Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 03:30 AM EDT

PDB ID	:	4FF3 / pdb_00004ff3
Title	:	N4 mini-vRNAP transcription initiation complex, 3 min after soaking GTP, ATP and Mn
Authors	:	Murakami, K.S.; Basu, R.S.
Deposited on	:	2012-05-30
Resolution	:	2.00 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:

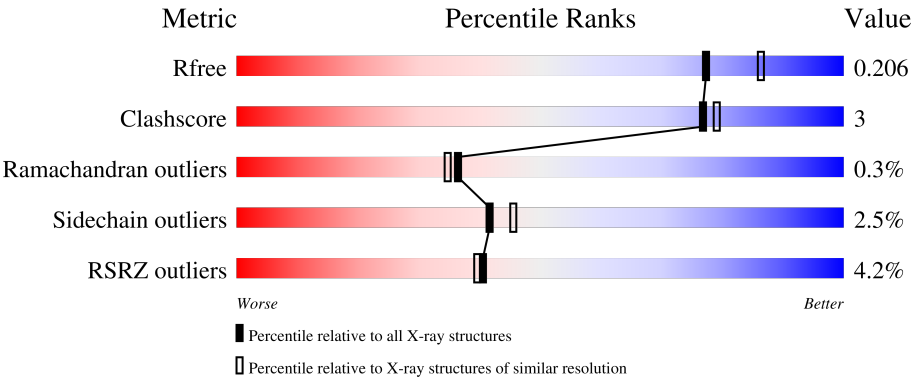
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1118	4% 88% 9%
1	B	1118	4% 89% 8%
2	C	36	42% 14% 44%
2	D	36	44% 8% 44%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19046 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			

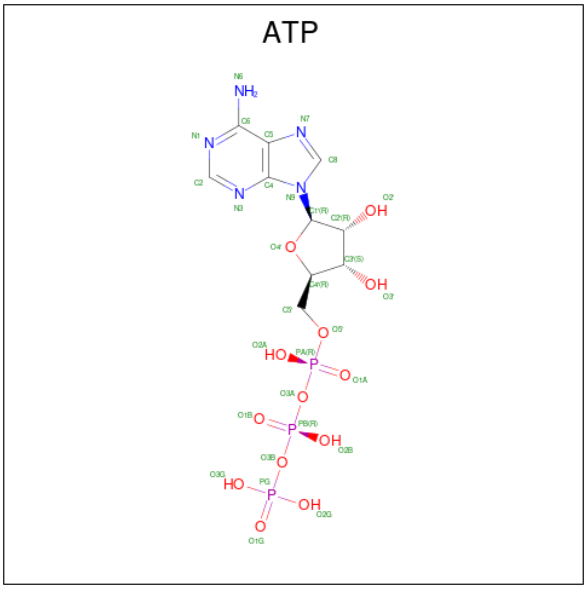
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q859P9
A	-10	GLY	-	expression tag	UNP Q859P9
A	-9	GLY	-	expression tag	UNP Q859P9
A	-8	SER	-	expression tag	UNP Q859P9
A	-7	HIS	-	expression tag	UNP Q859P9
A	-6	HIS	-	expression tag	UNP Q859P9
A	-5	HIS	-	expression tag	UNP Q859P9
A	-4	HIS	-	expression tag	UNP Q859P9
A	-3	HIS	-	expression tag	UNP Q859P9
A	-2	HIS	-	expression tag	UNP Q859P9
A	-1	ARG	-	expression tag	UNP Q859P9
A	0	SER	-	expression tag	UNP Q859P9
B	-11	MET	-	expression tag	UNP Q859P9
B	-10	GLY	-	expression tag	UNP Q859P9
B	-9	GLY	-	expression tag	UNP Q859P9
B	-8	SER	-	expression tag	UNP Q859P9
B	-7	HIS	-	expression tag	UNP Q859P9
B	-6	HIS	-	expression tag	UNP Q859P9
B	-5	HIS	-	expression tag	UNP Q859P9
B	-4	HIS	-	expression tag	UNP Q859P9
B	-3	HIS	-	expression tag	UNP Q859P9
B	-2	HIS	-	expression tag	UNP Q859P9
B	-1	ARG	-	expression tag	UNP Q859P9
B	0	SER	-	expression tag	UNP Q859P9

- Molecule 2 is a DNA chain called Bacteriophage N4 P2 promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			
2	D	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

