



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 04:46 pm GMT

PDB ID : 5LJ7
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 : 4.02b-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

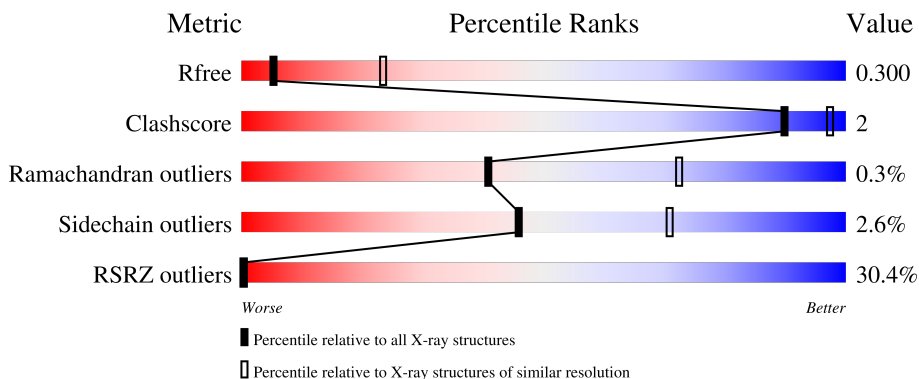
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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	
1	B	664	

2 Entry composition [i](#)

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	
			Total	C	H	N	O				S
1	A	592	9207	2856	4690	775	865	21	0	0	0
1	B	599	9265	2864	4724	781	875	21	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

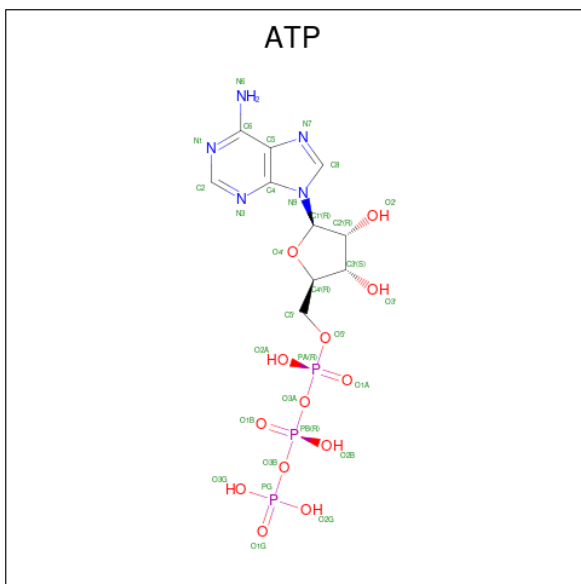
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2EHL8
A	-18	GLY	-	expression tag	UNP Q2EHL8
A	-17	SER	-	expression tag	UNP Q2EHL8
A	-16	SER	-	expression tag	UNP Q2EHL8
A	-15	HIS	-	expression tag	UNP Q2EHL8
A	-14	HIS	-	expression tag	UNP Q2EHL8
A	-13	HIS	-	expression 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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
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 (three-letter code: 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

