



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:58 PM UTC

PDB ID : 5LIL / pdb_00005lil
Title : Structure of Aggregatibacter actinomycetemcomitans MacB bound to ATPyS (P21)
Authors : Crow, A.
Deposited on : 2016-07-15
Resolution : 3.35 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

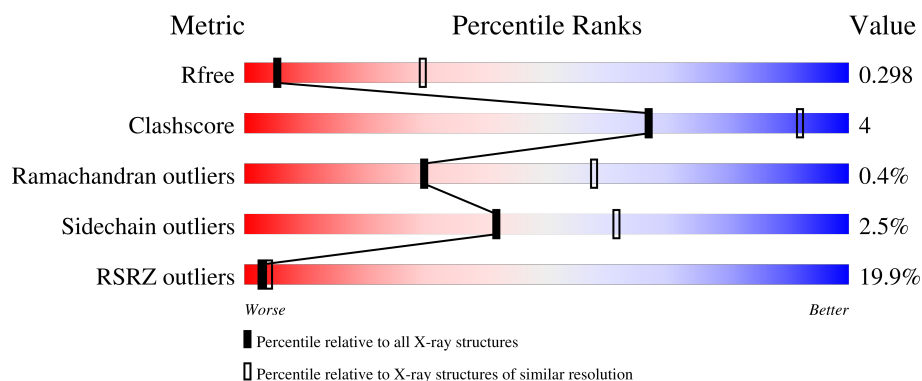
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	664	 16% 81% 10% 7%
1	B	664	 20% 82% 8% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18962 atoms, of which 9639 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 Macrolide export ATP-binding/permease protein MacB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	615	Total	C	H	N	O	S	0	0	0
			9529	2954	4853	802	899	21			
1	B	604	Total	C	H	N	O	S	0	0	0
			9341	2888	4762	787	883	21			

There are 42 discrepancies between the modelled and reference sequences:

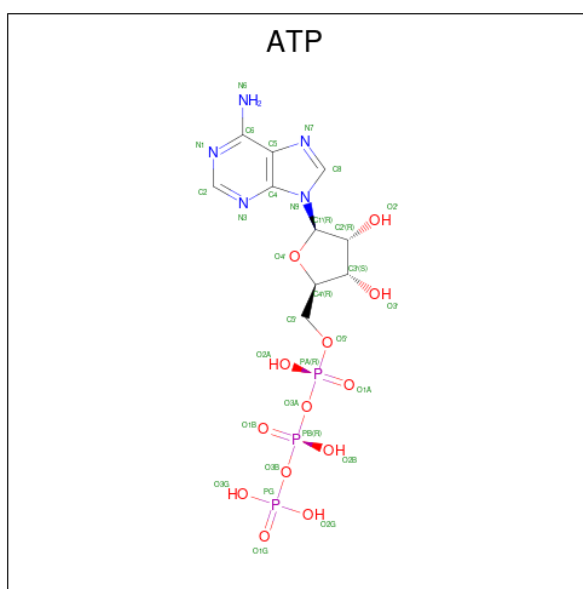
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2EHL8
A	-18	GLY	-	expression tag	UNP Q2EHL8
A	-17	SER	-	expression tag	UNP Q2EHL8
A	-16	SER	-	expression tag	UNP Q2EHL8
A	-15	HIS	-	expression tag	UNP Q2EHL8
A	-14	HIS	-	expression tag	UNP Q2EHL8
A	-13	HIS	-	expression tag	UNP Q2EHL8
A	-12	HIS	-	expression tag	UNP Q2EHL8
A	-11	HIS	-	expression tag	UNP Q2EHL8
A	-10	HIS	-	expression tag	UNP Q2EHL8
A	-9	SER	-	expression tag	UNP Q2EHL8
A	-8	SER	-	expression tag	UNP Q2EHL8
A	-7	GLY	-	expression tag	UNP Q2EHL8
A	-6	LEU	-	expression tag	UNP Q2EHL8
A	-5	VAL	-	expression tag	UNP Q2EHL8
A	-4	PRO	-	expression tag	UNP Q2EHL8
A	-3	ARG	-	expression tag	UNP Q2EHL8
A	-2	GLY	-	expression tag	UNP Q2EHL8
A	-1	SER	-	expression tag	UNP Q2EHL8
A	0	HIS	-	expression tag	UNP Q2EHL8
A	169	GLN	GLU	engineered mutation	UNP Q2EHL8
B	-19	MET	-	initiating methionine	UNP Q2EHL8
B	-18	GLY	-	expression tag	UNP Q2EHL8
B	-17	SER	-	expression tag	UNP Q2EHL8
B	-16	SER	-	expression tag	UNP Q2EHL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q2EHL8
B	-14	HIS	-	expression tag	UNP Q2EHL8
B	-13	HIS	-	expression tag	UNP Q2EHL8
B	-12	HIS	-	expression tag	UNP Q2EHL8
B	-11	HIS	-	expression tag	UNP Q2EHL8
B	-10	HIS	-	expression tag	UNP Q2EHL8
B	-9	SER	-	expression tag	UNP Q2EHL8
B	-8	SER	-	expression tag	UNP Q2EHL8
B	-7	GLY	-	expression tag	UNP Q2EHL8
B	-6	LEU	-	expression tag	UNP Q2EHL8
B	-5	VAL	-	expression tag	UNP Q2EHL8
B	-4	PRO	-	expression tag	UNP Q2EHL8
B	-3	ARG	-	expression tag	UNP Q2EHL8
B	-2	GLY	-	expression tag	UNP Q2EHL8
B	-1	SER	-	expression tag	UNP Q2EHL8
B	0	HIS	-	expression tag	UNP Q2EHL8
B	169	GLN	GLU	engineered mutation	UNP Q2EHL8

