



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:02 AM UTC

PDB ID : 5LJ7 / pdb_00005lj7
Title : Structure of Aggregatibacter actinomycetemcomitans MacB bound to ATP (P21)
Authors : Crow, A.
Deposited on : 2016-07-18
Resolution : 3.25 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

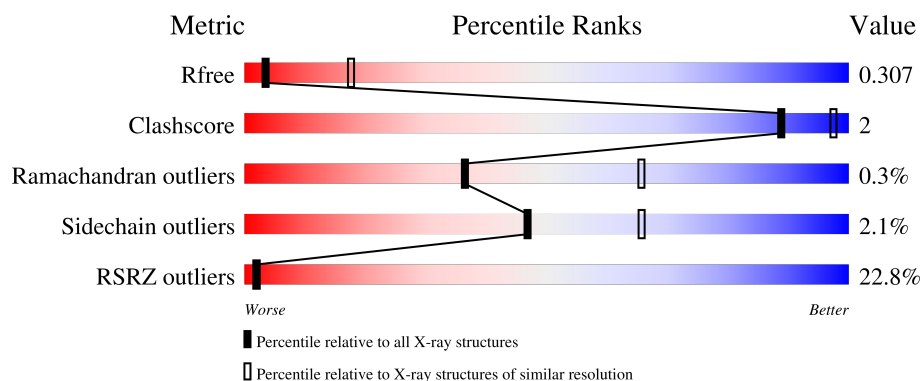
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	24% 82% 6% 11%
1	B	664	17% 86% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18564 atoms, of which 9438 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	592	Total	C	H	N	O	S	0	0	0
			9207	2856	4690	775	865	21			
1	B	599	Total	C	H	N	O	S	0	0	0
			9265	2864	4724	781	875	21			

There are 42 discrepancies between the modelled and reference sequences:

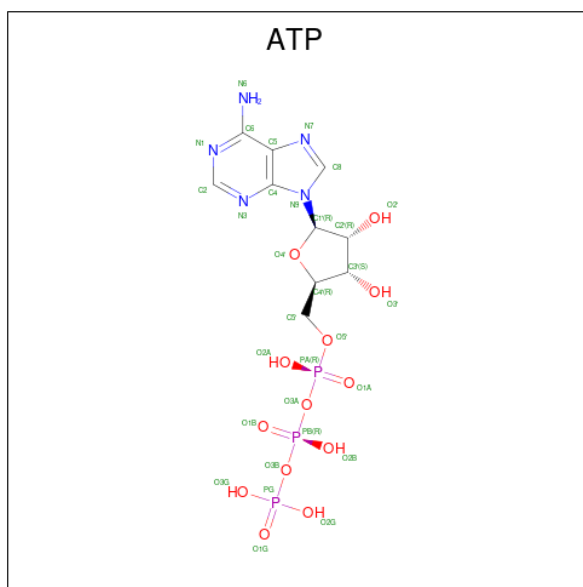
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2EHL8
A	-18	GLY	-	expression tag	UNP Q2EHL8
A	-17	SER	-	expression tag	UNP Q2EHL8
A	-16	SER	-	expression tag	UNP Q2EHL8
A	-15	HIS	-	expression tag	UNP Q2EHL8
A	-14	HIS	-	expression tag	UNP Q2EHL8
A	-13	HIS	-	expression 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	conflict	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	conflict	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
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

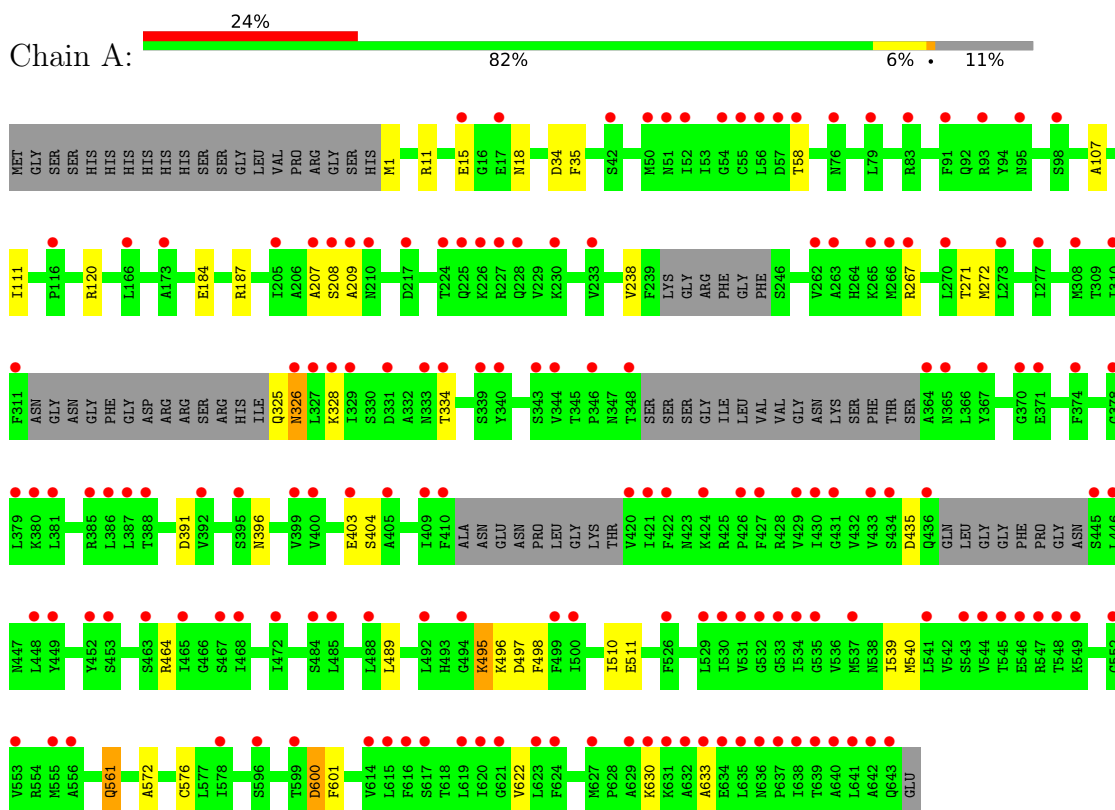
- Molecule 4 is water.