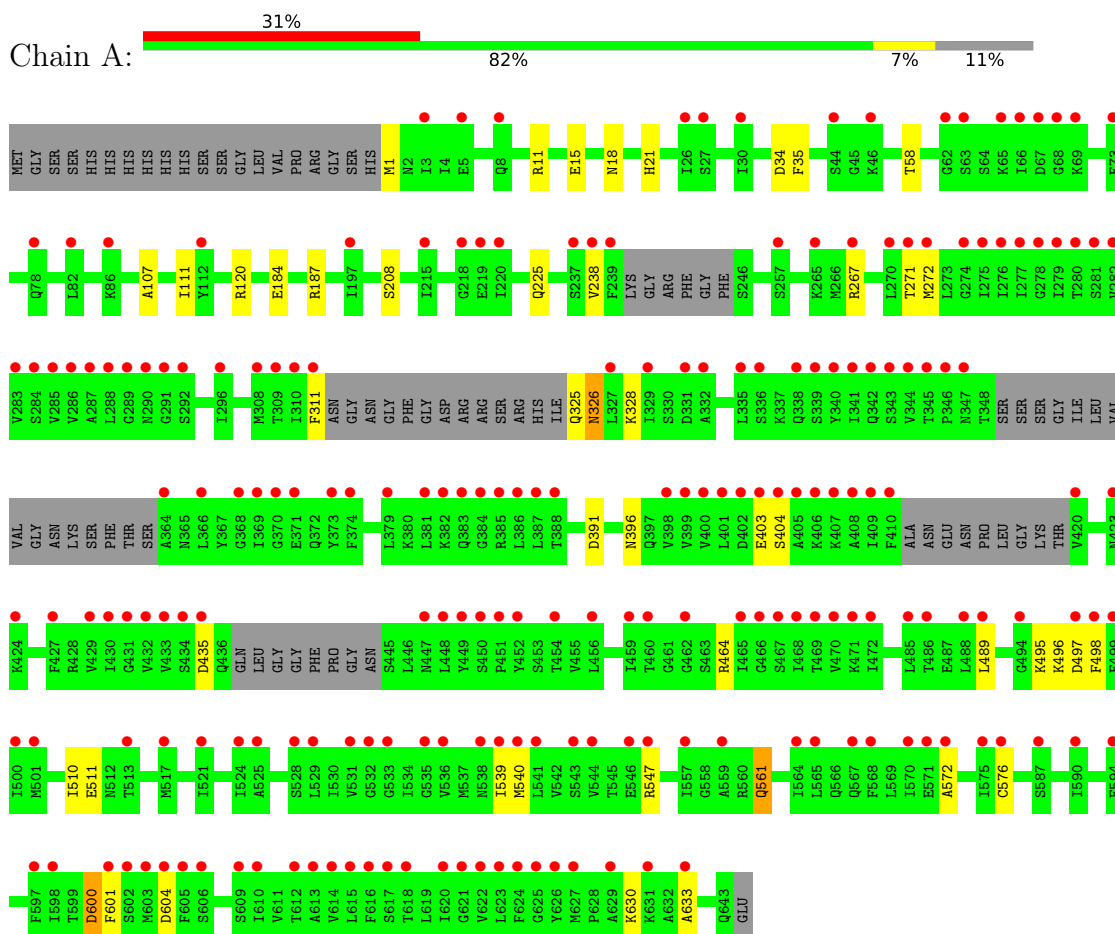
- Molecule 4 is water.

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

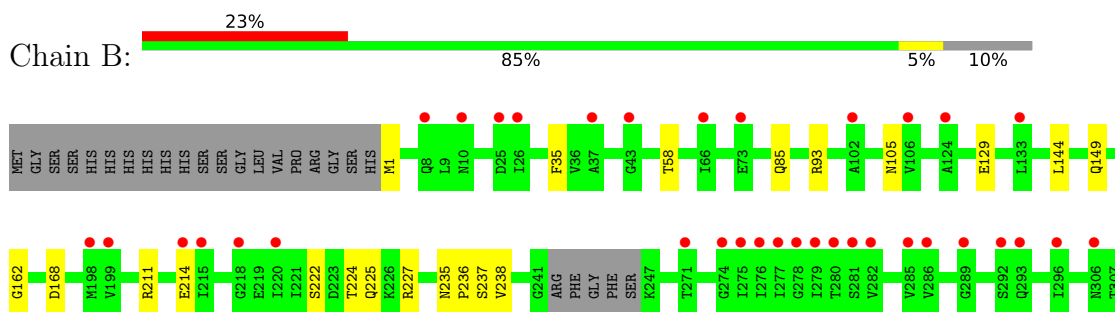
3 Residue-property plots i

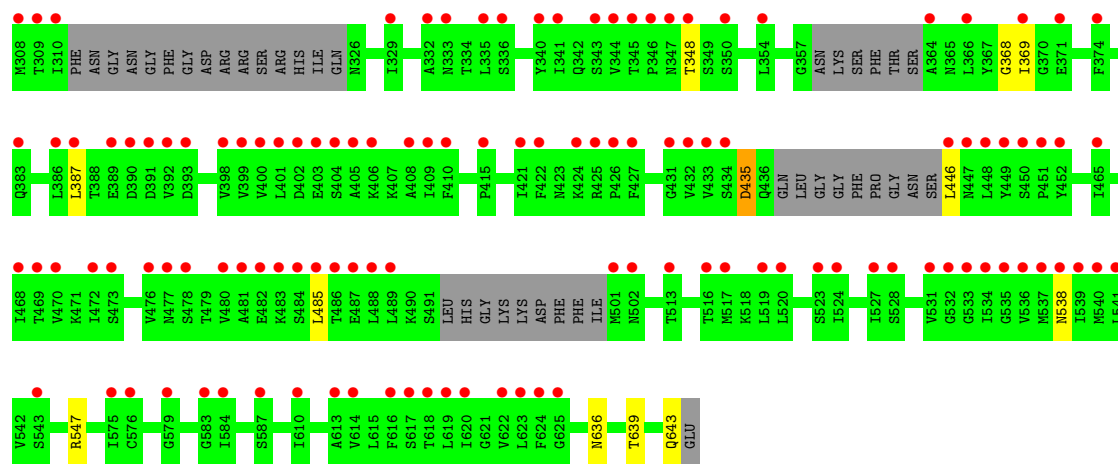
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	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)	Xtrriage
Refinement program	PHENIX (dev_2196: ???)	Depositor
R, R_{free}	0.246 , 0.299 0.246 , 0.300	Depositor DCC
R_{free} test set	1758 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18564	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage'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: MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/4562	0.42	0/6142
1	B	0.25	0/4583	0.43	0/6173
All	All	0.24	0/9145	0.43	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	21	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	33	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 (33) 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: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
1:A:11:ARG:NH1	1:A:58:THR:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASP:OD1	1:A:396:ASN:ND2	2.52	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: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 [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	580/664 (87%)	542 (93%)	36 (6%)	2 (0%)	41	72
1	B	587/664 (88%)	550 (94%)	36 (6%)	1 (0%)	47	77
All	All	1167/1328 (88%)	1092 (94%)	72 (6%)	3 (0%)	41	72