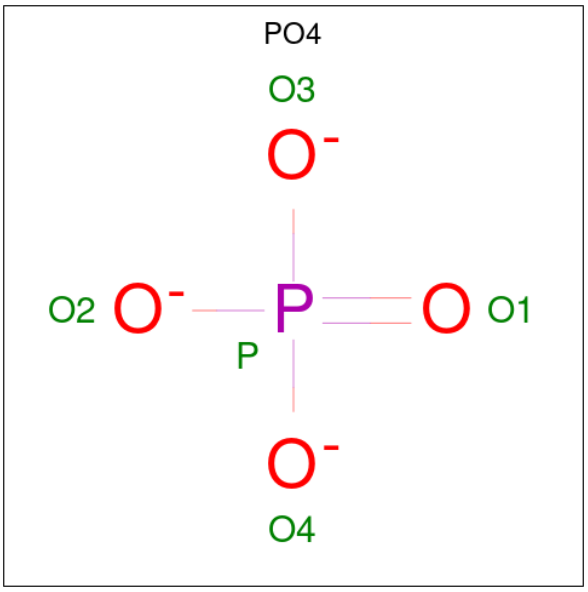


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

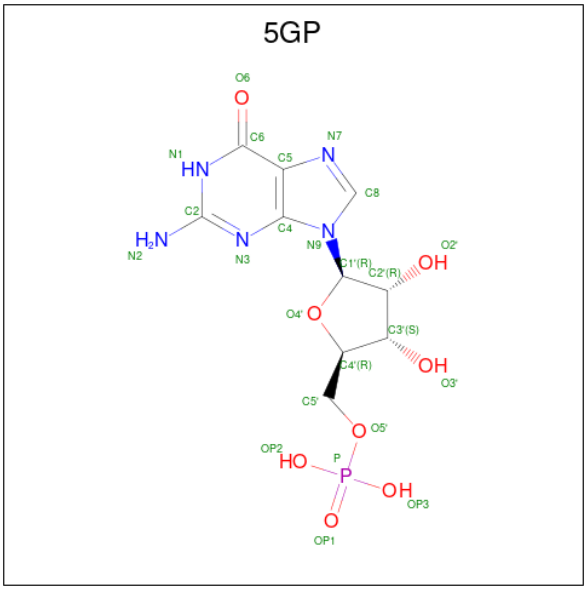
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P 24 10 5 8 1	0	0

- Molecule 7 is water.

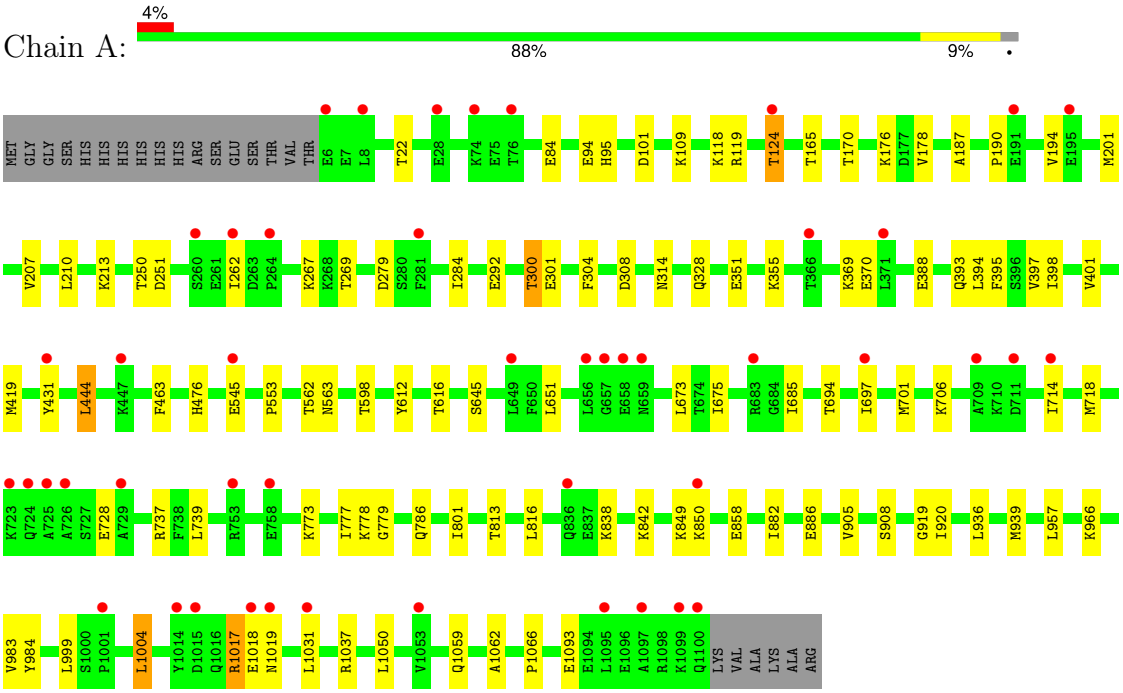
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	546	Total O 546 546	0	0
7	C	42	Total O 42 42	0	0
7	B	624	Total O 624 624	0	0
7	D	33	Total O 33 33	0	0

