



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:06 am BST

PDB ID : 4KOD  
Title : Structure of p97 N-D1 R155H mutant in complex with ADP  
Authors : Xia, D.; Tang, W.K.  
Deposited on : 2013-05-11  
Resolution : 2.96 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 : 2.11  
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) : 2.11

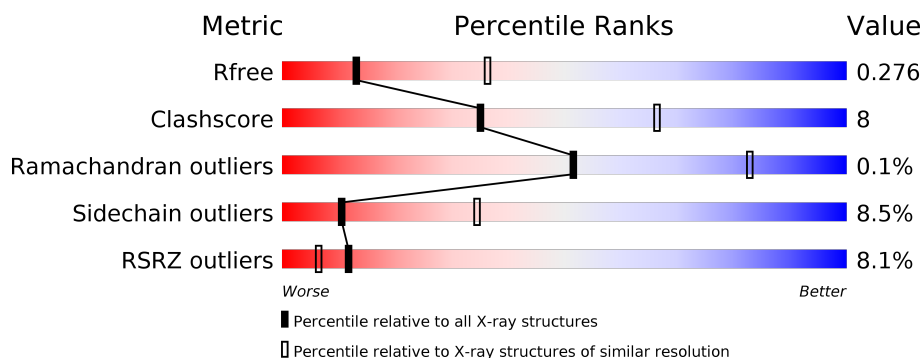
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on 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	489	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	489	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	489	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	489	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	489	<div> <div>12%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	F	489	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	489	<div><div></div><div>6%</div><div>71%</div><div>17%</div><div>•</div><div>11%</div></div>
1	H	489	<div><div></div><div>4%</div><div>71%</div><div>16%</div><div>•</div><div>10%</div></div>
1	I	489	<div><div></div><div>7%</div><div>71%</div><div>17%</div><div>•</div><div>10%</div></div>
1	J	489	<div><div></div><div>3%</div><div>73%</div><div>16%</div><div>•</div><div>9%</div></div>
1	K	489	<div><div></div><div>18%</div><div>61%</div><div>23%</div><div>5%</div><div>•</div><div>10%</div></div>
1	L	489	<div><div></div><div>9%</div><div>71%</div><div>18%</div><div>•</div><div>10%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41760 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3430	2154	607	651	18			
1	B	439	Total	C	N	O	S	0	0	0
			3438	2158	609	653	18			
1	C	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	D	439	Total	C	N	O	S	0	0	0
			3438	2158	609	653	18			
1	E	439	Total	C	N	O	S	0	0	0
			3434	2157	606	653	18			
1	F	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	G	437	Total	C	N	O	S	0	0	0
			3419	2148	603	650	18			
1	H	438	Total	C	N	O	S	0	0	0
			3430	2154	607	651	18			
1	I	440	Total	C	N	O	S	0	0	0
			3447	2164	611	654	18			
1	J	445	Total	C	N	O	S	0	0	0
			3486	2187	619	662	18			
1	K	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	L	442	Total	C	N	O	S	0	0	0
			3465	2175	615	657	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
A	482	ARG	-	EXPRESSION TAG	UNP P55072
A	483	SER	-	EXPRESSION TAG	UNP P55072
A	484	HIS	-	EXPRESSION TAG	UNP P55072
A	485	HIS	-	EXPRESSION TAG	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	HIS	-	EXPRESSION TAG	UNP P55072
A	487	HIS	-	EXPRESSION TAG	UNP P55072
A	488	HIS	-	EXPRESSION TAG	UNP P55072
A	489	HIS	-	EXPRESSION TAG	UNP P55072
B	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
B	482	ARG	-	EXPRESSION TAG	UNP P55072
B	483	SER	-	EXPRESSION TAG	UNP P55072
B	484	HIS	-	EXPRESSION TAG	UNP P55072
B	485	HIS	-	EXPRESSION TAG	UNP P55072
B	486	HIS	-	EXPRESSION TAG	UNP P55072
B	487	HIS	-	EXPRESSION TAG	UNP P55072
B	488	HIS	-	EXPRESSION TAG	UNP P55072
B	489	HIS	-	EXPRESSION TAG	UNP P55072
C	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
C	482	ARG	-	EXPRESSION TAG	UNP P55072
C	483	SER	-	EXPRESSION TAG	UNP P55072
C	484	HIS	-	EXPRESSION TAG	UNP P55072
C	485	HIS	-	EXPRESSION TAG	UNP P55072
C	486	HIS	-	EXPRESSION TAG	UNP P55072
C	487	HIS	-	EXPRESSION TAG	UNP P55072
C	488	HIS	-	EXPRESSION TAG	UNP P55072
C	489	HIS	-	EXPRESSION TAG	UNP P55072
D	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
D	482	ARG	-	EXPRESSION TAG	UNP P55072
D	483	SER	-	EXPRESSION TAG	UNP P55072
D	484	HIS	-	EXPRESSION TAG	UNP P55072
D	485	HIS	-	EXPRESSION TAG	UNP P55072
D	486	HIS	-	EXPRESSION TAG	UNP P55072
D	487	HIS	-	EXPRESSION TAG	UNP P55072
D	488	HIS	-	EXPRESSION TAG	UNP P55072
D	489	HIS	-	EXPRESSION TAG	UNP P55072
E	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
E	482	ARG	-	EXPRESSION TAG	UNP P55072
E	483	SER	-	EXPRESSION TAG	UNP P55072
E	484	HIS	-	EXPRESSION TAG	UNP P55072
E	485	HIS	-	EXPRESSION TAG	UNP P55072
E	486	HIS	-	EXPRESSION TAG	UNP P55072
E	487	HIS	-	EXPRESSION TAG	UNP P55072
E	488	HIS	-	EXPRESSION TAG	UNP P55072
E	489	HIS	-	EXPRESSION TAG	UNP P55072
F	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
F	482	ARG	-	EXPRESSION TAG	UNP P55072