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

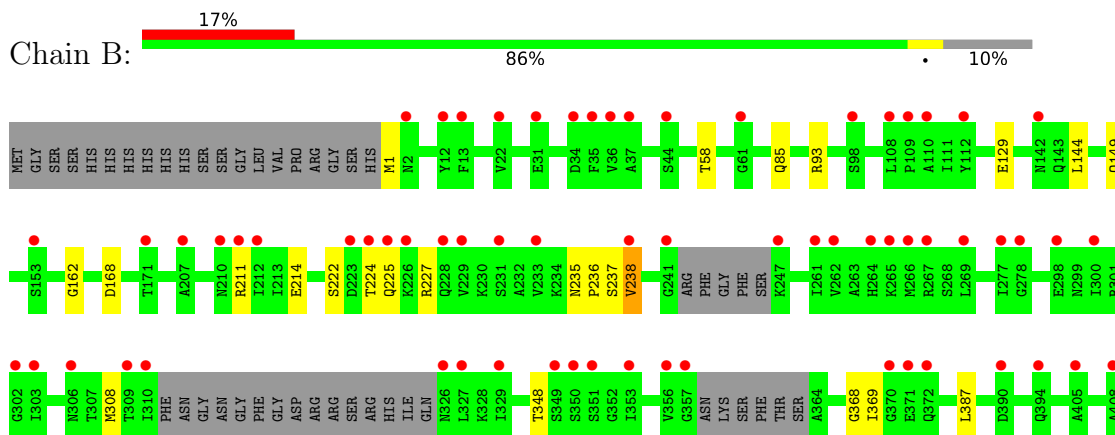
3 Residue-property plots

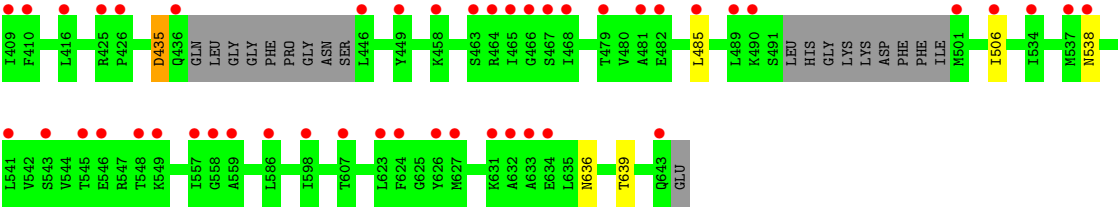
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	112.33Å 82.61Å 125.17Å 90.00° 93.54° 90.00°	Depositor
Resolution (Å)	86.13 – 3.25 86.13 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (86.13-3.25) 99.3 (86.13-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.26Å)	Xtriage
Refinement program	PHENIX (dev_2196: ???)	Depositor
R, R_{free}	0.246 , 0.299 0.252 , 0.307	Depositor DCC
R_{free} test set	1758 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.4	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	18564	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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	0.12	0/4562	0.30	0/6142
1	B	0.12	0/4583	0.30	0/6173
All	All	0.12	0/9145	0.30	0/12315

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	4517	4690	4692	24	1
1	B	4541	4724	4726	12	1
2	A	31	12	12	1	0
2	B	31	12	12	0	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	1	0
All	All	9126	9438	9442	36	1

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 2.

