lengths



Bond angles

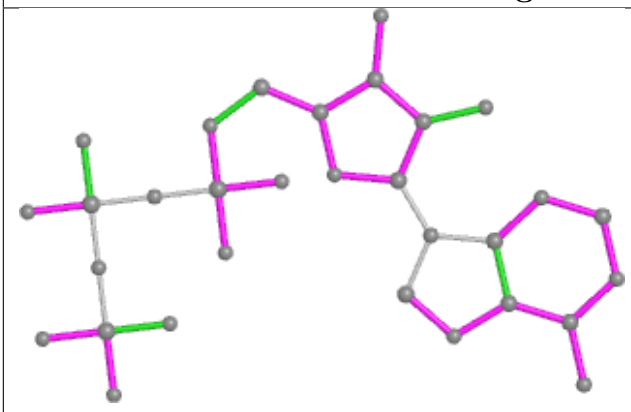


Torsions

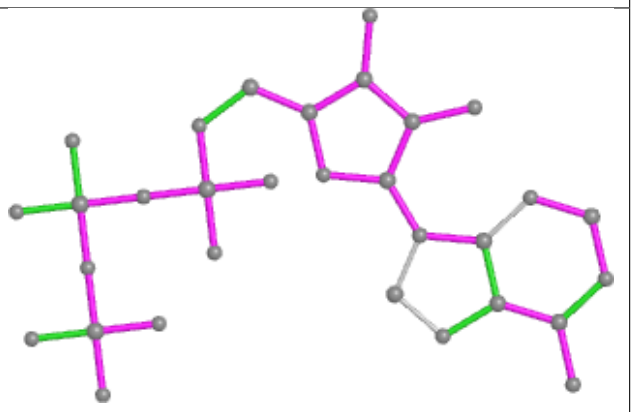


Rings

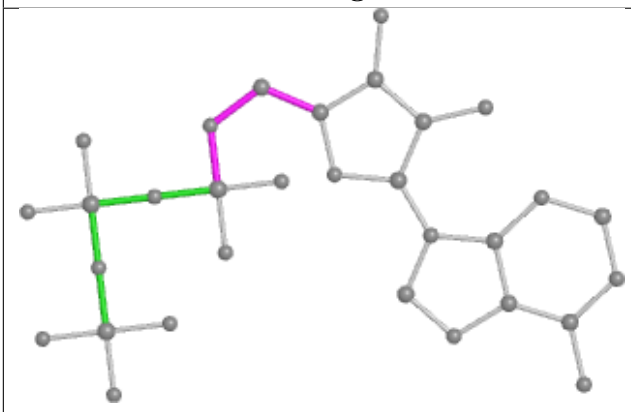
Ligand ATP C 1666



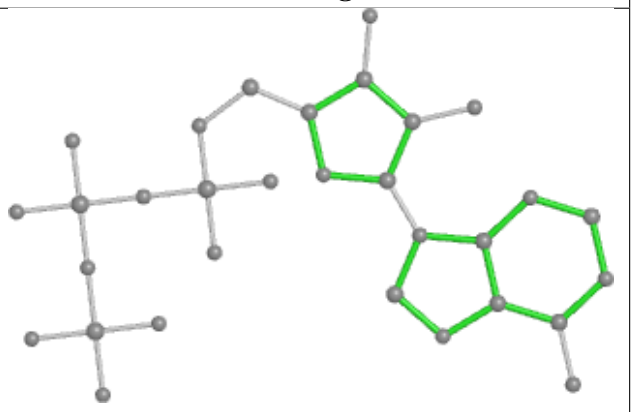
Bond lengths



Bond angles

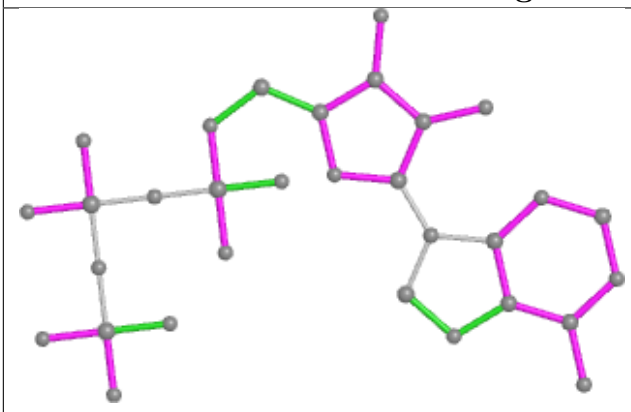


Torsions

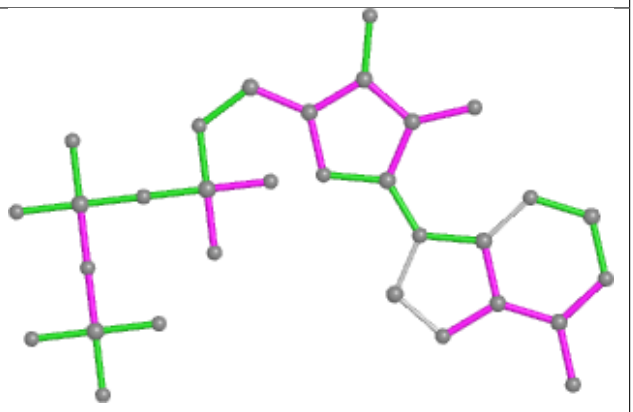


Rings

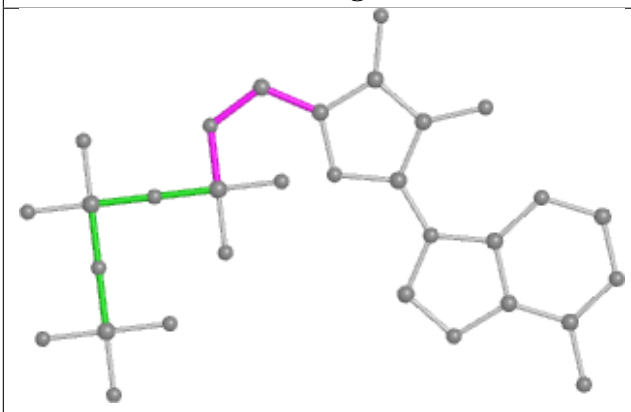
Ligand ATP A 1666



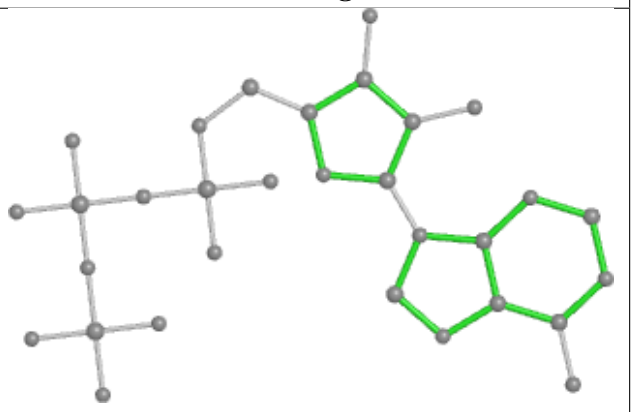
Bond lengths



Bond angles

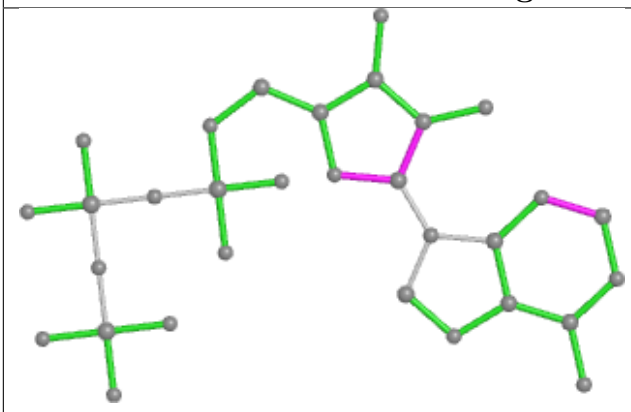