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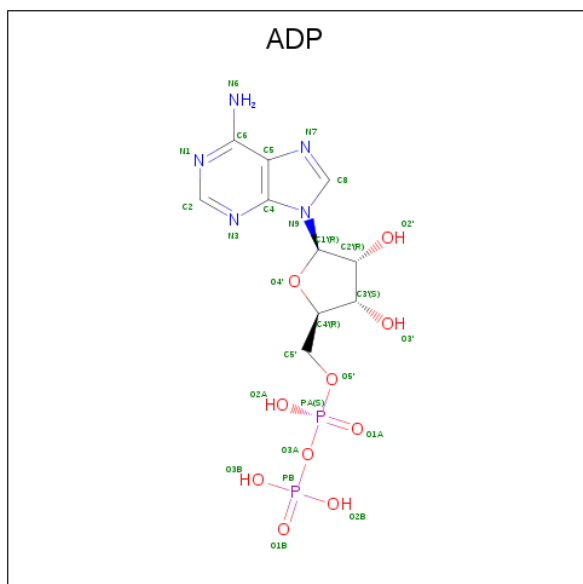
Chain	Residue	Modelled	Actual	Comment	Reference
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F	484	HIS	-	EXPRESSION TAG	UNP P55072
F	485	HIS	-	EXPRESSION TAG	UNP P55072
F	486	HIS	-	EXPRESSION TAG	UNP P55072
F	487	HIS	-	EXPRESSION TAG	UNP P55072
F	488	HIS	-	EXPRESSION TAG	UNP P55072
F	489	HIS	-	EXPRESSION TAG	UNP P55072
G	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
G	482	ARG	-	EXPRESSION TAG	UNP P55072
G	483	SER	-	EXPRESSION TAG	UNP P55072
G	484	HIS	-	EXPRESSION TAG	UNP P55072
G	485	HIS	-	EXPRESSION TAG	UNP P55072
G	486	HIS	-	EXPRESSION TAG	UNP P55072
G	487	HIS	-	EXPRESSION TAG	UNP P55072
G	488	HIS	-	EXPRESSION TAG	UNP P55072
G	489	HIS	-	EXPRESSION TAG	UNP P55072
H	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
H	482	ARG	-	EXPRESSION TAG	UNP P55072
H	483	SER	-	EXPRESSION TAG	UNP P55072
H	484	HIS	-	EXPRESSION TAG	UNP P55072
H	485	HIS	-	EXPRESSION TAG	UNP P55072
H	486	HIS	-	EXPRESSION TAG	UNP P55072
H	487	HIS	-	EXPRESSION TAG	UNP P55072
H	488	HIS	-	EXPRESSION TAG	UNP P55072
H	489	HIS	-	EXPRESSION TAG	UNP P55072
I	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
I	482	ARG	-	EXPRESSION TAG	UNP P55072
I	483	SER	-	EXPRESSION TAG	UNP P55072
I	484	HIS	-	EXPRESSION TAG	UNP P55072
I	485	HIS	-	EXPRESSION TAG	UNP P55072
I	486	HIS	-	EXPRESSION TAG	UNP P55072
I	487	HIS	-	EXPRESSION TAG	UNP P55072
I	488	HIS	-	EXPRESSION TAG	UNP P55072
I	489	HIS	-	EXPRESSION TAG	UNP P55072
J	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
J	482	ARG	-	EXPRESSION TAG	UNP P55072
J	483	SER	-	EXPRESSION TAG	UNP P55072
J	484	HIS	-	EXPRESSION TAG	UNP P55072
J	485	HIS	-	EXPRESSION TAG	UNP P55072
J	486	HIS	-	EXPRESSION TAG	UNP P55072
J	487	HIS	-	EXPRESSION TAG	UNP P55072
J	488	HIS	-	EXPRESSION TAG	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
J	489	HIS	-	EXPRESSION TAG	UNP P55072
K	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
K	482	ARG	-	EXPRESSION TAG	UNP P55072
K	483	SER	-	EXPRESSION TAG	UNP P55072
K	484	HIS	-	EXPRESSION TAG	UNP P55072
K	485	HIS	-	EXPRESSION TAG	UNP P55072
K	486	HIS	-	EXPRESSION TAG	UNP P55072
K	487	HIS	-	EXPRESSION TAG	UNP P55072
K	488	HIS	-	EXPRESSION TAG	UNP P55072
K	489	HIS	-	EXPRESSION TAG	UNP P55072
L	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
L	482	ARG	-	EXPRESSION TAG	UNP P55072
L	483	SER	-	EXPRESSION TAG	UNP P55072
L	484	HIS	-	EXPRESSION TAG	UNP P55072
L	485	HIS	-	EXPRESSION TAG	UNP P55072
L	486	HIS	-	EXPRESSION TAG	UNP P55072
L	487	HIS	-	EXPRESSION TAG	UNP P55072
L	488	HIS	-	EXPRESSION TAG	UNP P55072
L	489	HIS	-	EXPRESSION TAG	UNP P55072

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	9	Total	O	0	0
			9	9		
3	C	14	Total	O	0	0
			14	14		
3	D	17	Total	O	0	0
			17	17		
3	E	17	Total	O	0	0
			17	17		
3	F	15	Total	O	0	0
			15	15		
3	G	11	Total	O	0	0
			11	11		
3	H	16	Total	O	0	0
			16	16		

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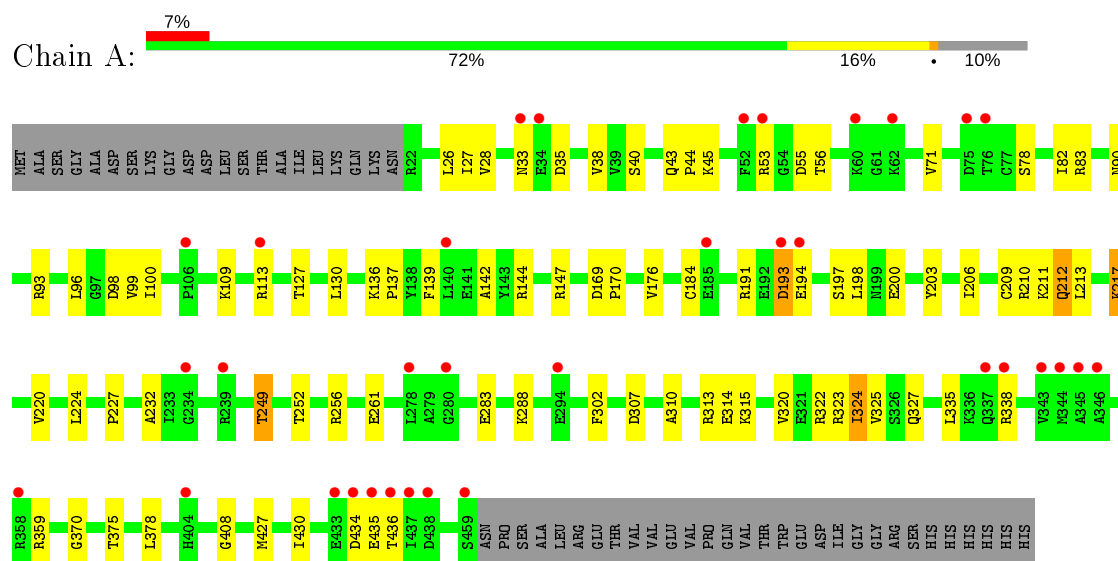
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total 11	O 11	0	0
3	J	17	Total 17	O 17	0	0
3	K	11	Total 11	O 11	0	0
3	L	16	Total 16	O 16	0	0