All (36) 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:A:701:ATP:O2B	4:A:801:HOH:O	2.03	0.76
1:B:168:ASP:OD1	4:B:801:HOH:O	2.10	0.68
1:A:496:LYS:HB3	1:A:497:ASP:HA	1.77	0.65
1:B:435:ASP:N	1:B:435:ASP:OD1	2.31	0.62
1:B:348:THR:O	1:B:368:GLY:N	2.36	0.56
1:A:15:GLU:O	1:A:18:ASN:N	2.39	0.54
1:A:600:ASP:OD1	1:A:601:PHE:N	2.42	0.53
1:A:561:GLN:NE2	1:A:633:ALA:O	2.42	0.53
1:A:326:ASN:N	1:A:326:ASN:OD1	2.41	0.51
1:A:496:LYS:CB	1:A:497:ASP:HA	2.40	0.51
1:B:85:GLN:HB2	1:B:238:VAL:HG11	1.93	0.51
1:B:85:GLN:CB	1:B:238:VAL:HG11	2.42	0.50
1:A:403:GLU:N	1:A:435:ASP:OD1	2.46	0.48
1:B:235:ASN:HB3	1:B:236:PRO:HD2	1.95	0.48
1:B:636:ASN:O	1:B:639:THR:OG1	2.28	0.48
1:A:572:ALA:O	1:A:576:CYS:N	2.47	0.48
1:A:489:LEU:HB3	1:A:498:PHE:CZ	2.50	0.47
1:A:539:ILE:HD13	1:B:538:ASN:HB3	1.96	0.47
1:B:85:GLN:O	1:B:162:GLY:HA2	2.16	0.45
1:A:34:ASP:OD1	1:A:35:PHE:N	2.44	0.45
1:B:144:LEU:O	1:B:149:GLN:NE2	2.48	0.45
1:A:111:ILE:CD1	1:A:120:ARG:CZ	2.97	0.43
1:A:207:ALA:C	1:A:209:ALA:H	2.27	0.43
1:A:184:GLU:OE1	1:A:187:ARG:NH2	2.38	0.43
1:A:238:VAL:HG13	1:A:238:VAL:O	2.19	0.43
1:A:325:GLN:HG3	1:A:464:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH1	1:A:58:THR:O	2.53	0.41
1:A:391:ASP:OD1	1:A:396:ASN:ND2	2.52	0.41
1:A:403:GLU:HB3	1:A:435:ASP:CG	2.46	0.41
1:B:369:ILE:HD11	1:B:387:LEU:HD12	2.03	0.41
1:B:211:ARG:HA	1:B:224:THR:O	2.21	0.41
1:A:404:SER:N	1:A:435:ASP:OD2	2.54	0.41
1:A:510:ILE:HG13	1:A:511:GLU:N	2.36	0.41
1:A:495:LYS:HA	1:A:496:LYS:C	2.46	0.40
1:A:107:ALA:HB1	1:A:120:ARG:HB3	2.02	0.40
1:A:267:ARG:O	1:A:271:THR:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:OE2	1:B:227:ARG:NH2[2_556]	2.15	0.05

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	580/664 (87%)	542 (93%)	36 (6%)	2 (0%)	36	66
1	B	587/664 (88%)	550 (94%)	36 (6%)	1 (0%)	43	70
All	All	1167/1328 (88%)	1092 (94%)	72 (6%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	ASP
1	B	237	SER
1	A	208	SER

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	506/563 (90%)	496 (98%)	10 (2%)	48	66
1	B	509/563 (90%)	498 (98%)	11 (2%)	45	65
All	All	1015/1126 (90%)	994 (98%)	21 (2%)	47	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	272	MET
1	A	326	ASN
1	A	328	LYS
1	A	334	THR
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	129	GLU
1	B	214	GLU
1	B	222	SER
1	B	225	GLN
1	B	238	VAL
1	B	308	MET
1	B	435	ASP
1	B	485	LEU
1	B	506	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	160	ASN
1	A	181	ASN
1	A	235	ASN
1	A	249	GLN
1	A	299	ASN
1	A	333	ASN
1	A	566	GLN
1	A	567	GLN
1	B	2	ASN
1	B	181	ASN
1	B	293	GLN
1	B	333	ASN
1	B	394	GLN
1	B	512	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	1.38	5 (15%)	48,52,52	1.77	10 (20%)
2	ATP	A	701	3	32,33,33	1.42	5 (15%)	48,52,52	1.80	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	-	4/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ATP	C5-C4	4.58	1.47	1.39
2	A	701	ATP	C5-C4	4.57	1.47	1.39
2	B	701	ATP	C5-C6	2.64	1.48	1.41
2	A	701	ATP	C5-C6	2.55	1.48	1.41
2	A	701	ATP	PB-O3B	2.40	1.62	1.59
2	A	701	ATP	C8-N7	2.32	1.36	1.31
2	A	701	ATP	C5-N7	-2.31	1.34	1.39
2	B	701	ATP	C5-N7	-2.29	1.34	1.39
2	B	701	ATP	C8-N7	2.29	1.36	1.31
2	B	701	ATP	PB-O3B	2.15	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	-5.73	118.83	126.72
2	B	701	ATP	C5-C4-N3	-5.60	119.00	126.72
2	A	701	ATP	N3-C4-N9	4.72	135.20	127.17
2	B	701	ATP	N3-C4-N9	4.67	135.11	127.17
2	A	701	ATP	C2-N3-C4	3.84	121.21	111.83
2	A	701	ATP	N3-C2-N1	-3.78	122.86	128.58
2	B	701	ATP	C2-N3-C4	3.73	120.93	111.83
2	B	701	ATP	N3-C2-N1	-3.67	123.02	128.58
2	B	701	ATP	C4-C5-N7	-3.34	106.76	110.58
2	A	701	ATP	C4-C5-N7	-3.26	106.85	110.58
2	B	701	ATP	C4-N9-C8	3.19	109.09	105.74
2	A	701	ATP	C4-N9-C8	3.01	108.89	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ATP	C5-N7-C8	2.74	107.76	103.45
2	A	701	ATP	C5-N7-C8	2.65	107.61	103.45
2	B	701	ATP	N9-C8-N7	-2.42	110.51	113.94
2	A	701	ATP	N9-C8-N7	-2.30	110.67	113.94
2	B	701	ATP	C2-N1-C6	2.16	122.28	118.73
2	A	701	ATP	C2-N1-C6	2.10	122.18	118.73
2	A	701	ATP	C6-C5-N7	2.06	136.05	132.09
2	B	701	ATP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

