



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2021 – 07:03 PM JST

PDB ID : 7COR  
Title : Hexameric Ring Complex of Engineered V1-ATPase bound to 5 ADPs: A3(D  
e)3\_(ADP-Pi)1cat(ADP)2cat,2non-cat  
Authors : Kosugi, T.; Tanabe, M.; Koga, N.  
Deposited on : 2020-08-05  
Resolution : 2.90 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

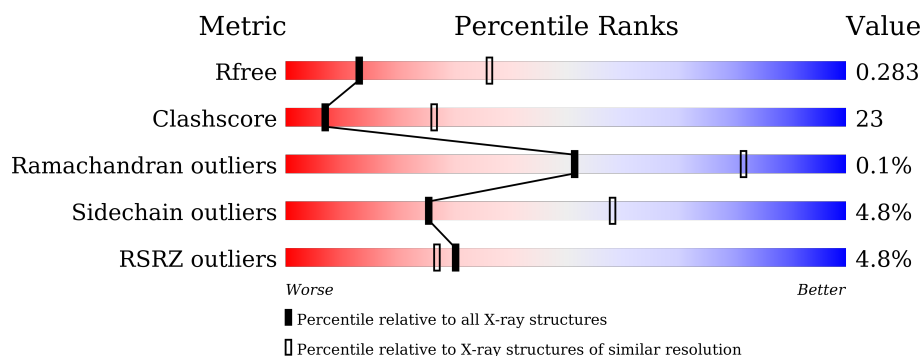
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	596	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div>..</div> </div> </div>
1	B	596	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>37%</div> <div>..</div> </div> </div>
1	C	596	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>32%</div> <div>..</div> </div> </div>
2	D	458	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>. .</div> </div> </div>
2	E	458	<div> <div>9%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>. .</div> </div> </div>
2	F	458	<div> <div>12%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>. 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	602	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24282 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4571	2871	767	907	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	0	0
			4549	2858	764	901	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

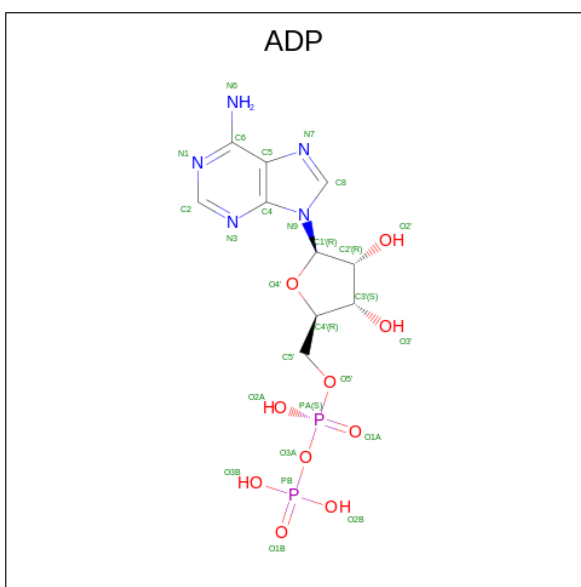
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	444	Total	C	N	O	S	0	0	0
			3471	2196	596	665	14			
2	E	440	Total	C	N	O	S	0	0	0
			3450	2186	592	658	14			
2	F	433	Total	C	N	O	S	0	1	0
			3402	2154	586	648	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

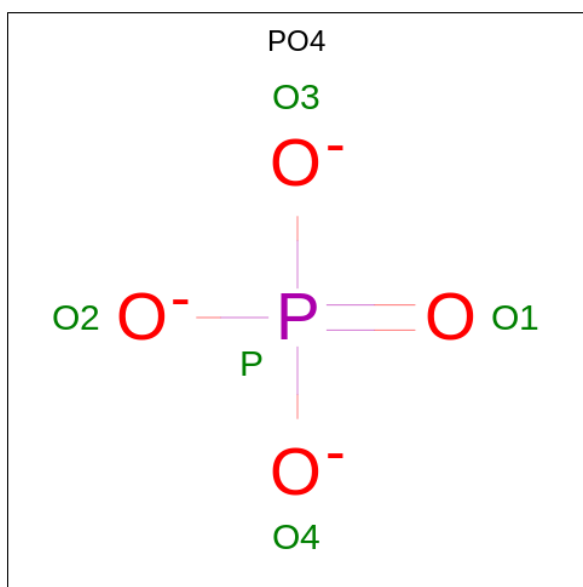


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



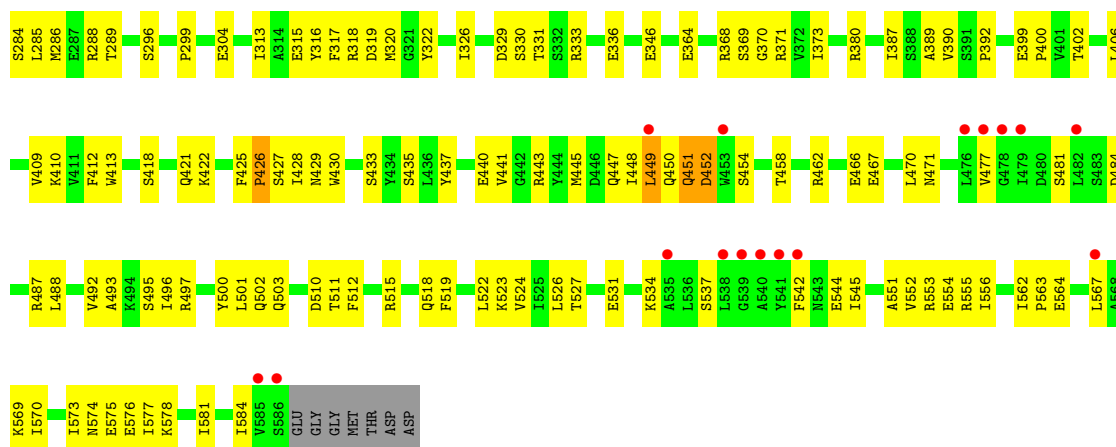
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

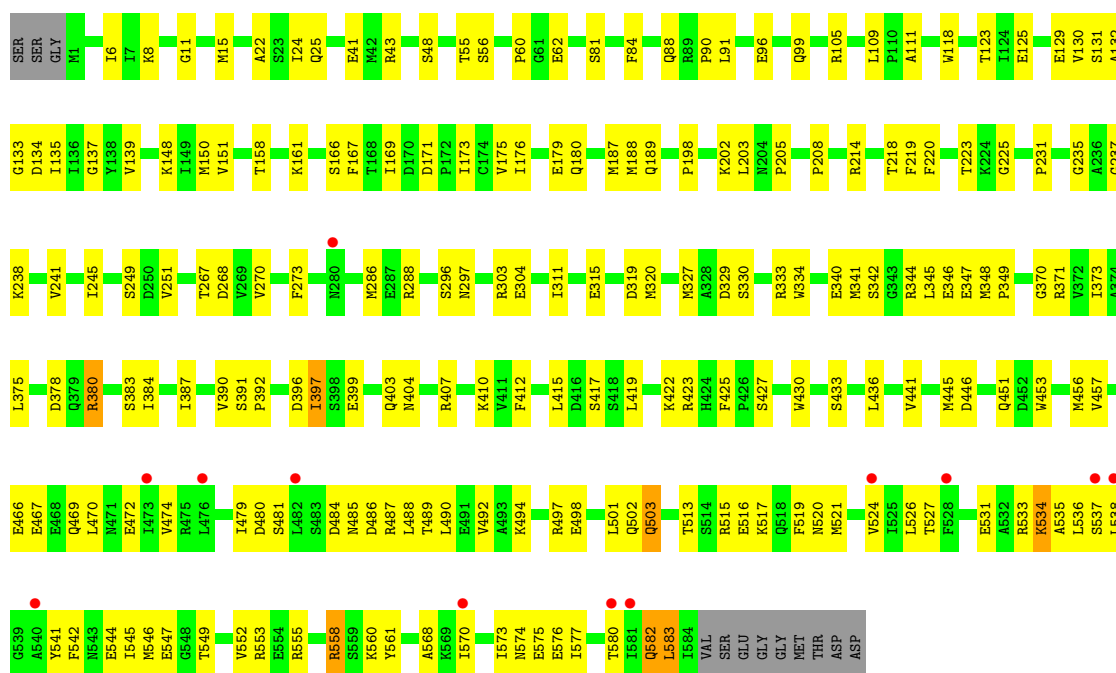
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	11	Total	O	0	0
			11	11		
6	C	35	Total	O	0	0
			35	35		
6	D	23	Total	O	0	0
			23	23		
6	E	15	Total	O	0	0
			15	15		
6	F	12	Total	O	0	0
			12	12		