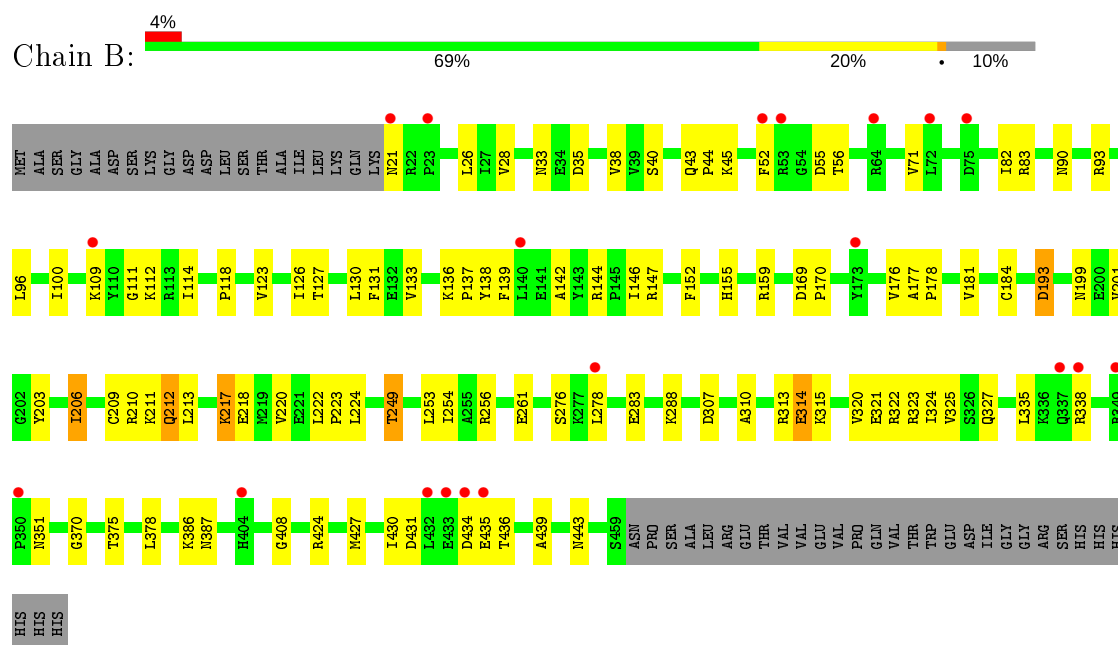
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

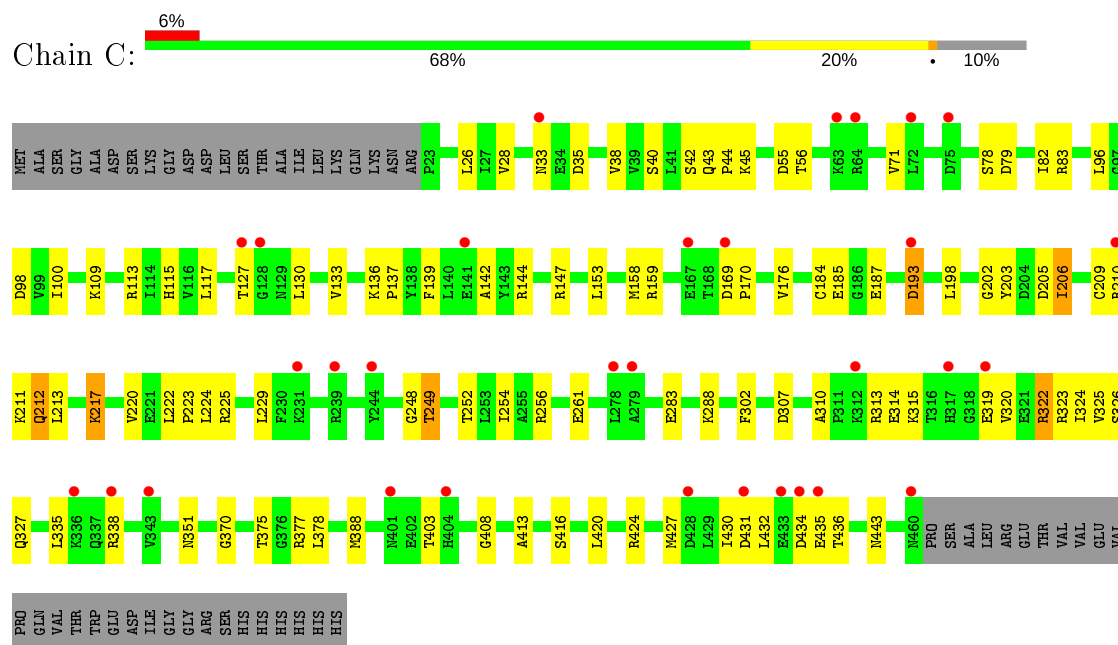
- Molecule 1: Transitional endoplasmic reticulum ATPase



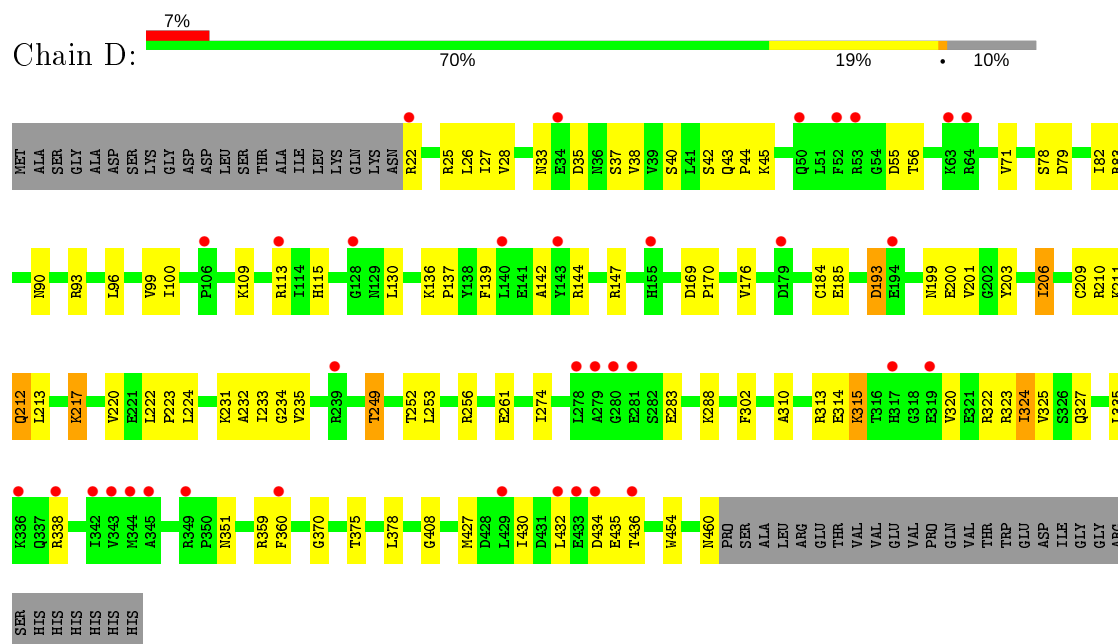
- Molecule 1: Transitional endoplasmic reticulum ATPase



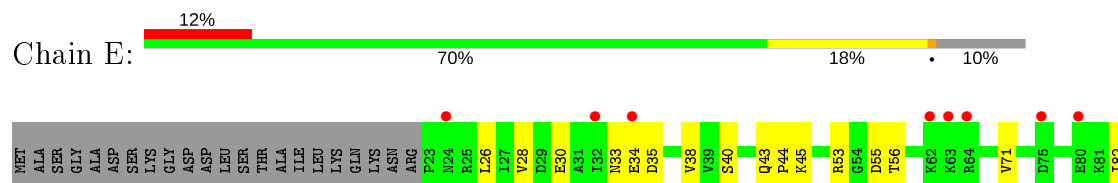
- Molecule 1: Transitional endoplasmic reticulum ATPase