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 [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	506/563 (90%)	493 (97%)	13 (3%)	46	71
1	B	509/563 (90%)	496 (97%)	13 (3%)	46	71
All	All	1015/1126 (90%)	989 (97%)	26 (3%)	46	71

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	HIS
1	A	225	GLN
1	A	272	MET
1	A	311	PHE
1	A	326	ASN
1	A	328	LYS
1	A	495	LYS
1	A	540	MET
1	A	547	ARG
1	A	561	GLN
1	A	604	ASP
1	A	630	LYS
1	B	1	MET
1	B	35	PHE
1	B	58	THR
1	B	105	ASN
1	B	129	GLU
1	B	214	GLU
1	B	222	SER
1	B	225	GLN
1	B	435	ASP
1	B	446	LEU
1	B	485	LEU
1	B	547	ARG
1	B	643	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	A	701	3	26,33,33	0.93	1 (3%)	31,52,52	1.41	5 (16%)
2	ATP	B	701	3	26,33,33	0.93	1 (3%)	31,52,52	1.48	6 (19%)

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	A	701	3	-	5/18/38/38	0/3/3/3
2	ATP	B	701	3	-	8/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ATP	C5-C4	2.39	1.47	1.40
2	A	701	ATP	C5-C4	2.38	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	N3-C2-N1	-3.72	122.86	128.68
2	B	701	ATP	N3-C2-N1	-3.62	123.02	128.68
2	B	701	ATP	PA-O3A-PB	-3.43	121.04	132.83
2	B	701	ATP	C4-C5-N7	-2.53	106.76	109.40
2	A	701	ATP	PB-O3B-PG	-2.45	124.40	132.83
2	A	701	ATP	C4-C5-N7	-2.45	106.85	109.40
2	A	701	ATP	C3'-C2'-C1'	2.44	104.65	100.98
2	B	701	ATP	PB-O3B-PG	-2.40	124.59	132.83
2	B	701	ATP	C3'-C2'-C1'	2.34	104.50	100.98
2	B	701	ATP	C2-N1-C6	2.06	122.28	118.75
2	A	701	ATP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

