



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 08:54 am BST

PDB ID : 4BLO  
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI6 IN COMPLEX WITH ADP  
Authors : El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.  
Deposited on : 2013-05-04  
Resolution : 2.80 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>.

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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 : 2.36.2  
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) : 2.36.2

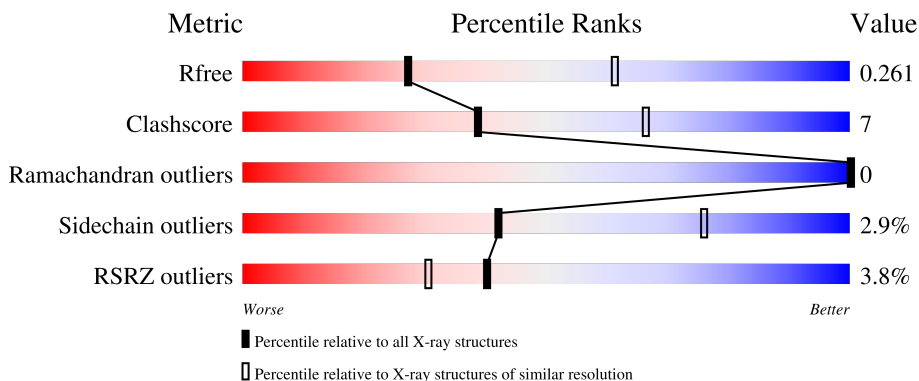
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	309	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      75%      11%      •      13%</p>
1	B	309	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      73%      12%      •      13%</p>
1	C	309	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      72%      13%      •      13%</p>
1	D	309	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6%      70%      15%      •      13%</p>
1	E	309	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      71%      15%      •      13%</p>

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Mol	Chain	Length	Quality of chain
1	F	309	<p>4% 72% 14% • 13%</p>
1	G	309	<p>5% 71% 14% • 13%</p>
1	H	309	<p>3% 71% 15% • 13%</p>
1	I	309	<p>2% 72% 13% • 13%</p>
1	J	309	<p>3% 72% 14% • 13%</p>
1	K	309	<p>2% 72% 13% • 13%</p>
1	L	309	<p>2% 70% 17% • 11%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24437 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PACKAGING ENZYME P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2003	1276	335	382	10	0	0	0
1	B	270	2011	1281	336	383	11	0	0	0
1	C	270	2011	1281	336	383	11	0	0	0
1	D	270	2011	1281	336	383	11	0	0	0
1	E	269	2006	1278	335	382	11	0	0	0
1	F	269	2006	1278	335	382	11	0	0	0
1	G	268	1998	1274	333	380	11	0	0	0
1	H	269	2003	1276	335	382	10	0	0	0
1	I	269	2003	1276	335	382	10	0	0	0
1	J	269	2006	1278	335	382	11	0	0	0
1	K	269	2003	1276	335	382	10	0	0	0
1	L	275	2040	1300	341	388	11	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

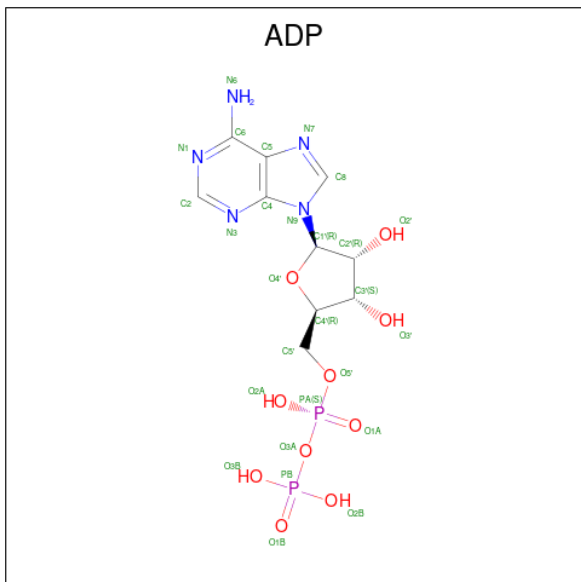
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0

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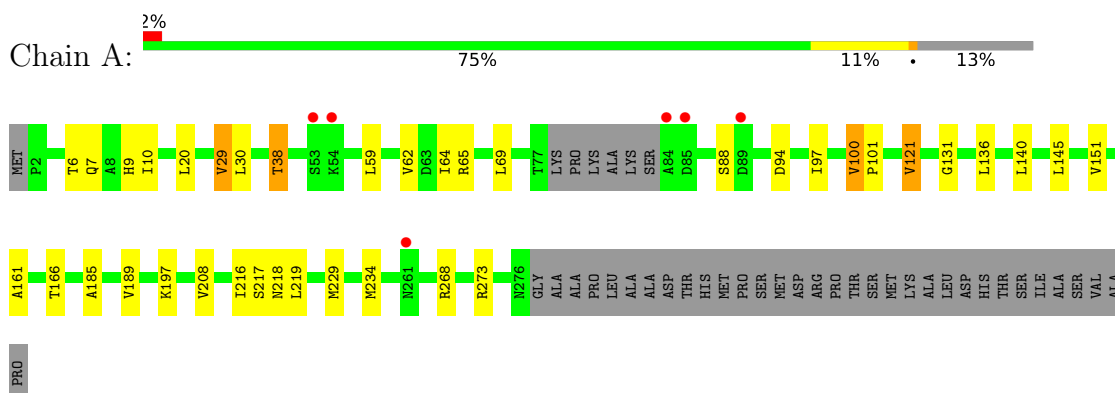
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

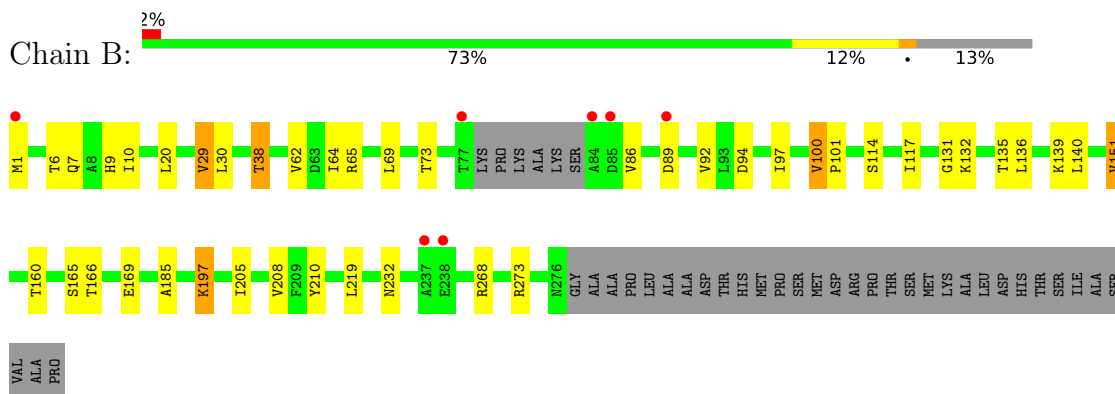
### 3 Residue-property plots [i](#)

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.