3 Residue-property plots (i)

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

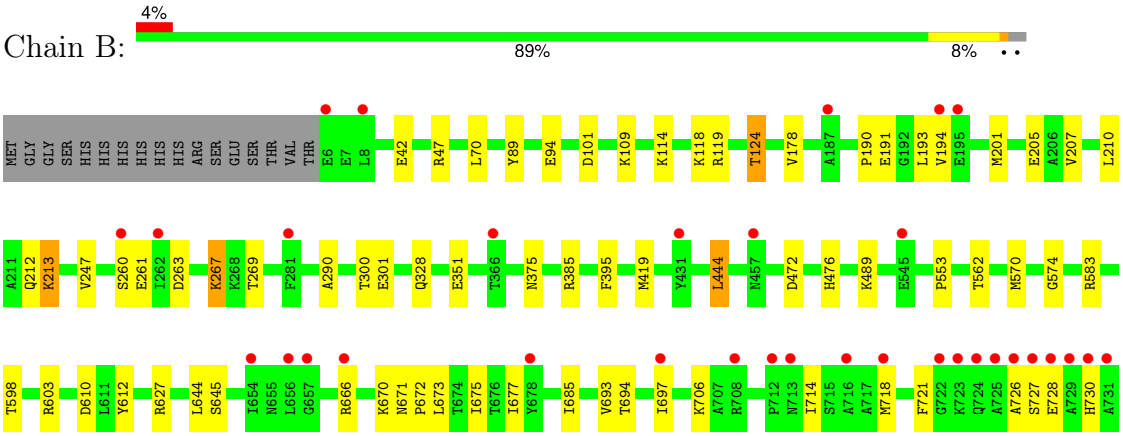
• Molecule 1: Virion RNA polymerase

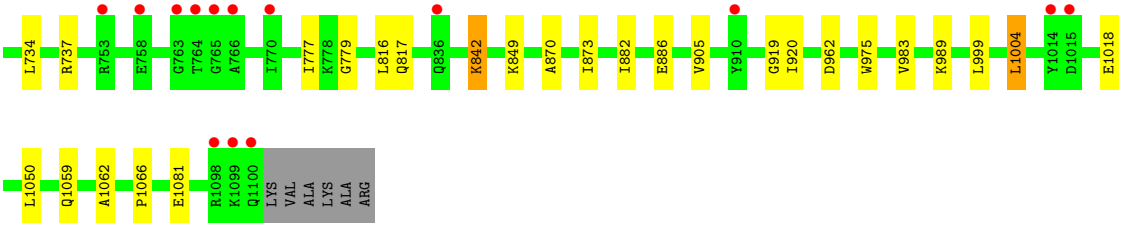
Chain A:



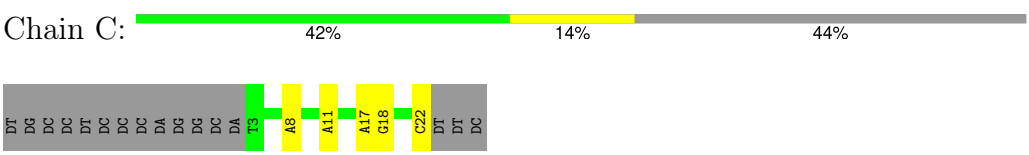
• Molecule 1: Virion RNA polymerase

Chain B:

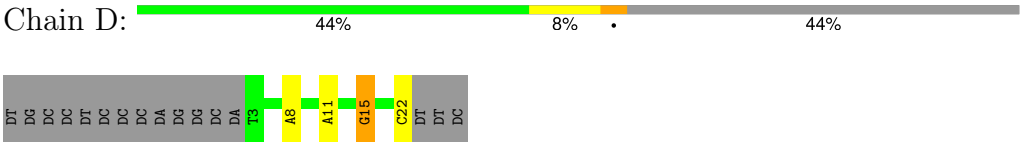




• Molecule 2: Bacteriophage N4 P2 promoter



• Molecule 2: Bacteriophage N4 P2 promoter



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.02Å 111.65Å 276.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 2.00 42.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (42.38-2.00) 84.7 (42.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.182 , 0.211 0.175 , 0.206	Depositor DCC
R_{free} test set	2000 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19046	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: MN, PO4, 5GP, 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	0.34	0/8583	0.70	1/11609 (0.0%)
1	B	0.34	0/8583	0.70	0/11609
2	C	0.15	0/464	0.67	0/714
2	D	0.16	0/464	0.68	1/714 (0.1%)
All	All	0.33	0/18094	0.70	2/24646 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	15	DG	C2'-C3'-O3'	-5.98	102.52	111.50
1	A	563	ASN	N-CA-C	5.33	116.78	110.97