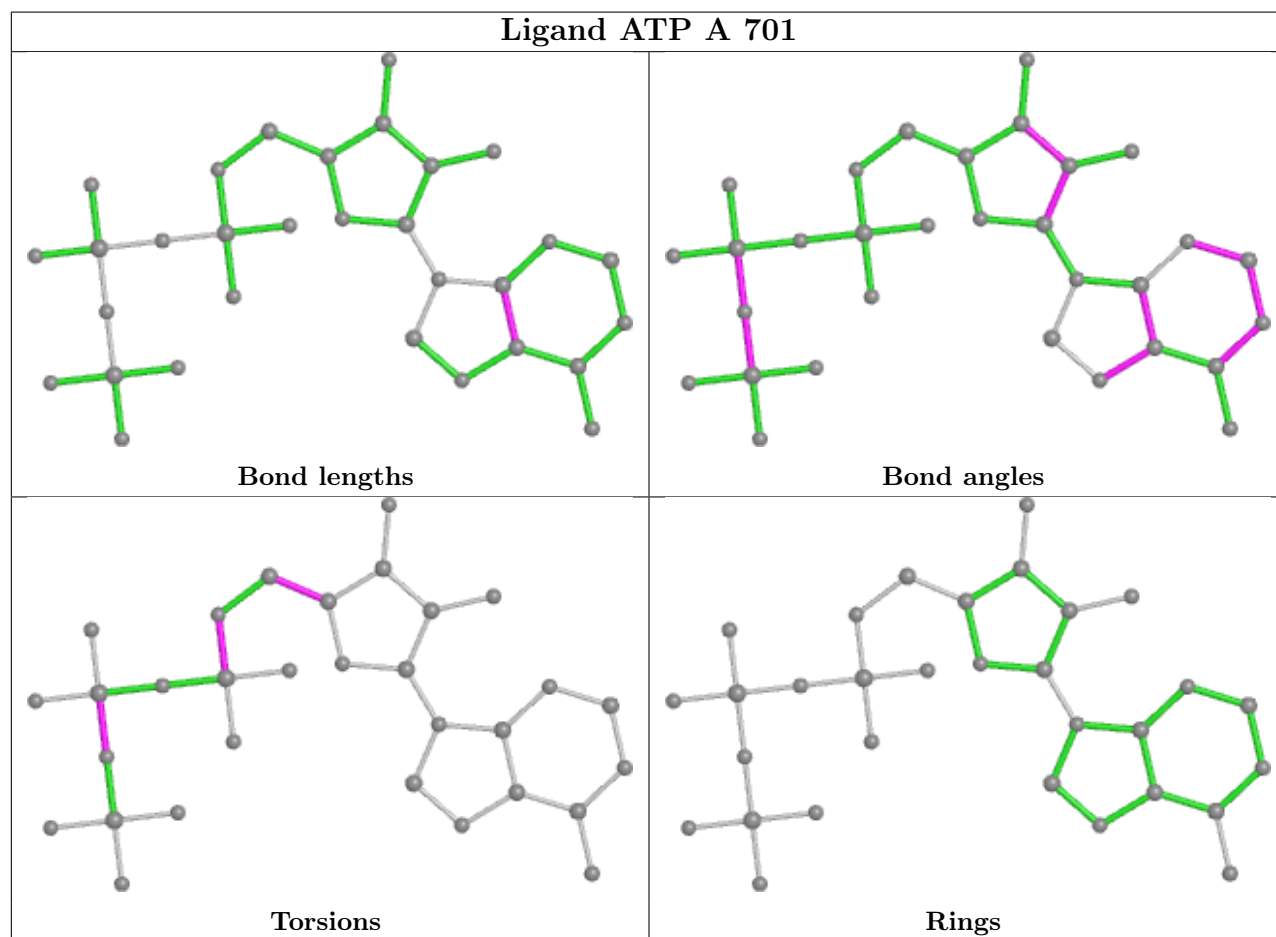
Mol	Chain	Res	Type	Atoms
2	B	701	ATP	PB-O3B-PG-O3G
2	B	701	ATP	C5'-O5'-PA-O2A
2	A	701	ATP	O4'-C4'-C5'-O5'
2	A	701	ATP	C3'-C4'-C5'-O5'
2	B	701	ATP	O4'-C4'-C5'-O5'
2	B	701	ATP	C3'-C4'-C5'-O5'
2	B	701	ATP	C5'-O5'-PA-O3A
2	B	701	ATP	PG-O3B-PB-O1B
2	A	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O1A
2	A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