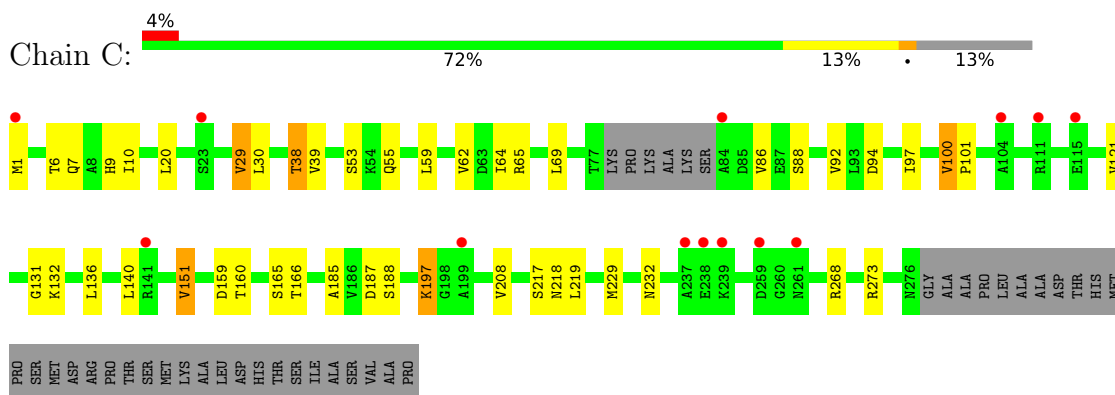
- Molecule 1: PACKAGING ENZYME P4



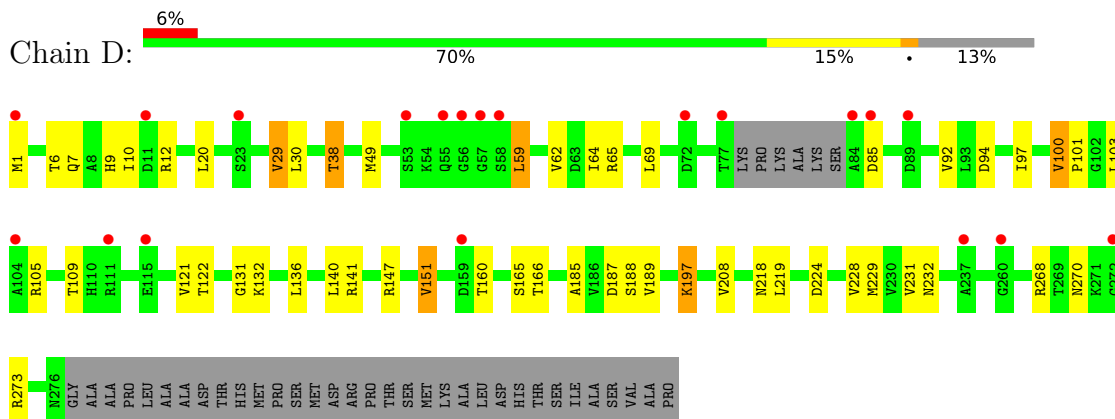
- Molecule 1: PACKAGING ENZYME P4



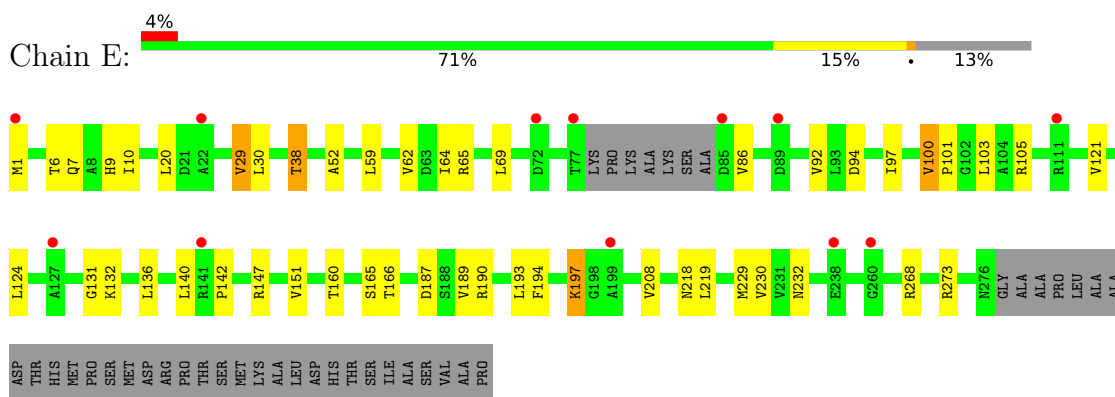
- Molecule 1: PACKAGING ENZYME P4



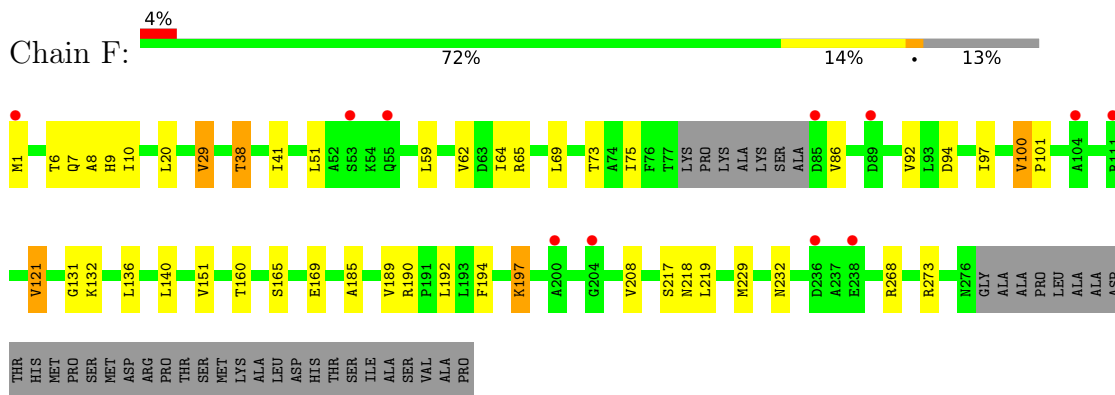
- Molecule 1: PACKAGING ENZYME P4



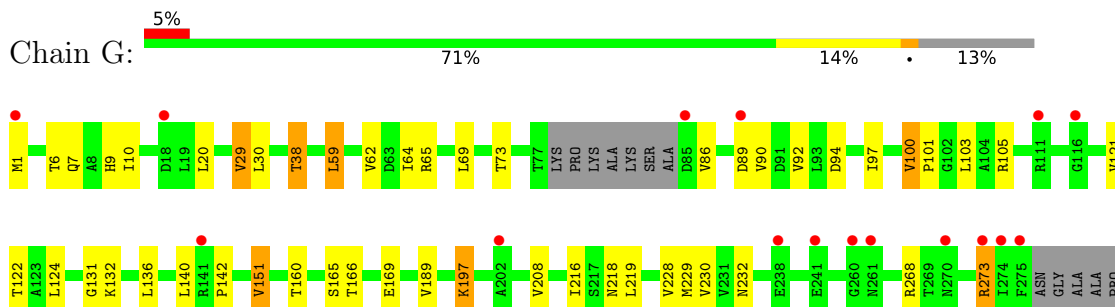
- Molecule 1: PACKAGING ENZYME P4



- Molecule 1: PACKAGING ENZYME P4



- Molecule 1: PACKAGING ENZYME P4





LEU  
ALA  
ALA  
ASP  
THR  
HIS  
MET  
PRO  
SER  
MET  
MET  
ASP  
ARG  
PRO  
THR  
MET  
MET  
ALA  
LEU  
ASP  
HIS  
SER  
THR  
SER  
ILE  
ALA  
SER  
VAL  
ALA  
PRO

● Molecule 1: PACKAGING ENZYME P4

Chain H: 3% 71% 15% 13%

MET F2 T6 Q7 A8 H9 I10 L20 D21 A22 V29 L30 T38 T33 I41 V62 D63 I64 R65 L69 L70 K71 D72 T73 A74 I75 F76 T77 LYS PRO LYS PRO LYS LYS ALA LYS SER A84 D85 V86 E87 S88 D89 V92 V93 D94 I97 V100 P101 G102 L103 A104 R105

R111 V121 L124 Q131 K132 L136 L140 G149 E150 V151 S165 T166 E169 P191 K197 V208 L216 S217 N218 L219 M229 V230 V231 M232 A237 T265 R268 K271 G272 E273 F275 N276 GLY ALA PRO LEU ALA THR ASP THR HIS

MET PRO SER MET ASP ARG PRO THR SER MET MET LYS ALA ASP HIS THR SER ILE VAL PRO

● Molecule 1: PACKAGING ENZYME P4

Chain I: 2% 72% 13% 13%

MET F2 T6 Q7 A8 H9 I10 L20 D21 A22 V29 T38 E50 L51 R64 Q65 L69 V62 D63 I64 R65 L69 T77 LYS PRO LYS LYS ALA LYS SER A84 D85 V86 E87 S88 D89 V90 D91 V92 L93 D94 I97 V100 P101 W112 V121

K132 L136 L140 G149 E150 V151 S165 M163 V184 A185 P191 K197 V208 N218 L219 F220 T221 V228 M229 N232 E238 M261 R268 R273 N276 GLY ALA PRO LEU ALA ASP THR HIS MET SER SER ASP ARG THR PRO SER

MET LYS ALA LEU ASP HIS THR SER ILE VAL ALA PRO

● Molecule 1: PACKAGING ENZYME P4

Chain J: 3% 72% 14% 13%

M1 T6 Q7 A8 H9 I10 L20 D21 A22 V29 L30 T38 T33 I41 V62 D63 I64 R65 L69 T73 A74 I75 F76 T77 LYS PRO LYS ALA LYS SER SER ALA D85 V86 E87 S88 D89 V90 D94 I97 V100 P101 G102 L103 A104 R105 R111 W112 P113

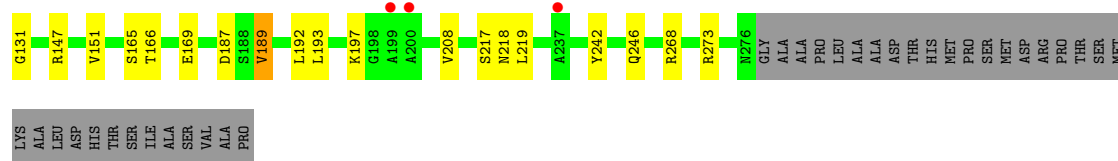
V121 G131 K132 L136 L140 V151 A152 T160 S165 T166 E169 A185 K197 V208 N218 L219 M229 N232 E238 V262 R268 K271 G272 R273 N276 GLY ALA PRO LEU ALA ASP THR MET MET ASP PRO

THR SER MET LYS ALA LEU ASP HIS THR SER SER ILE ALA SER VAL ALA PRO

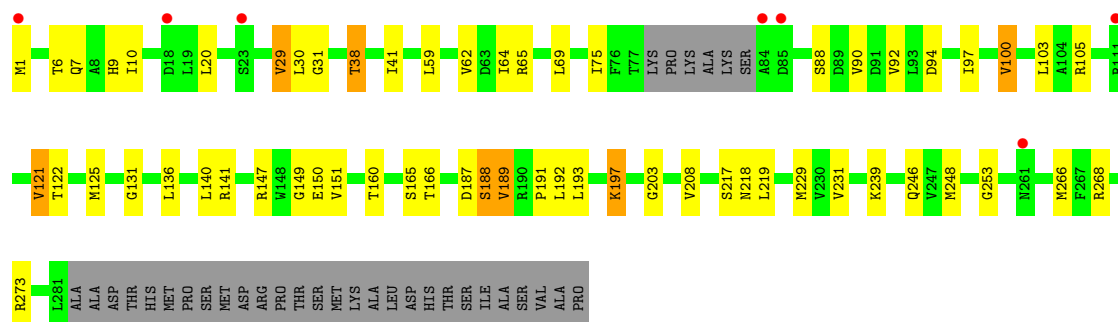
● Molecule 1: PACKAGING ENZYME P4

Chain K: 2% 72% 13% 13%

MET F2 T6 Q7 A8 H9 I10 L20 V29 T38 A52 L59 V62 D63 I64 R65 L69 L70 K71 D72 T73 T77 LYS PRO LYS ALA LYS SER SER A84 D85 V86 E87 S88 D89 V92 V93 D94 I97 V98 S99 V100 P101 G102 L103 A104 R105 V121



- Molecule 1: PACKAGING ENZYME P4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.84Å 95.26Å 98.33Å 82.46° 86.17° 64.85°	Depositor
Resolution (Å)	19.99 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.80) 96.9 (20.00-2.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.79Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.217 , 0.244 0.235 , 0.261	Depositor DCC
$R_{free}$ test set	3664 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.657	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24437	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 11.71% 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: CA, ADP

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	0.47	0/2033	0.66	2/2767 (0.1%)
1	B	0.48	0/2041	0.67	2/2778 (0.1%)
1	C	0.44	0/2041	0.67	2/2778 (0.1%)
1	D	0.45	0/2041	0.66	2/2778 (0.1%)
1	E	0.44	0/2036	0.66	2/2771 (0.1%)
1	F	0.46	0/2036	0.66	2/2771 (0.1%)
1	G	0.46	0/2028	0.68	2/2760 (0.1%)
1	H	0.46	0/2033	0.66	2/2767 (0.1%)
1	I	0.48	0/2033	0.70	2/2767 (0.1%)
1	J	0.47	0/2036	0.68	2/2771 (0.1%)
1	K	0.46	0/2033	0.68	2/2767 (0.1%)
1	L	0.54	1/2071 (0.0%)	0.70	2/2820 (0.1%)
All	All	0.47	1/24462 (0.0%)	0.67	24/33295 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	31	GLY	C-N	10.48	1.58	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	VAL	CB-CA-C	-7.84	96.51	111.40
1	I	29	VAL	CB-CA-C	-7.83	96.53	111.40
1	J	29	VAL	CB-CA-C	-7.83	96.53	111.40
1	G	29	VAL	CB-CA-C	-7.82	96.53	111.40
1	K	29	VAL	CB-CA-C	-7.82	96.53	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2003	0	2052	28	0
1	B	2011	0	2063	37	0
1	C	2011	0	2063	35	0
1	D	2011	0	2063	36	0
1	E	2006	0	2058	30	0
1	F	2006	0	2058	37	0
1	G	1998	0	2052	39	0
1	H	2003	0	2052	40	0
1	I	2003	0	2052	32	0
1	J	2006	0	2058	40	0
1	K	2003	0	2052	40	0
1	L	2040	0	2094	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	1	0
3	H	27	0	12	1	0
3	I	27	0	12	0	0
3	J	27	0	12	1	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
All	All	24437	0	24861	368	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 7.

The worst 5 of 368 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:29:VAL:O	1:A:208:VAL:HG21	1.42	1.18
1:F:29:VAL:O	1:F:208:VAL:HG21	1.45	1.17
1:L:29:VAL:O	1:L:208:VAL:HG21	1.43	1.17
1:K:29:VAL:O	1:K:208:VAL:HG21	1.42	1.16
1:H:29:VAL:O	1:H:208:VAL:HG21	1.47	1.13

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	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	B	266/309 (86%)	261 (98%)	5 (2%)	0	100	100
1	C	266/309 (86%)	258 (97%)	8 (3%)	0	100	100
1	D	266/309 (86%)	257 (97%)	9 (3%)	0	100	100
1	E	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	F	265/309 (86%)	259 (98%)	6 (2%)	0	100	100
1	G	264/309 (85%)	257 (97%)	7 (3%)	0	100	100
1	H	265/309 (86%)	259 (98%)	6 (2%)	0	100	100
1	I	265/309 (86%)	261 (98%)	4 (2%)	0	100	100
1	J	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	K	265/309 (86%)	256 (97%)	9 (3%)	0	100	100
1	L	271/309 (88%)	266 (98%)	5 (2%)	0	100	100
All	All	3188/3708 (86%)	3114 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	219/250 (88%)	213 (97%)	6 (3%)	44	78
1	B	220/250 (88%)	216 (98%)	4 (2%)	59	86
1	C	220/250 (88%)	215 (98%)	5 (2%)	50	82
1	D	220/250 (88%)	213 (97%)	7 (3%)	39	73
1	E	220/250 (88%)	215 (98%)	5 (2%)	50	82
1	F	220/250 (88%)	213 (97%)	7 (3%)	39	73
1	G	219/250 (88%)	210 (96%)	9 (4%)	30	64
1	H	219/250 (88%)	214 (98%)	5 (2%)	50	82
1	I	219/250 (88%)	213 (97%)	6 (3%)	44	78
1	J	220/250 (88%)	216 (98%)	4 (2%)	59	86
1	K	219/250 (88%)	212 (97%)	7 (3%)	39	73
1	L	222/250 (89%)	211 (95%)	11 (5%)	24	56
All	All	2637/3000 (88%)	2561 (97%)	76 (3%)	42	76