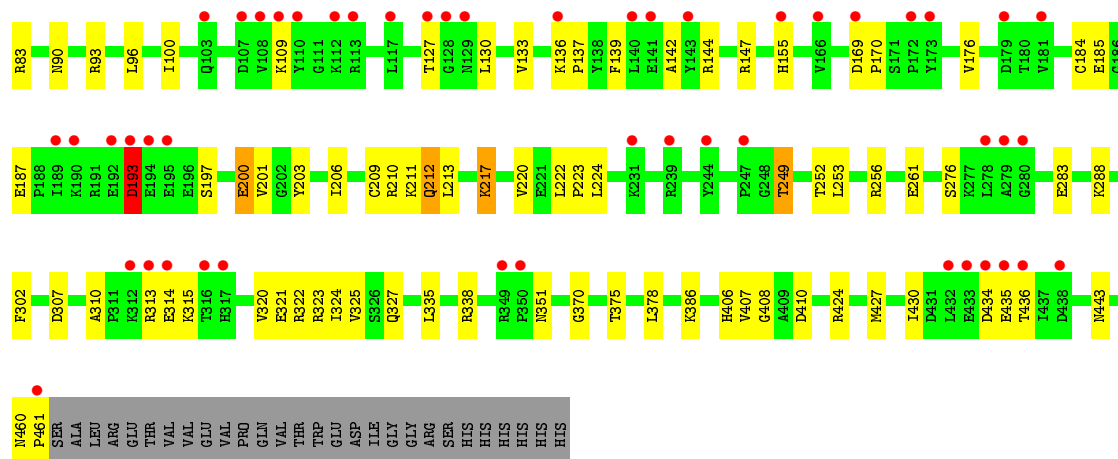


- Molecule 1: Transitional endoplasmic reticulum ATPase

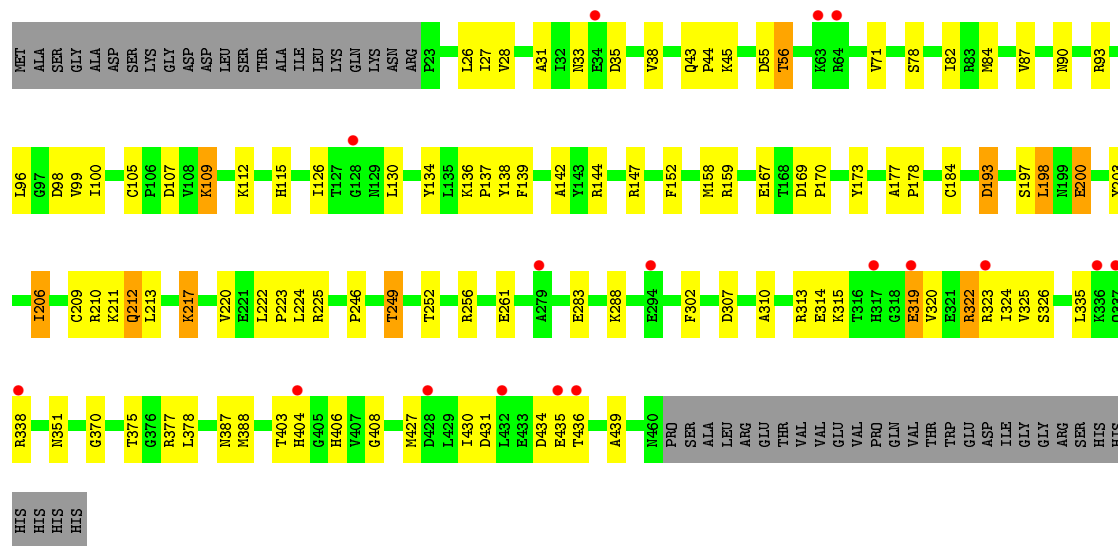


- Molecule 1: Transitional endoplasmic reticulum ATPase

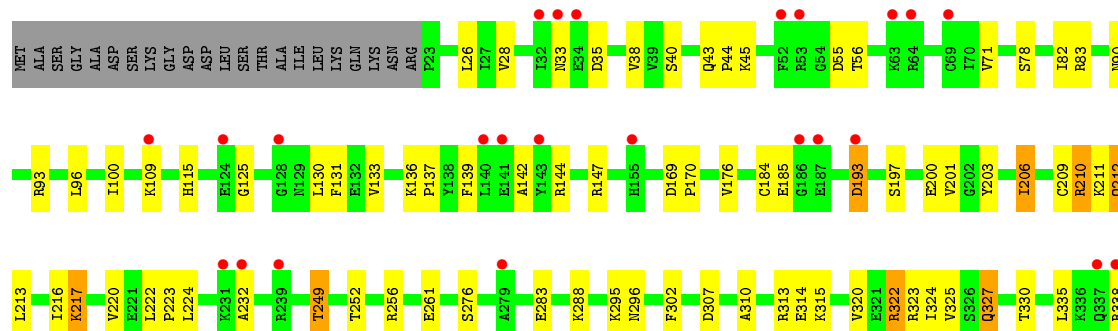


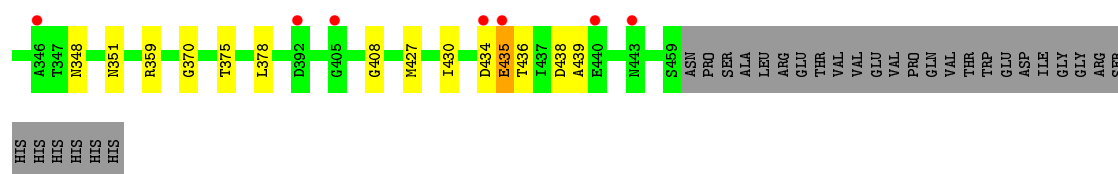


• Molecule 1: Transitional endoplasmic reticulum ATPase

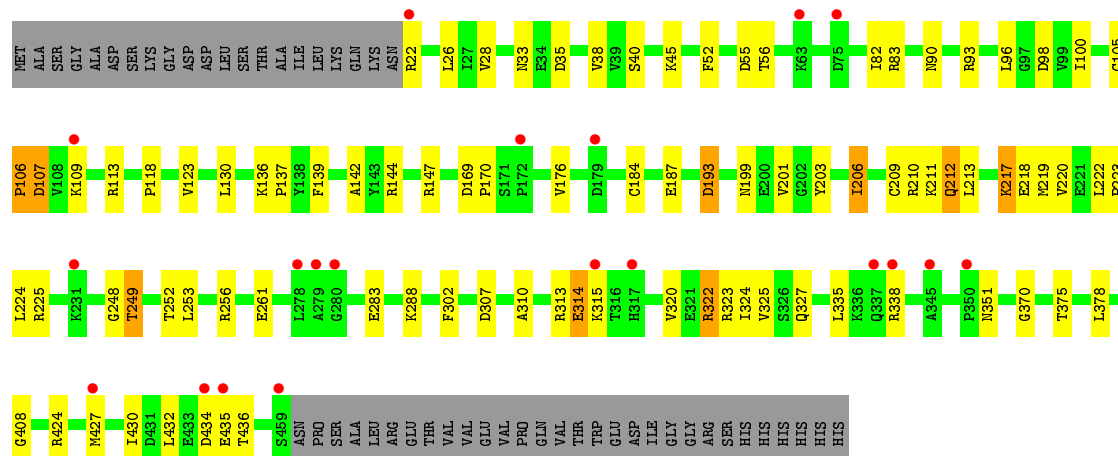


• Molecule 1: Transitional endoplasmic reticulum ATPase

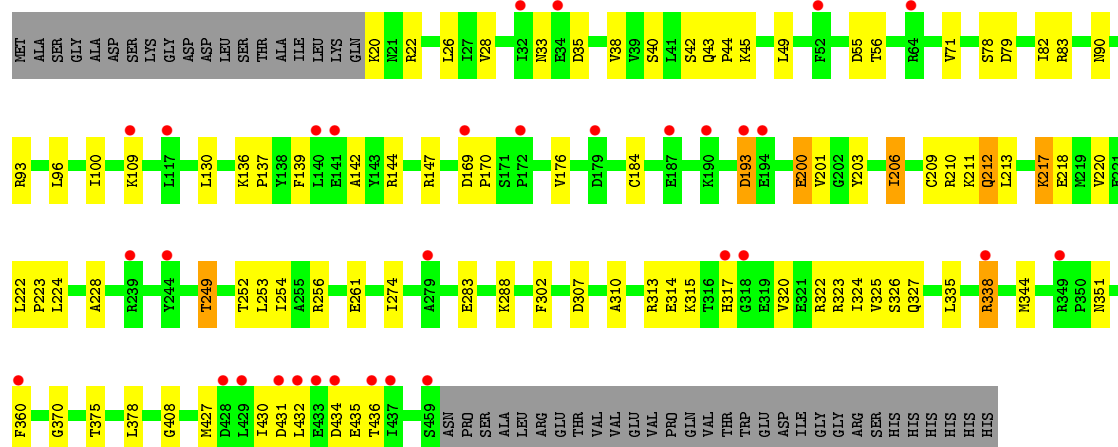




• Molecule 1: Transitional endoplasmic reticulum ATPase

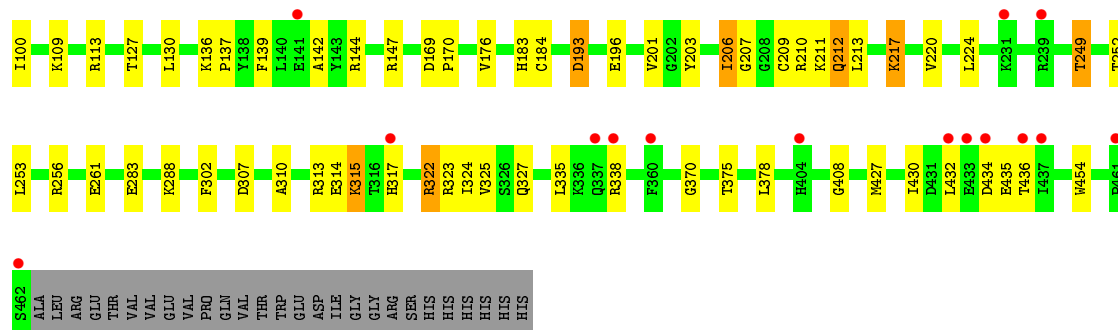


• Molecule 1: Transitional endoplasmic reticulum ATPase

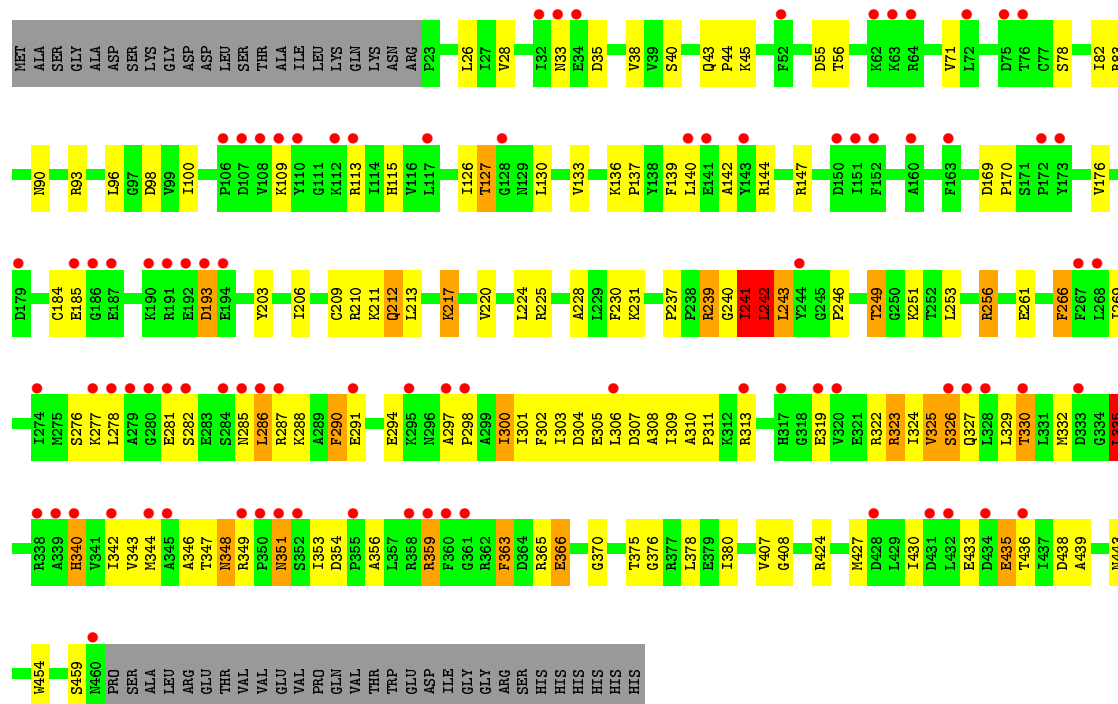


• Molecule 1: Transitional endoplasmic reticulum ATPase

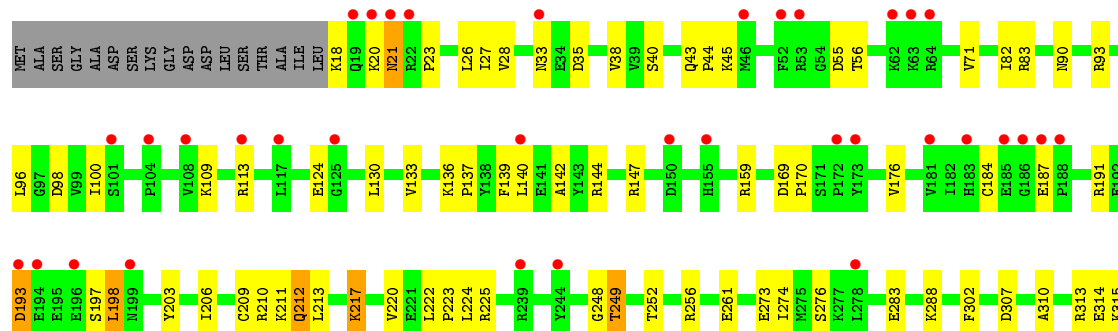


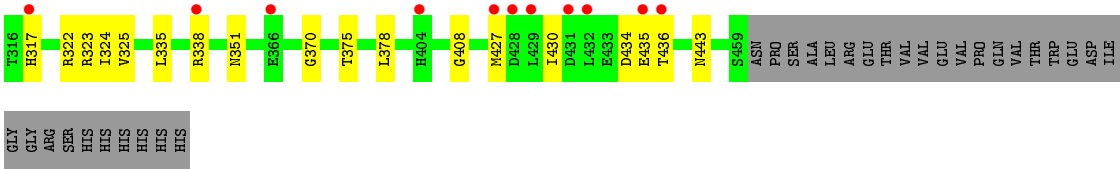


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.52Å 170.74Å 256.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.99 – 2.96 21.99 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.0 (21.99-2.96) 88.3 (21.99-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.268 , 0.291 0.250 , 0.276	Depositor DCC
$R_{free}$ test set	5937 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 26.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: 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	0.37	0/3484	0.63	0/4708
1	B	0.47	0/3492	0.67	0/4719
1	C	0.38	0/3481	0.62	0/4704
1	D	0.39	0/3492	0.64	0/4719
1	E	0.40	1/3489 (0.0%)	0.68	3/4716 (0.1%)
1	F	0.48	0/3481	0.70	1/4704 (0.0%)
1	G	0.43	2/3473 (0.1%)	0.64	0/4693
1	H	0.42	0/3484	0.66	0/4708
1	I	0.40	0/3501	0.64	2/4730 (0.0%)