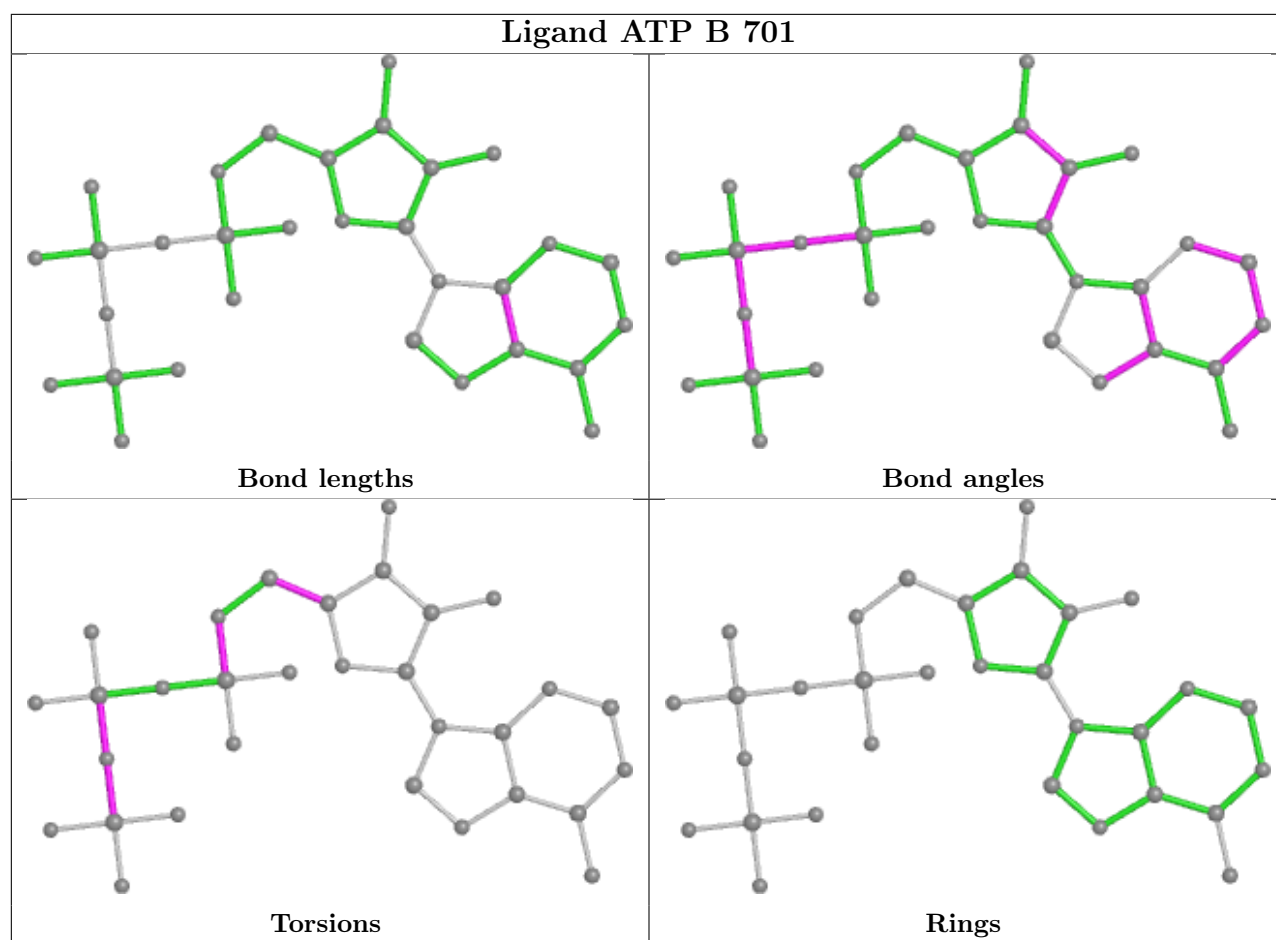
There are no ring outliers.