Torsions

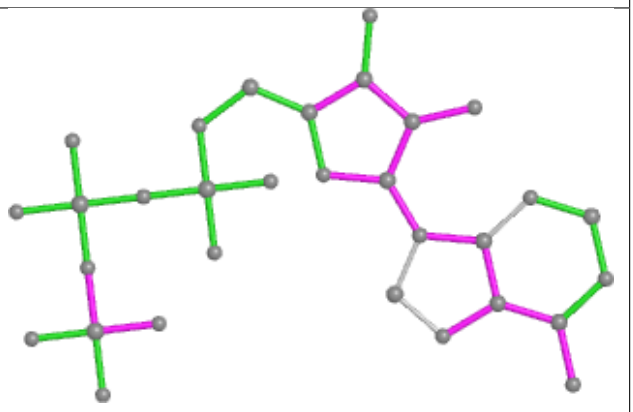


Rings

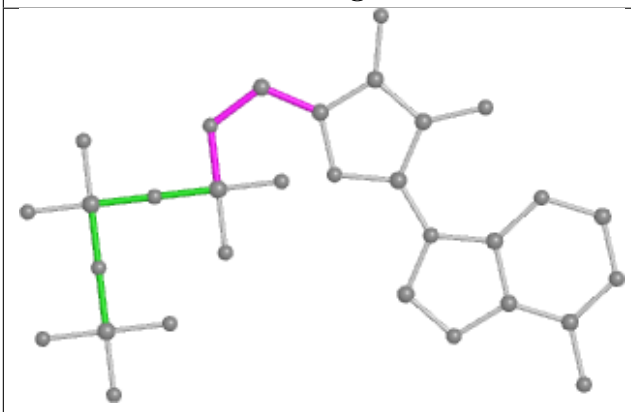
Ligand ATP B 1666



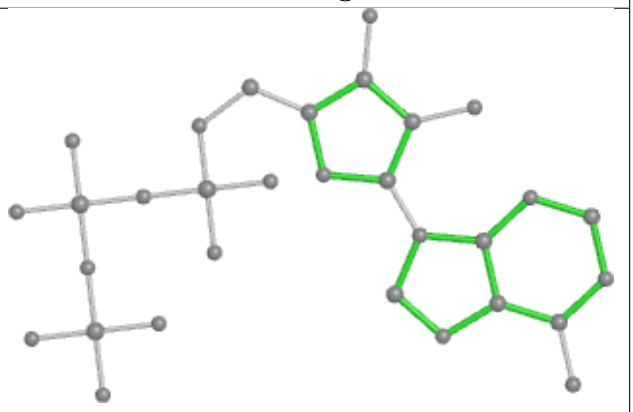
Bond lengths



Bond angles

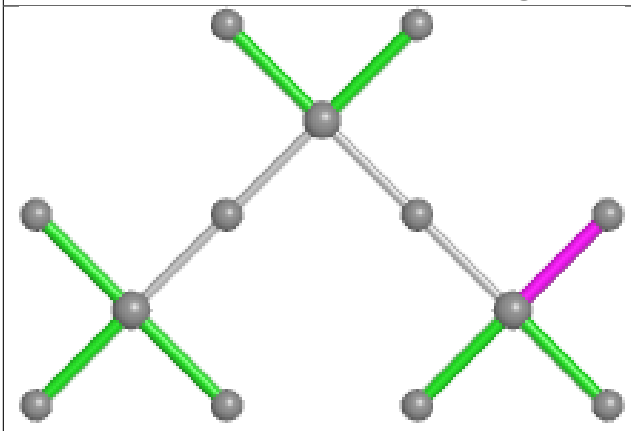


Torsions

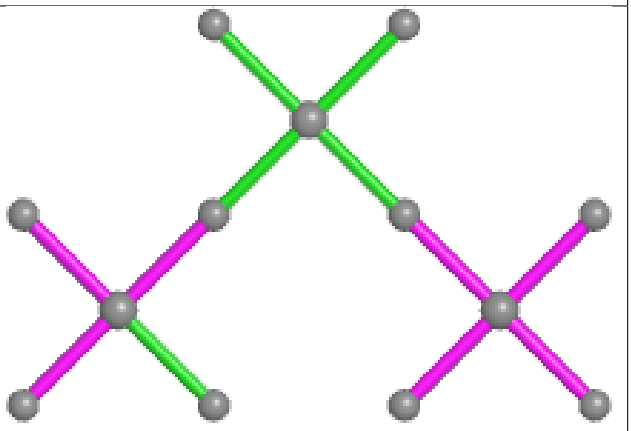


Rings

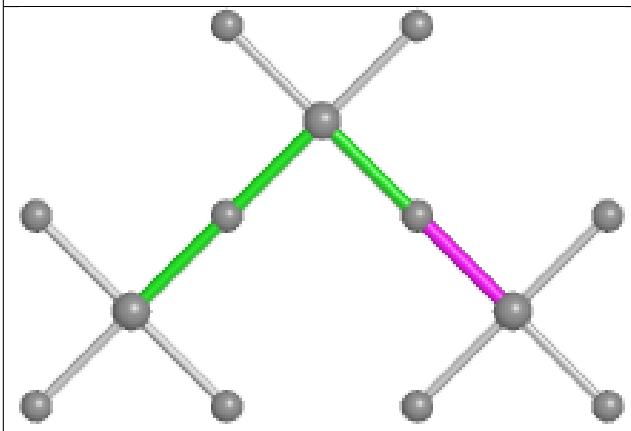
Ligand ATP A 1667



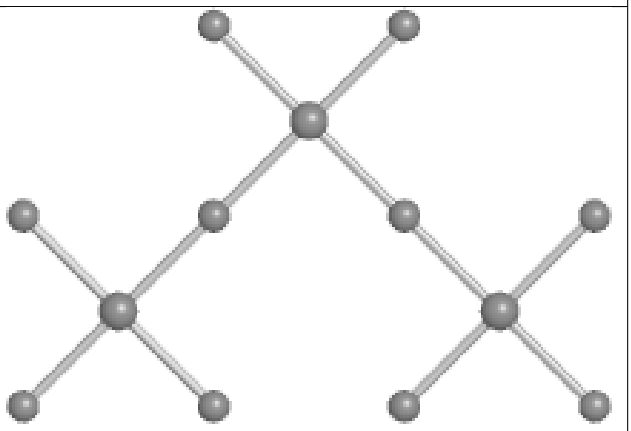
Bond lengths



Bond angles

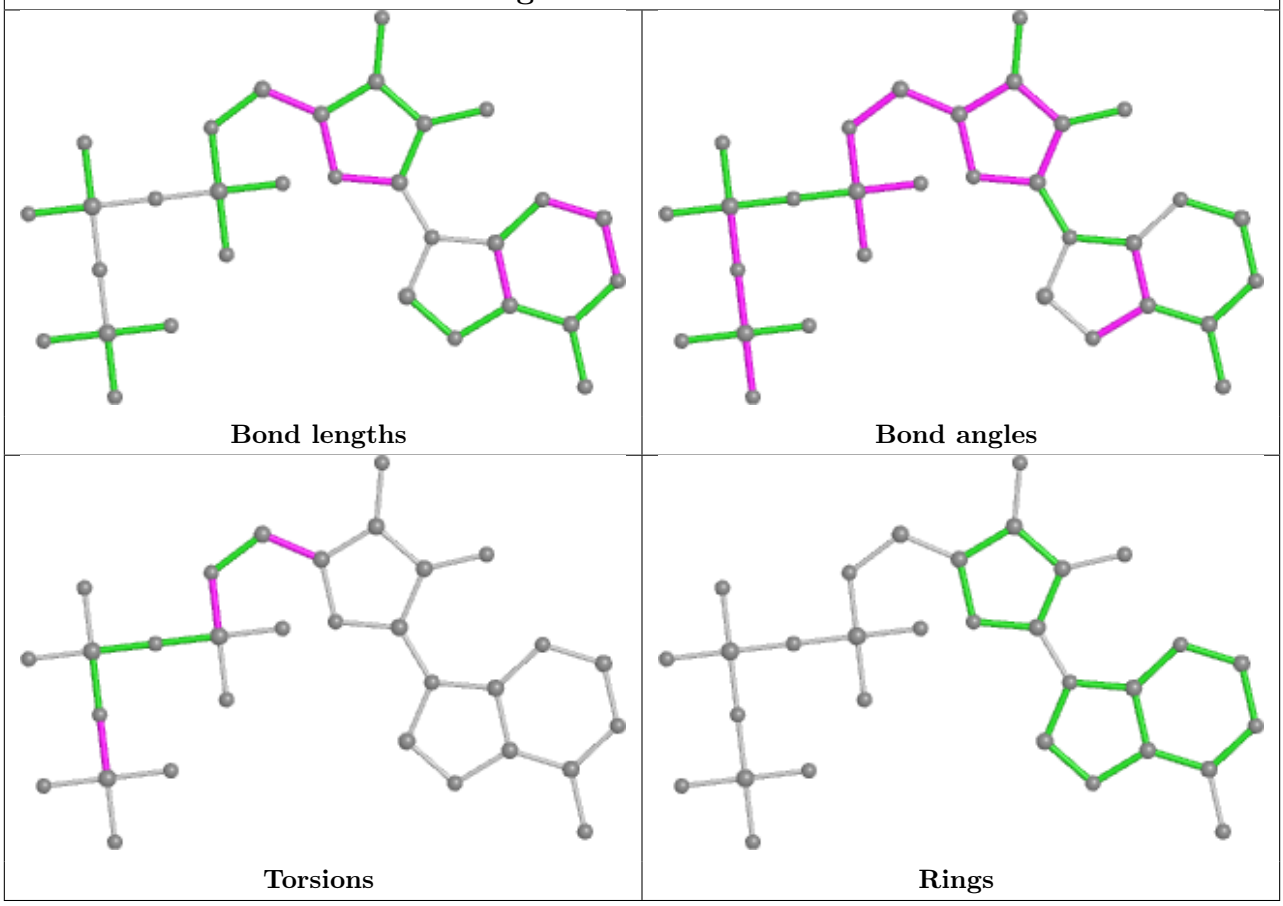


Torsions



Rings