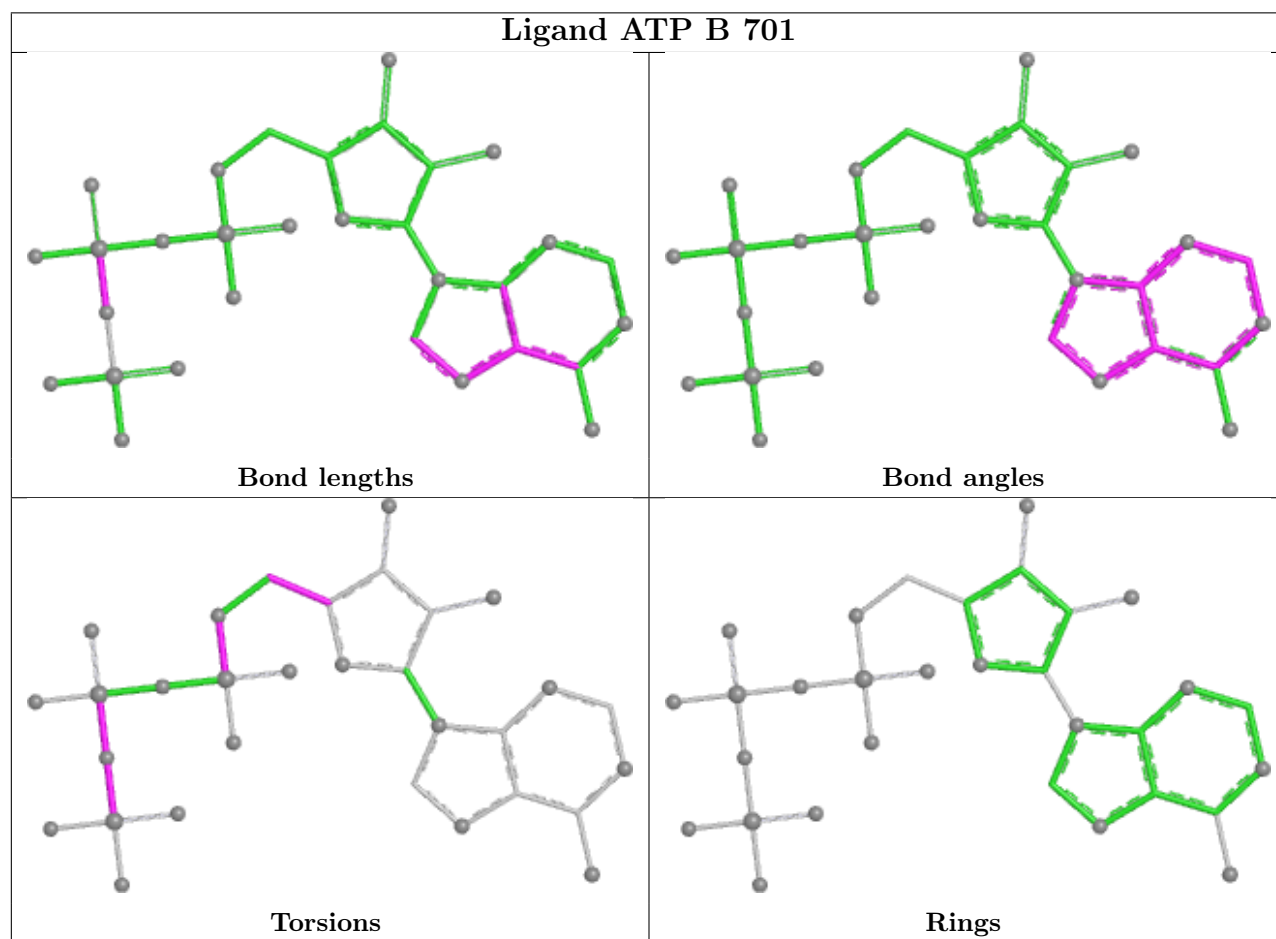
There are no ring outliers.