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%)	1.99	206 (34%) 0 0	43, 85, 176, 197	0
1	B	599/664 (90%)	1.47	156 (26%) 0 0	40, 82, 137, 164	0
All	All	1191/1328 (89%)	1.73	362 (30%) 0 0	40, 83, 167, 197	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	GLN	15.4
1	A	431	GLY	14.6
1	A	399	VAL	13.3
1	A	387	LEU	13.3
1	A	401	LEU	13.0
1	A	432	VAL	12.0
1	A	410	PHE	11.9
1	A	386	LEU	11.8
1	A	400	VAL	10.8
1	A	409	ILE	9.7
1	A	284	SER	9.5
1	A	278	GLY	8.7
1	A	617	SER	8.7
1	B	405	ALA	8.5
1	A	433	VAL	8.4
1	A	288	LEU	8.3
1	B	489	LEU	8.3
1	B	481	ALA	8.3
1	B	432	VAL	8.2
1	A	343	SER	8.1
1	A	279	ILE	8.0
1	A	341	ILE	8.0
1	B	485	LEU	7.8
1	B	424	LYS	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	483	LYS	7.8
1	A	402	ASP	7.6
1	A	332	ALA	7.6
1	B	401	LEU	7.4
1	A	405	ALA	7.4
1	B	617	SER	7.4
1	A	471	LYS	7.4
1	A	625	GLY	7.3
1	A	335	LEU	7.2
1	A	470	VAL	6.9
1	A	371	GLU	6.6
1	A	280	THR	6.4
1	A	450	SER	6.4
1	B	523	SER	6.2
1	A	282	VAL	6.2
1	B	433	VAL	6.2
1	A	281	SER	6.1
1	A	285	VAL	6.1
1	A	403	GLU	6.1
1	B	278	GLY	6.1
1	A	603	MET	6.1
1	B	488	LEU	6.1
1	A	309	THR	6.0
1	A	374	PHE	6.0
1	B	472	ILE	6.0
1	B	448	LEU	6.0
1	B	482	GLU	6.0
1	A	605	PHE	6.0
1	B	409	ILE	5.9
1	A	621	GLY	5.9
1	A	536	VAL	5.9
1	B	383	GLN	5.8
1	A	489	LEU	5.8
1	A	594	PHE	5.7
1	A	468	ILE	5.7
1	A	275	ILE	5.7
1	A	382	LYS	5.6
1	B	308	MET	5.6
1	B	310	ILE	5.5
1	A	336	SER	5.5
1	A	373	TYR	5.5
1	A	613	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	485	LEU	5.4
1	A	597	PHE	5.4
1	A	406	LYS	5.4
1	A	366	LEU	5.3
1	A	331	ASP	5.3
1	A	404	SER	5.2
1	A	283	VAL	5.2
1	A	344	VAL	5.2
1	B	426	PRO	5.2
1	A	338	GLN	5.2
1	B	402	ASP	5.1
1	A	498	PHE	5.1
1	B	275	ILE	5.1
1	A	287	ALA	5.1
1	A	429	VAL	5.1
1	B	480	VAL	5.0
1	A	292	SER	5.0
1	B	387	LEU	5.0
1	A	342	GLN	5.0
1	A	448	LEU	5.0
1	A	517	MET	5.0
1	B	279	ILE	5.0
1	B	579	GLY	4.9
1	A	620	ILE	4.9
1	B	613	ALA	4.9
1	B	390	ASP	4.9
1	A	452	TYR	4.8
1	A	238	VAL	4.8
1	B	366	LEU	4.8
1	B	449	TYR	4.8
1	A	601	PHE	4.7
1	A	277	ILE	4.7
1	A	626	TYR	4.7
1	B	584	ILE	4.7
1	A	466	GLY	4.7
1	B	468	ILE	4.6
1	A	451	PRO	4.6
1	B	341	ILE	4.6
1	A	345	THR	4.6
1	B	422	PHE	4.6
1	A	590	ILE	4.5
1	B	534	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	4.5
1	A	276	ILE	4.5
1	B	392	VAL	4.5
1	A	27	SER	4.4
1	B	369	ILE	4.4
1	A	571	GLU	4.4
1	A	290	ASN	4.4
1	A	598	ILE	4.4
1	A	616	PHE	4.3
1	B	470	VAL	4.3
1	B	469	THR	4.3
1	B	576	CYS	4.3
1	B	406	LYS	4.2
1	B	487	GLU	4.2
1	A	469	THR	4.2
1	B	532	GLY	4.2
1	B	427	PHE	4.2
1	A	388	THR	4.2
1	B	540	MET	4.2
1	A	624	PHE	4.2
1	A	499	PHE	4.2
1	A	533	GLY	4.2
1	B	336	SER	4.2
1	A	614	VAL	4.2
1	B	450	SER	4.2
1	A	486	THR	4.2
1	B	274	GLY	4.1
1	A	627	MET	4.1
1	B	399	VAL	4.1
1	A	543	SER	4.1
1	A	568	PHE	4.1
1	A	239	PHE	4.1
1	B	536	VAL	4.0
1	B	620	ILE	4.0
1	A	532	GLY	4.0
1	A	602	SER	4.0
1	B	476	VAL	4.0
1	B	477	ASN	4.0
1	A	587	SER	4.0
1	B	484	SER	4.0
1	A	622	VAL	3.9
1	A	459	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	575	ILE	3.9
1	A	329	ILE	3.9
1	B	616	PHE	3.9
1	A	528	SER	3.9
1	A	629	ALA	3.9
1	B	289	GLY	3.8
1	B	408	ALA	3.8
1	A	424	LYS	3.8
1	A	310	ILE	3.8
1	B	486	THR	3.8
1	B	452	TYR	3.8
1	A	384	GLY	3.8
1	B	451	PRO	3.8
1	A	267	ARG	3.8
1	A	567	GLN	3.7
1	B	371	GLU	3.7
1	A	5	GLU	3.7
1	B	296	ILE	3.7
1	B	277	ILE	3.7
1	B	446	LEU	3.7
1	A	220	ILE	3.6
1	B	400	VAL	3.6
1	B	410	PHE	3.6
1	B	614	VAL	3.6
1	A	8	GLN	3.6
1	B	386	LEU	3.6
1	A	488	LEU	3.6
1	A	529	LEU	3.6
1	B	527	ILE	3.6
1	B	618	THR	3.6
1	A	218	GLY	3.6
1	A	610	ILE	3.6
1	A	68	GLY	3.6
1	B	276	ILE	3.5
1	B	329	ILE	3.5
1	A	340	TYR	3.5
1	B	431	GLY	3.5
1	B	346	PRO	3.5
1	A	430	ILE	3.5
1	A	65	LYS	3.5
1	B	403	GLU	3.5
1	A	289	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	564	ILE	3.4
1	A	576	CYS	3.4
1	B	340	TYR	3.4
1	B	531	VAL	3.4
1	B	541	LEU	3.4
1	B	292	SER	3.3
1	A	544	VAL	3.3
1	A	521	ILE	3.3
1	A	497	ASP	3.3
1	B	501	MET	3.3
1	A	311	PHE	3.3
1	A	296	ILE	3.3
1	B	502	ASN	3.3
1	B	332	ALA	3.3
1	B	374	PHE	3.3
1	A	286	VAL	3.3
1	B	106	VAL	3.3
1	A	435	ASP	3.3
1	A	237	SER	3.2
1	B	524	ILE	3.2
1	A	513	THR	3.2
1	B	133	LEU	3.2
1	B	309	THR	3.2
1	A	540	MET	3.2
1	A	369	ILE	3.2
1	A	467	SER	3.2
1	B	389	GLU	3.2
1	B	354	LEU	3.2
1	B	391	ASP	3.1
1	A	500	ILE	3.1
1	A	69	LYS	3.1
1	A	449	TYR	3.1
1	A	215	ILE	3.1
1	A	420	VAL	3.1
1	A	408	ALA	3.1
1	A	618	THR	3.1
1	B	624	PHE	3.1
1	B	425	ARG	3.1
1	A	370	GLY	3.1
1	B	583	GLY	3.1
1	A	531	VAL	3.1
1	A	472	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	407	LYS	3.1
1	A	327	LEU	3.1
1	B	214	GLU	3.0
1	B	215	ILE	3.0
1	B	404	SER	3.0
1	B	528	SER	3.0
1	B	344	VAL	3.0
1	B	73	GLU	3.0
1	A	434	SER	3.0
1	A	501	MET	3.0
1	A	63	SER	2.9
1	B	293	GLN	2.9
1	A	219	GLU	2.9
1	B	513	THR	2.9
1	B	533	GLY	2.9
1	A	385	ARG	2.9
1	B	271	THR	2.9
1	B	625	GLY	2.9
1	B	282	VAL	2.9
1	B	285	VAL	2.9
1	A	347	ASN	2.9
1	B	478	SER	2.9
1	A	381	LEU	2.9
1	A	535	GLY	2.9
1	B	286	VAL	2.8
1	A	82	LEU	2.8
1	A	570	ILE	2.8
1	A	274	GLY	2.8
1	B	26	ILE	2.8
1	B	415	PRO	2.8
1	A	112	TYR	2.8
1	B	348	THR	2.8
1	A	44	SER	2.8
1	B	281	SER	2.8
1	B	343	SER	2.8
1	A	3	ILE	2.8
1	A	539	ILE	2.8
1	A	66	ILE	2.7
1	A	575	ILE	2.7
1	A	623	LEU	2.7
1	B	25	ASP	2.7
1	B	218	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	2.7
1	A	197	ILE	2.6
1	B	537	MET	2.6
1	B	517	MET	2.6
1	A	423	ASN	2.6
1	A	86	LYS	2.6
1	B	434	SER	2.6
1	A	604	ASP	2.6
1	A	612	THR	2.6
1	A	565	LEU	2.6
1	A	265	LYS	2.6
1	B	350	SER	2.6
1	B	623	LEU	2.5
1	B	465	ILE	2.5
1	A	633	ALA	2.5
1	B	124	ALA	2.5
1	A	398	VAL	2.5
1	B	333	ASN	2.5
1	B	538	ASN	2.5
1	A	30	ILE	2.5
1	A	572	ALA	2.5
1	A	62	GLY	2.5
1	B	421	ILE	2.5
1	B	619	LEU	2.4
1	A	257	SER	2.4
1	A	456	LEU	2.4
1	B	539	ILE	2.4
1	A	615	LEU	2.4
1	B	398	VAL	2.4
1	A	559	ALA	2.4
1	B	364	ALA	2.4
1	A	427	PHE	2.4
1	A	339	SER	2.4
1	B	199	VAL	2.4
1	B	10	ASN	2.4
1	A	465	ILE	2.3
1	A	73	GLU	2.3
1	A	308	MET	2.3
1	B	37	ALA	2.3
1	A	271	THR	2.3
1	A	272	MET	2.3
1	A	379	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	519	LEU	2.3
1	A	546	GLU	2.3
1	A	460	THR	2.3
1	B	345	THR	2.3
1	B	198	MET	2.3
1	B	587	SER	2.3
1	A	454	THR	2.2
1	A	631	LYS	2.2
1	A	538	ASN	2.2
1	A	346	PRO	2.2
1	B	8	GLN	2.2
1	A	462	GLY	2.2
1	A	606	SER	2.2
1	A	291	GLY	2.2
1	A	494	GLY	2.2
1	B	473	SER	2.2
1	B	520	LEU	2.2
1	B	66	ILE	2.2
1	B	280	THR	2.2
1	A	541	LEU	2.2
1	B	393	ASP	2.2
1	B	535	GLY	2.2
1	B	335	LEU	2.1
1	A	525	ALA	2.1
1	B	43	GLY	2.1
1	A	46	LYS	2.1
1	B	610	ILE	2.1
1	A	547	ARG	2.1
1	A	447	ASN	2.1
1	B	516	THR	2.1
1	A	524	ILE	2.1
1	A	78	GLN	2.1
1	A	270	LEU	2.1
1	B	220	ILE	2.1
1	B	306	ASN	2.1
1	A	364	ALA	2.1
1	A	609	SER	2.1
1	A	368	GLY	2.1
1	B	447	ASN	2.0
1	B	622	VAL	2.0
1	A	557	ILE	2.0
1	B	543	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	102	ALA	2.0
1	B	347	ASN	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](#)