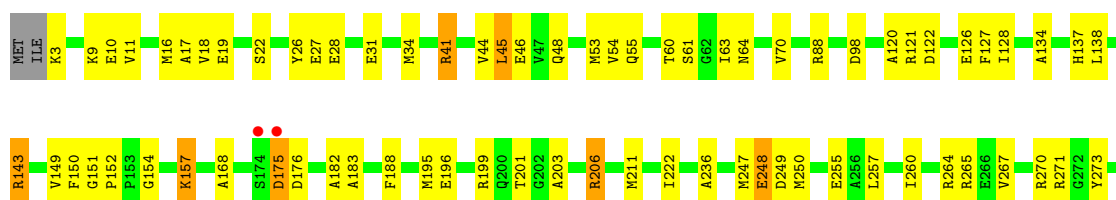


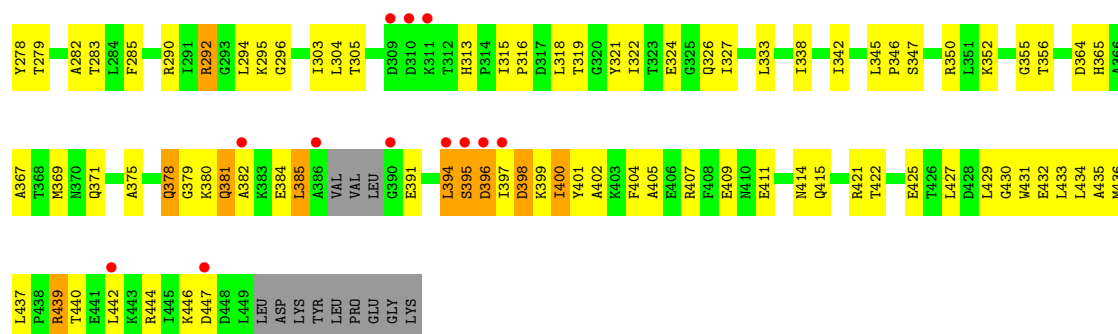


• Molecule 1: V-type sodium ATPase catalytic subunit A

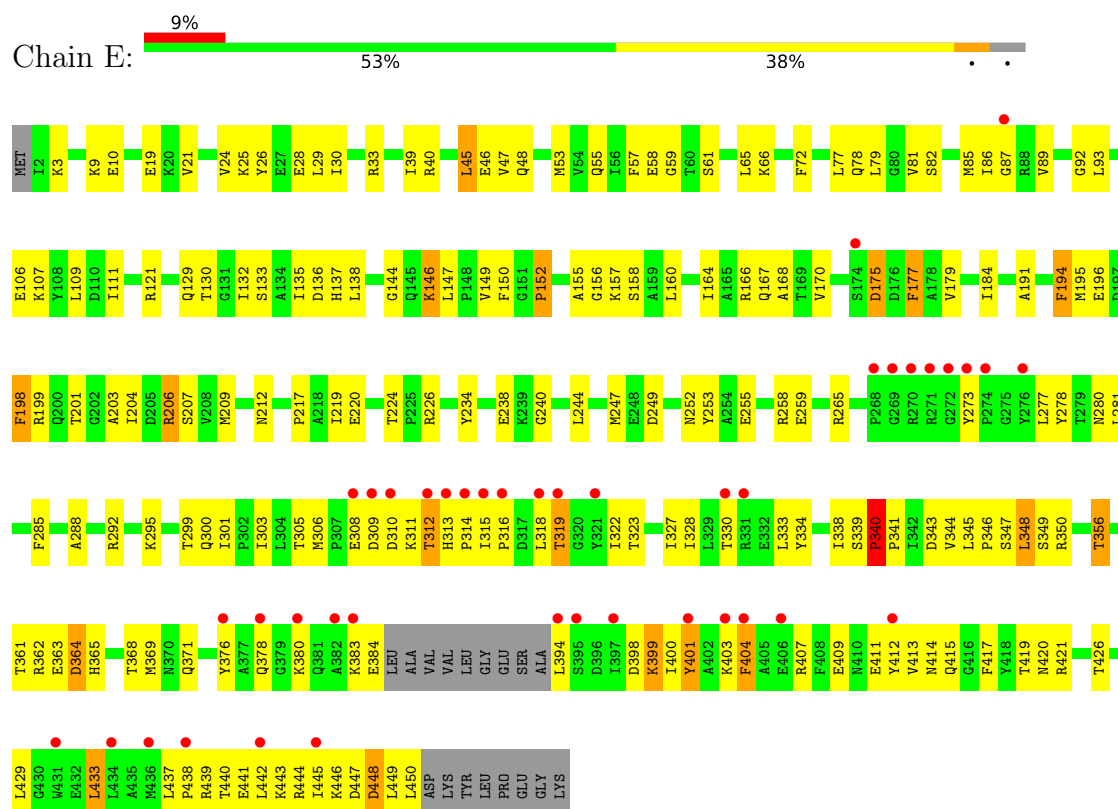


• Molecule 2: V-type sodium ATPase subunit B

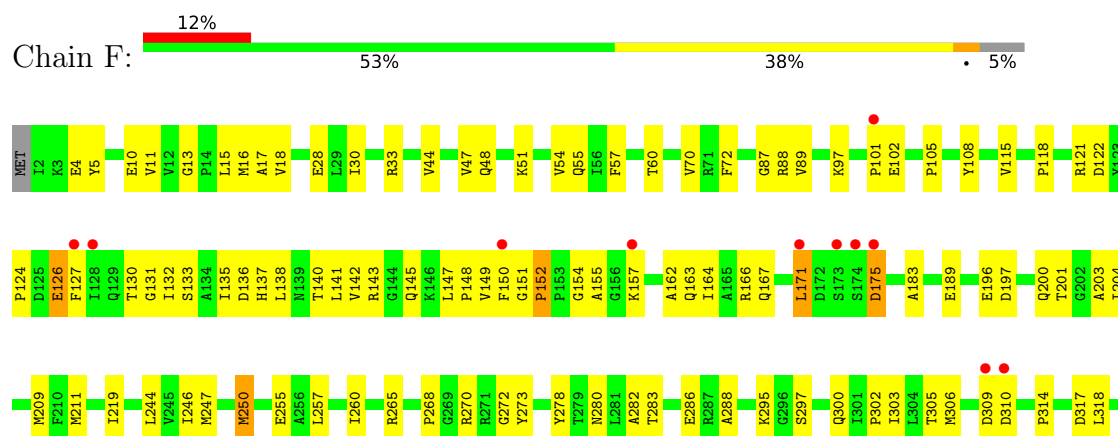




• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.76Å 126.73Å 123.81Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	44.62 – 2.90 44.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.62-2.90) 100.0 (44.58-2.90)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.231 , 0.287 0.232 , 0.283	Depositor DCC
$R_{free}$ test set	4066 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, PO4

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	0.55	1/4647 (0.0%)	0.55	5/6287 (0.1%)
1	B	0.51	0/4638	0.57	2/6275 (0.0%)
1	C	0.48	0/4625	0.52	0/6257
2	D	0.48	0/3531	0.58	0/4770
2	E	0.60	1/3510 (0.0%)	0.75	2/4742 (0.0%)
2	F	0.46	0/3461	0.61	0/4673
All	All	0.52	2/24412 (0.0%)	0.59	9/33004 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	GLU	CD-OE1	-5.25	1.19	1.25
2	E	28	GLU	CD-OE2	-5.06	1.20	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	340	PRO	CA-N-CD	-7.99	100.31	111.50
1	B	426	PRO	N-CA-C	-6.83	94.33	112.10
1	B	409	VAL	N-CA-C	6.26	127.90	111.00
1	A	237	GLY	N-CA-C	-5.47	99.42	113.10
1	A	236	ALA	N-CA-C	-5.46	96.27	111.00

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	4571	0	4533	168	1
1	B	4562	0	4528	176	0
1	C	4549	0	4513	163	0
2	D	3471	0	3485	154	0
2	E	3450	0	3471	242	1
2	F	3402	0	3418	238	0
3	A	27	0	12	4	0
3	B	27	0	12	1	0
3	C	27	0	12	4	0
3	D	27	0	12	2	0
3	E	27	0	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	5	0
6	A	36	0	0	1	0
6	B	11	0	0	1	0
6	C	35	0	0	1	0
6	D	23	0	0	0	0
6	E	15	0	0	1	0
6	F	12	0	0	1	0
All	All	24282	0	24008	1098	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 23.