- Molecule 2 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 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

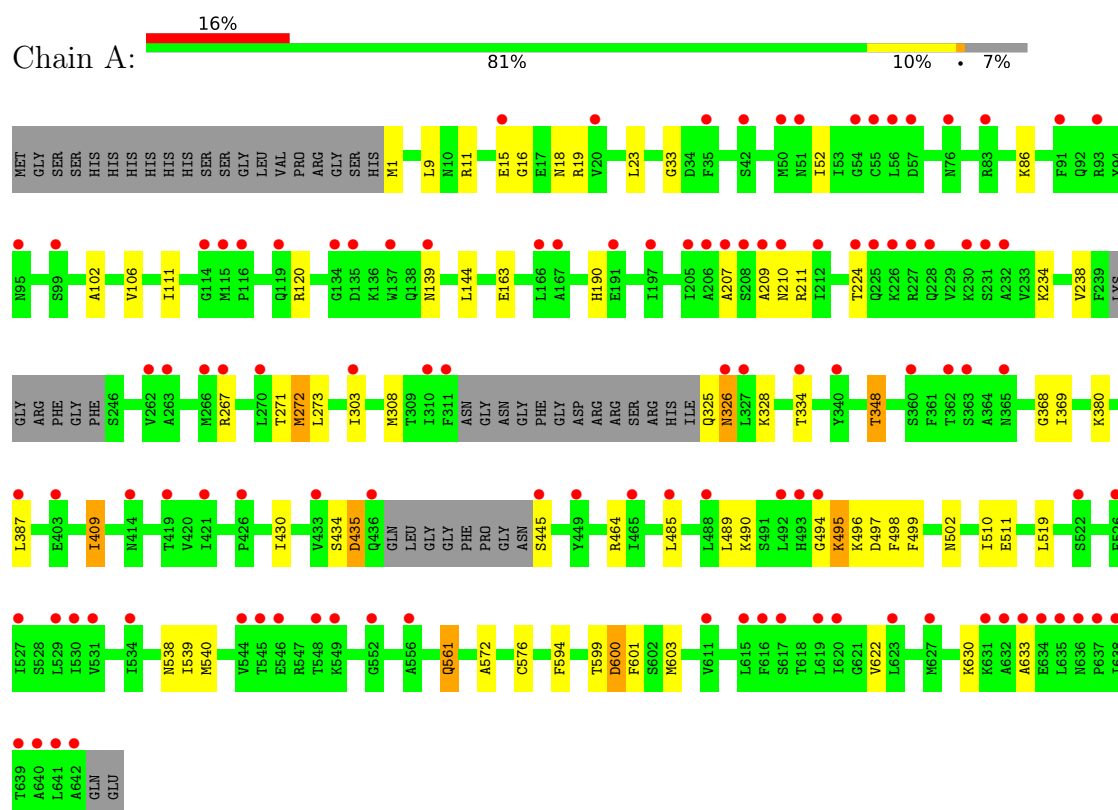
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0

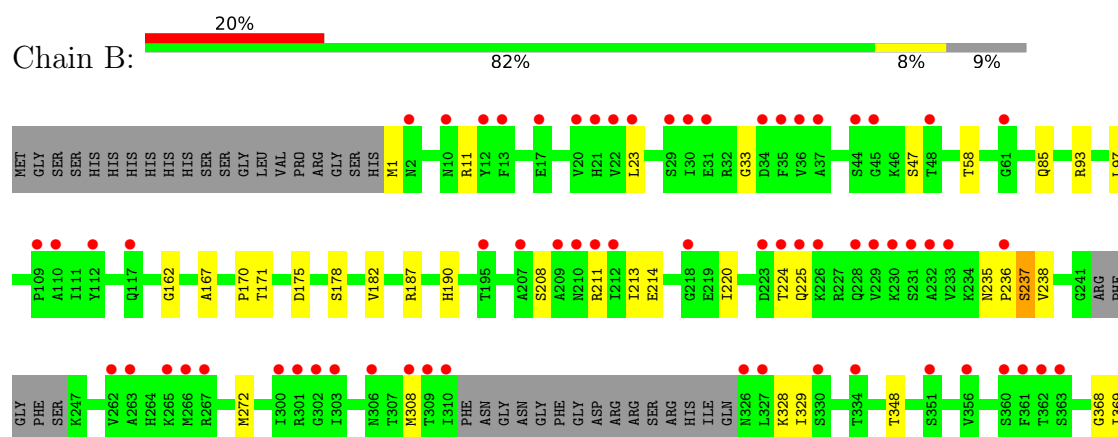
3 Residue-property plots [i](#)