Ligand ATP C 1665



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	664/665 (99%)	-0.03	4 (0%) 89 90	41, 73, 109, 140	0
1	B	664/665 (99%)	0.08	9 (1%) 75 75	43, 69, 101, 149	0
1	C	664/665 (99%)	-0.03	10 (1%) 73 72	38, 68, 104, 180	1 (0%)
2	G	4/4 (100%)	3.62	4 (100%) 0 0	171, 186, 187, 192	0
All	All	1996/1999 (99%)	0.02	27 (1%) 75 75	38, 70, 106, 192	1 (0%)

All (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
2	G	6	DC	4.4
1	B	629	GLN	4.2
1	B	604	SER	4.2
1	B	608	GLN	4.0
1	A	607	ARG	3.8
1	C	609	ALA	3.6
1	B	219	LYS	3.4
1	C	604	SER	3.3
1	A	219	LYS	3.1
1	A	425	ARG	2.4
1	B	492	HIS	2.4
1	C	479	LYS	2.4
1	B	664	ARG	2.4
1	B	393	SER	2.3
1	C	606	ALA	2.2
1	C	605	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	4	DA	2.2
2	G	5	DG	2.2
1	A	216	LYS	2.1
1	C	492	HIS	2.0
1	C	642	HIS	2.0
1	C	503	TYR	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)

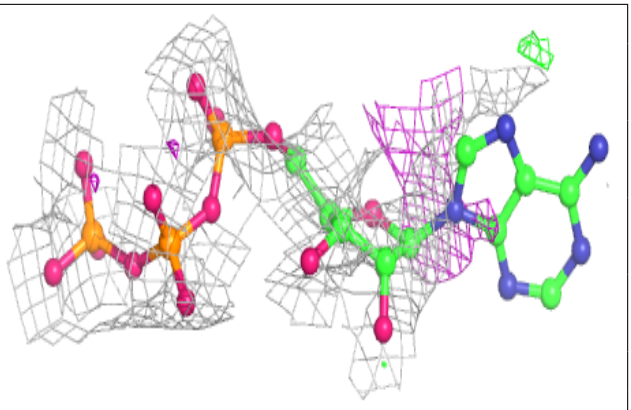
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

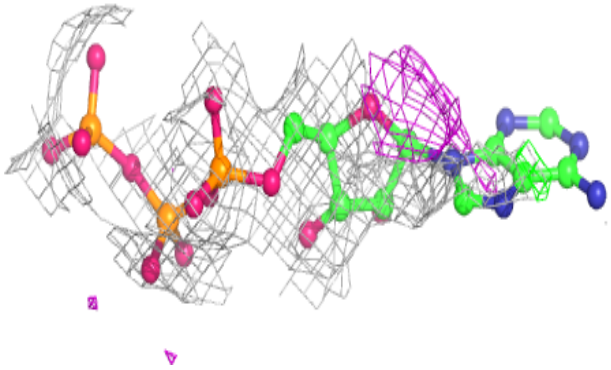
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	C	1665	31/31	0.57	0.48	176,178,179,181	0
4	ATP	B	1665	31/31	0.64	0.70	172,174,191,193	0
4	ATP	B	1666	31/31	0.68	0.57	170,172,179,180	0
4	ATP	C	1666	31/31	0.68	0.32	94,106,122,125	0
4	ATP	A	1666	31/31	0.69	0.37	89,104,131,133	0
3	MG	B	1667	1/1	0.70	0.35	49,49,49,49	0
3	MG	A	1665[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	A	1665[A]	1/1	0.76	0.60	29,29,29,29	1
3	MG	C	1667	1/1	0.93	0.27	56,56,56,56	0

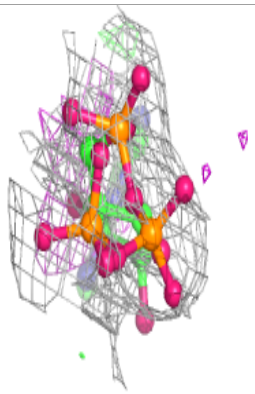
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