The worst 5 of 1098 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:E:277:LEU:CG	2:E:318:LEU:HD11	1.27	1.63
2:F:407:ARG:HH11	2:F:436:MET:CE	1.00	1.62
2:E:277:LEU:HG	2:E:318:LEU:CD1	1.33	1.55
2:D:401:TYR:HE1	2:D:437:LEU:CD2	1.32	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:TYR:CE1	2:D:437:LEU:HD21	1.55	1.40

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:544:GLU:OE1	2:E:446:LYS:NZ[2_555]	1.90	0.30

## 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	585/596 (98%)	564 (96%)	21 (4%)	0	100	100
1	B	584/596 (98%)	568 (97%)	16 (3%)	0	100	100
1	C	582/596 (98%)	565 (97%)	17 (3%)	0	100	100
2	D	440/458 (96%)	420 (96%)	20 (4%)	0	100	100
2	E	436/458 (95%)	409 (94%)	25 (6%)	2 (0%)	29	61
2	F	429/458 (94%)	402 (94%)	26 (6%)	1 (0%)	47	78
All	All	3056/3162 (97%)	2928 (96%)	125 (4%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	340	PRO
2	E	152	PRO
2	F	152	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/509 (99%)	497 (99%)	6 (1%)	71	91
1	B	502/509 (99%)	480 (96%)	22 (4%)	28	61
1	C	500/509 (98%)	481 (96%)	19 (4%)	33	67
2	D	367/380 (97%)	340 (93%)	27 (7%)	13	38
2	E	366/380 (96%)	341 (93%)	25 (7%)	16	42
2	F	360/380 (95%)	334 (93%)	26 (7%)	14	39
All	All	2598/2667 (97%)	2473 (95%)	125 (5%)	25	58

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	249	ASP
2	F	336	SER
2	D	439	ARG
2	F	309	ASP
2	F	436	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	414	ASN
2	F	137	HIS
2	F	300	GLN
2	F	163	GLN
1	A	424	HIS

### 5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	E	600	4	24,29,29	0.65	0	29,45,45	1.21	4 (13%)
3	ADP	D	600	4	24,29,29	0.56	0	29,45,45	1.27	3 (10%)
5	PO4	A	602	4	4,4,4	1.02	0	6,6,6	0.71	0
3	ADP	B	600	4	24,29,29	0.60	0	29,45,45	1.38	5 (17%)
3	ADP	A	600	4	24,29,29	0.65	0	29,45,45	1.39	3 (10%)
3	ADP	C	600	4	24,29,29	0.67	0	29,45,45	1.14	2 (6%)

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	E	600	4	-	3/12/32/32	0/3/3/3
3	ADP	D	600	4	-	2/12/32/32	0/3/3/3
3	ADP	B	600	4	-	5/12/32/32	0/3/3/3
3	ADP	A	600	4	-	6/12/32/32	0/3/3/3
3	ADP	C	600	4	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ADP	C3'-C2'-C1'	3.42	106.13	100.98
3	B	600	ADP	C3'-C2'-C1'	3.34	106.00	100.98
3	B	600	ADP	PA-O3A-PB	-3.23	121.75	132.83
3	E	600	ADP	C3'-C2'-C1'	2.74	105.11	100.98
3	E	600	ADP	C5-C6-N6	2.67	124.41	120.35

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

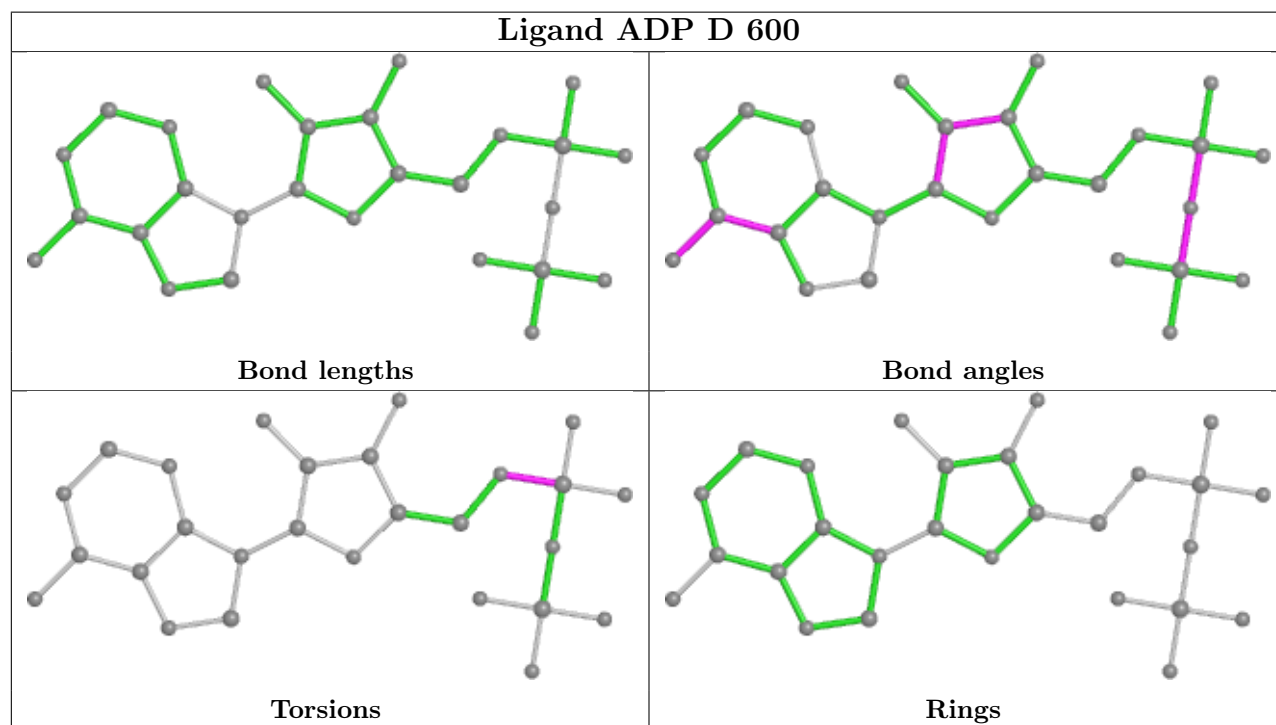
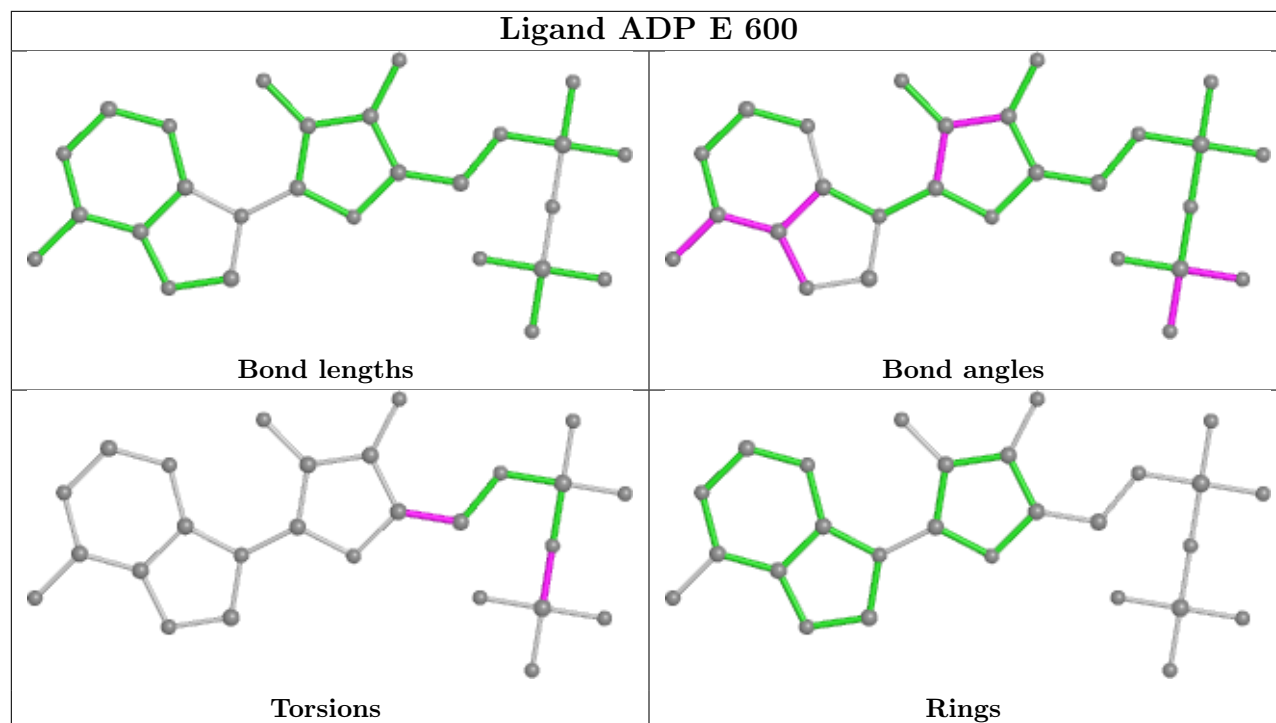
Mol	Chain	Res	Type	Atoms
3	A	600	ADP	PA-O3A-PB-O3B
3	A	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O2A
3	C	600	ADP	C5'-O5'-PA-O1A