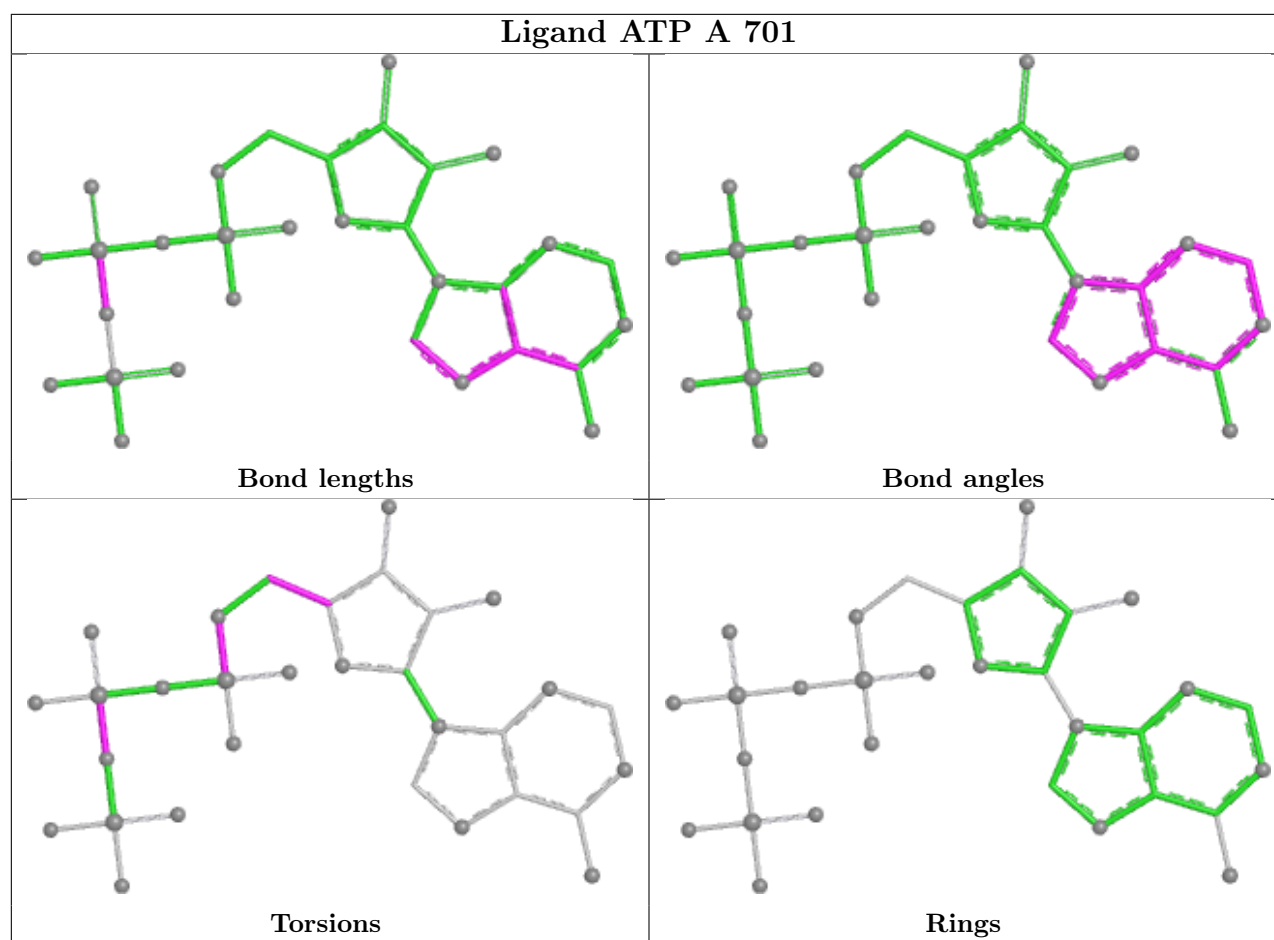
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	592/664 (89%)	1.51	159 (26%) 1 1	47, 93, 195, 217	0
1	B	599/664 (90%)	1.01	113 (18%) 3 3	44, 90, 151, 177	0
All	All	1191/1328 (89%)	1.26	272 (22%) 2 2	44, 92, 184, 217	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	643	GLN	17.6
1	A	639	THR	12.2
1	A	638	ILE	11.0
1	A	636	ASN	10.1
1	B	546	GLU	10.0
1	A	546	GLU	9.5
1	A	549	LYS	9.4
1	A	637	PRO	9.4
1	A	635	LEU	9.3
1	A	426	PRO	9.1
1	A	57	ASP	8.9
1	A	634	GLU	8.3
1	A	631	LYS	8.2
1	A	641	LEU	8.2
1	A	56	LEU	8.0
1	B	394	GLN	7.4
1	A	640	ALA	7.3
1	B	541	LEU	7.1
1	B	265	LYS	6.8
1	A	642	ALA	6.5
1	A	633	ALA	6.5
1	A	266	MET	6.3
1	A	327	LEU	6.2
1	A	265	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	409	ILE	6.1
1	A	387	LEU	6.1
1	A	530	ILE	6.0
1	B	534	ILE	5.9
1	A	334	THR	5.9
1	A	616	PHE	5.9
1	B	233	VAL	5.7
1	A	365	ASN	5.6
1	A	55	CYS	5.6
1	A	548	THR	5.6
1	A	599	THR	5.4
1	A	95	ASN	5.4
1	A	15	GLU	5.4
1	B	2	ASN	5.4
1	A	51	ASN	5.3
1	A	226	LYS	5.2
1	A	615	LEU	5.1
1	A	386	LEU	5.0
1	B	489	LEU	5.0
1	A	436	GLN	5.0
1	B	545	THR	5.0
1	A	399	VAL	5.0
1	A	632	ALA	4.9
1	A	494	GLY	4.9
1	B	466	GLY	4.7
1	B	537	MET	4.7
1	A	331	ASP	4.7
1	B	267	ARG	4.7
1	B	446	LEU	4.7
1	B	225	GLN	4.6
1	A	54	GLY	4.6
1	A	449	TYR	4.6
1	A	627	MET	4.6
1	A	529	LEU	4.5
1	B	241	GLY	4.5
1	B	266	MET	4.5
1	B	351	SER	4.4
1	B	357	GLY	4.4
1	A	465	ILE	4.4
1	A	421	ILE	4.4
1	A	348	THR	4.3
1	A	534	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	543	SER	4.2
1	A	262	VAL	4.2
1	B	34	ASP	4.2
1	B	549	LYS	4.2
1	B	631	LYS	4.2
1	B	309	THR	4.2
1	A	492	LEU	4.1
1	A	545	THR	4.1
1	A	485	LEU	4.1
1	A	620	ILE	4.1
1	A	364	ALA	4.1
1	A	448	LEU	4.0
1	B	31	GLU	4.0
1	A	429	VAL	4.0
1	B	37	ALA	3.9
1	A	446	LEU	3.9
1	A	452	TYR	3.8
1	B	465	ILE	3.8
1	A	58	THR	3.8
1	A	420	VAL	3.8
1	B	35	PHE	3.8
1	A	424	LYS	3.7
1	B	36	VAL	3.7
1	B	224	THR	3.7
1	B	464	ARG	3.7
1	B	409	ILE	3.7
1	A	310	ILE	3.7
1	A	210	ASN	3.7
1	A	227	ARG	3.7
1	A	225	GLN	3.6
1	B	643	GLN	3.6
1	A	488	LEU	3.6
1	B	109	PRO	3.6
1	A	270	LEU	3.6
1	A	378	GLY	3.5
1	B	627	MET	3.5
1	B	538	ASN	3.5
1	A	346	PRO	3.5
1	A	52	ILE	3.5
1	A	267	ARG	3.5
1	A	340	TYR	3.5
1	B	262	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	619	LEU	3.4
1	A	526	PHE	3.4
1	B	22	VAL	3.4
1	B	436	GLN	3.4
1	B	310	ILE	3.4
1	B	624	PHE	3.4
1	A	83	ARG	3.3
1	B	463	SER	3.3
1	B	485	LEU	3.3
1	A	76	ASN	3.3
1	A	91	PHE	3.3
1	A	116	PRO	3.3
1	A	410	PHE	3.3
1	B	300	ILE	3.3
1	A	614	VAL	3.3
1	A	374	PHE	3.3
1	A	623	LEU	3.3
1	B	623	LEU	3.3
1	A	209	ALA	3.2
1	A	629	ALA	3.2