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	151	VAL
1	L	151	VAL
1	K	92	VAL
1	L	38	THR
1	L	197	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	9	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	9	HIS
1	H	37	ASN
1	I	9	HIS
1	J	183	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	$\# Z  > 2$
3	ADP	C	401	2	24,29,29	0.69	0	29,45,45	0.73	1 (3%)
3	ADP	B	401	2	24,29,29	0.72	0	29,45,45	0.70	1 (3%)
3	ADP	H	401	2	24,29,29	0.70	0	29,45,45	0.76	1 (3%)
3	ADP	L	401	2	24,29,29	0.73	0	29,45,45	0.70	1 (3%)
3	ADP	E	401	2	24,29,29	0.73	0	29,45,45	0.71	1 (3%)
3	ADP	I	401	2	24,29,29	0.65	0	29,45,45	0.72	1 (3%)
3	ADP	D	401	2	24,29,29	0.68	0	29,45,45	0.70	1 (3%)
3	ADP	G	401	2	24,29,29	0.71	0	29,45,45	0.71	1 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	A	401	2	24,29,29	0.77	0	29,45,45	0.72	1 (3%)
3	ADP	J	401	2	24,29,29	0.70	0	29,45,45	0.72	1 (3%)
3	ADP	F	401	2	24,29,29	0.69	0	29,45,45	0.70	1 (3%)
3	ADP	K	401	2	24,29,29	0.72	1 (4%)	29,45,45	0.68	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	401	2	-	4/12/32/32	0/3/3/3
3	ADP	B	401	2	-	4/12/32/32	0/3/3/3
3	ADP	H	401	2	-	4/12/32/32	0/3/3/3
3	ADP	L	401	2	-	4/12/32/32	0/3/3/3
3	ADP	E	401	2	-	4/12/32/32	0/3/3/3
3	ADP	I	401	2	-	3/12/32/32	0/3/3/3
3	ADP	D	401	2	-	4/12/32/32	0/3/3/3
3	ADP	G	401	2	-	4/12/32/32	0/3/3/3
3	ADP	A	401	2	-	4/12/32/32	0/3/3/3
3	ADP	J	401	2	-	4/12/32/32	0/3/3/3
3	ADP	F	401	2	-	4/12/32/32	0/3/3/3
3	ADP	K	401	2	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	ADP	C8-N7	-2.01	1.31	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	401	ADP	C5-C6-N6	2.47	124.10	120.35
3	I	401	ADP	C5-C6-N6	2.43	124.05	120.35
3	A	401	ADP	C5-C6-N6	2.43	124.05	120.35
3	C	401	ADP	C5-C6-N6	2.43	124.04	120.35
3	H	401	ADP	C5-C6-N6	2.38	123.97	120.35

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

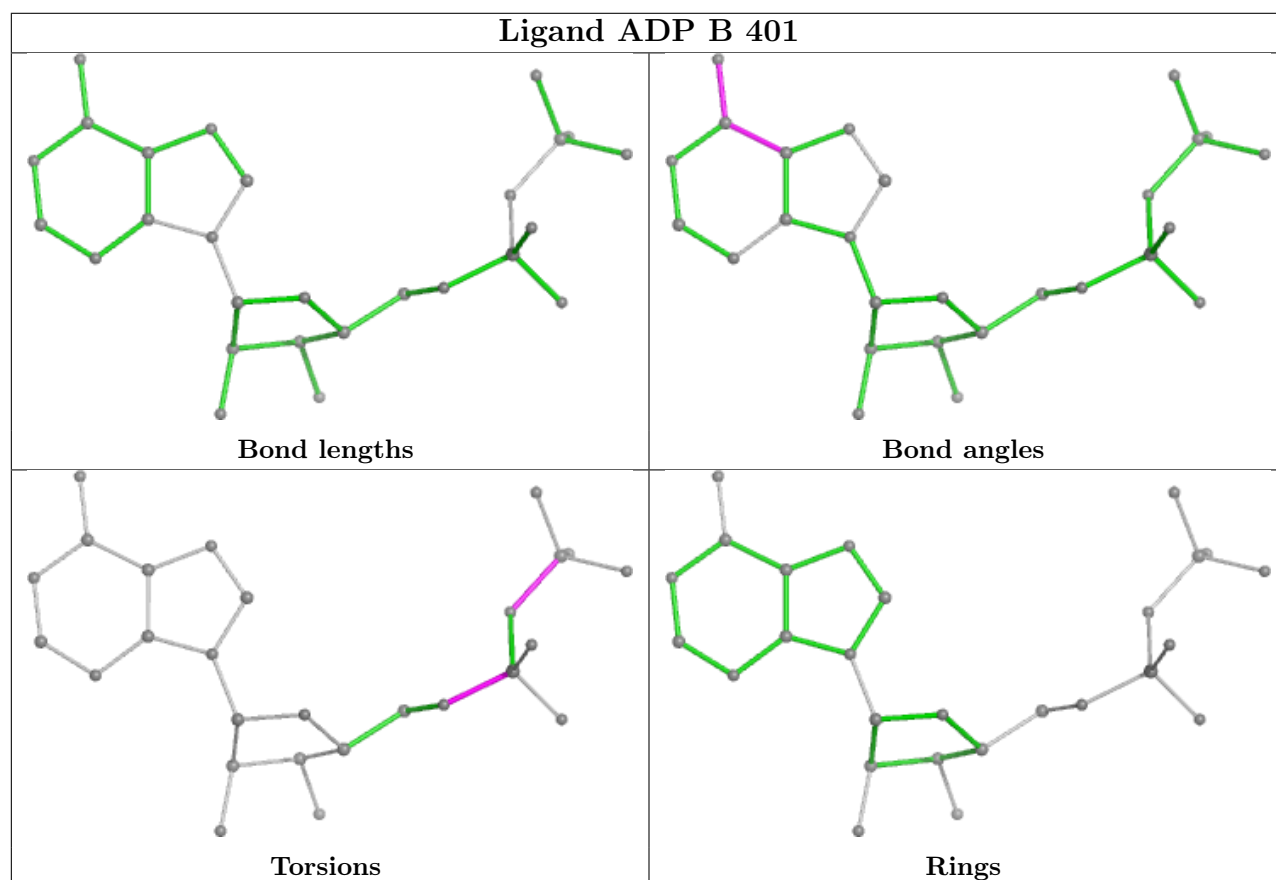
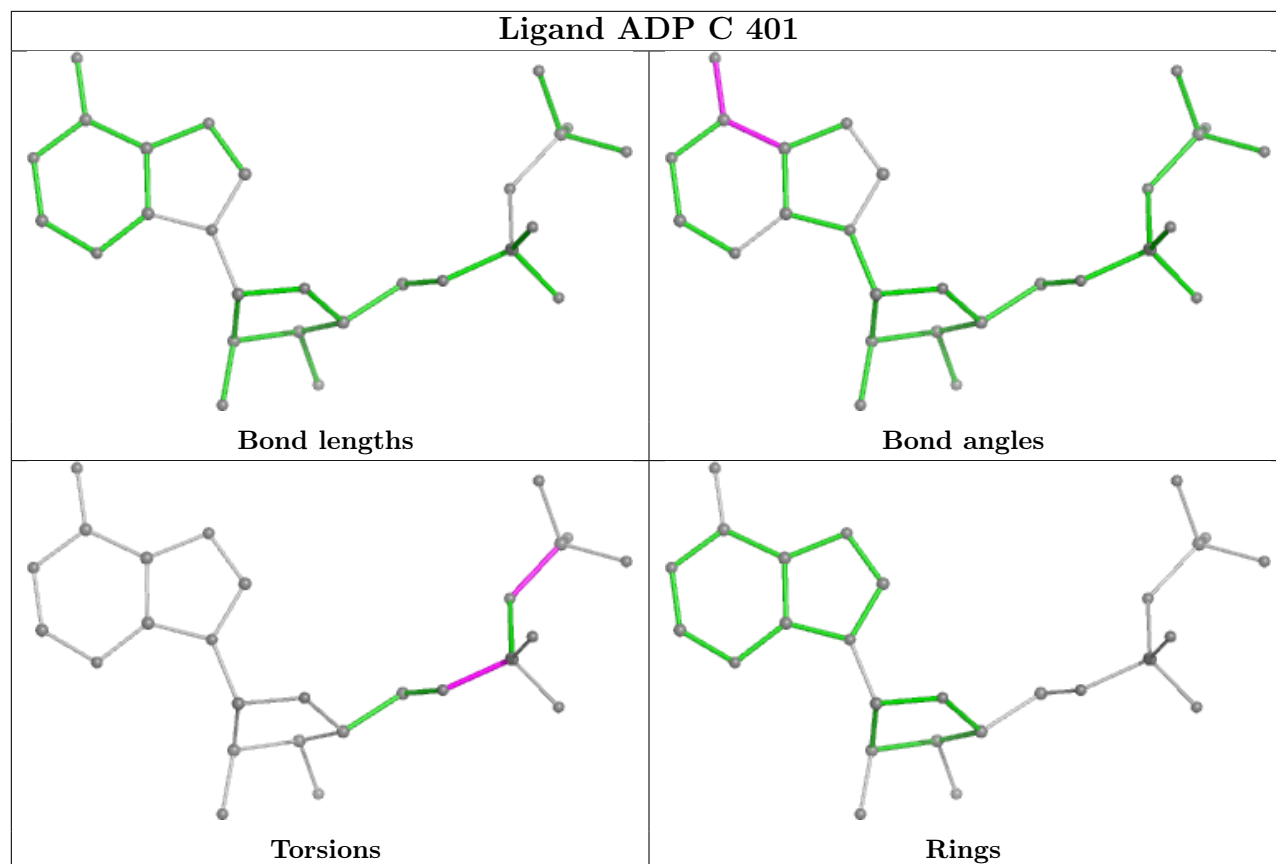
Mol	Chain	Res	Type	Atoms
3	A	401	ADP	PA-O3A-PB-O2B
3	A	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	PA-O3A-PB-O2B
3	B	401	ADP	C5'-O5'-PA-O3A
3	C	401	ADP	PA-O3A-PB-O2B