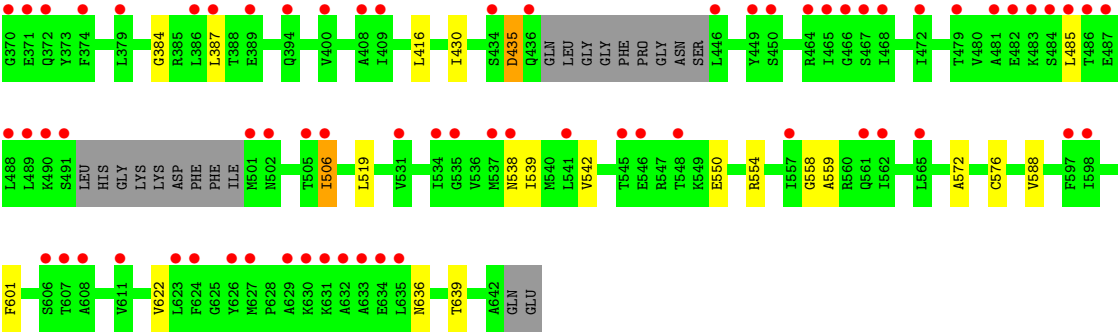
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Macrolide export ATP-binding/permease protein MacB



- Molecule 1: Macrolide export ATP-binding/permease protein MacB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.59Å 82.62Å 124.92Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	79.95 – 3.35 79.95 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (79.95-3.35) 99.1 (79.95-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.33Å)	Xtriage
Refinement program	PHENIX (dev_2196: ???)	Depositor
R, R_{free}	0.244 , 0.290 0.249 , 0.298	Depositor DCC
R_{free} test set	1592 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	18962	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.16	0/4725	0.39	0/6366
1	B	0.15	0/4623	0.36	0/6228
All	All	0.16	0/9348	0.38	0/12594

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	93	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4676	4853	4856	43	0
1	B	4579	4762	4764	33	0
2	A	31	12	12	1	0
2	B	31	12	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
All	All	9323	9639	9644	71	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 4.

All (71) 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:A:496:LYS:HB3	1:A:497:ASP:HA	1.76	0.67
1:A:489:LEU:HB3	1:A:498:PHE:CZ	2.38	0.59
1:A:325:GLN:HG3	1:A:464:ARG:HD3	1.85	0.58
1:B:435:ASP:N	1:B:435:ASP:OD1	2.35	0.58
1:A:600:ASP:OD1	1:A:601:PHE:N	2.38	0.56
1:A:599:THR:O	1:A:600:ASP:HB2	2.06	0.55
1:B:85:GLN:CB	1:B:238:VAL:HG11	2.36	0.55
1:A:519:LEU:HD23	1:B:601:PHE:CE1	2.42	0.54
1:B:47:SER:OG	2:B:701:ATP:O1B	2.25	0.54
1:B:187:ARG:NH1	1:B:208:SER:OG	2.42	0.53
2:A:701:ATP:O2B	4:A:801:HOH:O	2.19	0.52
1:A:539:ILE:HD13	1:B:538:ASN:HB3	1.91	0.52
1:B:97:LEU:HD22	1:B:550:GLU:HG3	1.91	0.51
1:B:211:ARG:HA	1:B:224:THR:O	2.11	0.51
1:A:380:LYS:O	1:A:434:SER:OG	2.29	0.51
1:A:15:GLU:O	1:A:18:ASN:N	2.43	0.50
1:A:434:SER:O	1:A:435:ASP:CB	2.59	0.50
1:B:550:GLU:O	1:B:554:ARG:HG3	2.12	0.49
1:A:308:MET:SD	1:A:502:ASN:ND2	2.85	0.49
1:A:434:SER:O	1:A:435:ASP:HB2	2.13	0.49
1:A:326:ASN:OD1	1:A:326:ASN:N	2.44	0.48
1:A:9:LEU:HD11	1:A:52:ILE:HG21	1.95	0.48
1:B:236:PRO:O	1:B:237:SER:CB	2.62	0.47
1:B:369:ILE:HD11	1:B:387:LEU:HD12	1.96	0.47
1:A:496:LYS:CB	1:A:497:ASP:HA	2.43	0.47
1:A:601:PHE:CE1	1:B:519:LEU:HD23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:THR:O	1:B:368:GLY:N	2.42	0.46
1:B:235:ASN:HB3	1:B:236:PRO:HD2	1.97	0.46
1:B:167:ALA:HB1	1:B:170:PRO:HG3	1.98	0.46
1:B:213:ILE:HG21	1:B:220:ILE:HD11	1.98	0.46
1:B:85:GLN:HB2	1:B:238:VAL:HG11	1.96	0.45
1:A:111:ILE:CD1	1:A:120:ARG:CZ	2.94	0.45
1:A:369:ILE:HD11	1:A:387:LEU:HD12	1.99	0.45
1:B:175:ASP:OD1	1:B:178:SER:N	2.42	0.45
1:B:11:ARG:HB3	1:B:23:LEU:HB2	1.99	0.45
1:A:387:LEU:HD23	1:A:430:ILE:HD11	1.99	0.44
1:A:539:ILE:HD11	1:B:542:VAL:HG21	1.98	0.44
1:B:85:GLN:HG3	1:B:238:VAL:HG11	1.98	0.44
1:A:272:MET:HG3	1:A:273:LEU:N	2.33	0.44
1:A:572:ALA:O	1:A:576:CYS:N	2.47	0.44
1:A:303:ILE:HD11	1:B:506:ILE:HD12	2.00	0.43
1:A:490:LYS:HD3	1:A:495:LYS:HG2	2.01	0.43
1:A:11:ARG:HB3	1:A:23:LEU:HB2	2.01	0.43
1:B:171:THR:HG22	1:B:171:THR:O	2.17	0.43
1:B:636:ASN:O	1:B:639:THR:OG1	2.33	0.43
1:A:211:ARG:HA	1:A:224:THR:O	2.19	0.43
1:B:85:GLN:O	1:B:162:GLY:HA2	2.19	0.43
1:A:16:GLY:N	1:A:19:ARG:HB2	2.34	0.42
1:A:139:ASN:HB2	1:A:144:LEU:HD21	2.01	0.42
1:B:572:ALA:O	1:B:576:CYS:N	2.49	0.42
1:A:594:PHE:HB3	1:A:603:MET:HE3	2.02	0.42
1:A:238:VAL:HG13	1:A:238:VAL:O	2.20	0.42
1:B:387:LEU:HD23	1:B:430:ILE:HD11	2.02	0.42
1:A:33:GLY:O	1:A:190:HIS:NE2	2.53	0.41
1:A:380:LYS:N	1:A:434:SER:OG	2.48	0.41
1:A:485:LEU:HD21	1:A:489:LEU:HD12	2.03	0.41
1:B:558:GLY:O	1:B:559:ALA:C	2.63	0.41
1:A:207:ALA:C	1:A:209:ALA:H	2.29	0.41
1:A:271:THR:HG22	1:A:539:ILE:HG23	2.02	0.41
1:A:409:ILE:N	1:A:409:ILE:CD1	2.84	0.41
1:A:499:PHE:O	1:A:499:PHE:CG	2.74	0.41
1:B:178:SER:O	1:B:182:VAL:HG23	2.20	0.41
1:A:102:ALA:O	1:A:106:VAL:HG23	2.21	0.41
1:A:348:THR:O	1:A:368:GLY:N	2.53	0.41
1:A:510:ILE:HG13	1:A:511:GLU:N	2.36	0.41
1:A:538:ASN:HB3	1:B:539:ILE:HD13	2.01	0.41
1:B:33:GLY:O	1:B:190:HIS:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LYS:HG3	1:B:329:ILE:H	1.87	0.40
1:A:86:LYS:NZ	1:A:163:GLU:OE2	2.47	0.40
1:A:561:GLN:NE2	1:A:633:ALA:O	2.55	0.40
1:B:384:GLY:HA3	1:B:416:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	607/664 (91%)	562 (93%)	41 (7%)	4 (1%)	18	46
1	B	594/664 (90%)	565 (95%)	28 (5%)	1 (0%)	43	70
All	All	1201/1328 (90%)	1127 (94%)	69 (6%)	5 (0%)	30	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	ASP
1	A	494	GLY
1	A	600	ASP
1	B	237	SER
1	A	348	THR