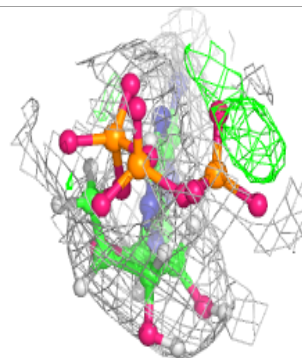
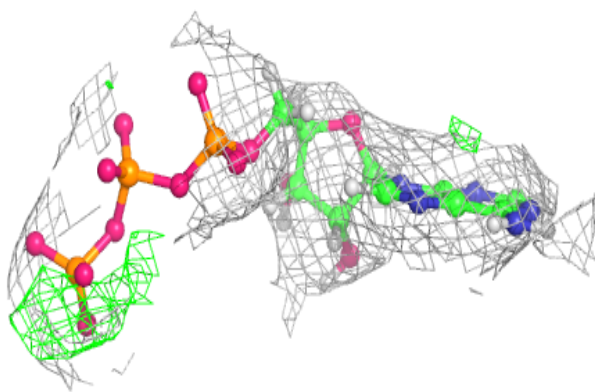
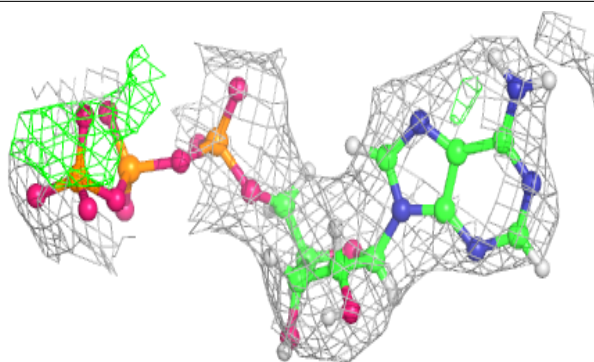
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.28	38,81,102,106	0
2	ATP	B	701	31/31	0.95	0.24	39,68,91,109	0
3	MG	A	702	1/1	0.95	0.27	51,51,51,51	0
3	MG	B	702	1/1	0.98	0.27	59,59,59,59	0