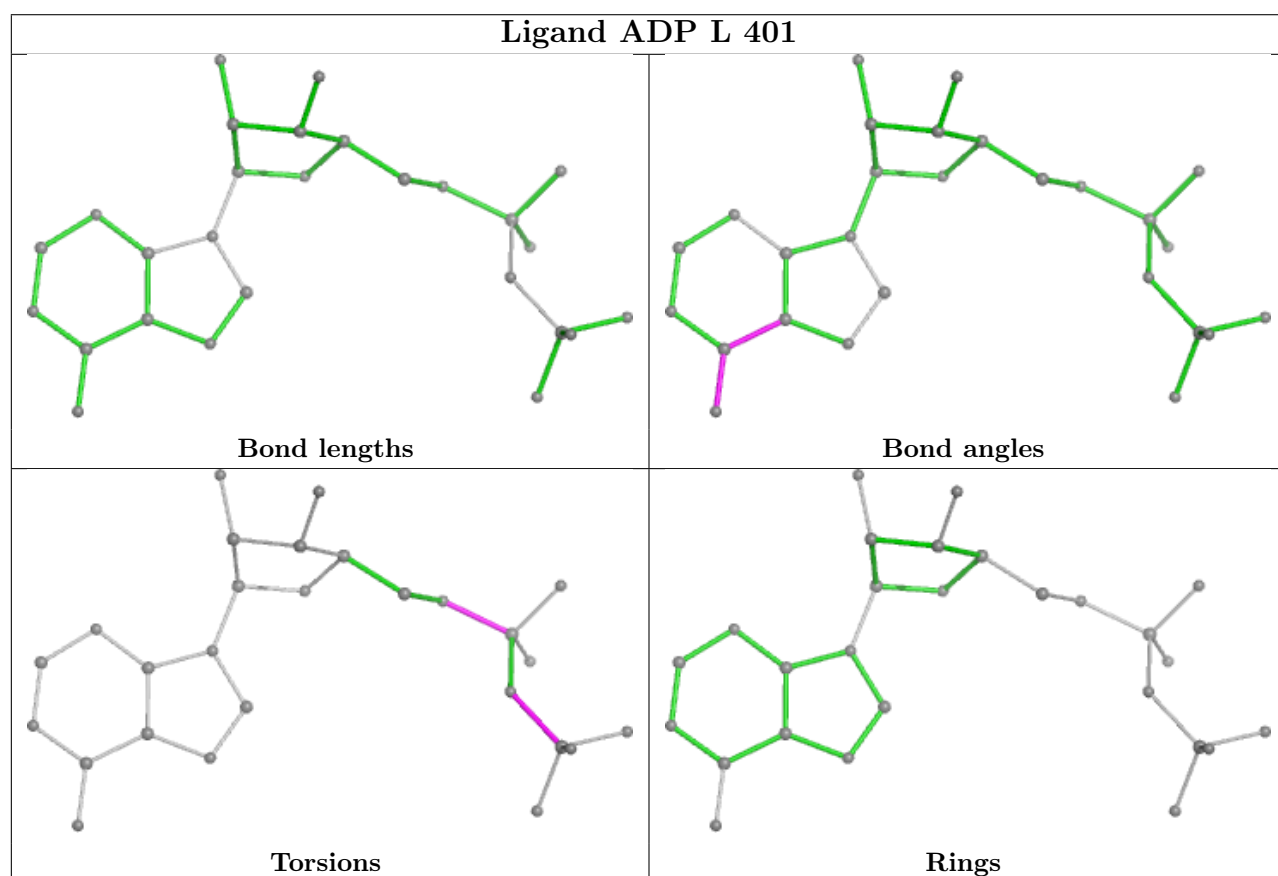
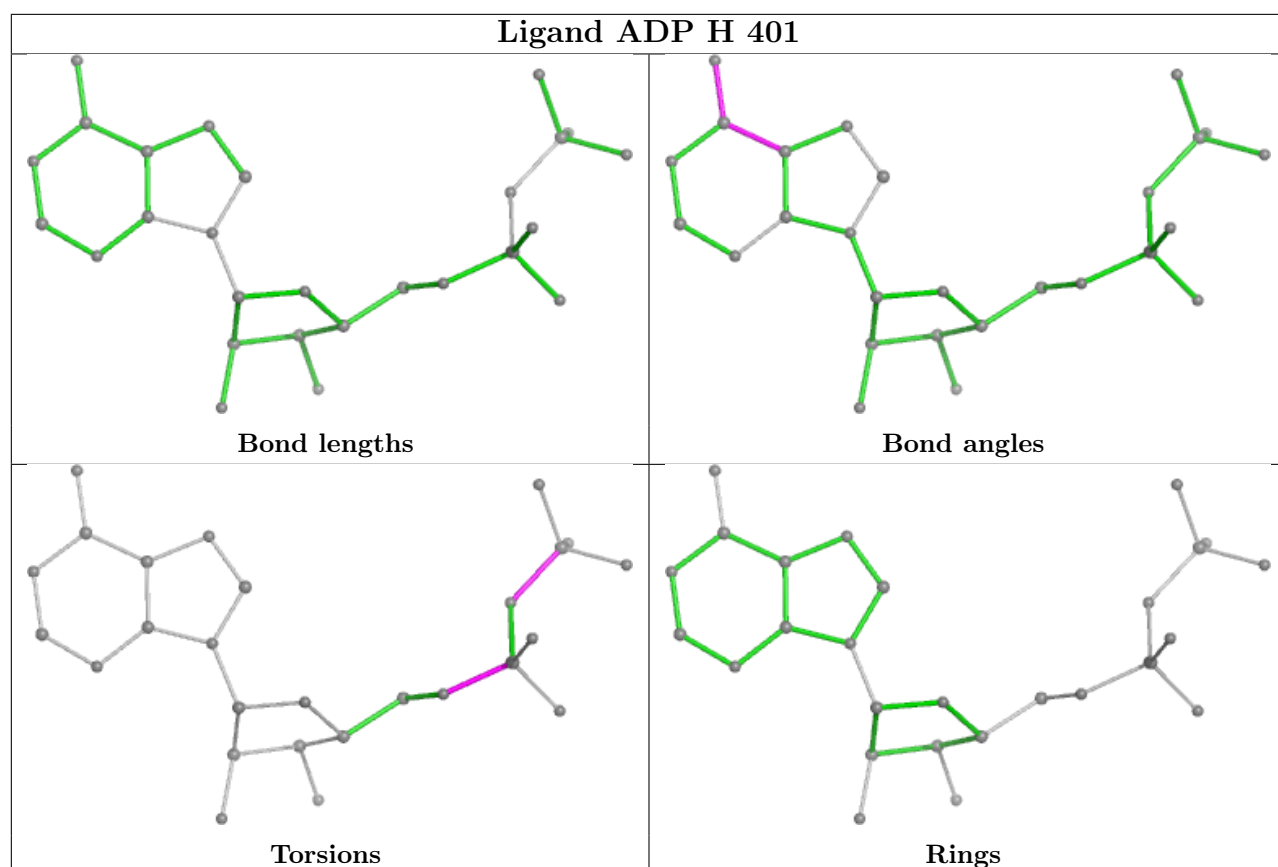
There are no ring outliers.

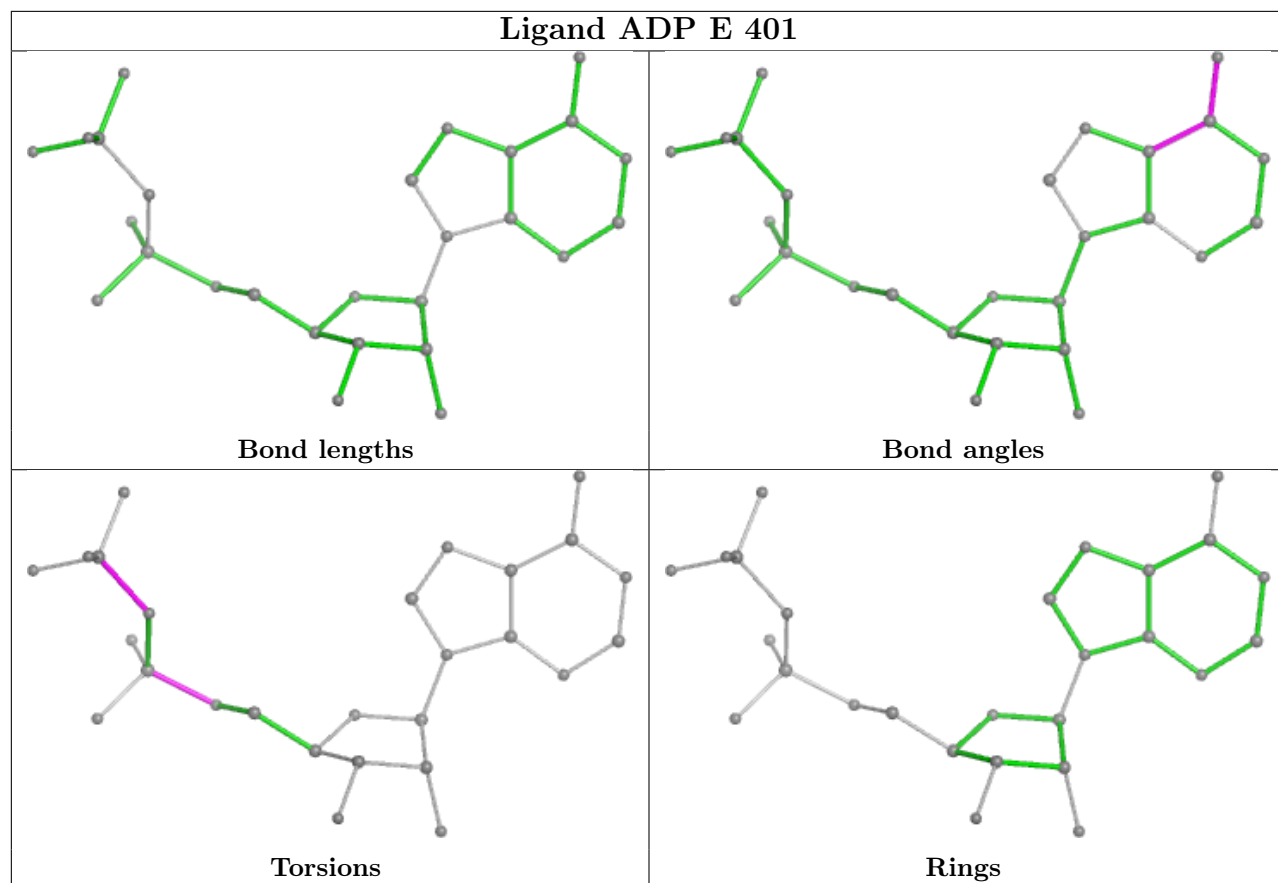
11 monomers are involved in 11 short contacts:

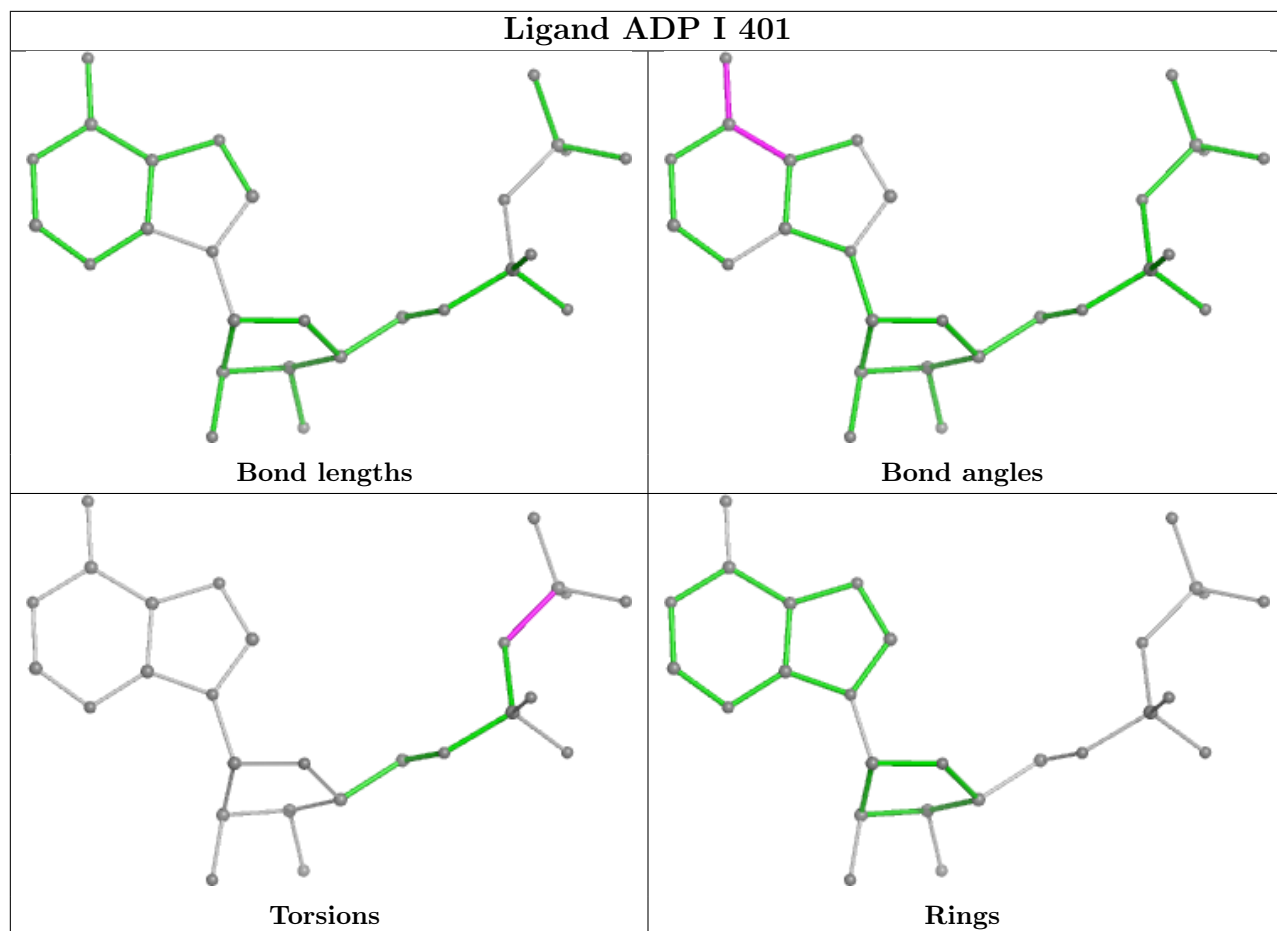
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ADP	1	0
3	B	401	ADP	1	0
3	H	401	ADP	1	0
3	L	401	ADP	1	0
3	E	401	ADP	1	0
3	D	401	ADP	1	0
3	G	401	ADP	1	0
3	A	401	ADP	1	0
3	J	401	ADP	1	0
3	F	401	ADP	1	0
3	K	401	ADP	1	0