1	J	0.44	0/3541	0.66	0/4784
1	K	0.44	1/3481 (0.0%)	0.71	2/4704 (0.0%)
1	L	0.36	0/3519	0.62	0/4753
All	All	0.42	4/41918 (0.0%)	0.66	8/56642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	459	SER	C-N	8.47	1.53	1.34
1	E	193	ASP	CB-CG	-8.24	1.34	1.51
1	G	296	ASN	CG-ND2	-6.77	1.16	1.32
1	G	296	ASN	CG-OD1	-5.05	1.12	1.24

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ASP	CB-CG-OD1	-16.01	103.89	118.30
1	E	193	ASP	CB-CG-OD2	7.36	124.93	118.30
1	I	360	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	K	242	LEU	CA-CB-CG	5.54	128.04	115.30
1	F	319	GLU	CB-CA-C	-5.48	99.43	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	239	ARG	Peptide

## 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	3430	0	3480	44	0
1	B	3438	0	3486	66	1
1	C	3427	0	3474	74	0
1	D	3438	0	3486	61	0
1	E	3434	0	3481	60	0
1	F	3427	0	3474	71	1
1	G	3419	0	3468	55	1
1	H	3430	0	3480	54	0
1	I	3447	0	3499	49	1
1	J	3486	0	3538	46	0
1	K	3427	0	3474	132	0
1	L	3465	0	3520	56	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	4	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
2	H	27	0	12	3	0
2	I	27	0	12	2	0
2	J	27	0	12	2	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	27	0	12	3	0
2	L	27	0	12	4	0
3	A	14	0	0	2	0
3	B	9	0	0	0	0
3	C	14	0	0	0	0
3	D	17	0	0	1	0
3	E	17	0	0	2	0
3	F	15	0	0	0	0
3	G	11	0	0	4	0
3	H	16	0	0	0	0
3	I	11	0	0	1	0
3	J	17	0	0	2	0
3	K	11	0	0	1	0
3	L	16	0	0	0	0
All	All	41760	0	42004	681	2

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 8.

The worst 5 of 681 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:K:433:GLU:HG3	1:K:436:THR:HG21	1.29	1.12
1:C:159:ARG:HD2	1:D:232:ALA:O	1.53	1.09
1:B:276:SER:HB3	1:F:326:SER:HB3	1.33	1.08