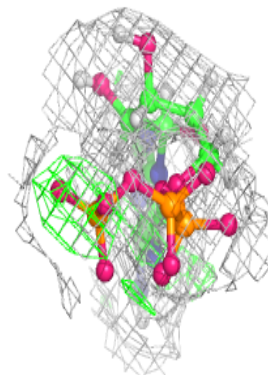
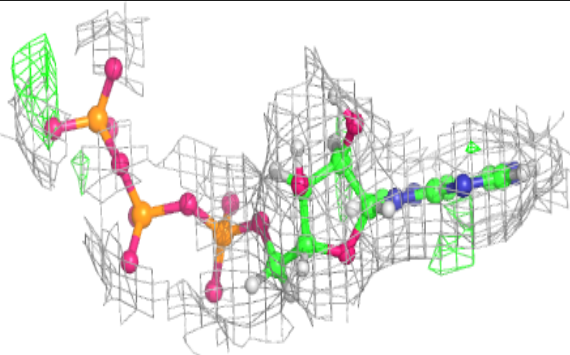
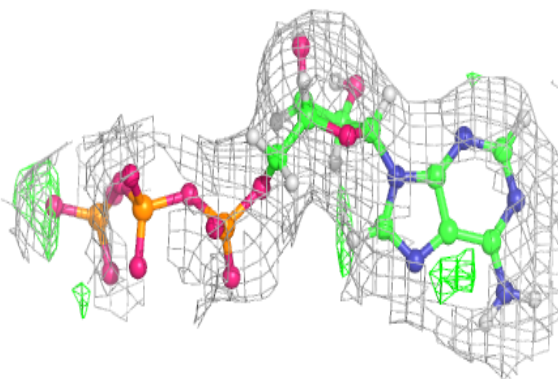
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP 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.