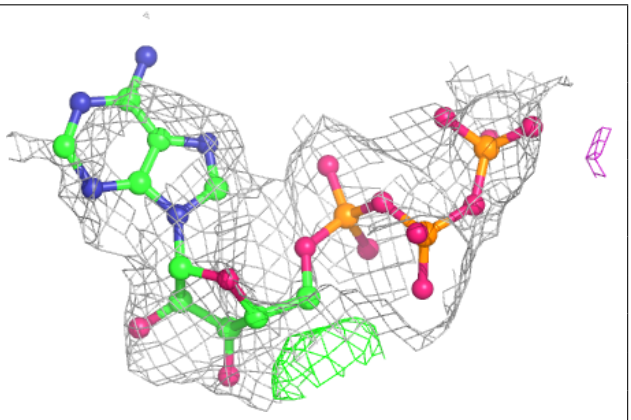


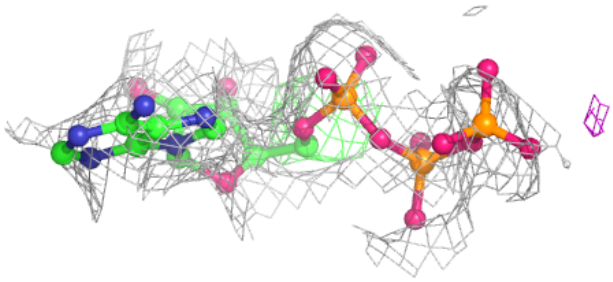


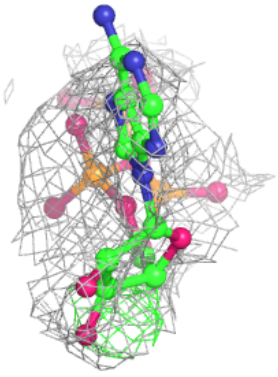


Electron density around ATP B 1665:

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

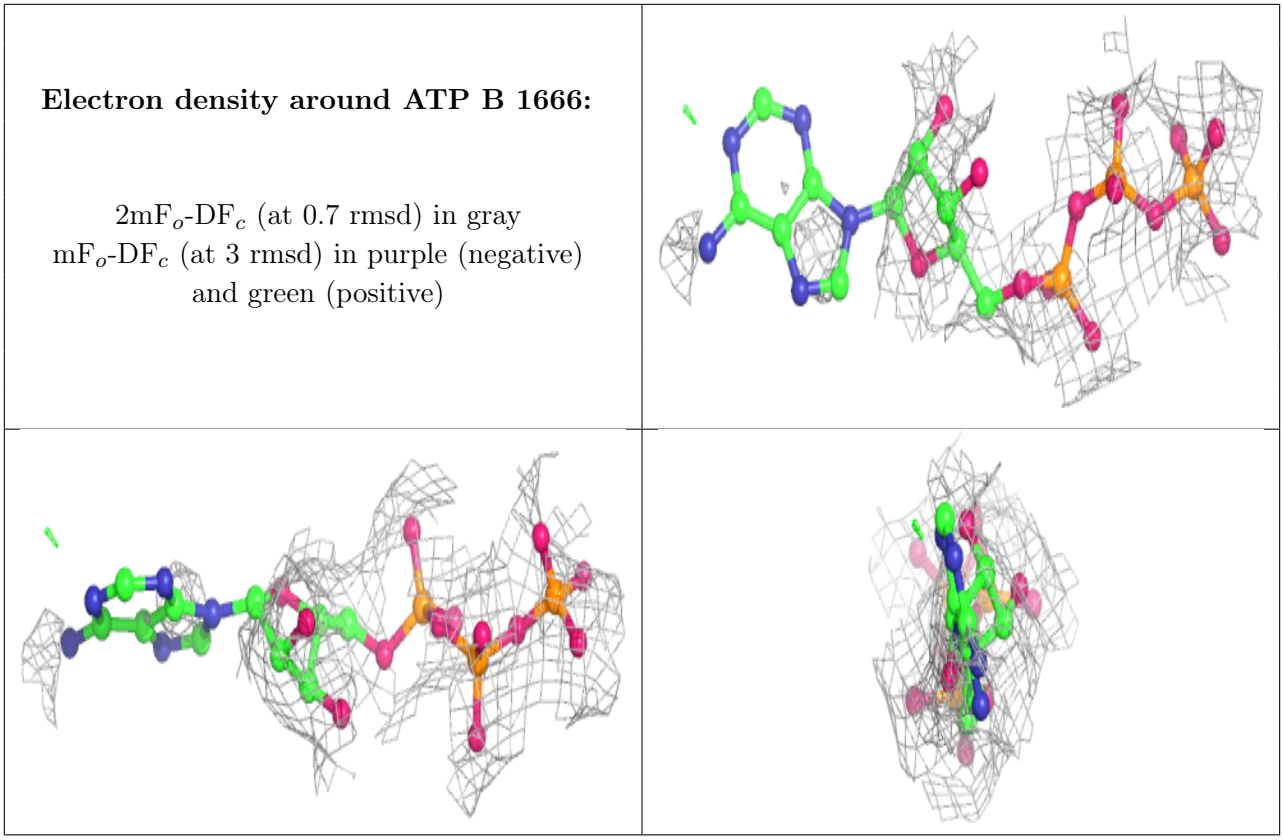






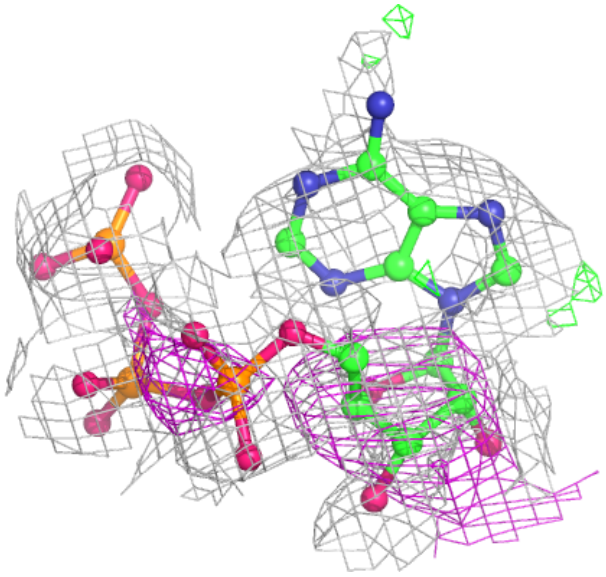
Electron density around ATP B 1666:

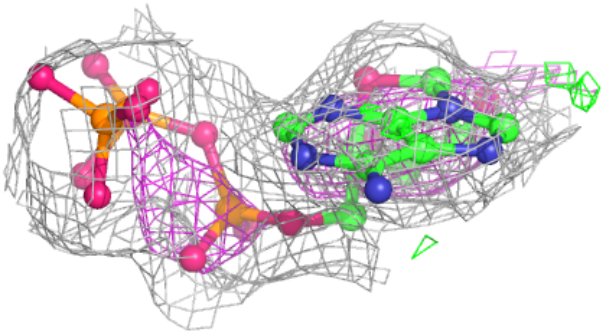
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ATP C 1666:

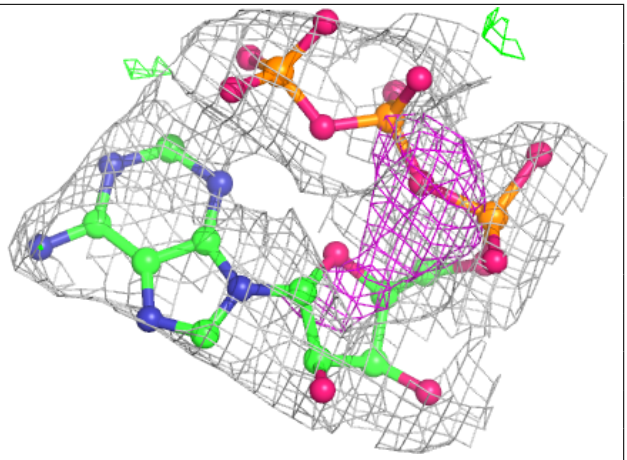
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

