



# wwPDB X-ray Structure Validation Summary Report

Mar 6, 2026 – 07:10 PM UTC

PDB ID : 4XTR / pdb\_00004xtr  
Title : Structure of Get3 bound to the transmembrane domain of Pep12  
Authors : Mateja, A.; Paduch, M.; Chang, H.-Y.; Szydłowska, A.; Kossiakoff, A.A.;  
Hegde, R.S.; Keenan, R.J.  
Deposited on : 2015-01-23  
Resolution : 2.05 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

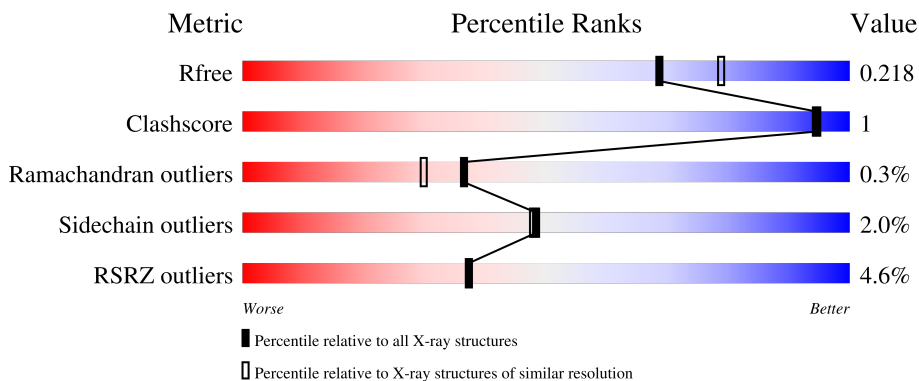
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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.



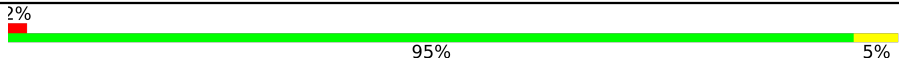
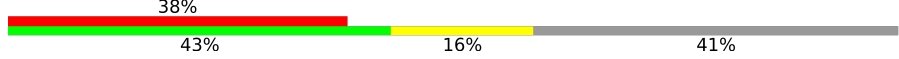
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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  $\geq 3$ , 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	354	 6% 81% 5% 14%
1	B	354	 4% 81% 6% 12%
2	C	230	 2% 91% 6% . 6%
2	E	230	 96% . .
3	D	217	 3% 94% 5%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	217	 <p>2% 95% 5%</p>
4	G	37	 <p>38% 43% 16% 41%</p>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 24293 atoms, of which 11564 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 ATPase GET3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	305	Total	C	H	N	O	S	0	2	0
			4815	1530	2400	401	466	18			
1	B	311	Total	C	H	N	O	S	0	1	0
			4873	1543	2432	404	476	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ASN	ASP	engineered mutation	UNP Q12154
B	57	ASN	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	217	Total	C	H	N	O	S	0	1	0
			3241	1037	1600	278	320	6			
2	E	222	Total	C	H	N	O	S	0	1	0
			3306	1055	1633	284	328	6			

- Molecule 3 is a protein called Antibody Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	D	216	Total	C	H	N	O	S	0	0	0
			3269	1038	1611	276	338	6			
3	F	216	Total	C	H	N	O	S	0	0	0
			3269	1038	1611	276	338	6			

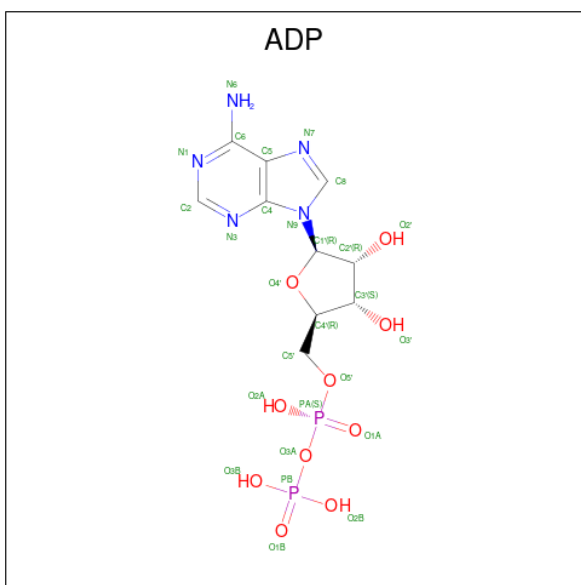
- Molecule 4 is a protein called Pep12p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	G	22	Total	C	H	N	O	S	0	0	0
			427	141	231	30	23	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	252	MET	-	initiating methionine	UNP E7M086
G	253	GLY	-	expression tag	UNP E7M086
G	254	SER	-	expression tag	UNP E7M086
G	255	HIS	-	expression tag	UNP E7M086
G	256	HIS	-	expression tag	UNP E7M086
G	257	HIS	-	expression tag	UNP E7M086
G	258	HIS	-	expression tag	UNP E7M086
G	259	HIS	-	expression tag	UNP E7M086
G	260	HIS	-	expression tag	UNP E7M086
G	261	SER	-	expression tag	UNP E7M086

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
5	A	1	Total	C	H	N	O	P	0	1
			38	10	11	5	10	2		
5	B	1	Total	C	H	N	O	P	0	1
			39	10	12	5	10	2		