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	8454	0	8479	50	0
1	B	8454	0	8479	53	0
2	C	413	0	225	5	0
2	D	413	0	225	4	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	C	24	0	12	0	0
7	A	546	0	0	0	0
7	B	624	0	0	4	0
7	C	42	0	0	0	0
7	D	33	0	0	1	0
All	All	19046	0	17432	101	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 (101) 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)
2:D:22:DC:O3'	7:D:109:HOH:O	2.10	0.69
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.75	0.67
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.77	0.66
1:B:583:ARG:NH2	1:B:1081:GLU:OE2	2.29	0.66
1:B:476:HIS:ND1	5:B:1201:PO4:O2	2.24	0.65
1:B:694:THR:HG22	1:B:777:ILE:HD12	1.79	0.65
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.80	0.63
1:A:101:ASP:OD1	1:B:109:LYS:NZ	2.28	0.62
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.82	0.62
1:A:999:LEU:HB2	1:A:1004:LEU:HD22	1.82	0.60
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.84	0.59
1:B:570:MET:HE2	1:B:975:TRP:HB3	1.85	0.58
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.87	0.56
1:A:694:THR:HG22	1:A:777:ILE:HD12	1.88	0.56
1:B:718:MET:HE2	1:B:728:GLU:HA	1.87	0.56
1:B:817:GLN:HB2	1:B:920:ILE:HD11	1.87	0.56
1:A:675:ILE:HD11	1:A:685:ILE:HG12	1.87	0.55
1:A:94:GLU:HG2	1:B:247:VAL:HG12	1.88	0.55
1:A:476:HIS:ND1	5:A:1204:PO4:O2	2.24	0.55
1:A:119:ARG:O	1:A:124:THR:HG23	2.07	0.55
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.89	0.54
1:A:718:MET:HE2	1:A:728:GLU:HA	1.89	0.54
1:B:119:ARG:O	1:B:124:THR:HG23	2.08	0.53
1:B:201:MET:HE2	1:B:205:GLU:HG2	1.91	0.52
1:B:726:ALA:HB3	1:B:730:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HG2	1:A:262:ILE:HG23	1.91	0.52
1:A:813:THR:O	1:A:920:ILE:HD11	2.09	0.52
1:B:213:LYS:HE2	1:B:301:GLU:OE2	2.09	0.52
1:A:328:GLN:HB3	1:A:419:MET:HE3	1.92	0.51
1:A:886:GLU:O	2:C:8:DA:H4'	2.10	0.51
1:B:610:ASP:OD2	1:B:666:ARG:NH1	2.43	0.51
1:A:645:SER:OG	1:A:737:ARG:HD2	2.11	0.50
1:B:191:GLU:HG2	1:B:375:ASN:O	2.12	0.50
1:B:114:LYS:NZ	2:D:15:DG:N7	2.59	0.49
1:A:849:LYS:NZ	2:C:17:DA:OP2	2.44	0.49
1:B:677:ILE:O	1:B:920:ILE:HG21	2.13	0.49
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	0.48
1:A:393:GLN:HG3	1:A:431:TYR:CD2	2.48	0.48
1:B:269:THR:O	2:D:11:DA:H5'	2.14	0.48
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.43	0.48
1:A:562:THR:HG22	1:A:612:TYR:CE1	2.50	0.47
1:A:187:ALA:HB1	1:A:786:GLN:HE22	1.79	0.47
1:B:886:GLU:O	2:D:8:DA:H4'	2.15	0.47
1:B:999:LEU:HB2	1:B:1004:LEU:HD22	1.96	0.47
1:B:612:TYR:CE2	1:B:673:LEU:HD23	2.50	0.46
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.50	0.46
1:A:351:GLU:HG3	1:A:395:PHE:CE2	2.50	0.46
1:B:574:GLY:O	7:B:1626:HOH:O	2.21	0.46
1:B:47:ARG:NH2	7:B:1374:HOH:O	2.40	0.46
1:B:693:VAL:O	1:B:697:ILE:HG23	2.16	0.46
1:B:645:SER:OG	1:B:737:ARG:HD2	2.16	0.45
1:B:714:ILE:HD11	1:B:718:MET:HB3	1.99	0.45
1:A:882:ILE:HD13	1:A:919:GLY:HA2	1.99	0.45
1:A:170:THR:HG22	1:A:201:MET:HE3	1.99	0.45
1:A:369:LYS:O	1:A:773:LYS:NZ	2.50	0.45
1:B:849:LYS:HE3	7:B:1777:HOH:O	2.17	0.45
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.52	0.45
1:B:444:LEU:HG	1:B:553:PRO:HB2	1.98	0.44
1:A:394:LEU:O	1:A:398:ILE:HG12	2.17	0.44
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.79	0.44
1:A:545:GLU:H	1:A:545:GLU:CD	2.25	0.44
1:B:882:ILE:HD13	1:B:919:GLY:HA2	2.00	0.44
1:A:673:LEU:HD12	1:A:801:ILE:HG12	2.00	0.44
1:A:463:PHE:HA	1:A:957:LEU:HD13	2.00	0.44
1:A:984:TYR:CE1	1:A:1037:ARG:HB2	2.53	0.44
1:B:721:PHE:HB3	1:B:734:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:GLN:HB3	1:B:419:MET:HE3	2.00	0.43
1:B:267:LYS:H	1:B:267:LYS:HG2	1.64	0.43
1:B:603:ARG:NH1	7:B:1413:HOH:O	2.22	0.43
1:A:95:HIS:NE2	1:A:251:ASP:OD2	2.41	0.43
1:B:727:SER:HB2	1:B:730:HIS:CE1	2.53	0.43
1:B:873:ILE:HD13	1:B:983:VAL:HG22	2.00	0.43
1:A:292:GLU:OE2	1:A:300:THR:HG23	2.19	0.43
1:A:714:ILE:HD11	1:A:718:MET:HB3	2.00	0.43
1:B:118:LYS:HB2	1:B:118:LYS:HE3	1.77	0.42
1:A:355:LYS:HD2	1:A:388:GLU:HG3	2.00	0.42
1:A:267:LYS:HD3	2:C:22:DC:C5	2.54	0.42
1:B:675:ILE:HD11	1:B:685:ILE:HG12	2.01	0.42
1:A:304:PHE:HB3	1:A:308:ASP:O	2.20	0.42
1:A:697:ILE:O	1:A:701:MET:HG2	2.20	0.42
1:B:842:LYS:HD2	1:B:842:LYS:HA	1.63	0.42
1:A:397:VAL:O	1:A:401:VAL:HG23	2.19	0.42
1:B:612:TYR:CZ	1:B:670:LYS:HG3	2.55	0.42
1:B:190:PRO:HD2	1:B:193:LEU:HD22	2.02	0.42
1:B:627:ARG:HH21	1:B:644:LEU:HD12	1.85	0.42
1:A:109:LYS:NZ	1:B:101:ASP:OD1	2.33	0.41
1:A:850:LYS:NZ	2:C:18:DG:OP1	2.37	0.41
1:A:842:LYS:HD3	1:A:842:LYS:HA	1.76	0.41
1:B:598:THR:HG22	1:B:1066:PRO:HD3	2.03	0.41
1:B:1004:LEU:HD13	1:B:1004:LEU:HA	1.94	0.41
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.02	0.41
1:B:260:SER:HA	1:B:263:ASP:O	2.20	0.41
1:A:1017:ARG:O	1:A:1019:ASN:N	2.53	0.41
1:B:42:GLU:H	1:B:42:GLU:HG2	1.75	0.41
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.56	0.41
1:A:939:MET:HE2	1:A:966:LYS:HD2	2.03	0.41
1:A:838:LYS:HE2	1:A:858:GLU:HG2	2.02	0.40
1:B:870:ALA:HB2	1:B:989:LYS:HD3	2.03	0.40
1:A:165:THR:OG1	1:A:301:GLU:OE1	2.39	0.40
1:A:187:ALA:HB1	1:A:786:GLN:NE2	2.36	0.40
1:A:269:THR:O	2:C:11:DA:H5'	2.22	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	1093/1118 (98%)	1068 (98%)	21 (2%)	4 (0%)	30	27
1	B	1093/1118 (98%)	1071 (98%)	20 (2%)	2 (0%)	43	42
All	All	2186/2236 (98%)	2139 (98%)	41 (2%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	A	1062	ALA
1	B	1062	ALA
1	A	779	GLY
1	A	1017	ARG
1	B	779	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	916/935 (98%)	891 (97%)	25 (3%)	39	42
1	B	916/935 (98%)	896 (98%)	20 (2%)	45	50
All	All	1832/1870 (98%)	1787 (98%)	45 (2%)	42	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	84	GLU
1	A	124	THR
1	A	176	LYS
1	A	210	LEU
1	A	213	LYS
1	A	250	THR
1	A	279	ASP
1	A	284	ILE
1	A	300	THR
1	A	314	ASN
1	A	370	GLU
1	A	444	LEU
1	A	616	THR
1	A	651	LEU
1	A	706	LYS
1	A	739	LEU
1	A	778	LYS
1	A	908	SER
1	A	936	LEU
1	A	1004	LEU
1	A	1031	LEU
1	A	1050	LEU
1	A	1059	GLN
1	A	1093	GLU
1	B	70	LEU
1	B	94	GLU
1	B	124	THR
1	B	210	LEU
1	B	212	GLN
1	B	213	LYS
1	B	261	GLU
1	B	267	LYS
1	B	300	THR
1	B	385	ARG
1	B	444	LEU
1	B	472	ASP
1	B	489	LYS
1	B	706	LYS
1	B	842	LYS
1	B	962	ASP
1	B	1004	LEU
1	B	1018	GLU