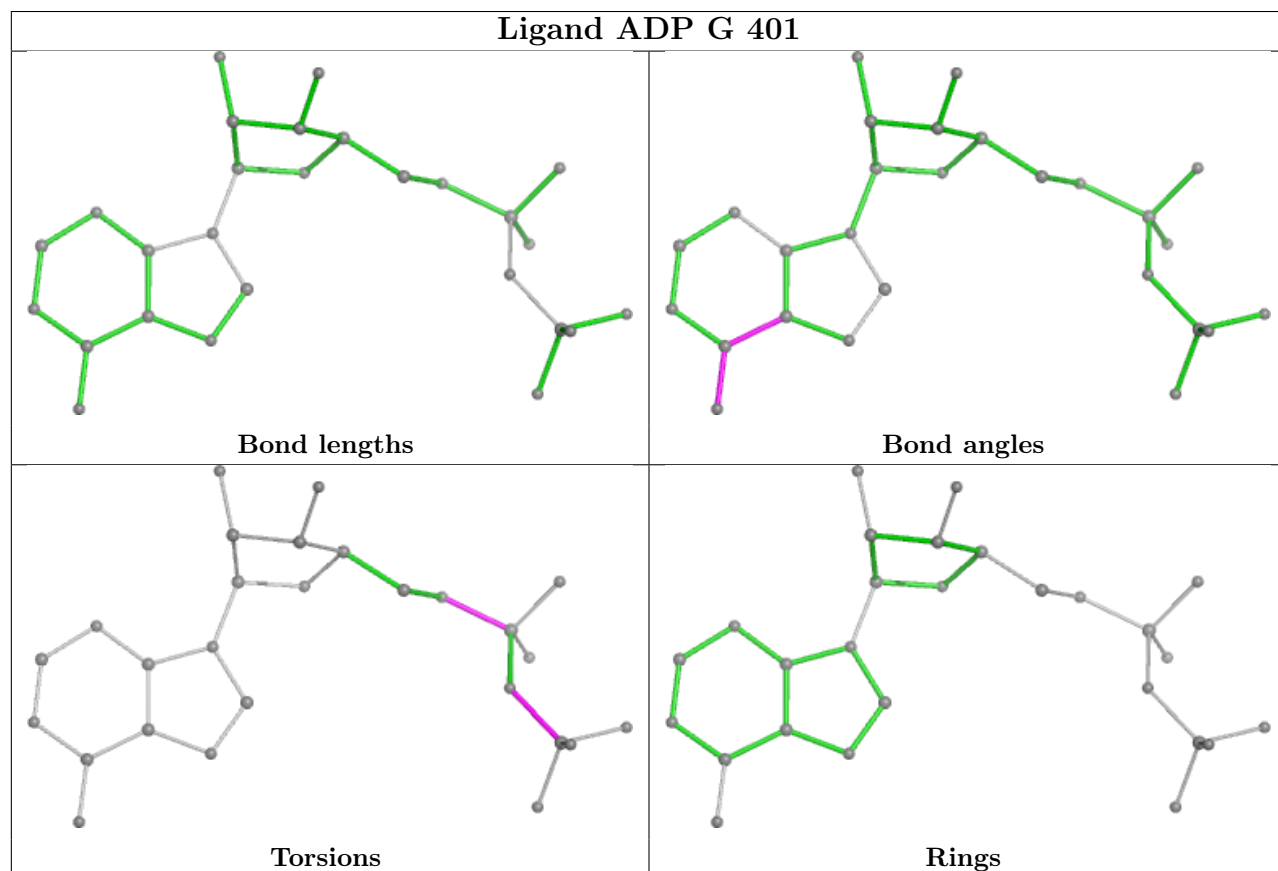
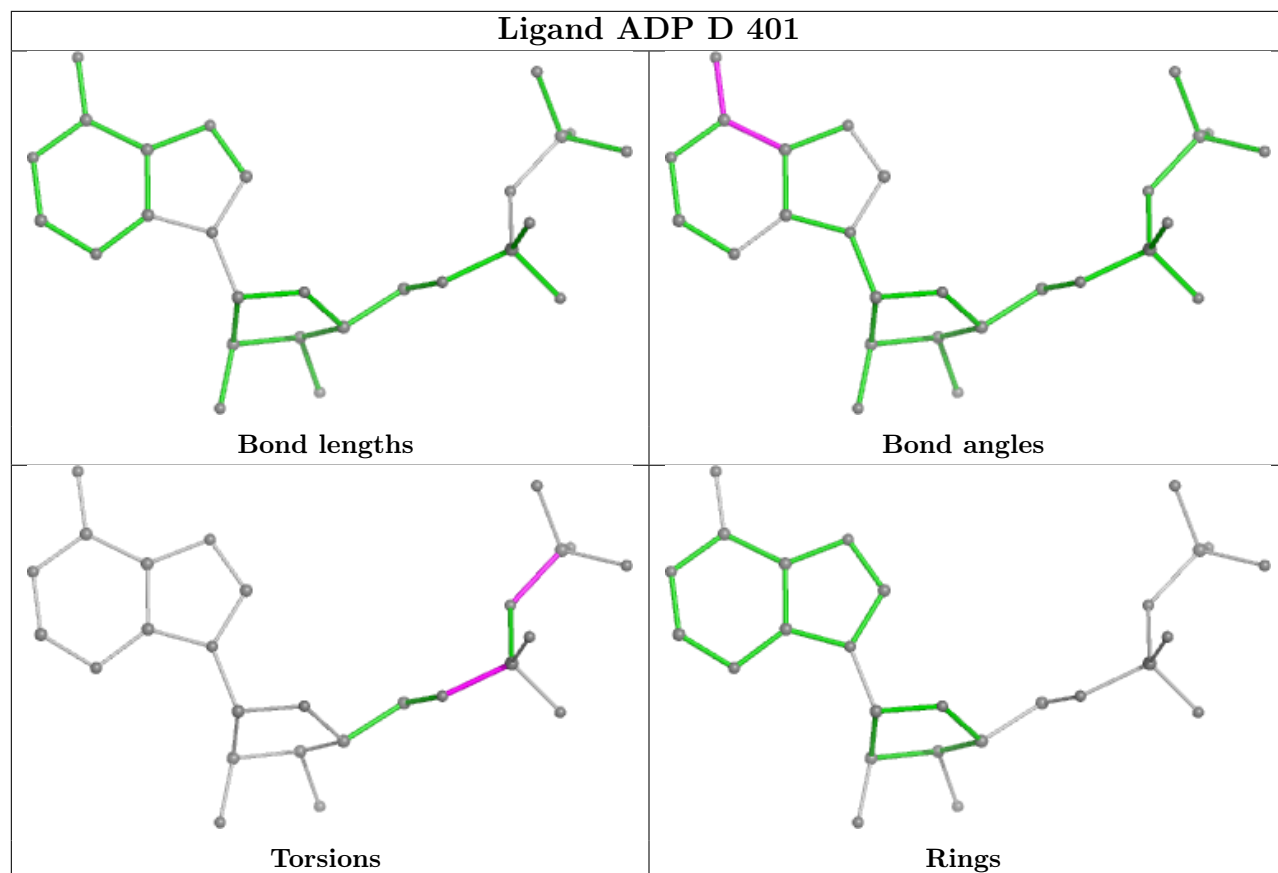
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

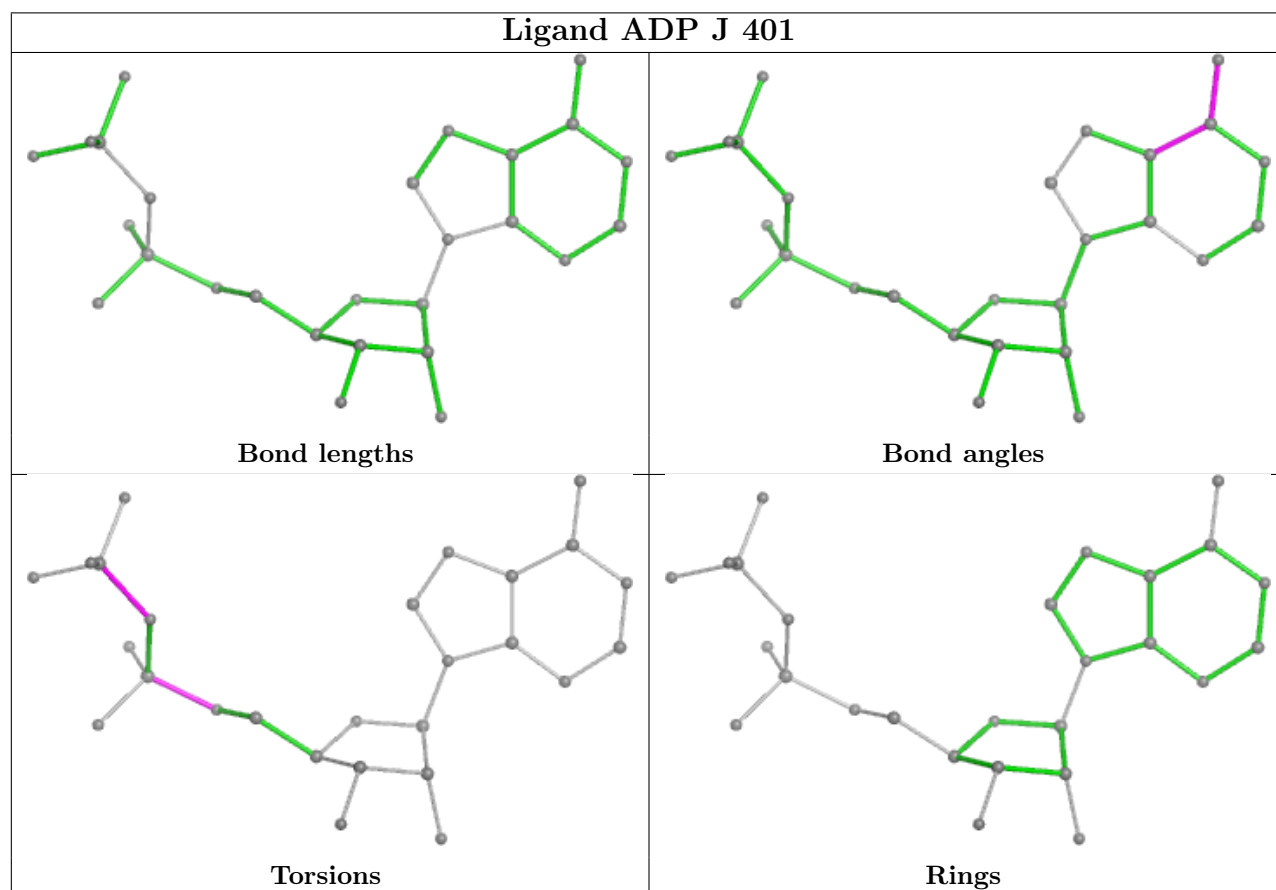
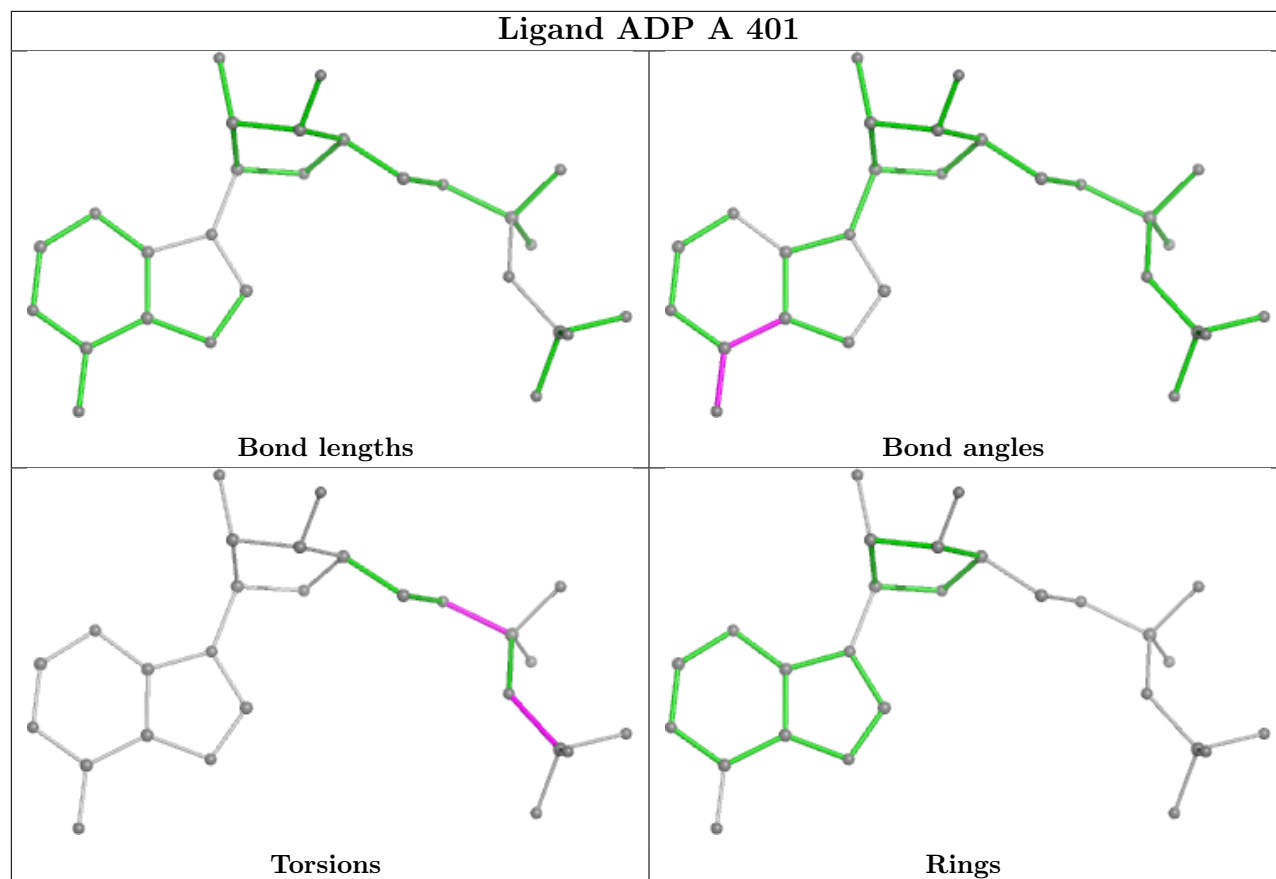