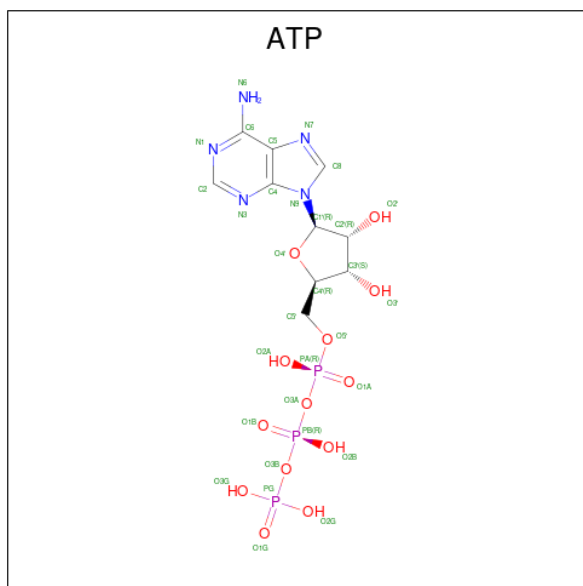
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	A	1	1	1	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
8	A	1	42	10	11	5	13	3	0	1
8	B	1	43	10	12	5	13	3	0	1

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	104	104	104	0	0
9	B	149	149	149	0	0
9	C	162	162	162	0	0
9	D	164	164	164	0	0
9	E	211	211	211	0	0
9	F	137	137	137	0	0

*Continued on next page...*

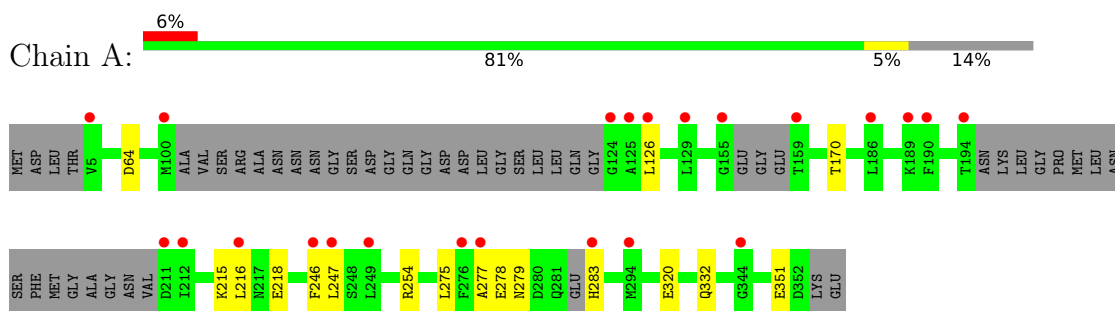
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
9	G	1	Total	O	0	0
			1	1		

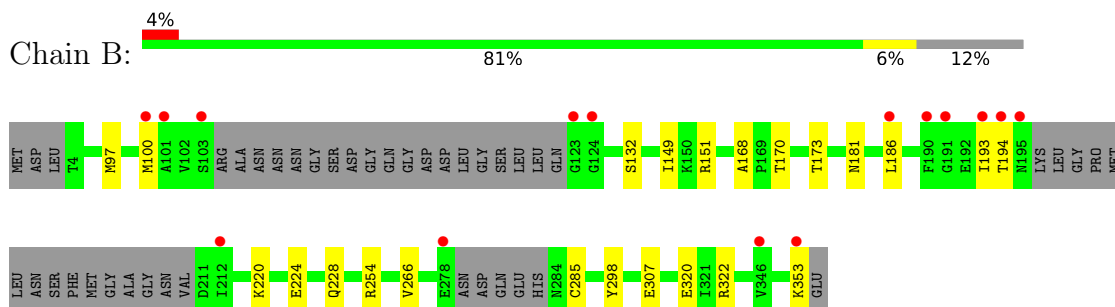
### 3 Residue-property plots [i](#)

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.

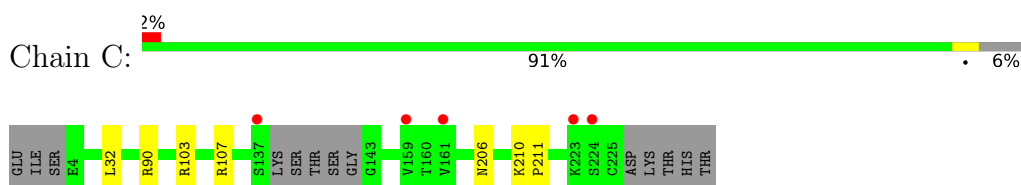
- Molecule 1: ATPase GET3



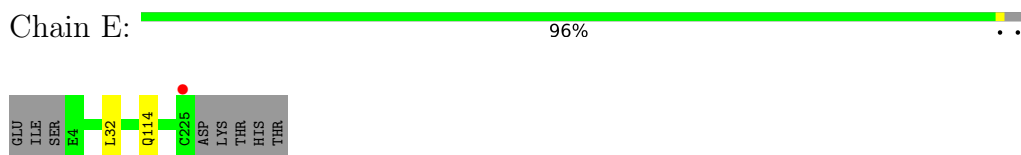
- Molecule 1: ATPase GET3



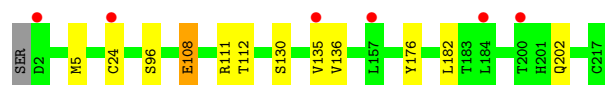
- Molecule 2: Antibody Heavy chain



- Molecule 2: Antibody Heavy chain



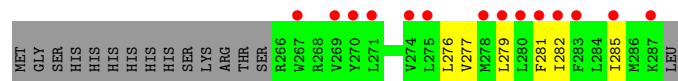
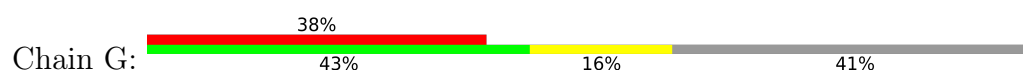
- Molecule 3: Antibody Light chain