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/563 (93%)	510 (97%)	15 (3%)	37	60
1	B	514/563 (91%)	503 (98%)	11 (2%)	47	64
All	All	1039/1126 (92%)	1013 (98%)	26 (2%)	42	61

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	210	ASN
1	A	234	LYS
1	A	267	ARG
1	A	272	MET
1	A	326	ASN
1	A	328	LYS
1	A	334	THR
1	A	409	ILE
1	A	445	SER
1	A	495	LYS
1	A	540	MET
1	A	561	GLN
1	A	622	VAL
1	A	630	LYS
1	B	1	MET
1	B	58	THR
1	B	214	GLU
1	B	225	GLN
1	B	272	MET
1	B	308	MET
1	B	435	ASP
1	B	485	LEU
1	B	506	ILE
1	B	588	VAL
1	B	622	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	51	ASN
1	A	181	ASN
1	A	201	HIS

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	249	GLN
1	A	333	ASN
1	A	383	GLN
1	A	412	ASN
1	A	566	GLN
1	B	2	ASN
1	B	10	ASN
1	B	21	HIS
1	B	181	ASN
1	B	293	GLN
1	B	394	GLN
1	B	412	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	ATP	B	701	3	32,33,33	1.40	5 (15%)	48,52,52	1.76	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	701	3	32,33,33	1.50	7 (21%)	48,52,52	1.81	10 (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
2	ATP	B	701	3	-	8/22/38/38	0/3/3/3
2	ATP	A	701	3	-	6/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ATP	C5-C4	4.51	1.47	1.39
2	A	701	ATP	C5-C4	4.47	1.47	1.39
2	A	701	ATP	PB-O3A	2.77	1.62	1.59
2	A	701	ATP	PB-O3B	2.70	1.62	1.59
2	B	701	ATP	C5-C6	2.58	1.48	1.41
2	A	701	ATP	C8-N7	2.47	1.36	1.31
2	A	701	ATP	C5-C6	2.44	1.47	1.41
2	A	701	ATP	PA-O3A	2.42	1.62	1.59
2	A	701	ATP	C5-N7	-2.38	1.34	1.39
2	B	701	ATP	C5-N7	-2.33	1.34	1.39
2	B	701	ATP	C8-N7	2.32	1.36	1.31
2	B	701	ATP	PB-O3B	2.09	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C5-C4-N3	-5.67	118.91	126.72
2	B	701	ATP	C5-C4-N3	-5.64	118.95	126.72
2	B	701	ATP	N3-C4-N9	4.75	135.25	127.17
2	A	701	ATP	N3-C4-N9	4.58	134.96	127.17
2	A	701	ATP	C2-N3-C4	3.88	121.31	111.83
2	A	701	ATP	N3-C2-N1	-3.85	122.75	128.58
2	B	701	ATP	C2-N3-C4	3.77	121.04	111.83
2	B	701	ATP	N3-C2-N1	-3.67	123.03	128.58
2	A	701	ATP	C4-C5-N7	-3.35	106.75	110.58
2	B	701	ATP	C4-N9-C8	3.33	109.23	105.74
2	B	701	ATP	C4-C5-N7	-3.21	106.91	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	C4-N9-C8	3.16	109.05	105.74
2	A	701	ATP	C5-N7-C8	2.73	107.74	103.45
2	B	701	ATP	C5-N7-C8	2.63	107.58	103.45
2	A	701	ATP	N9-C8-N7	-2.55	110.32	113.94
2	B	701	ATP	N9-C8-N7	-2.44	110.48	113.94
2	A	701	ATP	C6-C5-N7	2.17	136.27	132.09
2	A	701	ATP	C2-N1-C6	2.09	122.17	118.73
2	B	701	ATP	C2-N1-C6	2.03	122.07	118.73
2	B	701	ATP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	ATP	PB-O3B-PG-O3G
2	B	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O3A
2	A	701	ATP	O4'-C4'-C5'-O5'
2	B	701	ATP	O4'-C4'-C5'-O5'
2	B	701	ATP	C3'-C4'-C5'-O5'
2	A	701	ATP	C3'-C4'-C5'-O5'
2	A	701	ATP	PG-O3B-PB-O2B
2	B	701	ATP	PG-O3B-PB-O1B
2	B	701	ATP	C5'-O5'-PA-O1A
2	A	701	ATP	PG-O3B-PB-O1B
2	A	701	ATP	PB-O3A-PA-O1A
2	B	701	ATP	PG-O3B-PB-O2B
2	A	701	ATP	PB-O3A-PA-O2A