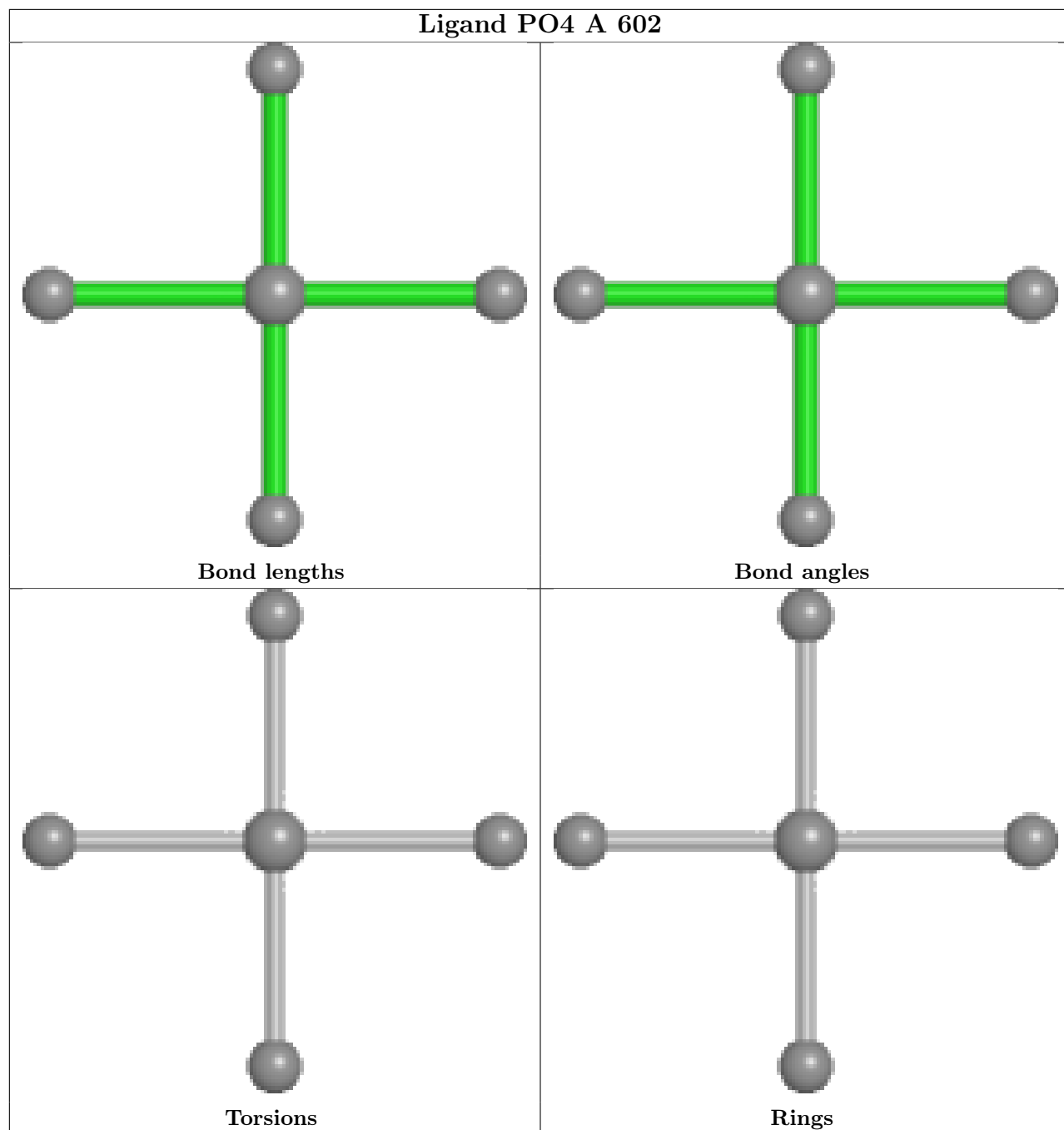
There are no ring outliers.

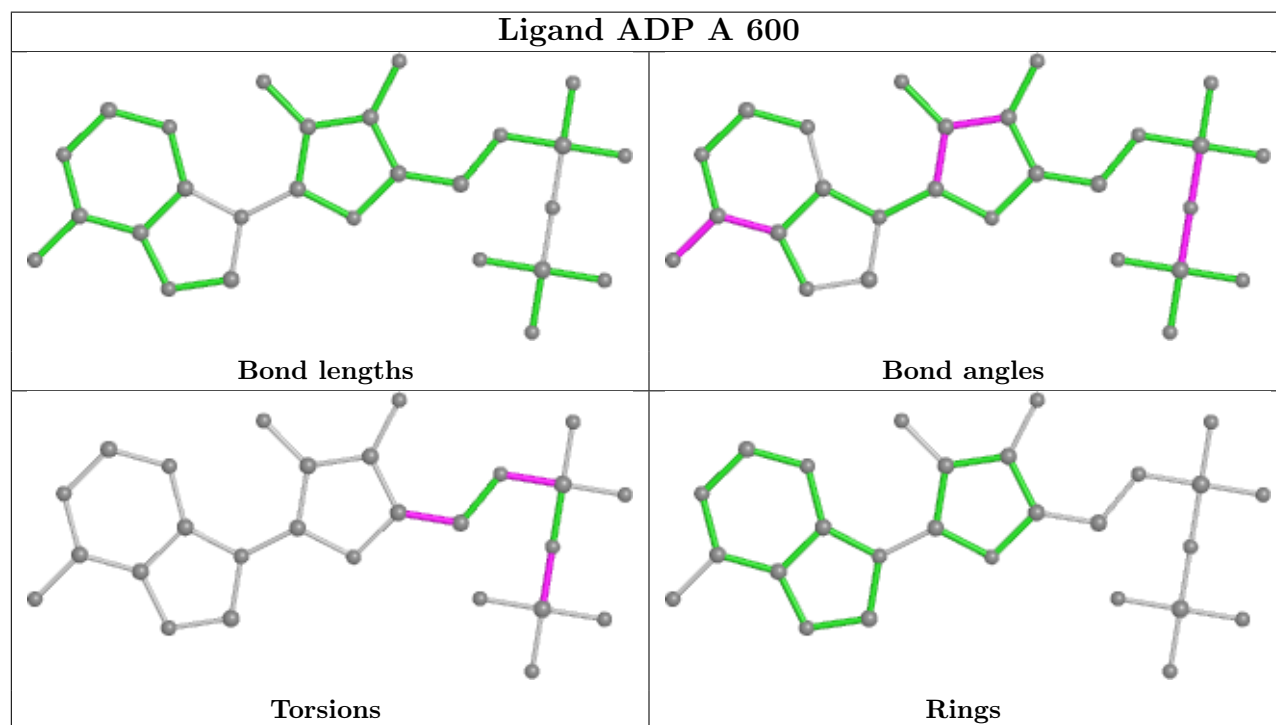
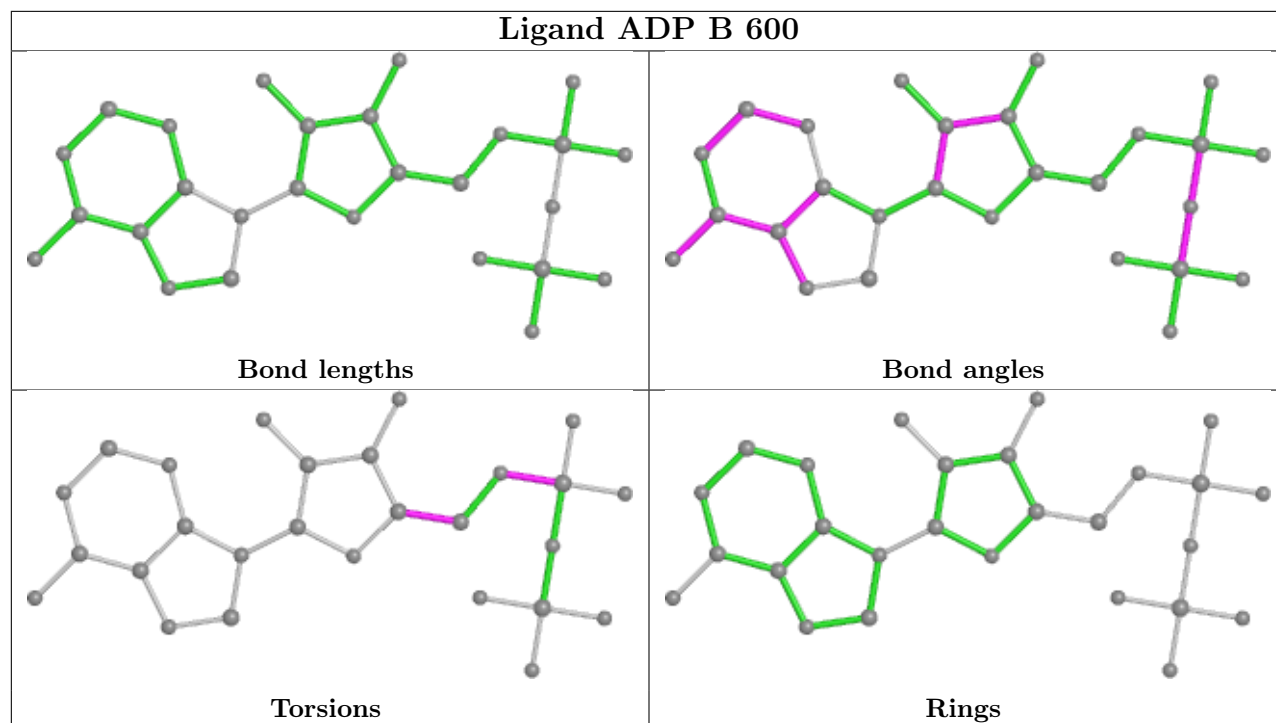
6 monomers are involved in 21 short contacts:

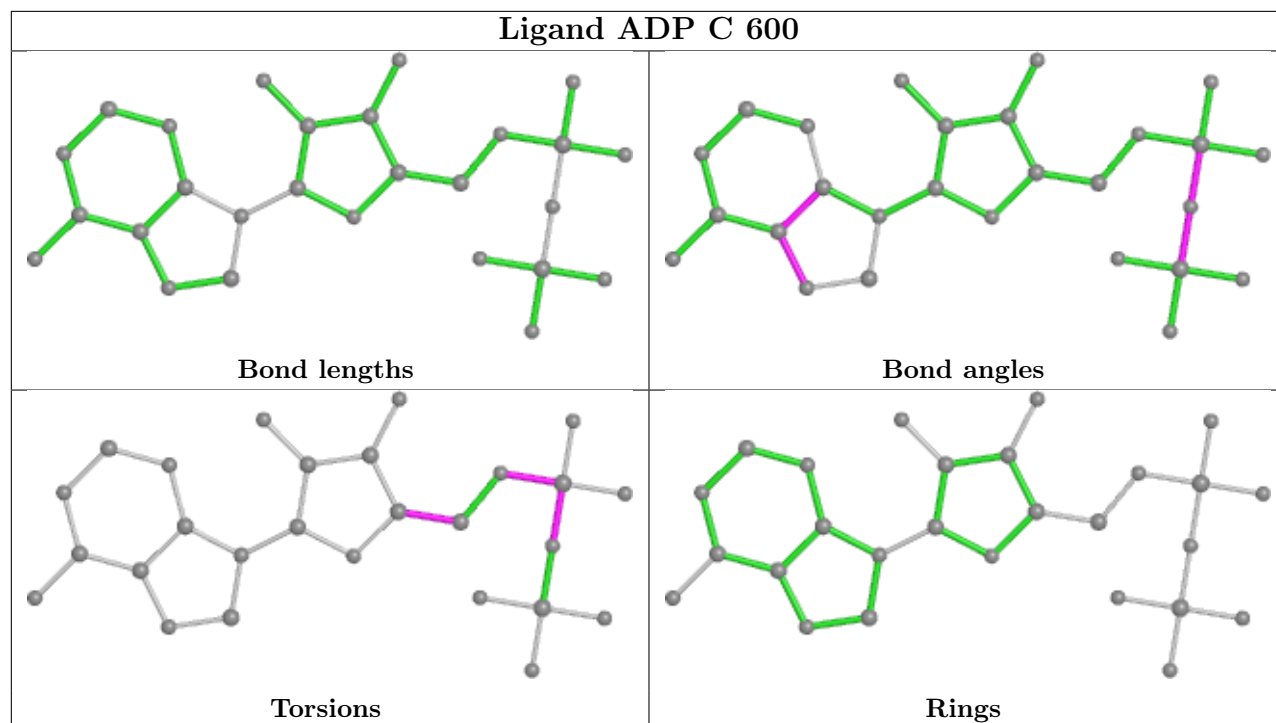
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	600	ADP	5	0
3	D	600	ADP	2	0
5	A	602	PO4	5	0
3	B	600	ADP	1	0
3	A	600	ADP	4	0
3	C	600	ADP	4	0

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	587/596 (98%)	-0.01	4 (0%) 87 87	28, 49, 80, 101	0
1	B	586/596 (98%)	0.19	21 (3%) 42 37	33, 69, 106, 130	0
1	C	584/596 (97%)	0.05	12 (2%) 63 61	25, 46, 107, 124	0
2	D	444/458 (96%)	0.00	14 (3%) 47 43	26, 44, 98, 145	0
2	E	440/458 (96%)	0.49	42 (9%) 8 6	33, 79, 133, 155	0
2	F	433/458 (94%)	0.60	55 (12%) 3 2	27, 67, 131, 154	0
All	All	3074/3162 (97%)	0.20	148 (4%) 30 27	25, 57, 115, 155	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	174	SER	6.6
2	F	401	TYR	6.6
2	E	394	LEU	6.2
2	F	431	TRP	6.0
2	E	318	LEU	6.0

### 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

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.

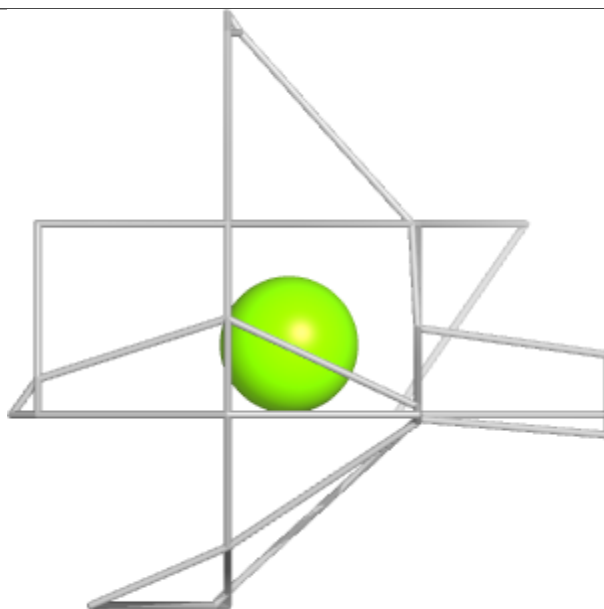
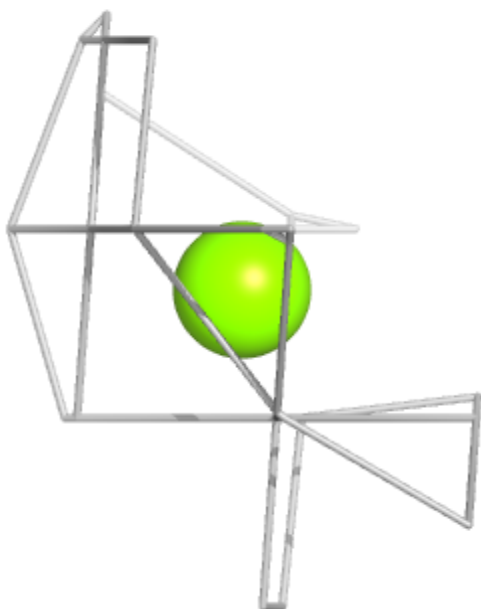
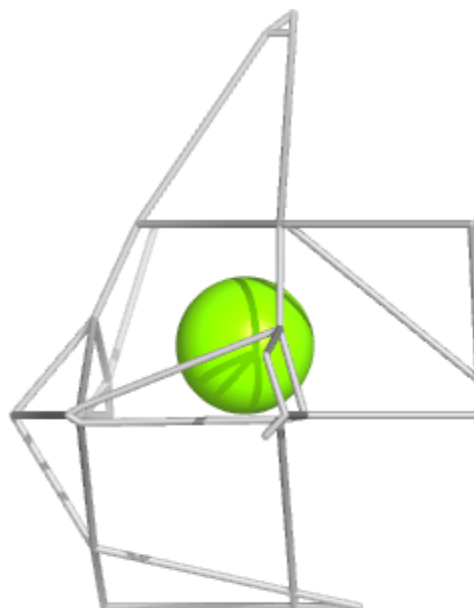
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	E	601	1/1	0.80	0.17	102,102,102,102	0
3	ADP	E	600	27/27	0.81	0.26	95,109,136,148	0
3	ADP	D	600	27/27	0.85	0.25	58,73,94,98	0
5	PO4	A	602	5/5	0.87	0.25	49,50,54,69	0
3	ADP	C	600	27/27	0.90	0.27	54,65,76,81	0
4	MG	A	601	1/1	0.90	0.48	39,39,39,39	0
4	MG	D	601	1/1	0.93	0.17	66,66,66,66	0
3	ADP	A	600	27/27	0.93	0.28	39,48,56,60	0
3	ADP	B	600	27/27	0.93	0.20	63,72,79,81	0
4	MG	C	601	1/1	0.97	0.51	48,48,48,48	0
4	MG	B	601	1/1	0.98	0.29	63,63,63,63	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.