- Molecule 3: Antibody Light chain



- Molecule 4: Pep12p



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.87Å 112.03Å 153.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.95 – 2.05 53.95 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (53.95-2.05) 92.1 (53.95-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.05Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.187 , 0.216 0.190 , 0.218	Depositor DCC
$R_{free}$ test set	5469 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	24293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ADP, MG, ZN

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	0.28	0/2457	0.60	0/3310
1	B	0.30	0/2482	0.61	0/3345
2	C	0.28	0/1682	0.57	0/2293
2	E	0.27	0/1715	0.59	0/2338
3	D	0.29	0/1694	0.57	0/2299
3	F	0.28	0/1694	0.57	0/2299
4	G	0.29	0/200	0.76	0/269
All	All	0.28	0/11924	0.59	0/16153

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2415	2400	2397	8	0
1	B	2441	2432	2431	9	0
2	C	1641	1600	1598	4	0
2	E	1673	1633	1632	0	0
3	D	1658	1611	1611	5	0
3	F	1658	1611	1611	6	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	196	231	230	4	0
5	A	27	11	12	0	0
5	B	27	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	31	11	12	0	0
8	B	31	12	12	0	0
9	A	104	0	0	0	0
9	B	149	0	0	1	0
9	C	162	0	0	2	0
9	D	164	0	0	0	0
9	E	211	0	0	0	0
9	F	137	0	0	2	0
9	G	1	0	0	0	0
All	All	12729	11564	11558	31	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 1.

The worst 5 of 31 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:B:320:GLU:OE1	1:B:322:ARG:NH1	2.01	0.93
3:D:111:ARG:NH1	3:D:112:THR:O	2.10	0.83
1:A:277:ALA:O	1:A:279:ASN:N	2.17	0.77
3:F:192:HIS:O	3:F:214:ARG:NH1	2.24	0.70
1:B:307:GLU:OE2	9:B:599:HOH:O	2.15	0.63

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	297/354 (84%)	285 (96%)	10 (3%)	2 (1%)	18	10
1	B	304/354 (86%)	297 (98%)	5 (2%)	2 (1%)	18	10
2	C	214/230 (93%)	208 (97%)	6 (3%)	0	100	100
2	E	221/230 (96%)	218 (99%)	3 (1%)	0	100	100
3	D	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
3	F	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
4	G	20/37 (54%)	19 (95%)	1 (5%)	0	100	100
All	All	1484/1639 (90%)	1446 (97%)	34 (2%)	4 (0%)	36	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	THR
1	A	170	THR
1	A	278	GLU
1	B	285	CYS

### 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	273/309 (88%)	267 (98%)	6 (2%)	45	44
1	B	276/309 (89%)	266 (96%)	10 (4%)	31	26
2	C	182/193 (94%)	179 (98%)	3 (2%)	55	56
2	E	186/193 (96%)	183 (98%)	3 (2%)	55	56
3	D	191/192 (100%)	187 (98%)	4 (2%)	47	46
3	F	191/192 (100%)	191 (100%)	0	100	100
4	G	22/36 (61%)	21 (96%)	1 (4%)	24	18
All	All	1321/1424 (93%)	1294 (98%)	27 (2%)	48	48

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	VAL
2	C	103	ARG
2	E	114[A]	GLN
2	C	32	LEU
2	C	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	85	GLN
2	E	87	ASN
1	B	301	GLN
1	B	335	ASN
2	C	173	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 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	ADP	B	401[B]	6	28,29,29	3.50	10 (35%)	43,45,45	2.13	10 (23%)
5	ADP	A	401[B]	6	28,29,29	3.50	10 (35%)	43,45,45	2.13	10 (23%)
8	ATP	B	403[A]	6	32,33,33	2.60	10 (31%)	48,52,52	2.21	12 (25%)
8	ATP	A	404[A]	6	32,33,33	2.62	12 (37%)	48,52,52	2.23	12 (25%)

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
5	ADP	B	401[B]	6	-	0/16/32/32	0/3/3/3
5	ADP	A	401[B]	6	-	0/16/32/32	0/3/3/3
8	ATP	B	403[A]	6	-	1/22/38/38	0/3/3/3
8	ATP	A	404[A]	6	-	0/22/38/38	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401[B]	ADP	PA-O3A	9.93	1.70	1.59
5	B	401[B]	ADP	PA-O3A	9.81	1.70	1.59
5	B	401[B]	ADP	O4'-C1'	8.64	1.62	1.42
5	A	401[B]	ADP	O4'-C1'	8.61	1.61	1.42
5	A	401[B]	ADP	C2'-C1'	-6.94	1.31	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	404[A]	ATP	C5-C4-N3	-7.60	116.26	126.72
8	B	403[A]	ATP	C5-C4-N3	-7.44	116.48	126.72
5	A	401[B]	ADP	N6-C6-N1	-6.28	104.39	118.38
5	B	401[B]	ADP	N6-C6-N1	-6.24	104.49	118.38
8	A	404[A]	ATP	N3-C4-N9	5.89	137.18	127.17

There are no chirality outliers.