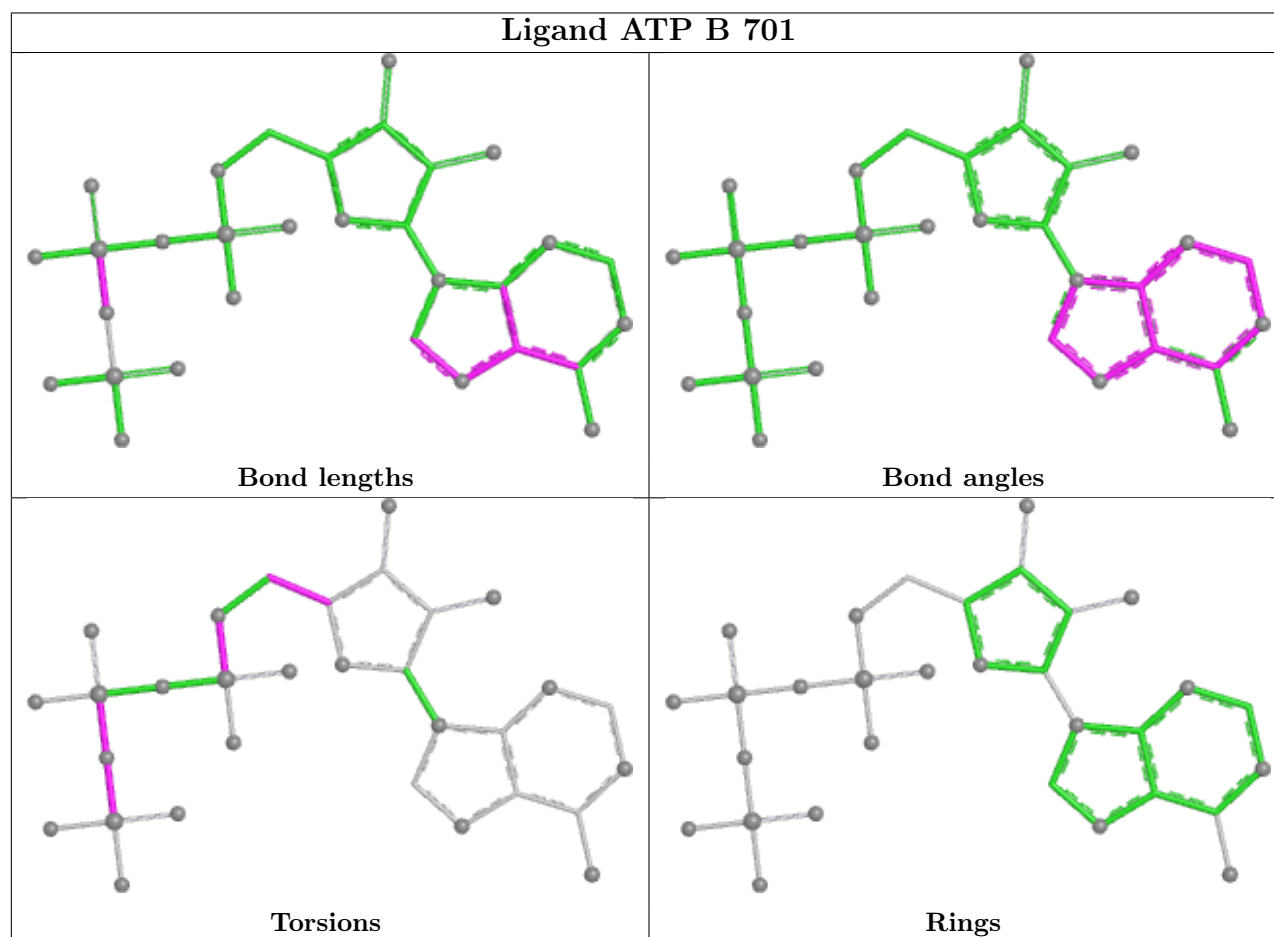
There are no ring outliers.