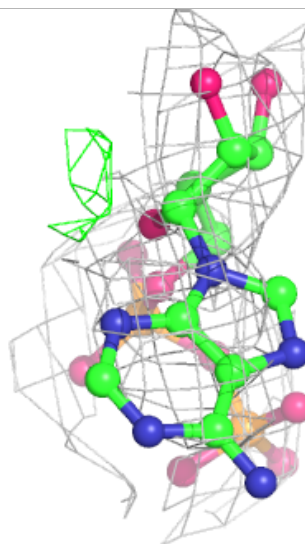
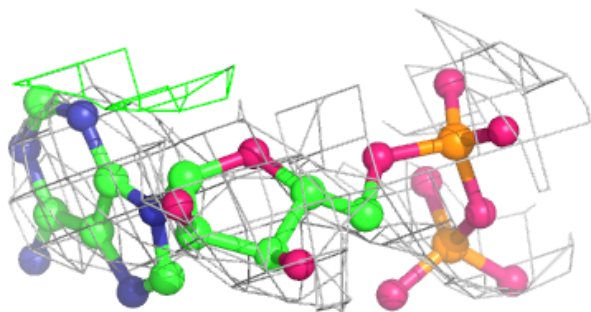
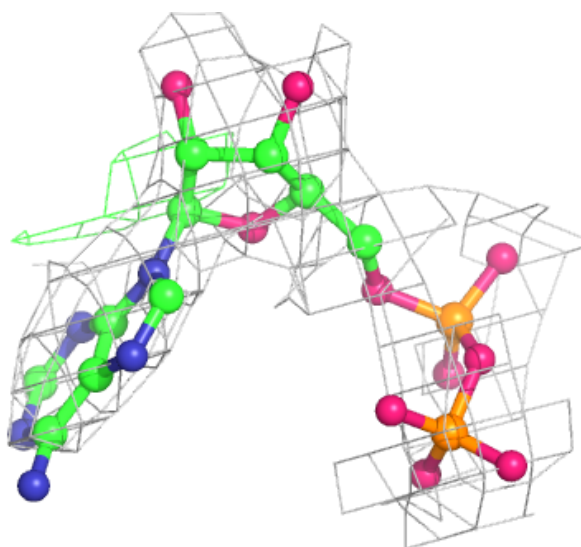
**Electron density around MG E 601:**

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



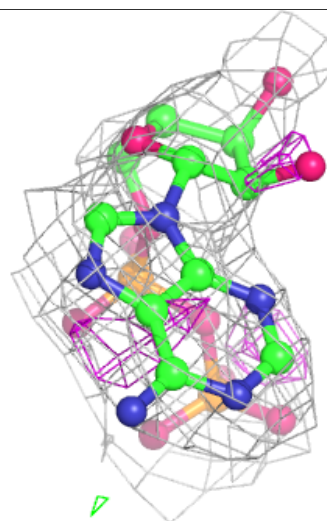
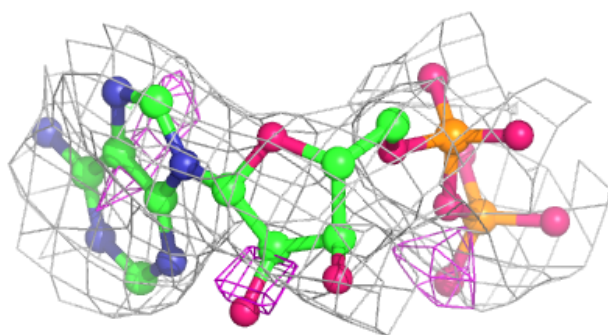
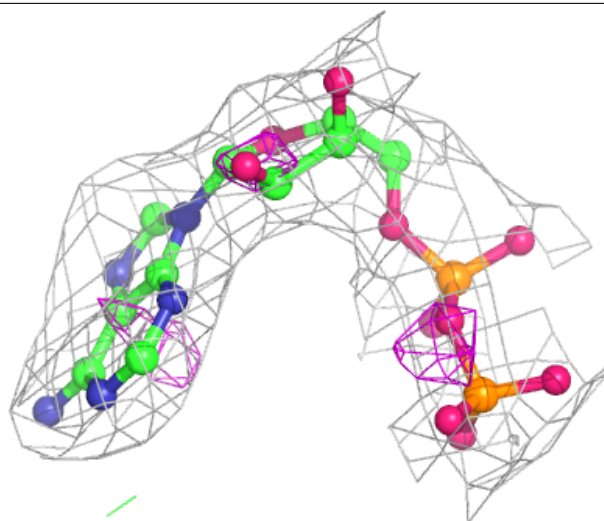
**Electron density around ADP E 600:**

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



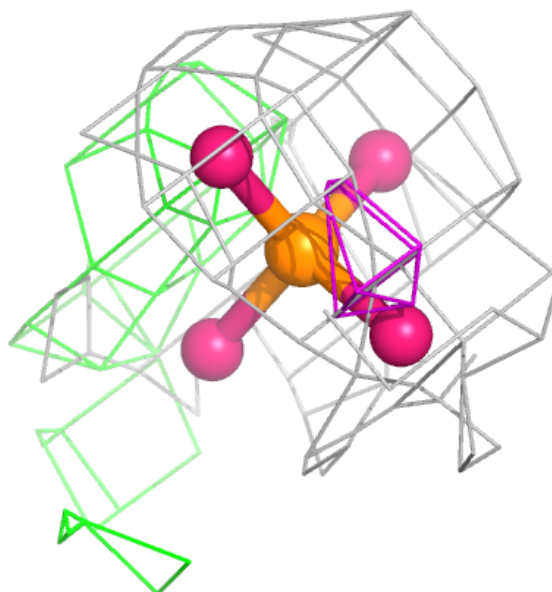
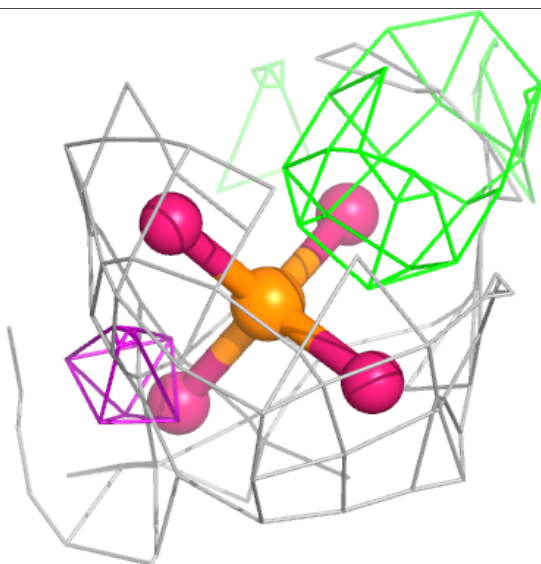
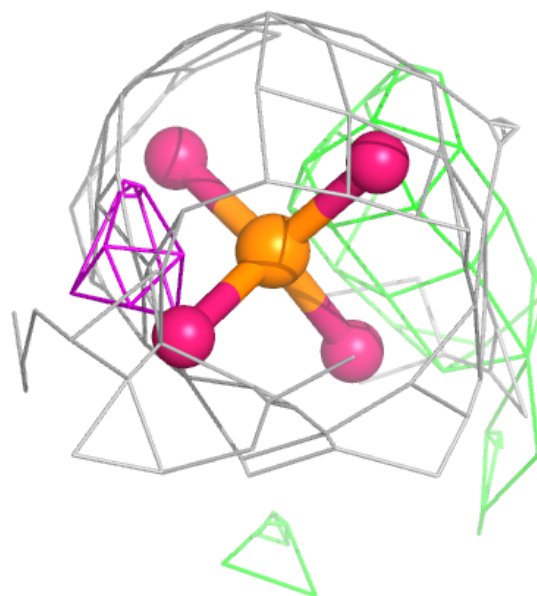
**Electron density around ADP D 600:**