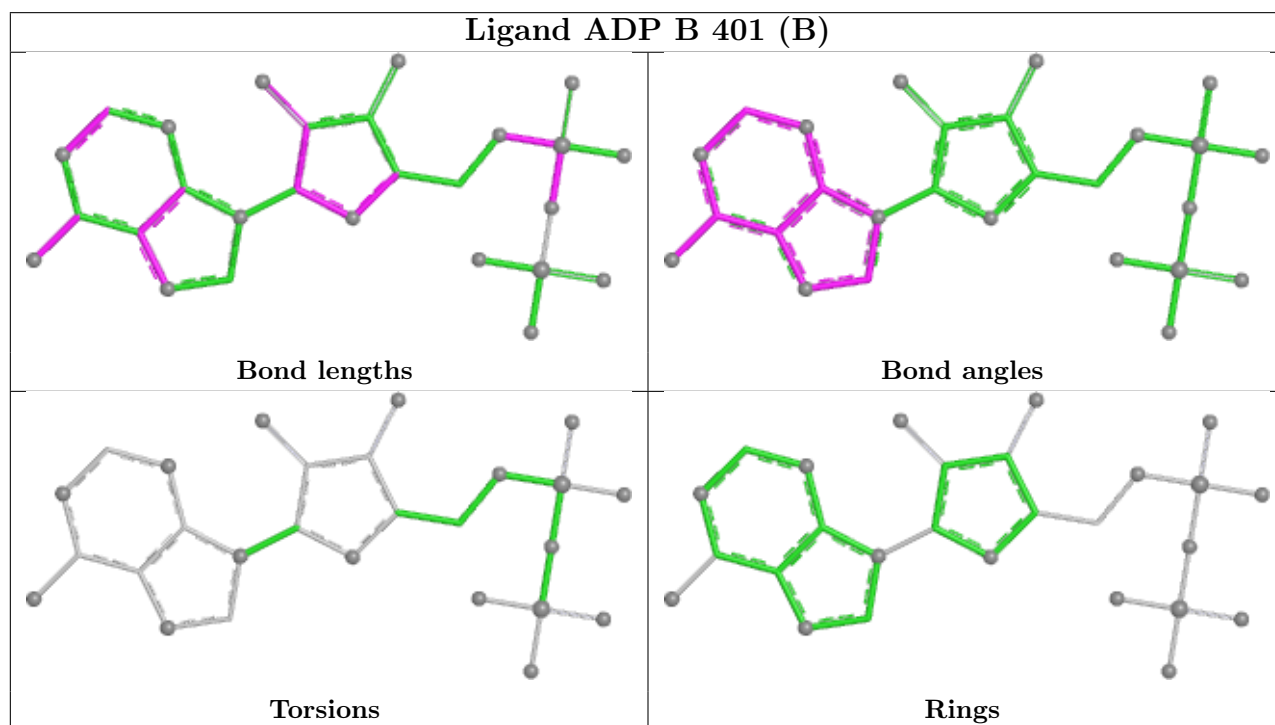
All (1) torsion outliers are listed below:

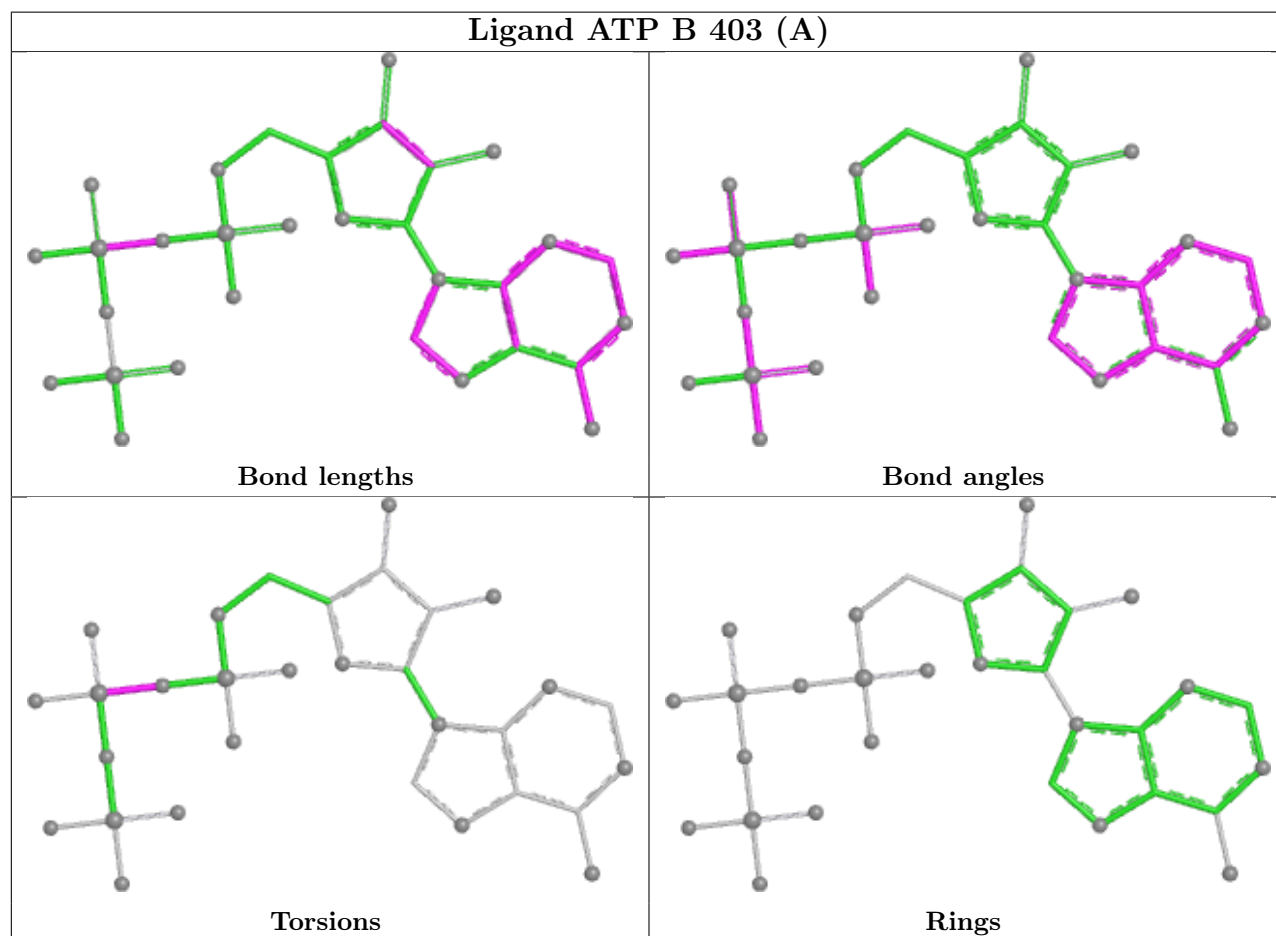
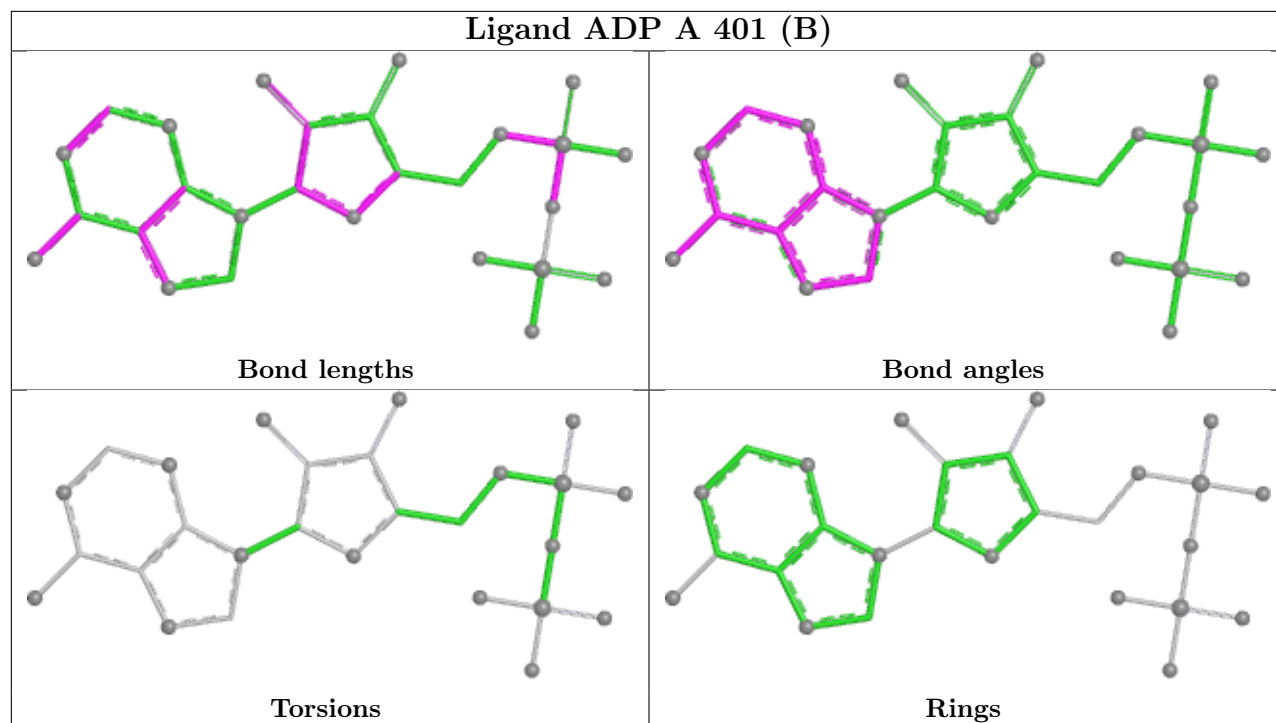
Mol	Chain	Res	Type	Atoms
8	B	403[A]	ATP	PA-O3A-PB-O2B