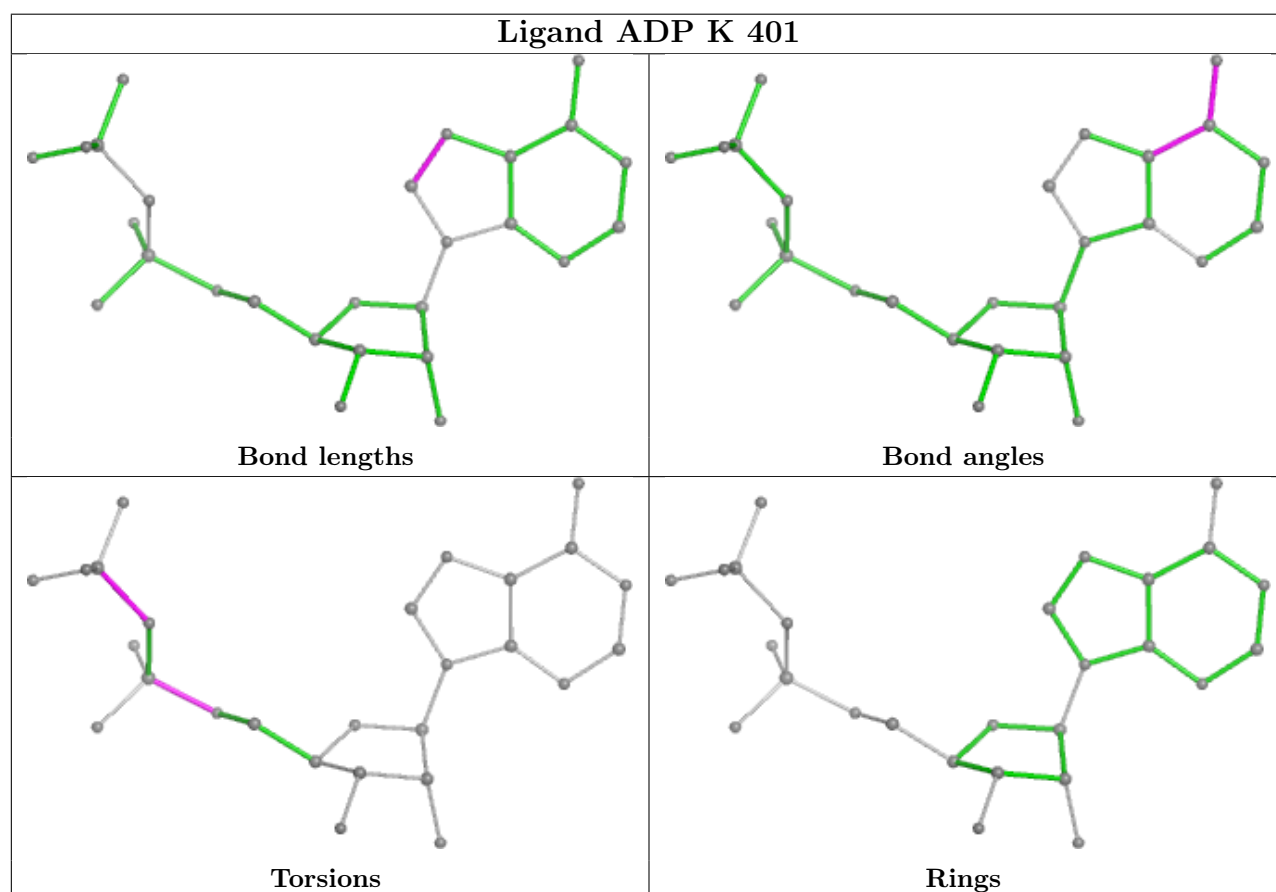
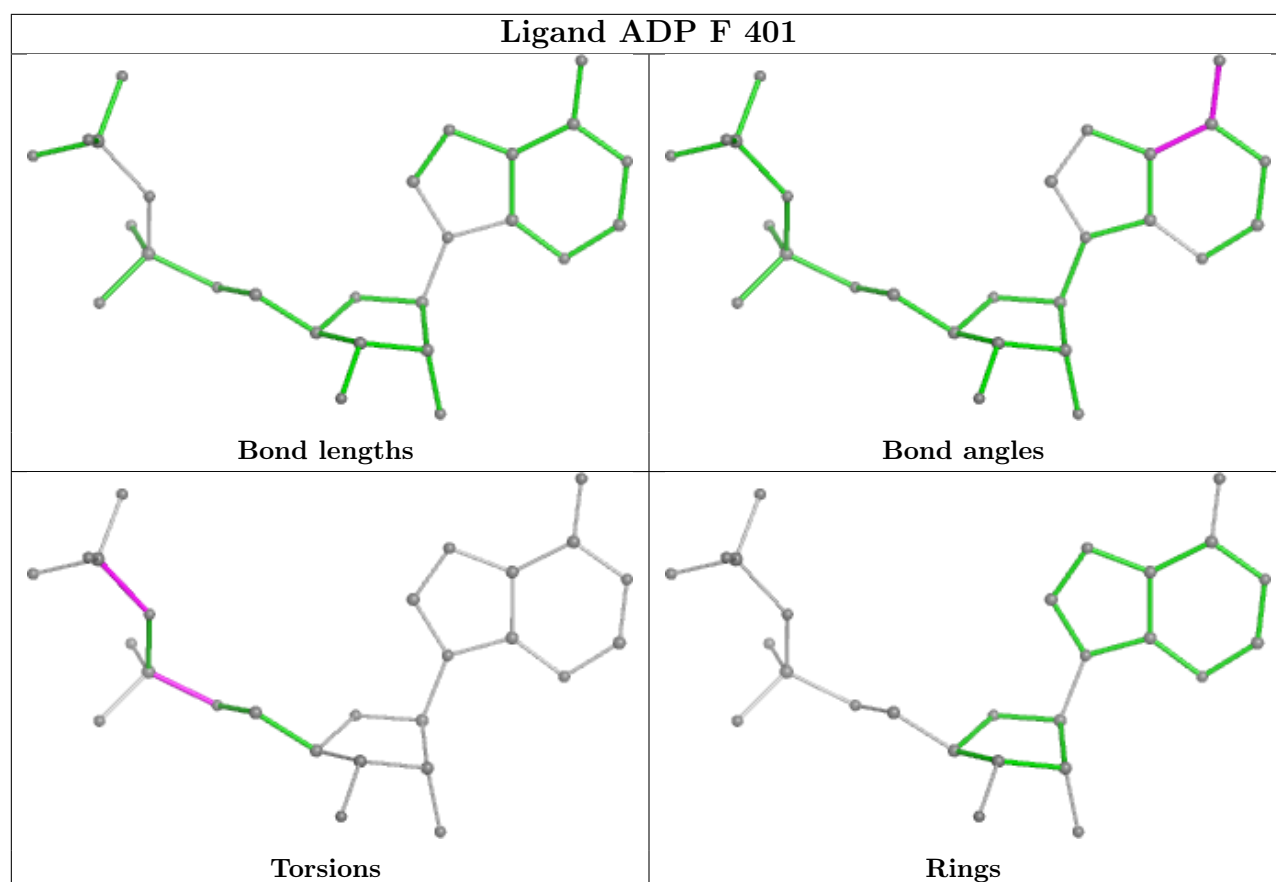












## 5.7 Other polymers [i](#)

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 [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	269/309 (87%)	-0.19	6 (2%) 62 52	22, 44, 77, 113	0
1	B	270/309 (87%)	-0.18	7 (2%) 56 46	23, 41, 73, 100	0
1	C	270/309 (87%)	0.25	13 (4%) 30 21	26, 64, 107, 130	0
1	D	270/309 (87%)	0.32	20 (7%) 14 8	26, 73, 112, 158	0
1	E	269/309 (87%)	0.17	12 (4%) 33 23	26, 63, 98, 115	0
1	F	269/309 (87%)	0.06	11 (4%) 37 27	26, 54, 87, 120	0
1	G	268/309 (86%)	0.08	16 (5%) 21 14	26, 52, 93, 137	0
1	H	269/309 (87%)	0.06	9 (3%) 46 36	26, 55, 92, 123	0
1	I	269/309 (87%)	-0.20	7 (2%) 56 46	25, 41, 73, 95	0
1	J	269/309 (87%)	-0.14	8 (2%) 50 40	26, 44, 80, 107	0
1	K	269/309 (87%)	-0.15	7 (2%) 56 46	26, 45, 81, 106	0
1	L	275/309 (88%)	-0.14	7 (2%) 57 47	26, 48, 82, 101	0
All	All	3236/3708 (87%)	-0.01	123 (3%) 40 30	22, 52, 93, 158	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	GLY	7.8
1	C	1	MET	6.3
1	J	1	MET	6.1
1	F	1	MET	6.1
1	I	84	ALA	5.9