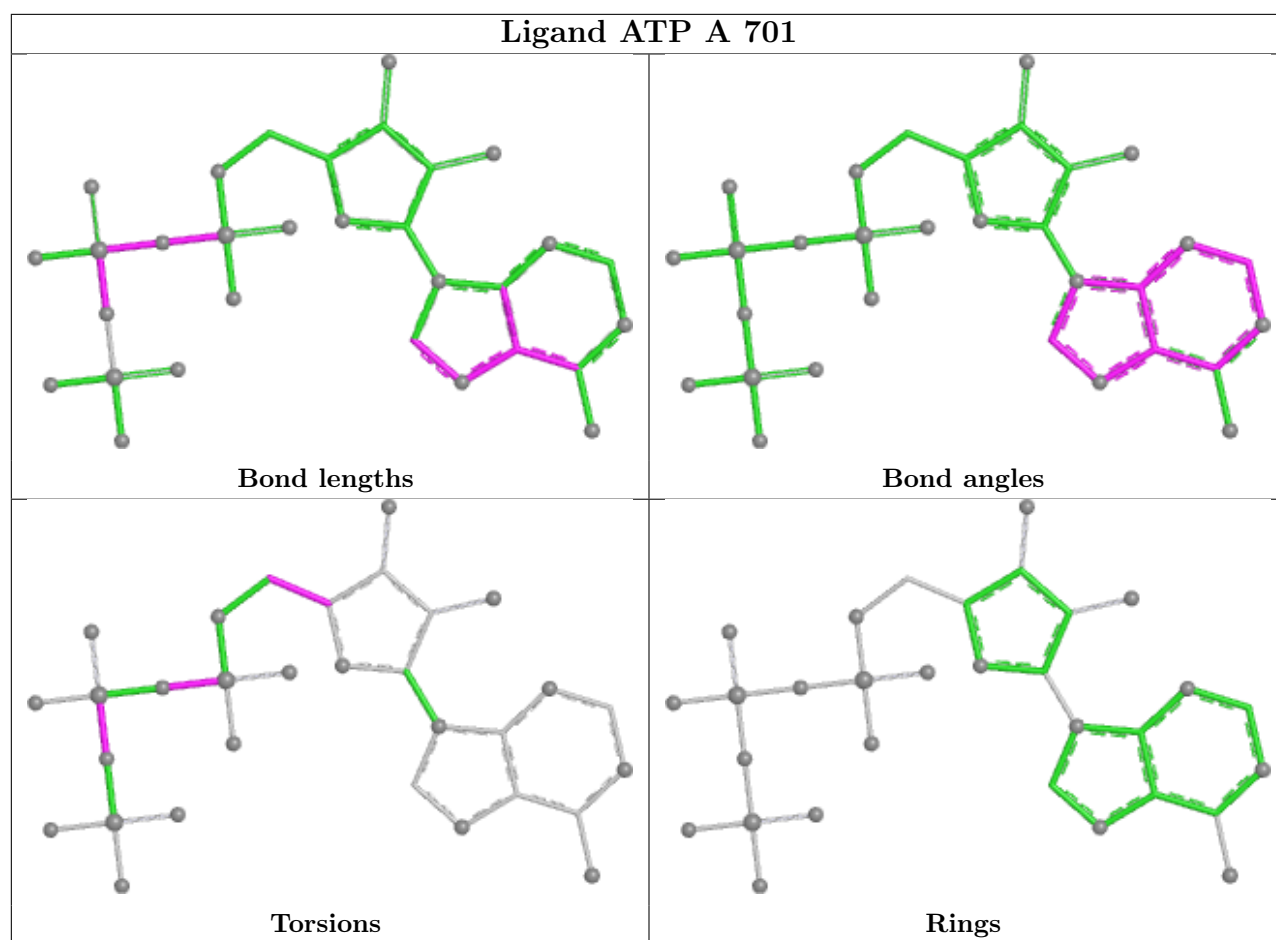
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ATP	1	0
2	A	701	ATP	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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	615/664 (92%)	0.98	109 (17%)  	50, 92, 174, 210	0
1	B	604/664 (90%)	1.04	134 (22%)  	54, 90, 146, 180	0
All	All	1219/1328 (91%)	1.01	243 (19%)  	50, 91, 163, 210	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	LYS	11.2
1	A	639	THR	10.1
1	A	638	ILE	9.1
1	A	637	PRO	8.9
1	A	226	LYS	8.9
1	B	233	VAL	8.7
1	A	641	LEU	8.1
1	A	635	LEU	7.6
1	A	640	ALA	7.5
1	B	607	THR	7.5
1	B	225	GLN	7.0
1	A	636	ASN	6.9
1	A	208	SER	6.8
1	B	226	LYS	6.7
1	B	485	LEU	6.5
1	A	56	LEU	6.2
1	A	548	THR	6.0
1	B	546	GLU	6.0
1	B	309	THR	5.9
1	B	541	LEU	5.9
1	B	501	MET	5.8
1	A	266	MET	5.8
1	B	466	GLY	5.8
1	A	327	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	530	ILE	5.6
1	A	116	PRO	5.6
1	B	631	LYS	5.6
1	A	210	ASN	5.4
1	B	482	GLU	5.3
1	A	209	ALA	5.2
1	B	486	THR	5.2
1	B	31	GLU	5.2
1	A	55	CYS	5.2
1	A	546	GLU	5.2
1	A	230	LYS	5.0
1	B	2	ASN	4.9
1	A	615	LEU	4.9
1	A	227	ARG	4.9
1	B	545	THR	4.9
1	A	95	ASN	4.9
1	A	616	PHE	4.9
1	B	534	ILE	4.8
1	B	310	ILE	4.8
1	A	642	ALA	4.8
1	B	489	LEU	4.7
1	B	634	GLU	4.7
1	A	426	PRO	4.6
1	B	229	VAL	4.6
1	B	228	GLN	4.5
1	A	634	GLU	4.5
1	B	224	THR	4.5
1	A	526	PHE	4.4
1	A	362	THR	4.4
1	A	205	ILE	4.3
1	B	34	ASP	4.3
1	B	598	ILE	4.3
1	B	531	VAL	4.2
1	B	632	ALA	4.2
1	A	529	LEU	4.2
1	B	303	ILE	4.1
1	A	91	PHE	4.1
1	A	231	SER	4.1
1	A	631	LYS	4.1
1	B	326	ASN	4.0
1	B	210	ASN	4.0
1	B	371	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	633	ALA	4.0
1	A	57	ASP	3.9
1	A	207	ALA	3.9
1	B	265	LYS	3.9
1	B	22	VAL	3.8
1	B	36	VAL	3.8
1	A	633	ALA	3.8
1	A	494	GLY	3.8
1	B	308	MET	3.7
1	B	464	ARG	3.6
1	B	300	ILE	3.6
1	B	37	ALA	3.6
1	A	51	ASN	3.6
1	B	266	MET	3.6
1	A	263	ALA	3.5
1	B	502	ASN	3.5
1	B	465	ILE	3.5
1	A	363	SER	3.5
1	B	370	GLY	3.5
1	B	627	MET	3.5
1	B	491	SER	3.5
1	A	620	ILE	3.4
1	A	225	GLN	3.3
1	A	492	LEU	3.3
1	A	232	ALA	3.3
1	B	449	TYR	3.3
1	B	481	ALA	3.3
1	A	83	ARG	3.2
1	A	556	ALA	3.2
1	A	267	ARG	3.2
1	A	493	HIS	3.2
1	A	119	GLN	3.2
1	B	232	ALA	3.2
1	B	608	ALA	3.2
1	A	228	GLN	3.1
1	B	387	LEU	3.1
1	A	365	ASN	3.1
1	B	23	LEU	3.1
1	B	374	PHE	3.0
1	B	467	SER	3.0
1	B	409	ILE	3.0
1	B	109	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	419	THR	3.0
1	B	548	THR	3.0
1	B	505	THR	3.0
1	A	632	ALA	2.9
1	A	445	SER	2.9
1	A	465	ILE	2.9
1	B	635	LEU	2.9
1	A	522	SER	2.9
1	B	306	ASN	2.9
1	B	362	THR	2.9
1	B	488	LEU	2.9
1	B	537	MET	2.9
1	A	35	PHE	2.9
1	A	449	TYR	2.9
1	B	207	ALA	2.8
1	A	485	LEU	2.8
1	B	12	TYR	2.8
1	B	446	LEU	2.8
1	A	433	VAL	2.8
1	B	212	ILE	2.8
1	A	206	ALA	2.8
1	B	231	SER	2.8
1	B	386	LEU	2.8
1	A	545	THR	2.8
1	B	327	LEU	2.8
1	A	552	GLY	2.8
1	B	61	GLY	2.8
1	B	302	GLY	2.8
1	B	490	LYS	2.7
1	A	20	VAL	2.7
1	B	372	GLN	2.7
1	A	527	ILE	2.7
1	A	114	GLY	2.7
1	B	44	SER	2.7
1	B	330	SER	2.7
1	B	450	SER	2.7
1	A	303	ILE	2.7
1	B	561	GLN	2.7
1	A	42	SER	2.6
1	A	488	LEU	2.6
1	A	619	LEU	2.6
1	A	135	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	310	ILE	2.6
1	A	534	ILE	2.6
1	B	468	ILE	2.6
1	B	484	SER	2.6
1	B	223	ASP	2.6
1	B	436	GLN	2.6
1	B	538	ASN	2.6
1	B	557	ILE	2.6
1	B	35	PHE	2.6
1	B	363	SER	2.6
1	B	487	GLU	2.6
1	A	531	VAL	2.6
1	B	262	VAL	2.6
1	A	212	ILE	2.5
1	B	506	ILE	2.5
1	B	626	TYR	2.5
1	B	29	SER	2.5
1	A	93	ARG	2.5
1	A	611	VAL	2.5
1	B	117	GLN	2.5
1	B	597	PHE	2.5
1	B	483	LYS	2.5
1	B	209	ALA	2.5
1	A	224	THR	2.5
1	B	211	ARG	2.5
1	A	15	GLU	2.5
1	A	115	MET	2.5
1	B	356	VAL	2.5
1	A	436	GLN	2.5
1	A	270	LEU	2.4
1	B	112	TYR	2.4
1	B	434	SER	2.4
1	B	13	PHE	2.4
1	B	334	THR	2.4
1	B	565	LEU	2.4
1	B	623	LEU	2.4
1	B	195	THR	2.4
1	B	479	THR	2.4
1	A	334	THR	2.4
1	A	360	SER	2.4
1	B	611	VAL	2.4
1	B	21	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	LEU	2.3
1	B	379	LEU	2.3
1	B	360	SER	2.3
1	A	544	VAL	2.3
1	A	197	ILE	2.3
1	A	340	TYR	2.3
1	A	414	ASN	2.3
1	B	394	GLN	2.3
1	A	617	SER	2.3
1	B	230	LYS	2.3
1	B	630	LYS	2.3
1	A	137	TRP	2.2
1	A	139	ASN	2.2
1	B	10	ASN	2.2
1	B	389	GLU	2.2
1	A	167	ALA	2.2
1	B	361	PHE	2.2
1	A	326	ASN	2.2
1	A	403	GLU	2.2
1	B	301	ARG	2.2
1	B	48	THR	2.2
1	B	400	VAL	2.2
1	A	421	ILE	2.2
1	B	472	ILE	2.2
1	B	408	ALA	2.2
1	A	262	VAL	2.2
1	A	99	SER	2.2
1	B	263	ALA	2.2
1	A	134	GLY	2.2
1	B	624	PHE	2.2
1	B	562	ILE	2.1
1	A	387	LEU	2.1
1	B	629	ALA	2.1
1	B	351	SER	2.1
1	B	267	ARG	2.1
1	B	535	GLY	2.1
1	B	606	SER	2.1
1	A	623	LEU	2.1
1	B	110	ALA	2.1
1	B	17	GLU	2.1
1	B	236	PRO	2.1
1	A	54	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	GLY	2.1
1	A	76	ASN	2.0
1	B	30	ILE	2.0
1	A	311	PHE	2.0
1	A	191	GLU	2.0
1	B	20	VAL	2.0
1	A	50	MET	2.0
1	A	627	MET	2.0
1	B	218	GLY	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](#)