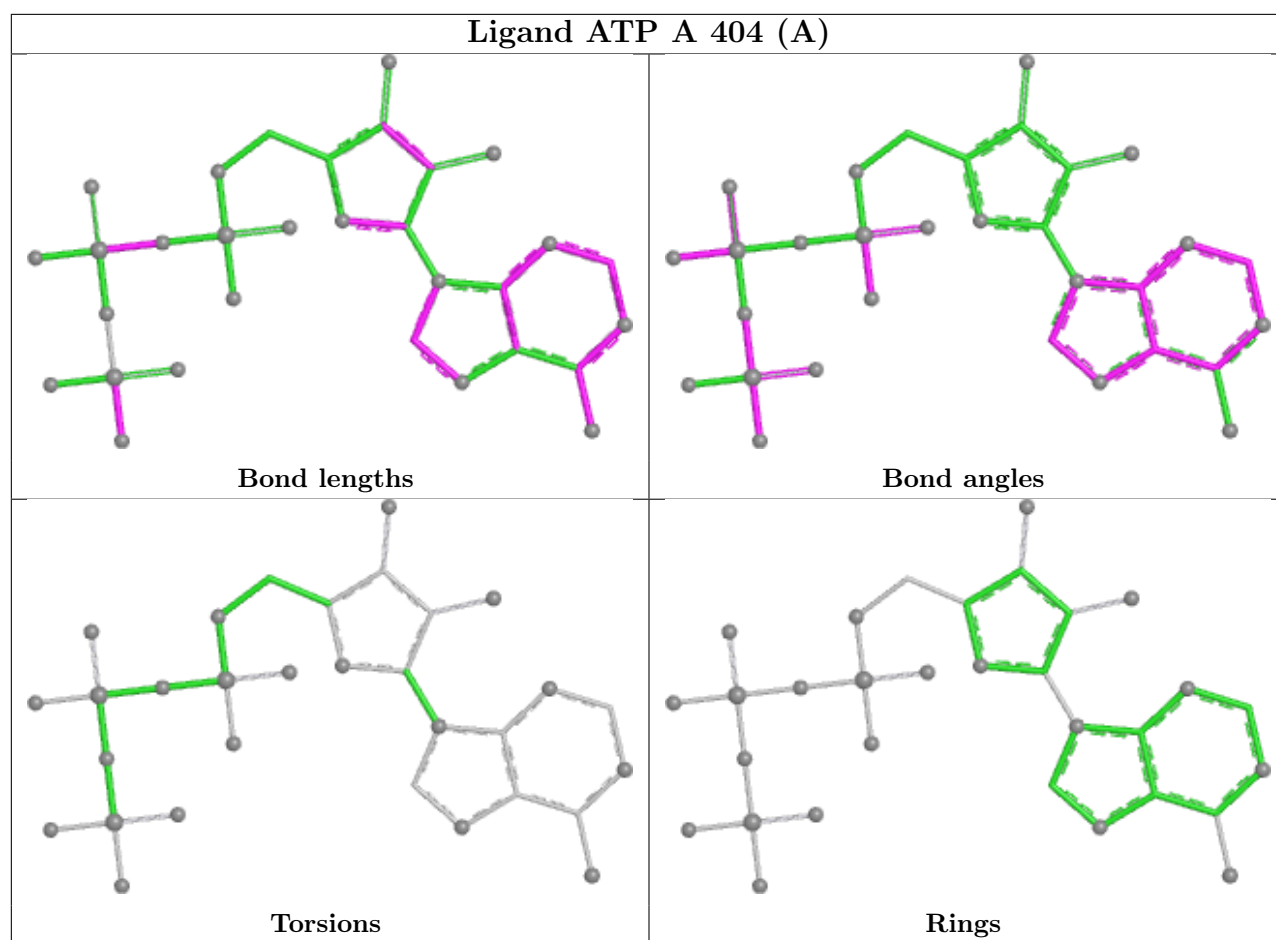
There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	305/354 (86%)	0.38	23 (7%) 20 20	24, 55, 134, 149	2 (0%)
1	B	311/354 (87%)	0.07	15 (4%) 35 36	20, 44, 110, 147	1 (0%)
2	C	217/230 (94%)	0.11	5 (2%) 61 63	19, 46, 105, 143	1 (0%)
2	E	222/230 (96%)	-0.31	1 (0%) 87 89	19, 38, 66, 110	1 (0%)
3	D	216/217 (99%)	0.16	6 (2%) 55 57	28, 52, 100, 145	0
3	F	216/217 (99%)	0.10	5 (2%) 61 63	30, 54, 78, 120	0
4	G	22/37 (59%)	2.50	14 (63%) 0 0	98, 125, 136, 155	0
All	All	1509/1639 (92%)	0.13	69 (4%) 37 37	19, 49, 112, 155	5 (0%)

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	279	LEU	5.8
1	A	246[A]	PHE	5.4
1	A	155	GLY	5.0
1	B	123	GLY	4.9
4	G	285	ILE	4.2

### 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](#)

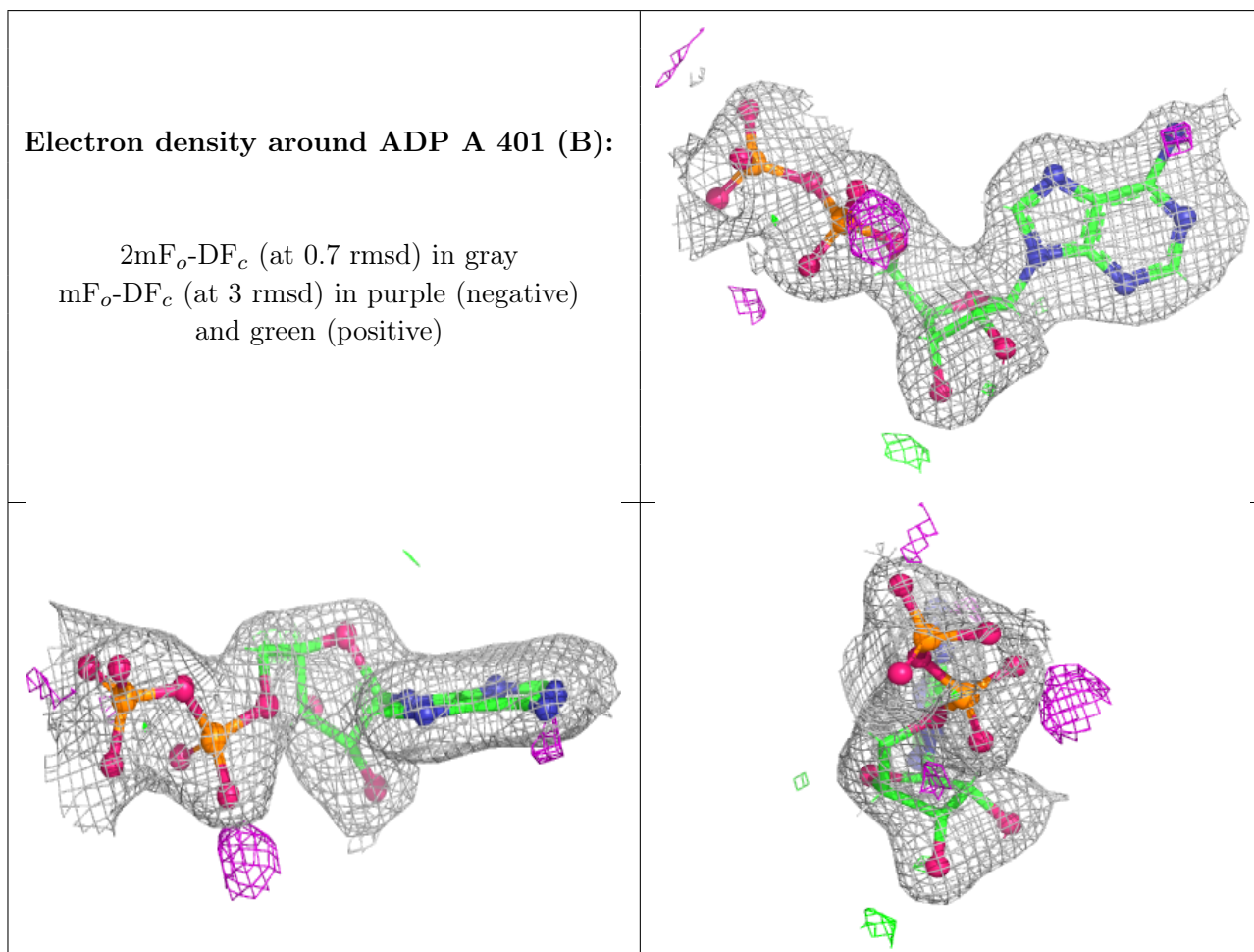
There are no oligosaccharides in this entry.