1:C:158:MET:HB2	1:D:233:ILE:HG22	1.36	1.07
1:I:209:CYS:HB2	1:I:212:GLN:HG2	1.36	1.03

All (2) 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:F:404:HIS:CG	1:G:210:ARG:NH1[3_645]	1.92	0.28
1:B:52:PHE:CZ	1:I:49:LEU:O[4_455]	2.09	0.11

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/489 (89%)	419 (96%)	17 (4%)	0	100	100
1	B	437/489 (89%)	416 (95%)	21 (5%)	0	100	100
1	C	436/489 (89%)	418 (96%)	18 (4%)	0	100	100
1	D	437/489 (89%)	417 (95%)	20 (5%)	0	100	100
1	E	437/489 (89%)	418 (96%)	19 (4%)	0	100	100
1	F	436/489 (89%)	417 (96%)	19 (4%)	0	100	100
1	G	435/489 (89%)	418 (96%)	17 (4%)	0	100	100
1	H	436/489 (89%)	416 (95%)	19 (4%)	1 (0%)	47	79
1	I	438/489 (90%)	418 (95%)	20 (5%)	0	100	100
1	J	443/489 (91%)	425 (96%)	18 (4%)	0	100	100
1	K	436/489 (89%)	398 (91%)	35 (8%)	3 (1%)	22	56
1	L	440/489 (90%)	419 (95%)	20 (4%)	1 (0%)	47	79
All	All	5247/5868 (89%)	4999 (95%)	243 (5%)	5 (0%)	51	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	23	PRO
1	K	241	ILE
1	K	277	LYS
1	K	359	ARG
1	H	106	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	375/418 (90%)	345 (92%)	30 (8%)	12	37
1	B	376/418 (90%)	346 (92%)	30 (8%)	12	37
1	C	375/418 (90%)	345 (92%)	30 (8%)	12	37
1	D	376/418 (90%)	345 (92%)	31 (8%)	11	36
1	E	376/418 (90%)	345 (92%)	31 (8%)	11	36
1	F	375/418 (90%)	343 (92%)	32 (8%)	10	34
1	G	374/418 (90%)	344 (92%)	30 (8%)	12	37
1	H	375/418 (90%)	344 (92%)	31 (8%)	11	35
1	I	377/418 (90%)	345 (92%)	32 (8%)	10	34
1	J	382/418 (91%)	349 (91%)	33 (9%)	10	34
1	K	375/418 (90%)	329 (88%)	46 (12%)	4	18
1	L	379/418 (91%)	349 (92%)	30 (8%)	12	37
All	All	4515/5016 (90%)	4129 (92%)	386 (8%)	10	34