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Mol	Chain	Res	Type
1	B	1050	LEU
1	B	1059	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	464	GLN
1	A	856	GLN
1	A	863	GLN
1	A	1035	ASN
1	B	225	ASN
1	B	375	ASN
1	B	404	GLN
1	B	506	ASN
1	B	815	GLN
1	B	856	GLN
1	B	878	GLN
1	B	976	GLN
1	B	1035	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	PO4	B	1201	-	4,4,4	0.93	0	6,6,6	0.46	0
3	ATP	A	1201	4	32,33,33	1.63	6 (18%)	48,52,52	1.76	11 (22%)
5	PO4	A	1204	-	4,4,4	0.96	0	6,6,6	0.40	0
6	5GP	C	101	4	26,26,26	0.98	2 (7%)	39,40,40	1.82	8 (20%)

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
3	ATP	A	1201	4	-	7/22/38/38	0/3/3/3
6	5GP	C	101	4	-	5/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ATP	C5-C4	4.56	1.47	1.39
3	A	1201	ATP	PB-O3A	3.69	1.63	1.59
3	A	1201	ATP	PA-O3A	3.22	1.63	1.59
3	A	1201	ATP	PB-O3B	2.90	1.62	1.59
3	A	1201	ATP	C5-C6	2.76	1.48	1.41
3	A	1201	ATP	C8-N7	2.54	1.36	1.31
6	C	101	5GP	C6-N1	-2.39	1.34	1.38
6	C	101	5GP	C5-N7	-2.09	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	101	5GP	C5-C4-N3	-6.26	118.43	128.39
3	A	1201	ATP	C5-C4-N3	-5.69	118.88	126.72
6	C	101	5GP	C2-N3-C4	4.83	120.61	112.30
3	A	1201	ATP	N3-C4-N9	4.42	134.68	127.17
6	C	101	5GP	N9-C4-N3	3.84	133.62	125.95
3	A	1201	ATP	C2-N3-C4	3.69	120.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	ATP	C4-C5-N7	-3.47	106.61	110.58
3	A	1201	ATP	N3-C2-N1	-3.47	123.34	128.58
3	A	1201	ATP	C2'-C1'-N9	-3.23	105.27	113.30
6	C	101	5GP	O6-C6-C5	-2.66	119.52	126.53
3	A	1201	ATP	C4-N9-C8	2.56	108.43	105.74
3	A	1201	ATP	C5-N7-C8	2.55	107.45	103.45
6	C	101	5GP	C5-C6-N1	2.44	119.46	113.25
3	A	1201	ATP	O2B-PB-O3A	2.43	113.83	107.27
6	C	101	5GP	OP2-P-O5'	-2.41	100.38	106.67
6	C	101	5GP	C2-N1-C6	-2.36	120.83	125.11
3	A	1201	ATP	C6-C5-N7	2.15	136.24	132.09
6	C	101	5GP	N9-C8-N7	-2.09	109.53	113.40
3	A	1201	ATP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	ATP	C5'-O5'-PA-O2A
3	A	1201	ATP	C5'-O5'-PA-O3A
6	C	101	5GP	C5'-O5'-P-OP1
6	C	101	5GP	C5'-O5'-P-OP3
6	C	101	5GP	C5'-O5'-P-OP2
6	C	101	5GP	C3'-C4'-C5'-O5'
6	C	101	5GP	O4'-C4'-C5'-O5'
3	A	1201	ATP	C5'-O5'-PA-O1A
3	A	1201	ATP	PB-O3B-PG-O1G
3	A	1201	ATP	PB-O3B-PG-O3G
3	A	1201	ATP	PA-O3A-PB-O1B
3	A	1201	ATP	PA-O3A-PB-O2B

There are no ring outliers.