## 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<sup>th</sup> 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.

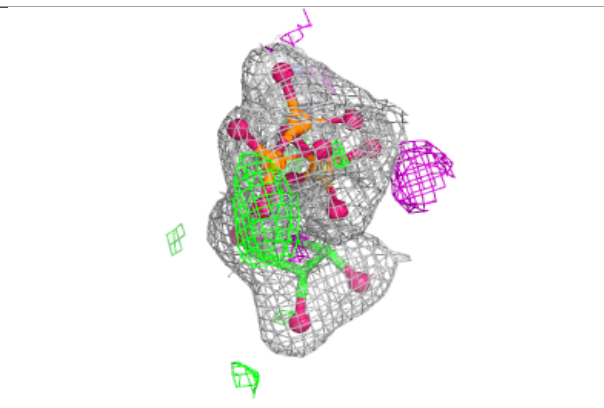
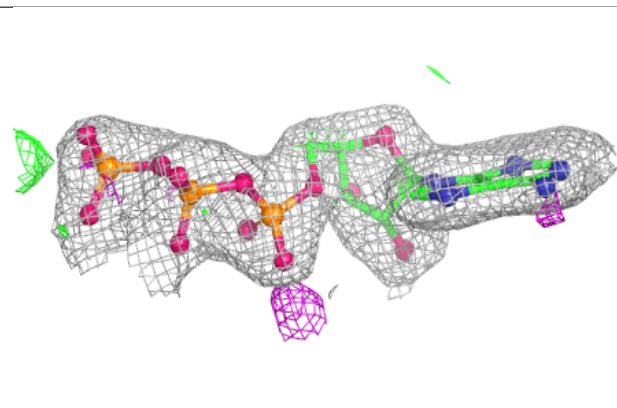
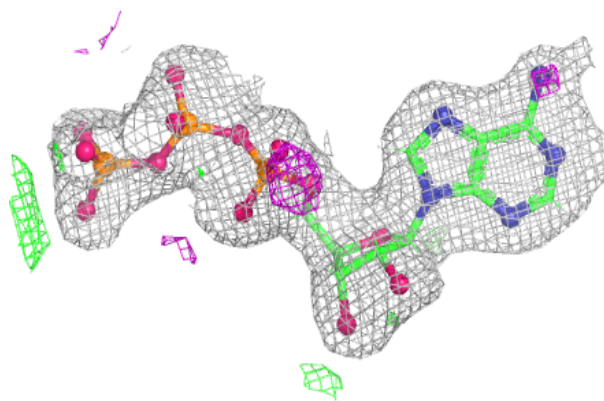
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ADP	A	401[B]	27/27	0.94	0.07	30,36,46,48	38
8	ATP	A	404[A]	31/31	0.94	0.08	30,36,45,48	42
8	ATP	B	403[A]	31/31	0.94	0.08	25,34,45,52	43
5	ADP	B	401[B]	27/27	0.95	0.08	30,36,45,50	39
6	MG	A	402	1/1	0.96	0.07	41,41,41,41	0
6	MG	B	402	1/1	0.96	0.05	35,35,35,35	0
7	ZN	A	403	1/1	0.97	0.04	68,68,68,68	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.