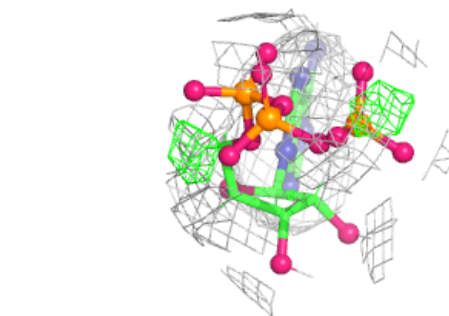
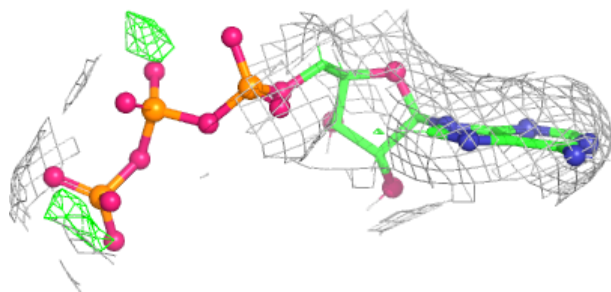
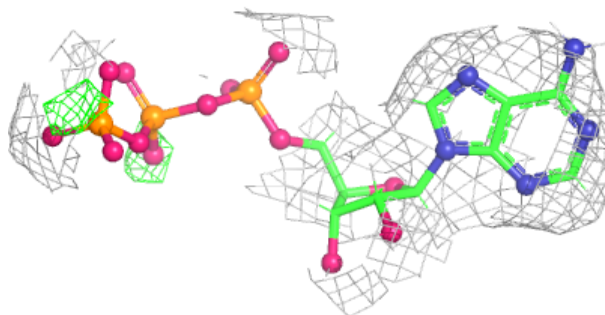
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	701	31/31	0.95	0.09	48,70,88,92	0
2	ATP	B	701	31/31	0.97	0.07	51,69,88,106	0
3	MG	A	702	1/1	0.98	0.06	54,54,54,54	0
3	MG	B	702	1/1	0.99	0.12	60,60,60,60	0