5 of 386 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	314	GLU
1	H	56	THR
1	L	18	LYS
1	F	338	ARG
1	G	211	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	33	ASN
1	G	212	GLN
1	L	50	GLN
1	F	183	HIS
1	G	327	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	L	800	-	24,29,29	0.91	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	B	800	-	24,29,29	0.99	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	C	800	-	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	A	800	-	24,29,29	0.89	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	G	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.41	4 (13%)
2	ADP	J	800	-	24,29,29	1.15	2 (8%)	29,45,45	1.46	3 (10%)
2	ADP	E	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	3 (10%)
2	ADP	K	800	-	24,29,29	0.83	1 (4%)	29,45,45	1.55	4 (13%)
2	ADP	I	800	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	F	800	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
2	ADP	D	800	-	24,29,29	1.02	2 (8%)	29,45,45	1.53	5 (17%)
2	ADP	H	800	-	24,29,29	0.87	0	29,45,45	1.46	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	L	800	-	-	3/12/32/32	0/3/3/3
2	ADP	B	800	-	-	4/12/32/32	0/3/3/3
2	ADP	C	800	-	-	4/12/32/32	0/3/3/3
2	ADP	A	800	-	-	4/12/32/32	0/3/3/3
2	ADP	G	800	-	-	4/12/32/32	0/3/3/3
2	ADP	J	800	-	-	4/12/32/32	0/3/3/3
2	ADP	E	800	-	-	3/12/32/32	0/3/3/3
2	ADP	K	800	-	-	4/12/32/32	0/3/3/3
2	ADP	I	800	-	-	3/12/32/32	0/3/3/3
2	ADP	F	800	-	-	4/12/32/32	0/3/3/3
2	ADP	D	800	-	-	4/12/32/32	0/3/3/3
2	ADP	H	800	-	-	2/12/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	800	ADP	C2'-C1'	-2.61	1.49	1.53
2	D	800	ADP	C5-C4	2.52	1.47	1.40
2	L	800	ADP	C5-C4	2.49	1.47	1.40
2	G	800	ADP	C5-C4	2.40	1.47	1.40
2	J	800	ADP	C5-C4	2.36	1.47	1.40

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	800	ADP	C3'-C2'-C1'	3.94	106.91	100.98
2	E	800	ADP	PA-O3A-PB	-3.84	119.66	132.83
2	D	800	ADP	PA-O3A-PB	-3.82	119.72	132.83
2	J	800	ADP	PA-O3A-PB	-3.80	119.80	132.83
2	H	800	ADP	N3-C2-N1	-3.79	122.76	128.68

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	800	ADP	C5'-O5'-PA-O1A
2	F	800	ADP	C5'-O5'-PA-O1A
2	J	800	ADP	C5'-O5'-PA-O3A
2	F	800	ADP	C5'-O5'-PA-O3A
2	D	800	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

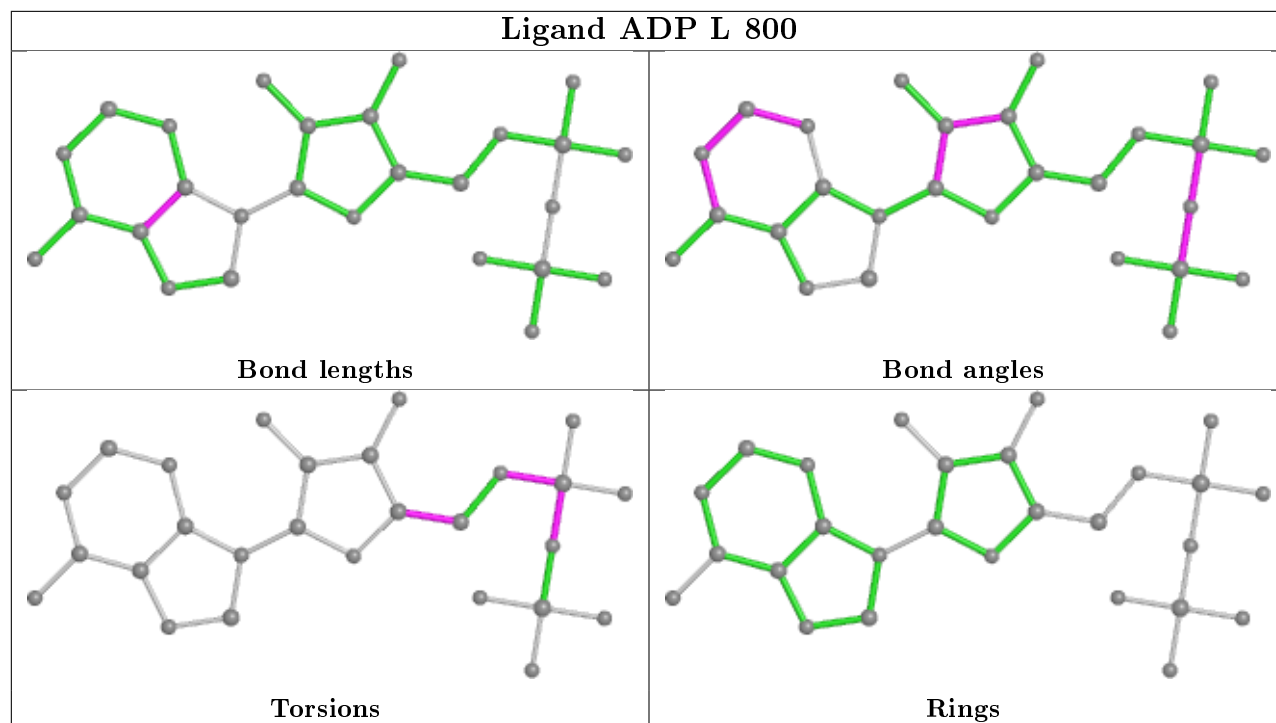
12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	800	ADP	4	0
2	B	800	ADP	2	0
2	C	800	ADP	4	0
2	A	800	ADP	2	0
2	G	800	ADP	2	0
2	J	800	ADP	2	0
2	E	800	ADP	2	0
2	K	800	ADP	3	0
2	I	800	ADP	2	0
2	F	800	ADP	3	0
2	D	800	ADP	2	0
2	H	800	ADP	3	0

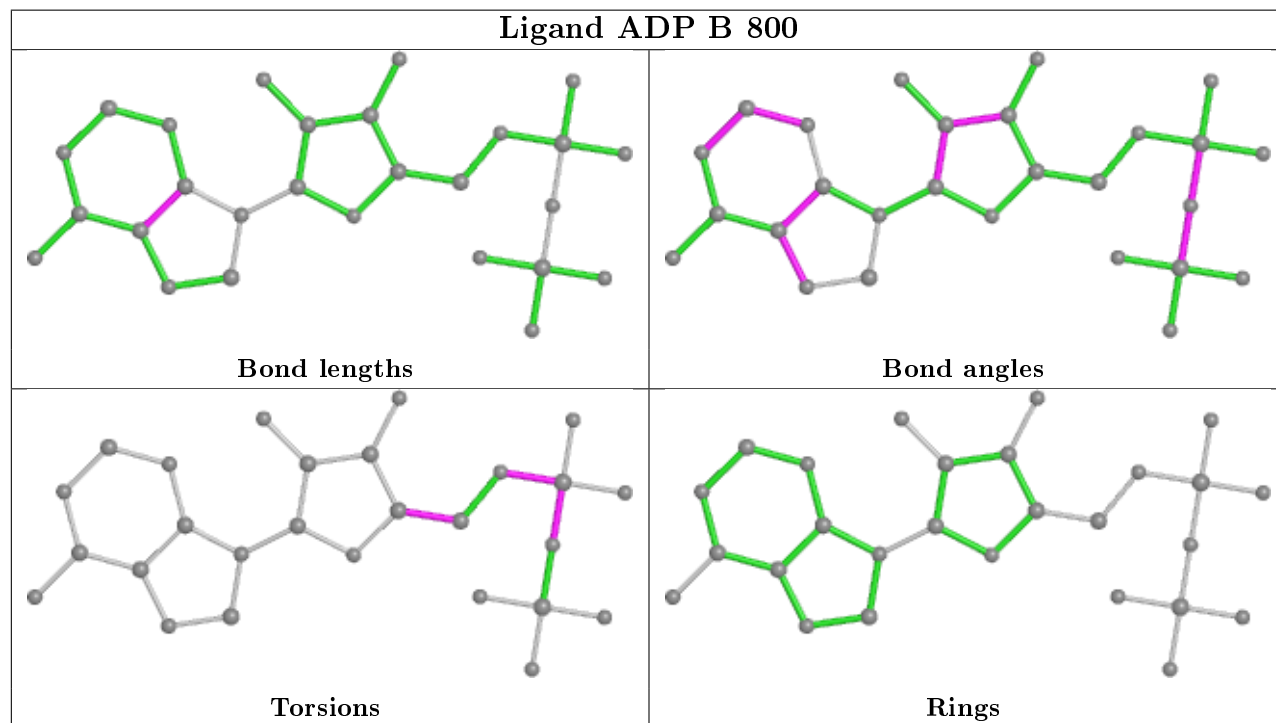
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