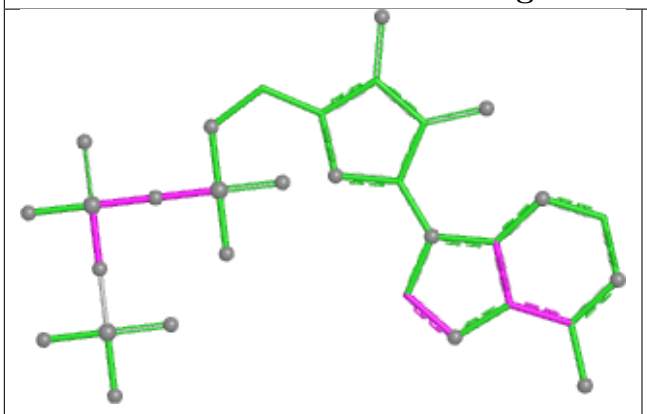
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	PO4	1	0
5	A	1204	PO4	1	0

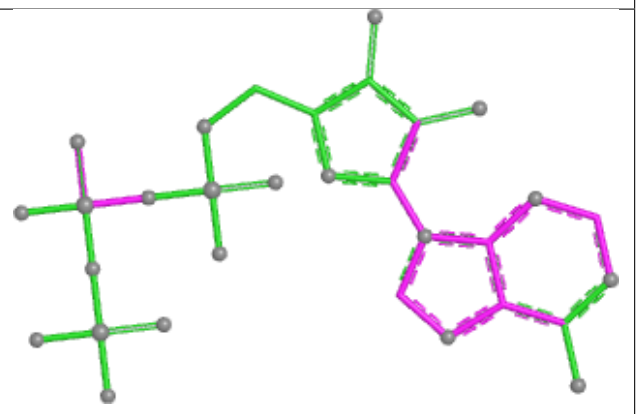
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