1	B	112	TYR	3.2
1	A	535	GLY	3.2
1	A	208	SER	3.2
1	A	463	SER	3.2
1	B	153	SER	3.2
1	A	533	GLY	3.1
1	B	226	LYS	3.1
1	B	278	GLY	3.1
1	A	205	ILE	3.1
1	B	210	ASN	3.0
1	A	434	SER	3.0
1	B	390	ASP	3.0
1	A	433	VAL	3.0
1	A	329	ILE	3.0
1	B	212	ILE	3.0
1	A	311	PHE	3.0
1	B	353	ILE	3.0
1	A	468	ILE	3.0
1	A	472	ILE	2.9
1	A	273	LEU	2.9
1	B	207	ALA	2.9
1	B	370	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	211	ARG	2.9
1	A	617	SER	2.8
1	A	556	ALA	2.8
1	A	624	PHE	2.8
1	A	42	SER	2.8
1	B	349	SER	2.8
1	A	207	ALA	2.8
1	B	269	LEU	2.8
1	A	541	LEU	2.8
1	B	598	ILE	2.8
1	B	633	ALA	2.8
1	A	484	SER	2.8
1	A	630	LYS	2.8
1	B	506	ILE	2.8
1	A	173	ALA	2.7
1	A	467	SER	2.7
1	B	231	SER	2.7
1	B	356	VAL	2.7
1	B	548	THR	2.7
1	B	142	ASN	2.7
1	B	264	HIS	2.7
1	B	632	ALA	2.7
1	B	327	LEU	2.7
1	B	302	GLY	2.7
1	A	328	LYS	2.7
1	A	224	THR	2.7
1	B	607	THR	2.7
1	A	427	PHE	2.6
1	B	12	TYR	2.6
1	B	626	TYR	2.6
1	B	247	LYS	2.6
1	A	422	PHE	2.6
1	A	544	VAL	2.6
1	A	578	ILE	2.6
1	B	467	SER	2.6
1	B	501	MET	2.6
1	A	531	VAL	2.6
1	B	426	PRO	2.6
1	A	379	LEU	2.6
1	A	367	TYR	2.5
1	A	553	VAL	2.5
1	B	223	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	468	ILE	2.5
1	A	532	GLY	2.5
1	A	98	SER	2.5
1	B	482	GLU	2.5
1	A	50	MET	2.5
1	B	634	GLU	2.4
1	B	108	LEU	2.4
1	A	343	SER	2.4
1	B	586	LEU	2.4
1	A	370	GLY	2.4
1	A	392	VAL	2.4
1	A	555	MET	2.4
1	B	98	SER	2.4
1	A	499	PHE	2.4
1	B	372	GLN	2.4
1	B	350	SER	2.4
1	B	479	THR	2.3
1	B	110	ALA	2.3
1	B	229	VAL	2.3
1	B	558	GLY	2.3
1	A	405	ALA	2.3
1	A	93	ARG	2.3
1	A	431	GLY	2.3
1	A	308	MET	2.3
1	B	303	ILE	2.3
1	B	557	ILE	2.3
1	B	416	LEU	2.3
1	B	405	ALA	2.3
1	B	481	ALA	2.2
1	B	228	GLN	2.2
1	B	238	VAL	2.2
1	A	430	ILE	2.2
1	A	263	ALA	2.2
1	A	381	LEU	2.2
1	B	13	PHE	2.2
1	A	326	ASN	2.2
1	A	371	GLU	2.2
1	B	329	ILE	2.2
1	A	537	MET	2.2
1	A	400	VAL	2.2
1	A	453	SER	2.2
1	A	17	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	2.2
1	B	277	ILE	2.2
1	B	61	GLY	2.2
1	B	458	LYS	2.2
1	B	410	PHE	2.2
1	A	344	VAL	2.1
1	B	261	ILE	2.1
1	A	445	SER	2.1
1	B	326	ASN	2.1
1	A	388	THR	2.1
1	B	449	TYR	2.1
1	A	339	SER	2.1
1	B	371	GLU	2.1
1	A	333	ASN	2.1
1	A	277	ILE	2.1
1	A	228	GLN	2.1
1	A	552	GLY	2.1
1	B	44	SER	2.1
1	A	230	LYS	2.1
1	B	490	LYS	2.1
1	A	79	LEU	2.1
1	B	408	ALA	2.1
1	B	298	GLU	2.1
1	A	596	SER	2.1
1	B	425	ARG	2.1
1	A	217	ASP	2.1
1	B	171	THR	2.1
1	A	395	SER	2.0
1	A	500	ILE	2.0
1	B	559	ALA	2.0
1	A	166	LEU	2.0
1	A	385	ARG	2.0
1	A	547	ARG	2.0
1	B	543	SER	2.0
1	A	621	GLY	2.0
1	A	380	LYS	2.0
1	A	233	VAL	2.0
1	A	403	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