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



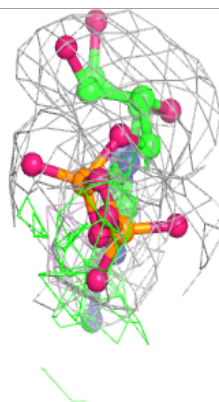
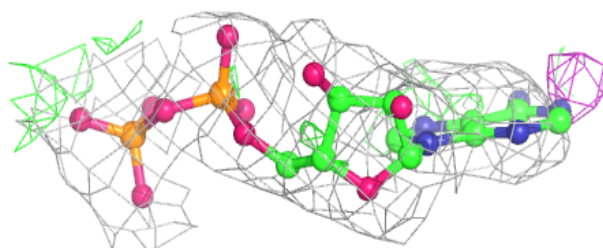
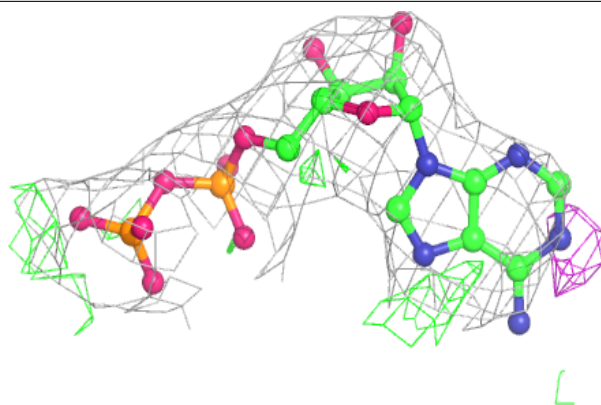
**Electron density around PO4 A 602:**

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



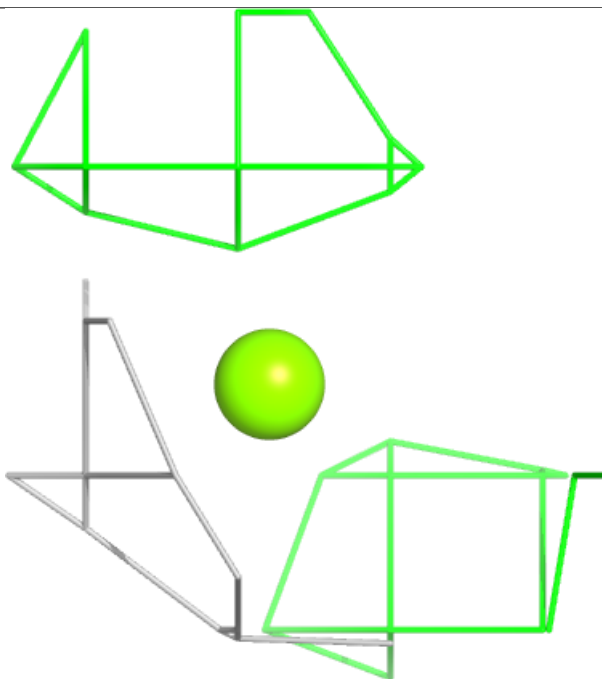
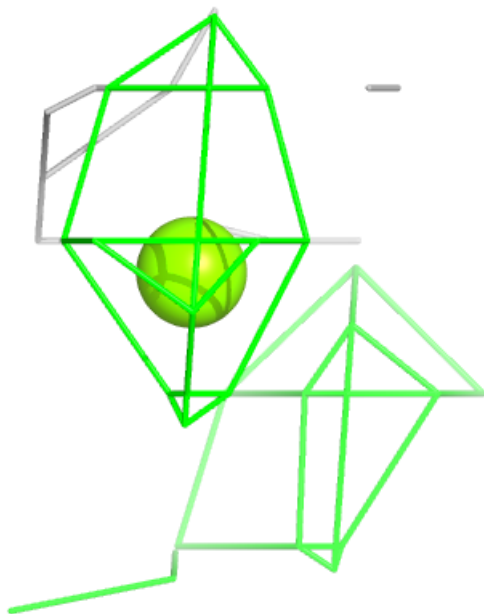
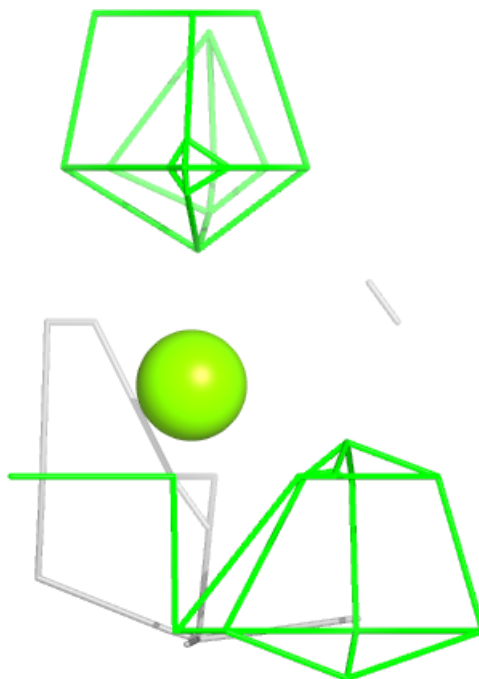
**Electron density around ADP C 600:**

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



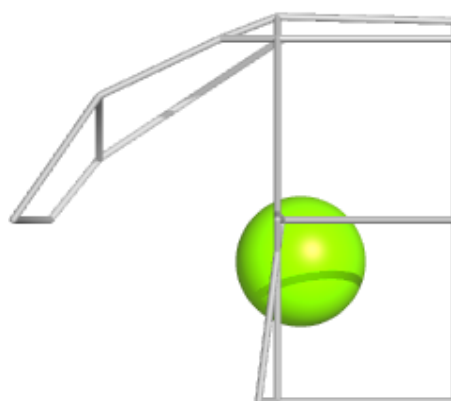
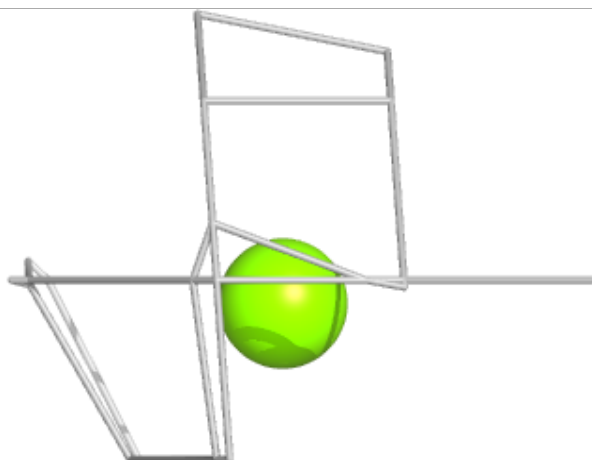
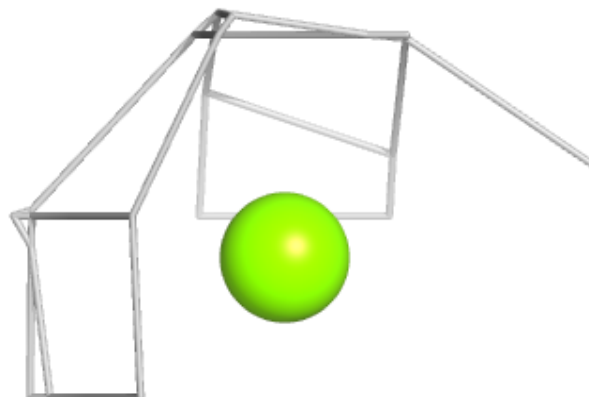
**Electron density around MG A 601:**

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



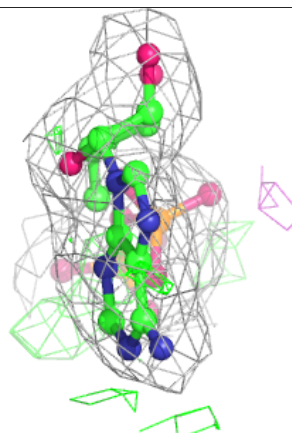
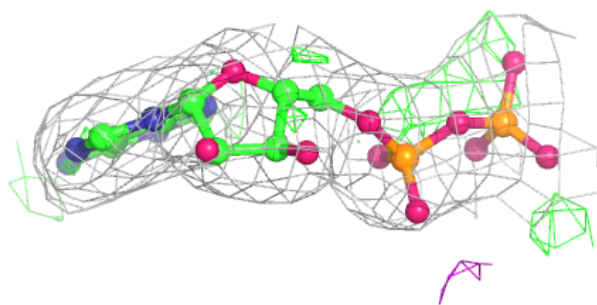
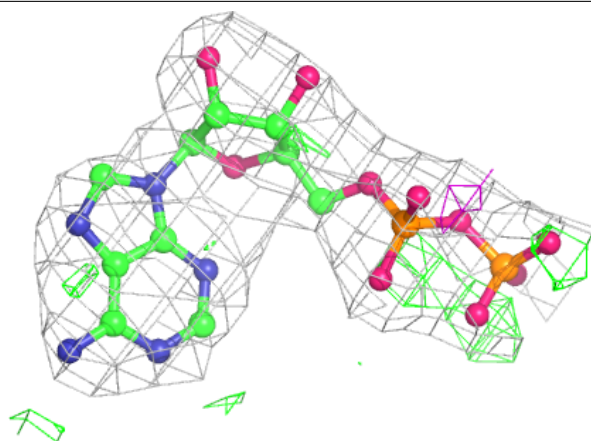
**Electron density around MG D 601:**