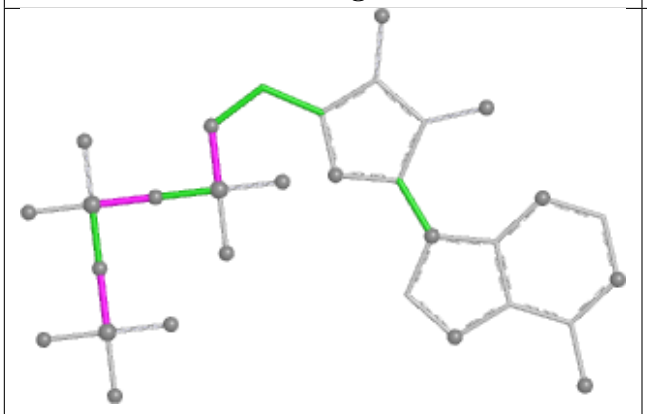
Ligand ATP A 1201



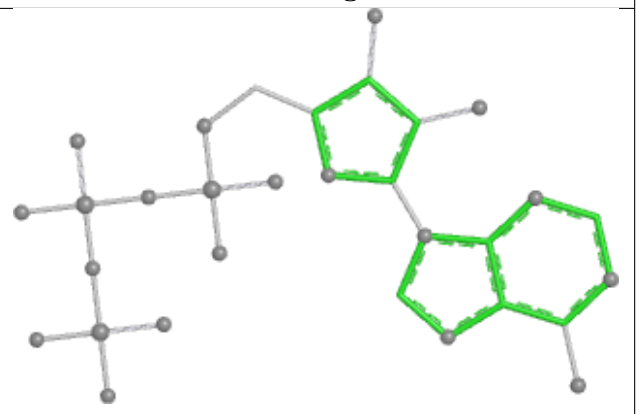
Bond lengths



Bond angles

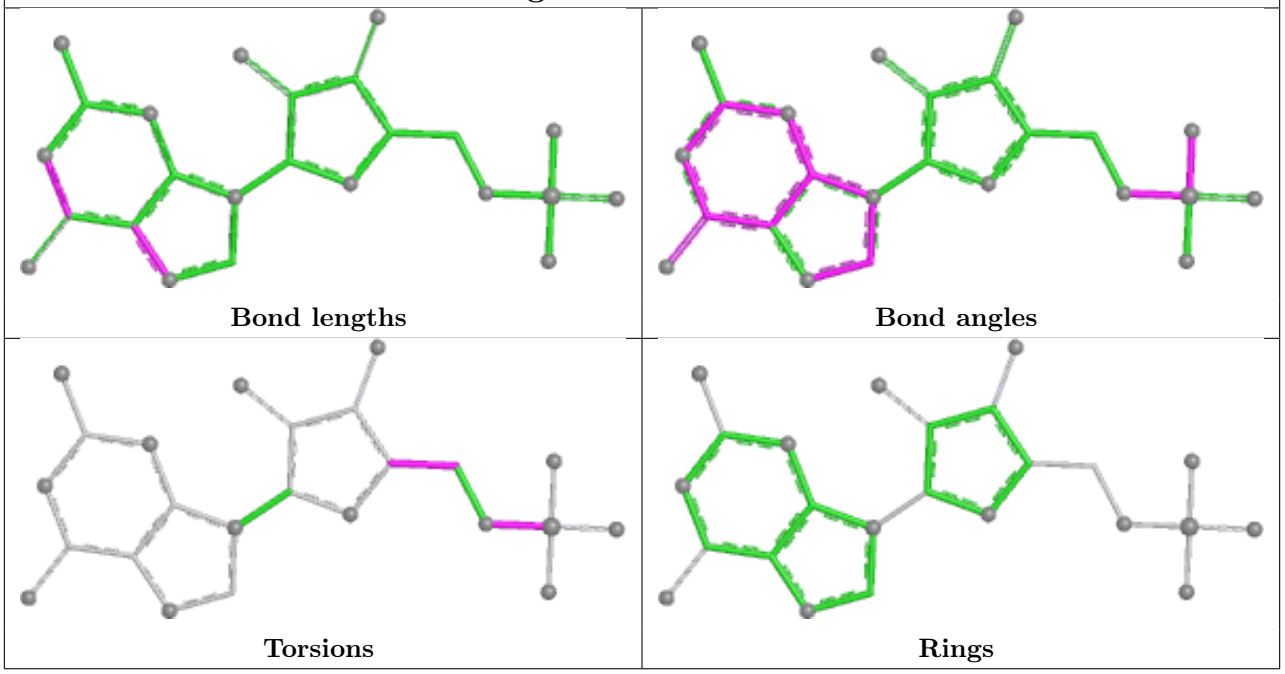


Torsions



Rings

Ligand 5GP C 101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	1095/1118 (97%)	0.07	47 (4%) 40 39	12, 29, 69, 107	0
1	B	1095/1118 (97%)	0.07	47 (4%) 40 39	13, 28, 69, 144	0
2	C	20/36 (55%)	-0.33	0 100 100	29, 36, 57, 60	0
2	D	20/36 (55%)	-0.29	0 100 100	22, 37, 53, 79	0
All	All	2230/2308 (96%)	0.06	94 (4%) 40 39	12, 29, 69, 144	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ALA	4.9
1	B	725	ALA	4.5
1	B	729	ALA	4.5
1	A	281	PHE	4.4
1	A	1014	TYR	4.4
1	A	447	LYS	4.3
1	A	726	ALA	3.9
1	A	758	GLU	3.7
1	A	262	ILE	3.7
1	B	1014	TYR	3.7
1	B	281	PHE	3.6
1	B	727	SER	3.6
1	B	697	ILE	3.6
1	B	431	TYR	3.5
1	B	195	GLU	3.5
1	A	725	ALA	3.4
1	A	1099	LYS	3.3
1	B	730	HIS	3.3
1	B	457	ASN	3.2
1	B	1099	LYS	3.2
1	B	722	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	763	GLY	3.1
1	B	718	MET	3.1
1	A	656	LEU	3.0
1	A	1097	ALA	3.0
1	A	431	TYR	3.0
1	A	659	ASN	3.0
1	A	6	GLU	3.0
1	B	6	GLU	3.0
1	A	709	ALA	3.0
1	A	729	ALA	2.9
1	B	716	ALA	2.9
1	A	657	GLY	2.9
1	B	654	ILE	2.9
1	B	656	LEU	2.9
1	B	1098	ARG	2.8
1	B	723	LYS	2.8
1	A	753	ARG	2.7
1	B	8	LEU	2.7
1	B	713	ASN	2.7
1	B	731	ALA	2.7
1	B	657	GLY	2.7
1	A	683	ARG	2.7
1	A	264	PRO	2.7
1	B	187	ALA	2.6
1	A	8	LEU	2.6
1	A	1019	ASN	2.6
1	B	1100	GLN	2.5
1	A	658	GLU	2.5
1	B	260	SER	2.5
1	B	708	ARG	2.5
1	B	194	VAL	2.5
1	B	728	GLU	2.5
1	B	765	GLY	2.5
1	B	724	GLN	2.4
1	A	191	GLU	2.4
1	B	545	GLU	2.4
1	B	758	GLU	2.4
1	A	260	SER	2.4
1	A	711	ASP	2.3
1	A	1018	GLU	2.3
1	A	850	LYS	2.3
1	A	1015	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	753	ARG	2.3
1	A	723	LYS	2.3
1	A	1031	LEU	2.3
1	A	1095	LEU	2.3
1	A	1001	PRO	2.2
1	B	678	TYR	2.2
1	B	262	ILE	2.2
1	A	1100	GLN	2.2
1	B	764	THR	2.2
1	A	724	GLN	2.2
1	B	910	TYR	2.2
1	A	28	GLU	2.2
1	A	76	THR	2.2
1	B	366	THR	2.2
1	B	766	ALA	2.2
1	B	1015	ASP	2.2
1	B	836	GLN	2.1
1	A	649	LEU	2.1
1	A	714	ILE	2.1
1	A	124	THR	2.1
1	A	1053	VAL	2.1
1	A	195	GLU	2.1
1	A	371	LEU	2.1
1	B	712	PRO	2.1
1	B	666	ARG	2.1
1	A	545	GLU	2.0
1	B	770	ILE	2.0
1	A	366	THR	2.0
1	A	836	GLN	2.0
1	A	74	LYS	2.0
1	A	697	ILE	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 oligosaccharides in this entry.