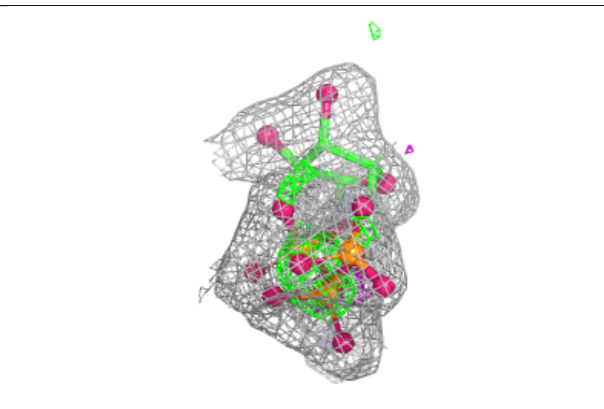
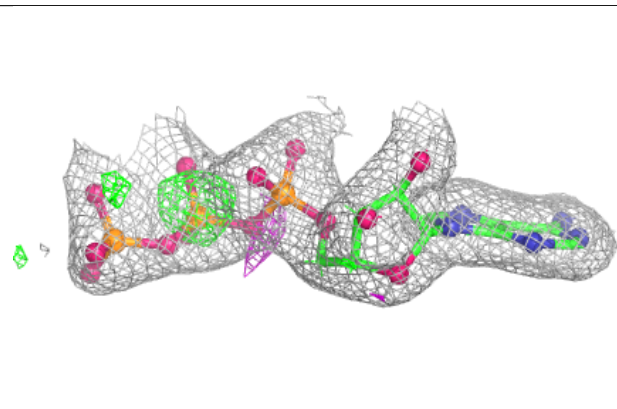
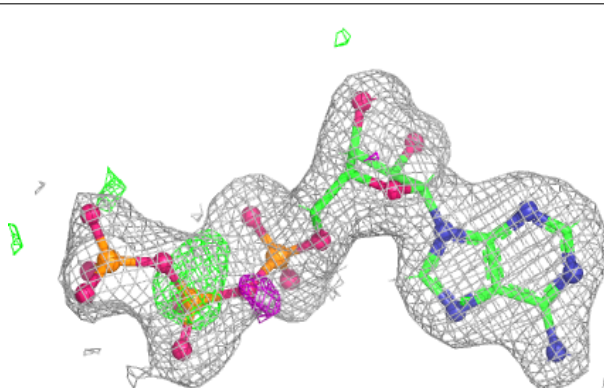


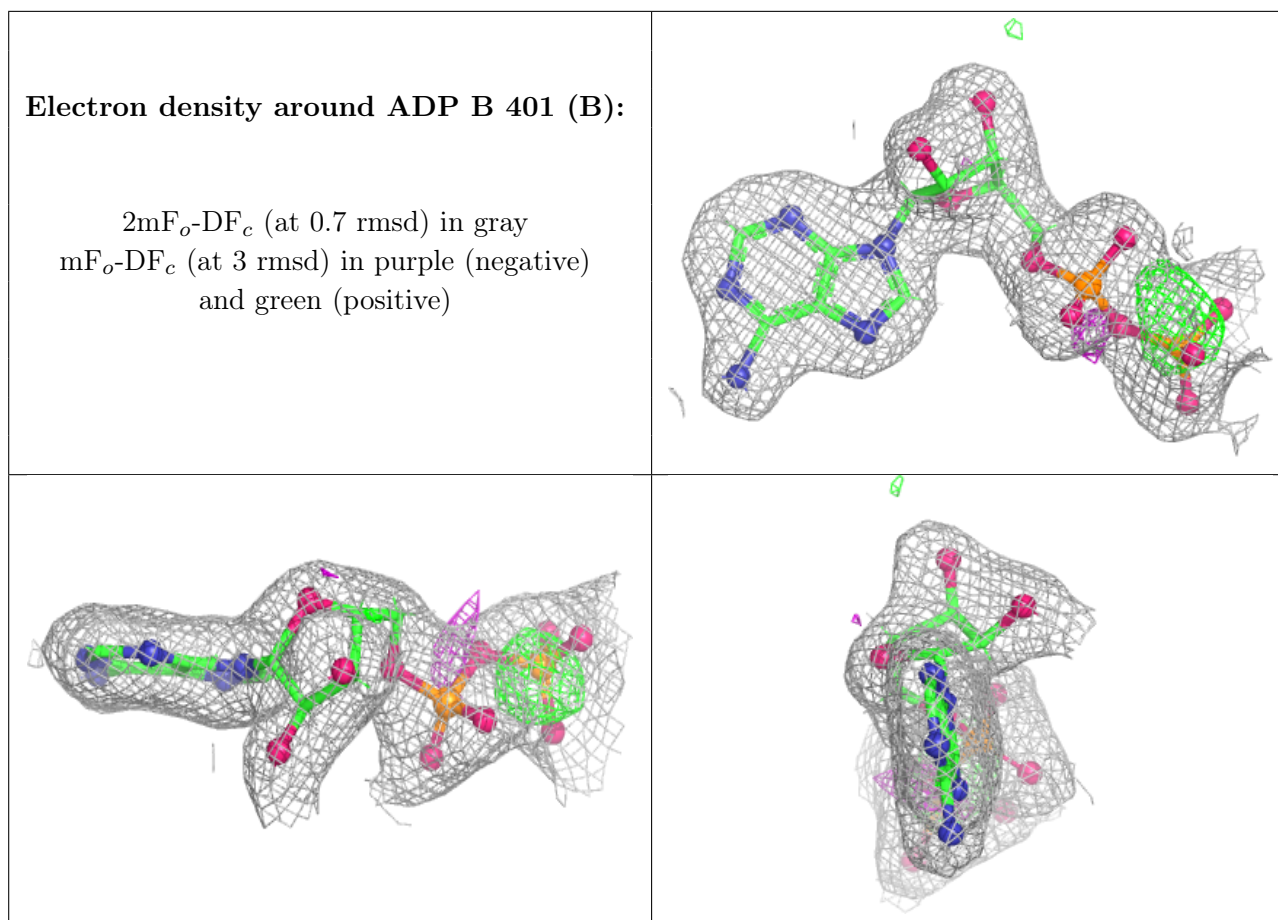
**Electron density around ATP A 404 (A):**

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

**Electron density around ATP B 403 (A):**

$2mF_o-DF_c$  (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.