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



**Electron density around ADP A 600:**

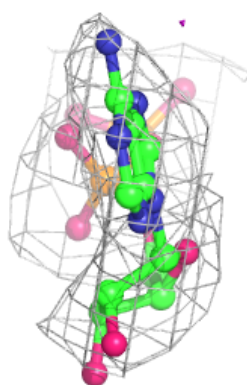
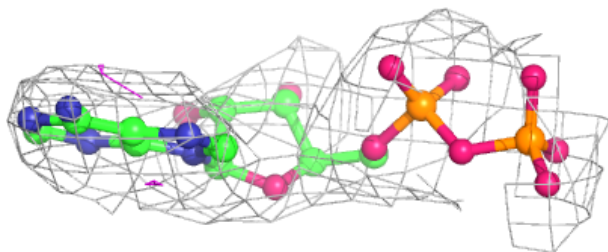
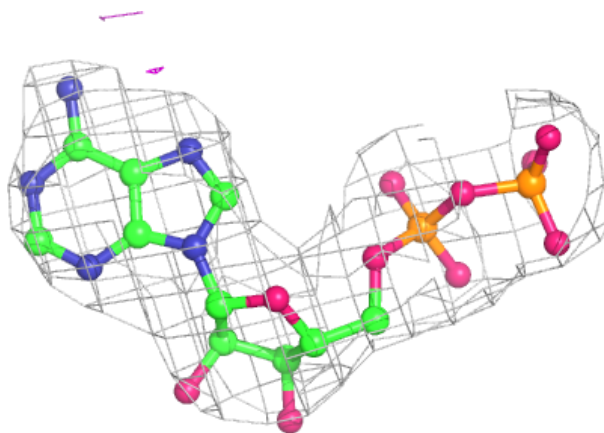
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





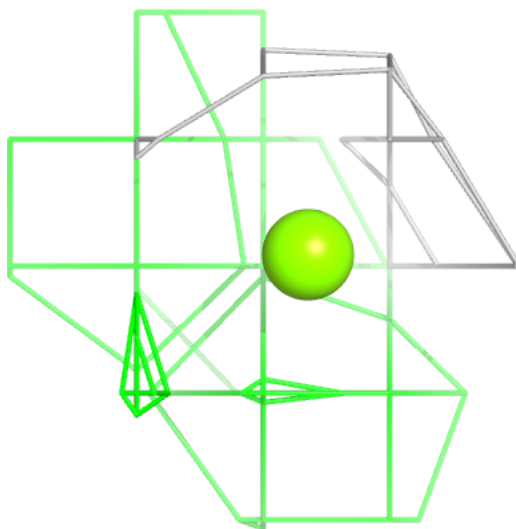
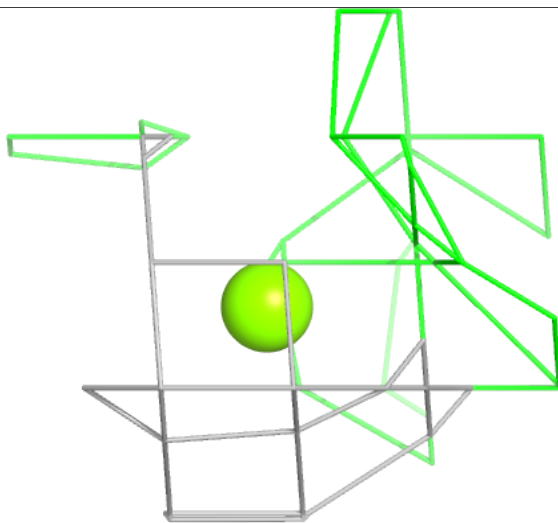
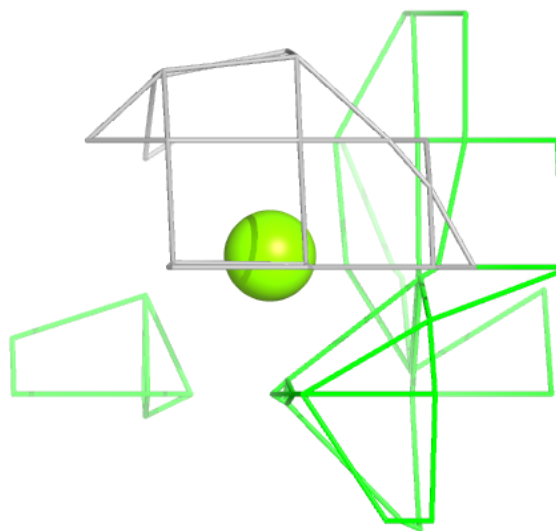
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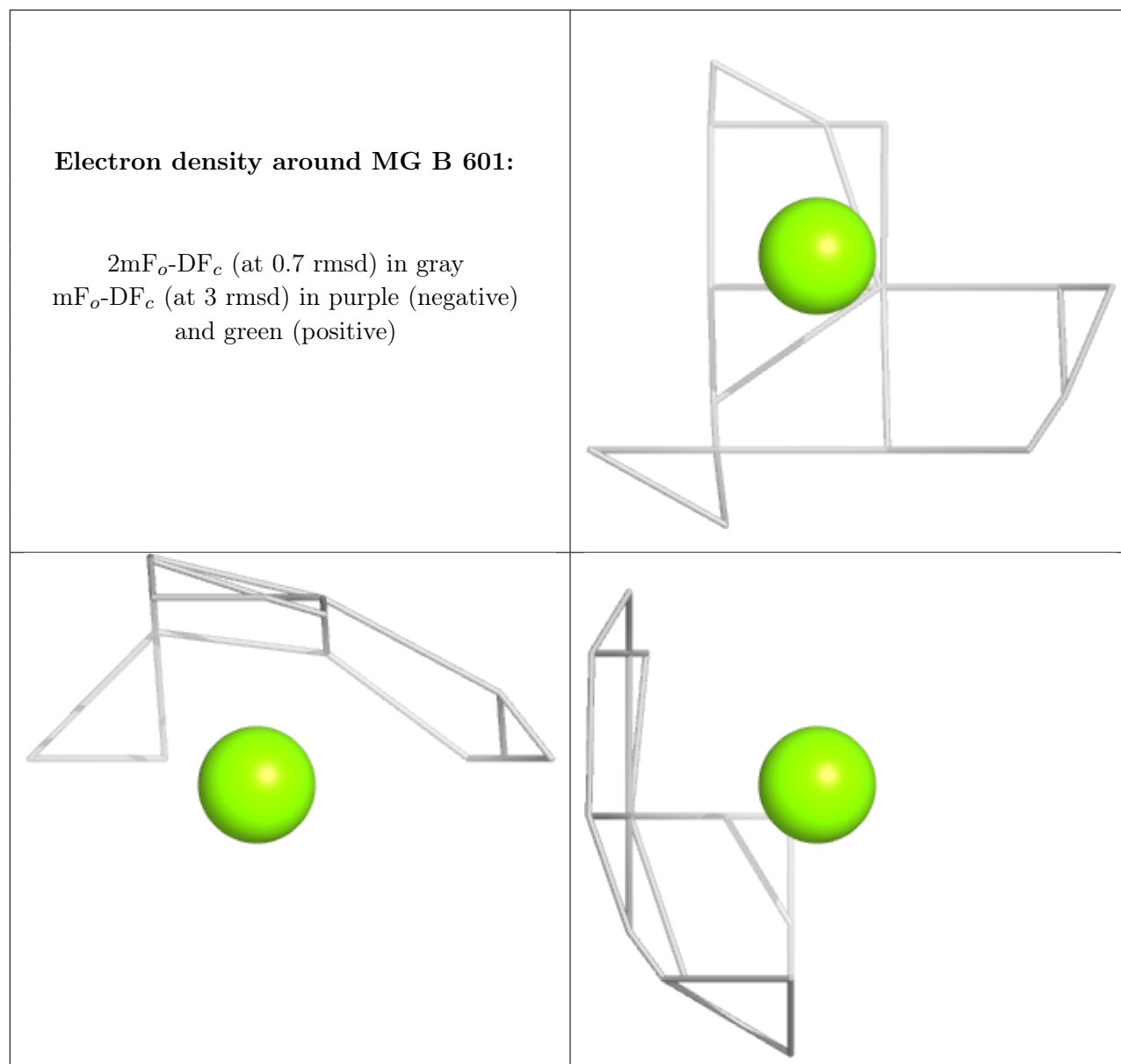
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 601:**

$2mF_o-DF_c$  (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.