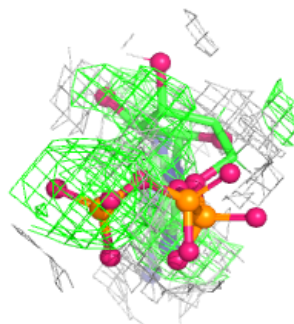
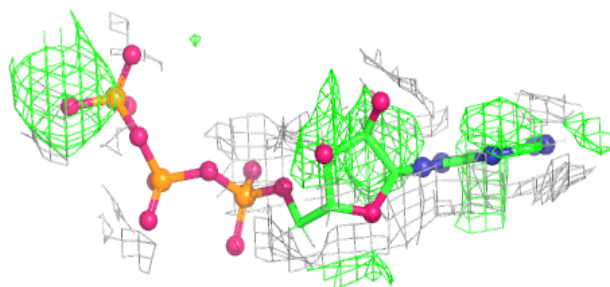
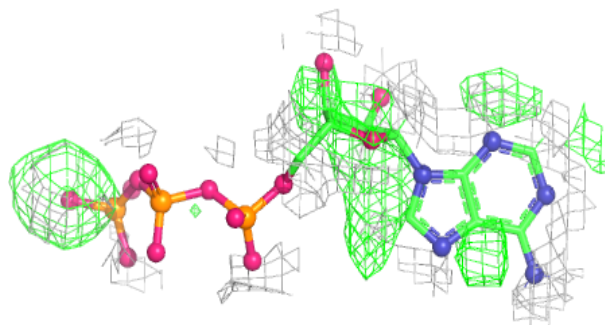
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