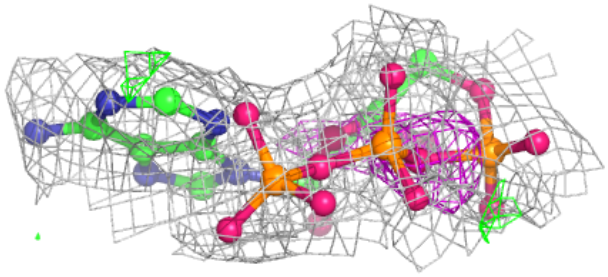


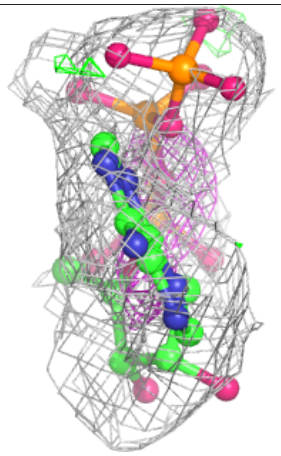


Electron density around ATP A 1666:

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

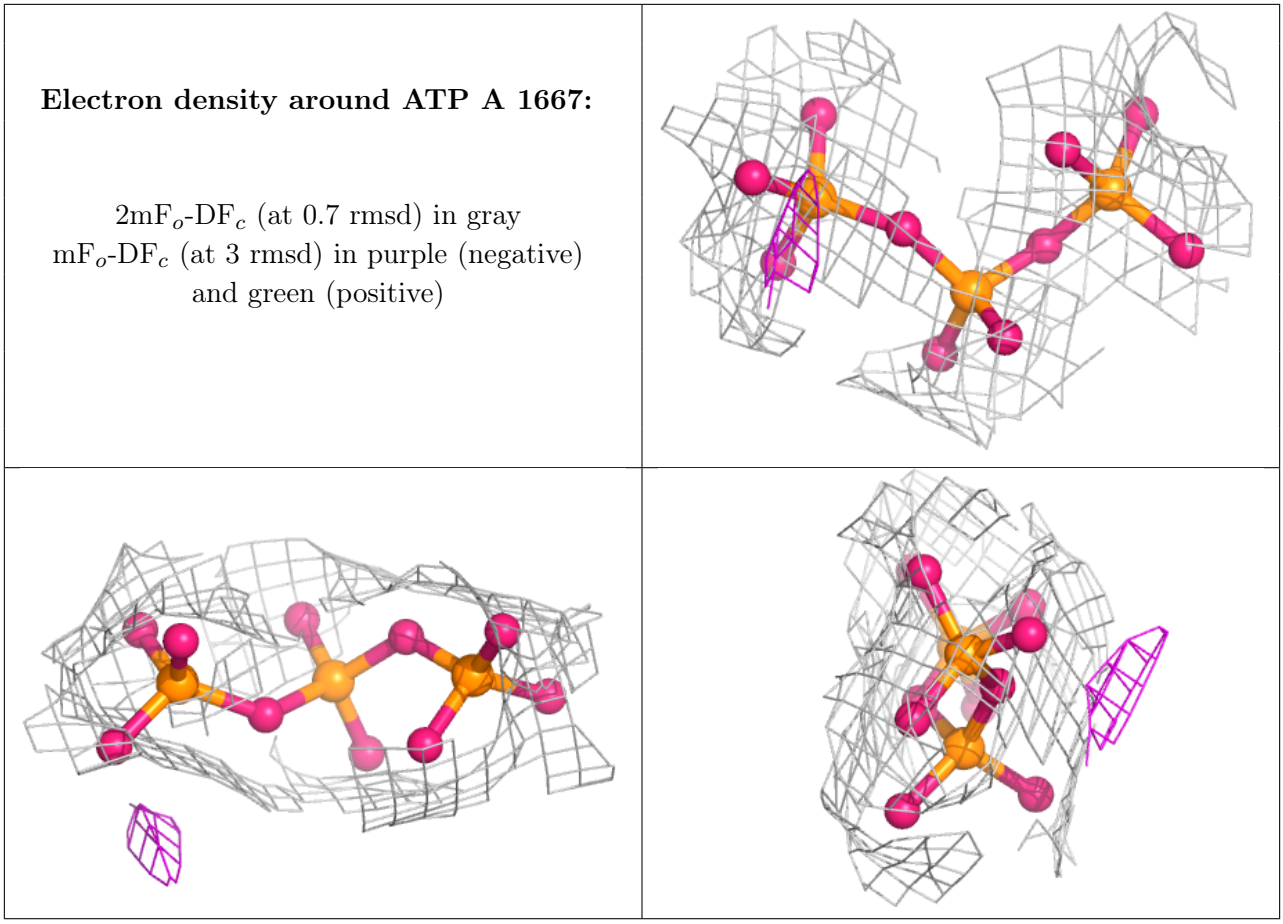






Electron density around ATP A 1667:

$2mF_o$-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.