6.4 Ligands (i)

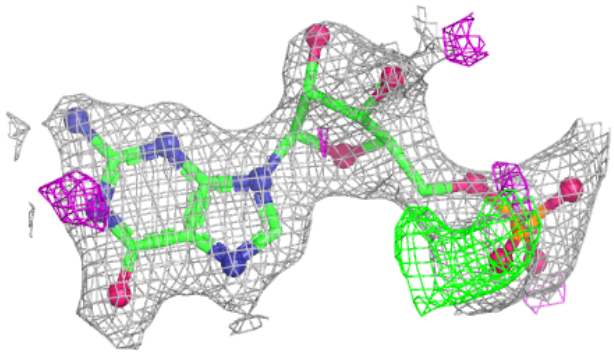
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

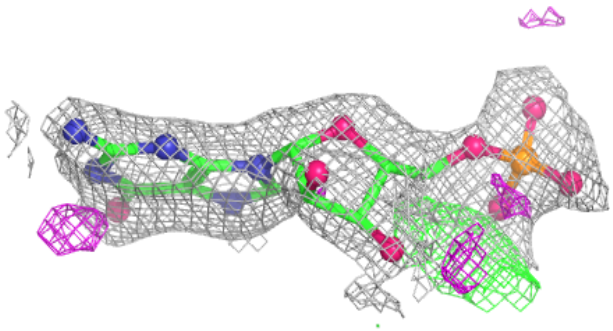
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	5GP	C	101	24/24	0.85	0.12	31,41,78,81	0
3	ATP	A	1201	31/31	0.92	0.09	16,26,42,124	0
5	PO4	B	1201	5/5	0.94	0.14	39,43,54,54	0
4	MN	A	1202	1/1	0.95	0.13	56,56,56,56	0
5	PO4	A	1204	5/5	0.97	0.10	28,34,37,44	0
4	MN	A	1203	1/1	0.98	0.09	35,35,35,35	0

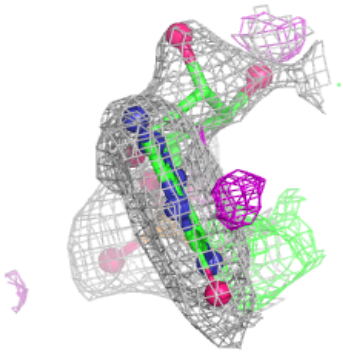
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP C 101:

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

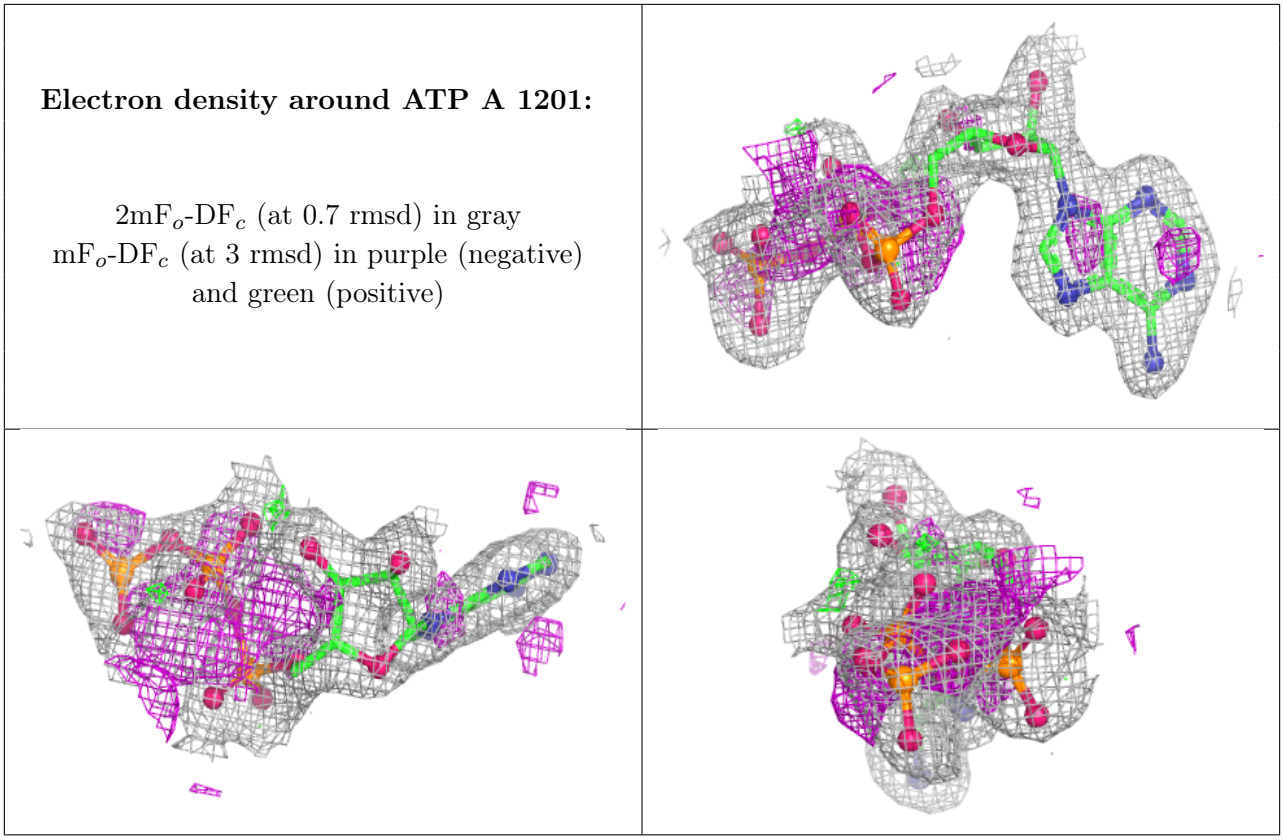






Electron density around ATP A 1201:

$2mF_o$-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.