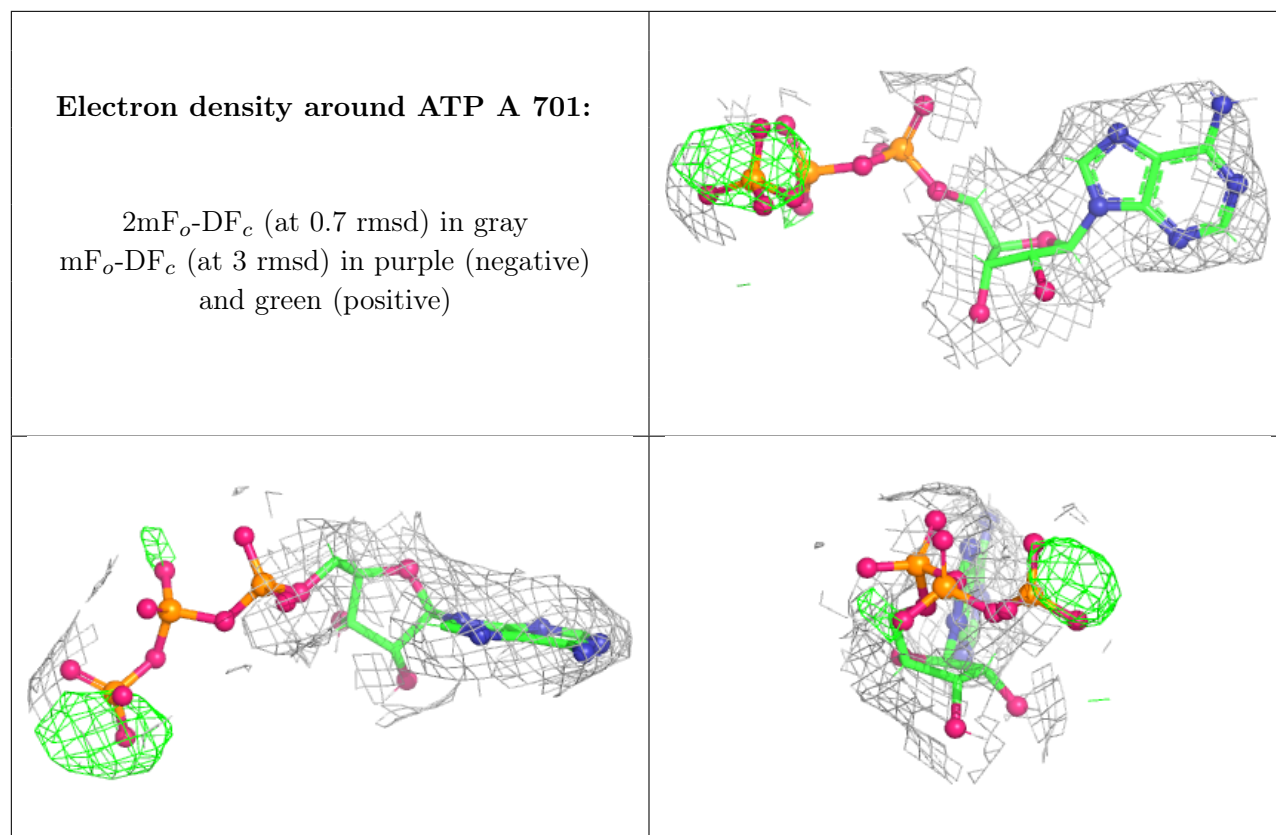
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	B	701	31/31	0.94	0.10	39,68,91,109	0
2	ATP	A	701	31/31	0.95	0.10	38,81,102,106	0
3	MG	A	702	1/1	0.99	0.07	51,51,51,51	0
3	MG	B	702	1/1	0.99	0.13	59,59,59,59	0

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 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.