### 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](#)

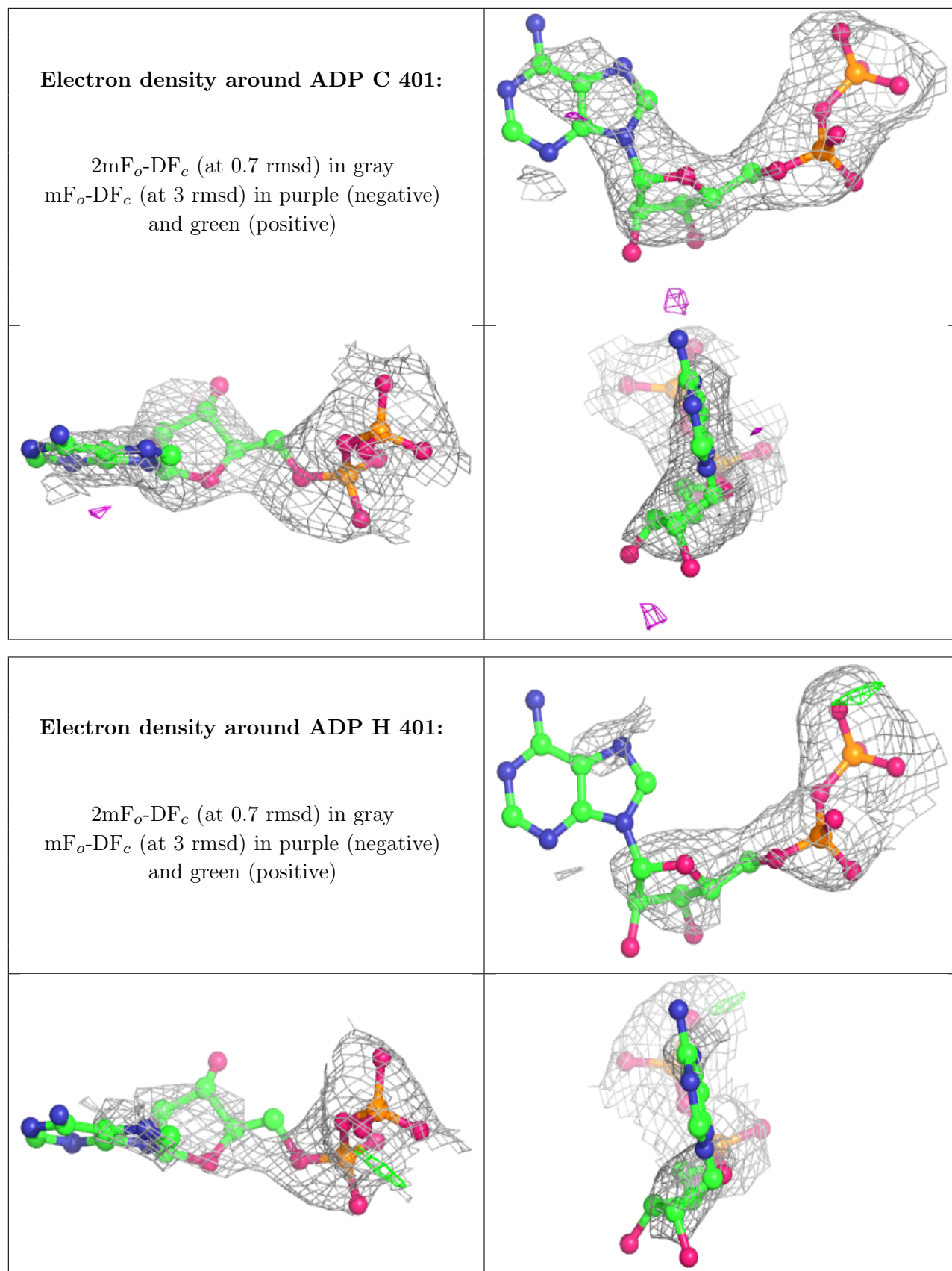
There are no monosaccharides in this entry.

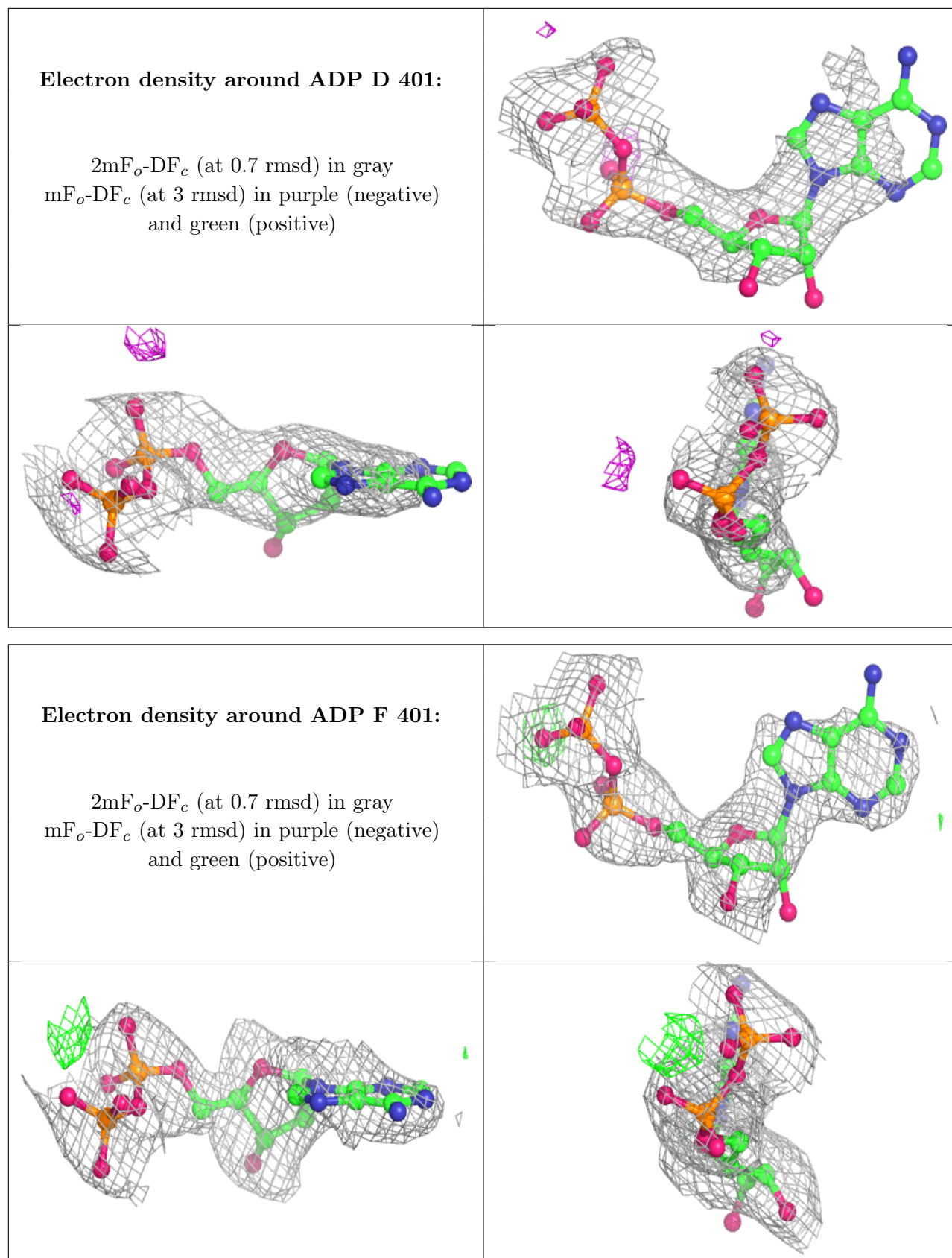
### 6.4 Ligands [i](#)

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, 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
3	ADP	C	401	27/27	0.82	0.28	70,100,119,121	0
3	ADP	H	401	27/27	0.82	0.41	77,127,140,143	0
3	ADP	D	401	27/27	0.83	0.27	82,120,135,138	0
3	ADP	F	401	27/27	0.85	0.25	62,91,106,108	0
2	CA	F	400	1/1	0.88	0.25	70,70,70,70	0
3	ADP	E	401	27/27	0.88	0.27	62,87,96,98	0
3	ADP	G	401	27/27	0.89	0.25	63,88,99,102	0
3	ADP	J	401	27/27	0.89	0.23	48,59,67,70	0
3	ADP	K	401	27/27	0.90	0.27	49,73,79,80	0
3	ADP	B	401	27/27	0.91	0.21	24,57,64,65	0
3	ADP	L	401	27/27	0.91	0.23	39,71,76,77	0
3	ADP	I	401	27/27	0.92	0.24	33,63,77,79	0
2	CA	I	400	1/1	0.92	0.13	49,49,49,49	0
2	CA	J	400	1/1	0.92	0.18	48,48,48,48	0
2	CA	B	400	1/1	0.92	0.19	55,55,55,55	0
3	ADP	A	401	27/27	0.93	0.19	33,57,62,63	0
2	CA	C	400	1/1	0.93	0.12	68,68,68,68	0
2	CA	A	400	1/1	0.93	0.25	65,65,65,65	0
2	CA	E	400	1/1	0.94	0.16	76,76,76,76	0
2	CA	H	400	1/1	0.96	0.15	68,68,68,68	0
2	CA	G	400	1/1	0.97	0.16	80,80,80,80	0
2	CA	D	400	1/1	0.97	0.17	70,70,70,70	0
2	CA	K	400	1/1	0.97	0.24	61,61,61,61	0
2	CA	L	400	1/1	0.98	0.15	50,50,50,50	0

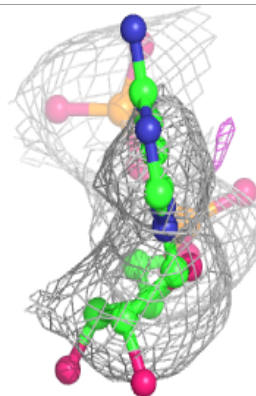
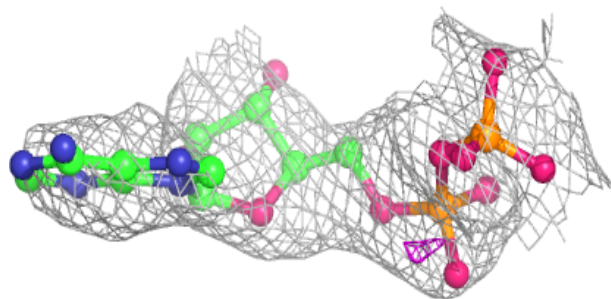
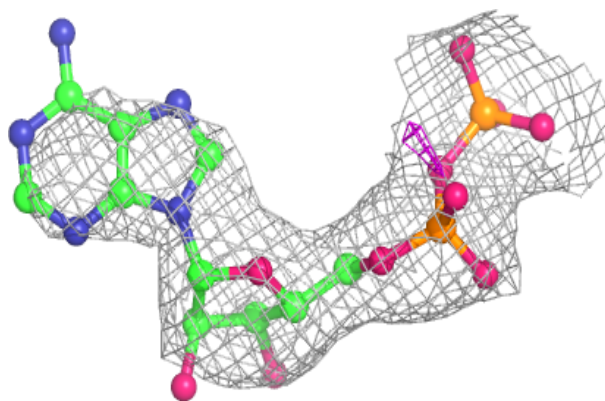
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



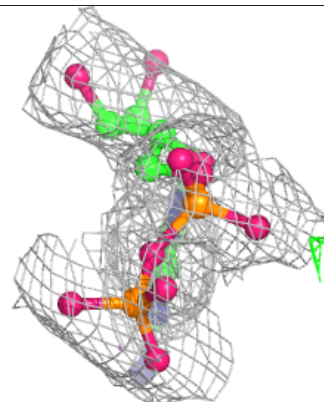
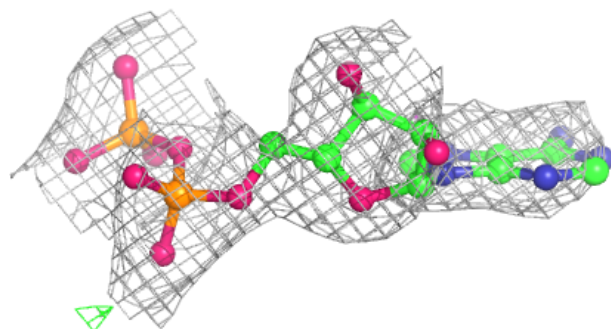
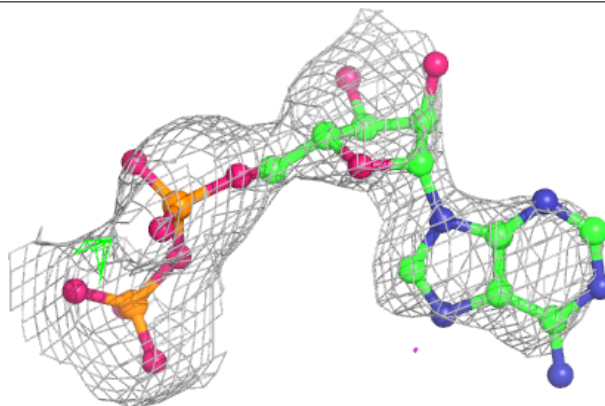