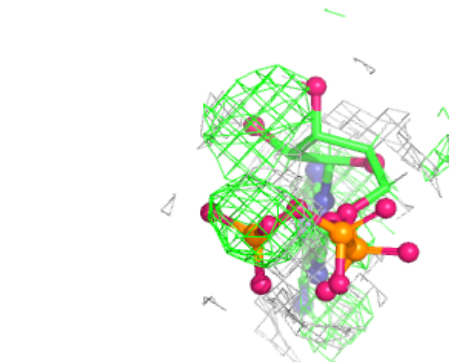
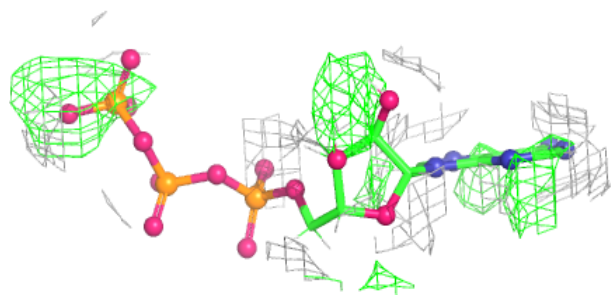
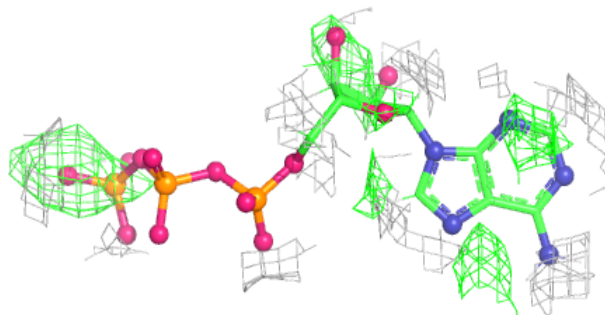
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 701:

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

**Electron density around ATP B 701:**

$2mF_o - DF_c$ (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.