**Electron density around ADP E 401:**

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

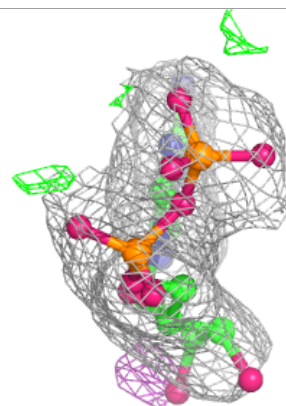
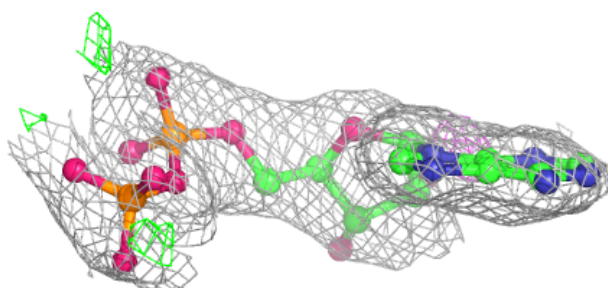
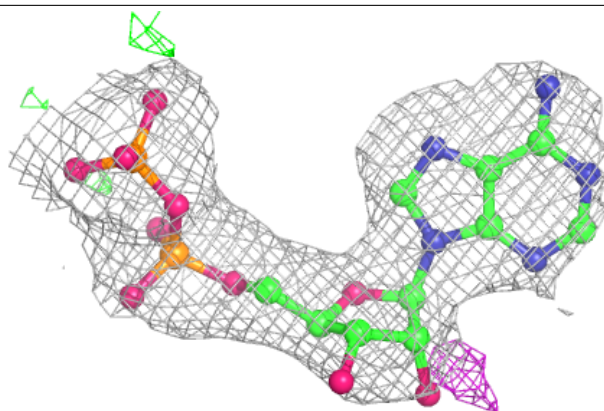
**Electron density around ADP G 401:**

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

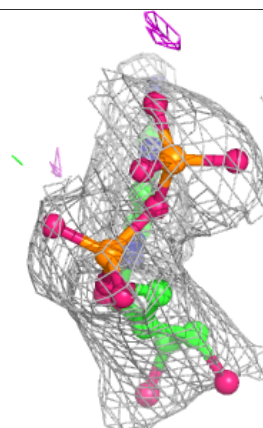
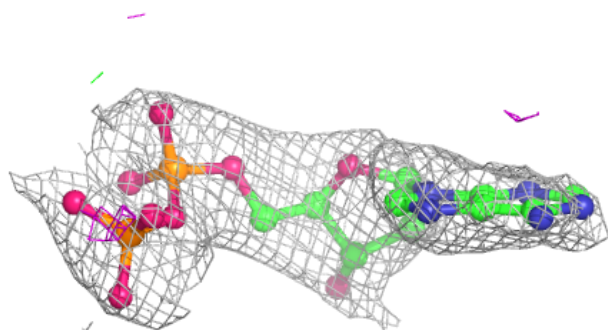
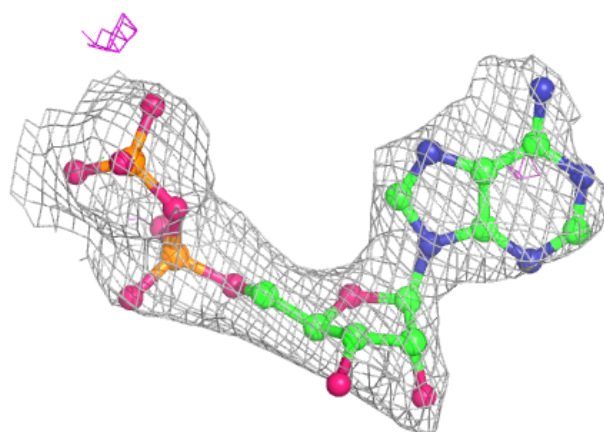


**Electron density around ADP J 401:**

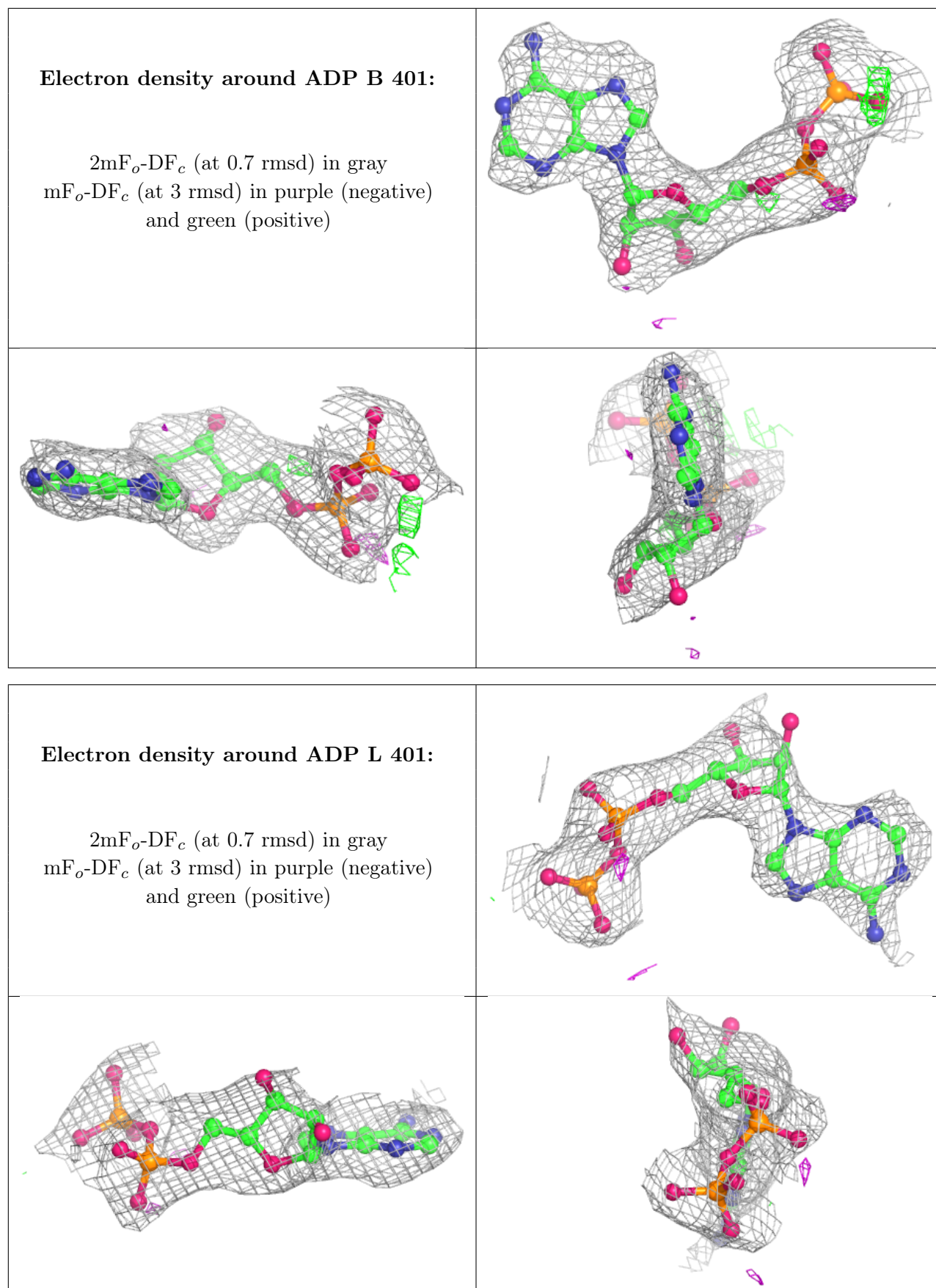
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP K 401:**

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

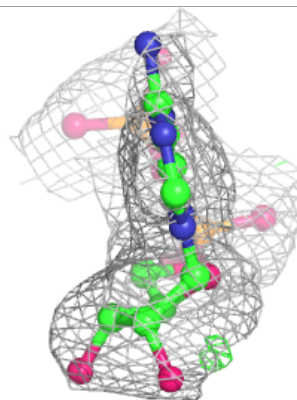
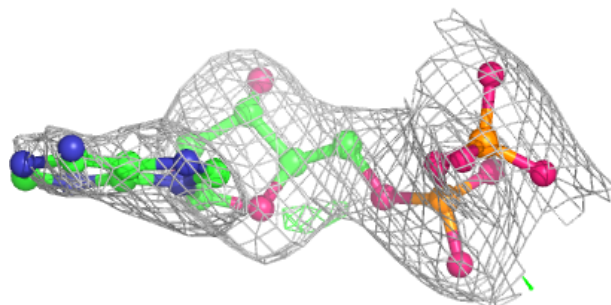
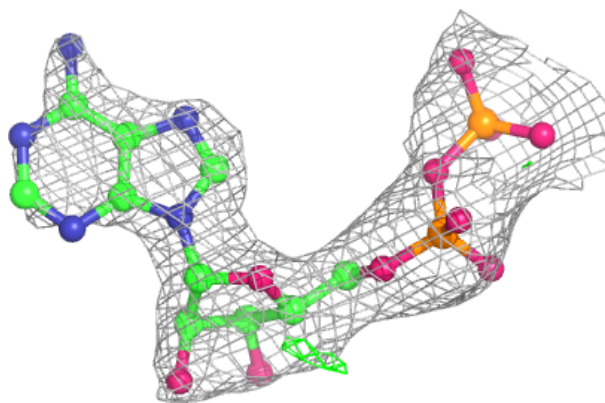




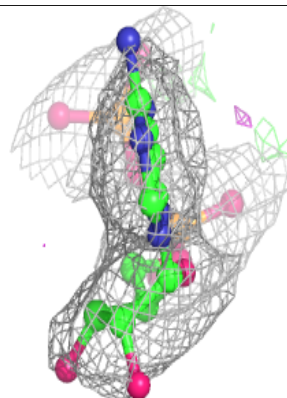
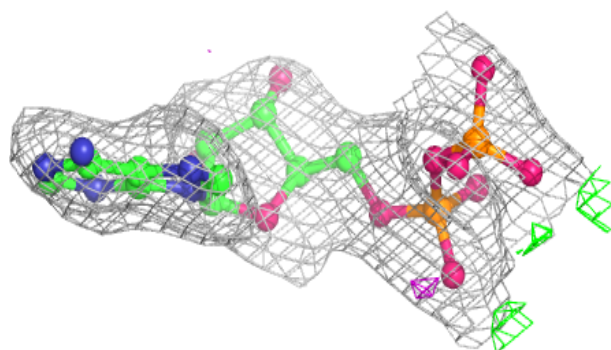
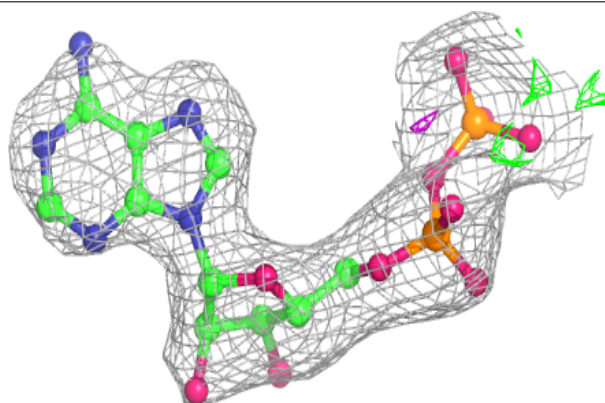


**Electron density around ADP I 401:**

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

**Electron density around ADP A 401:**

$2mF_o-DF_c$  (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.