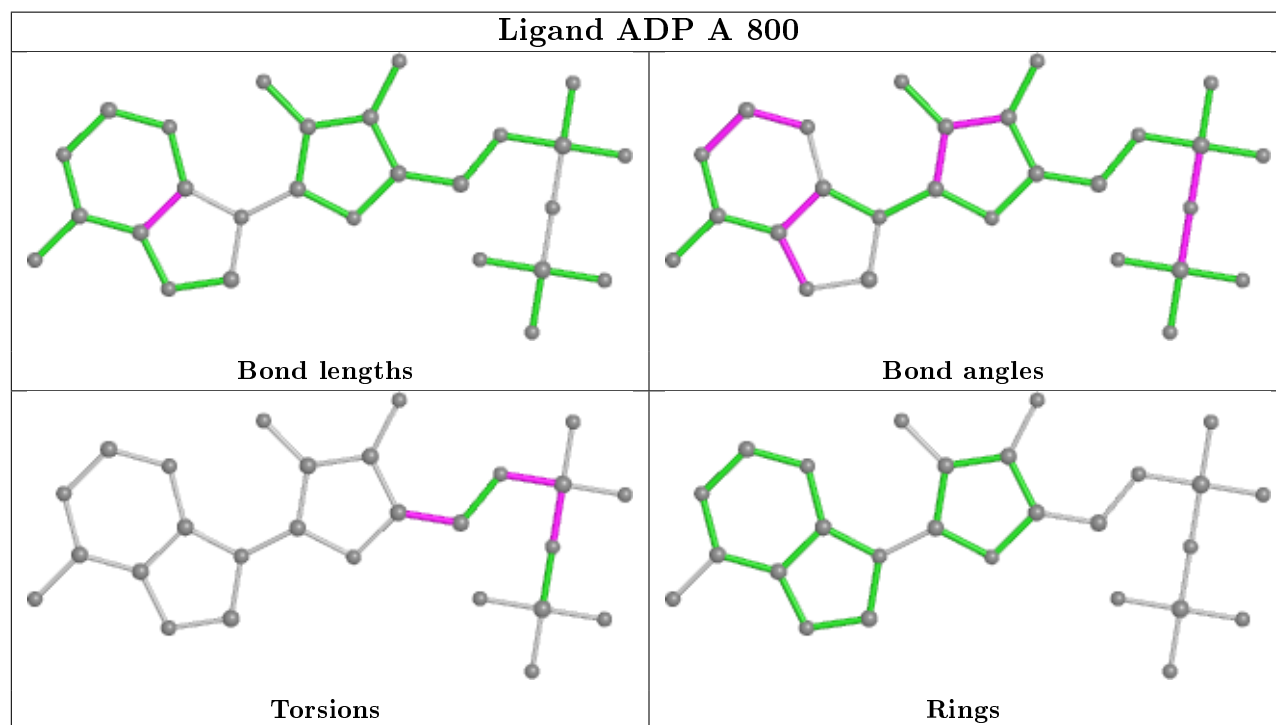
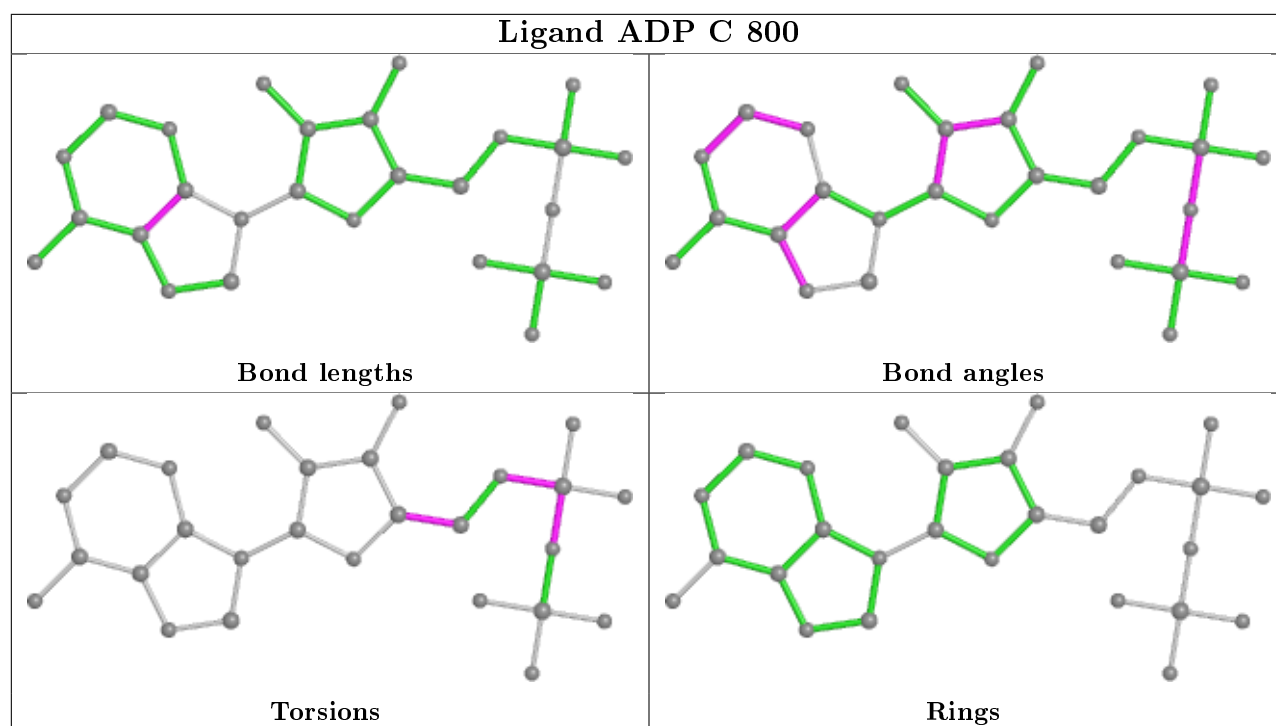


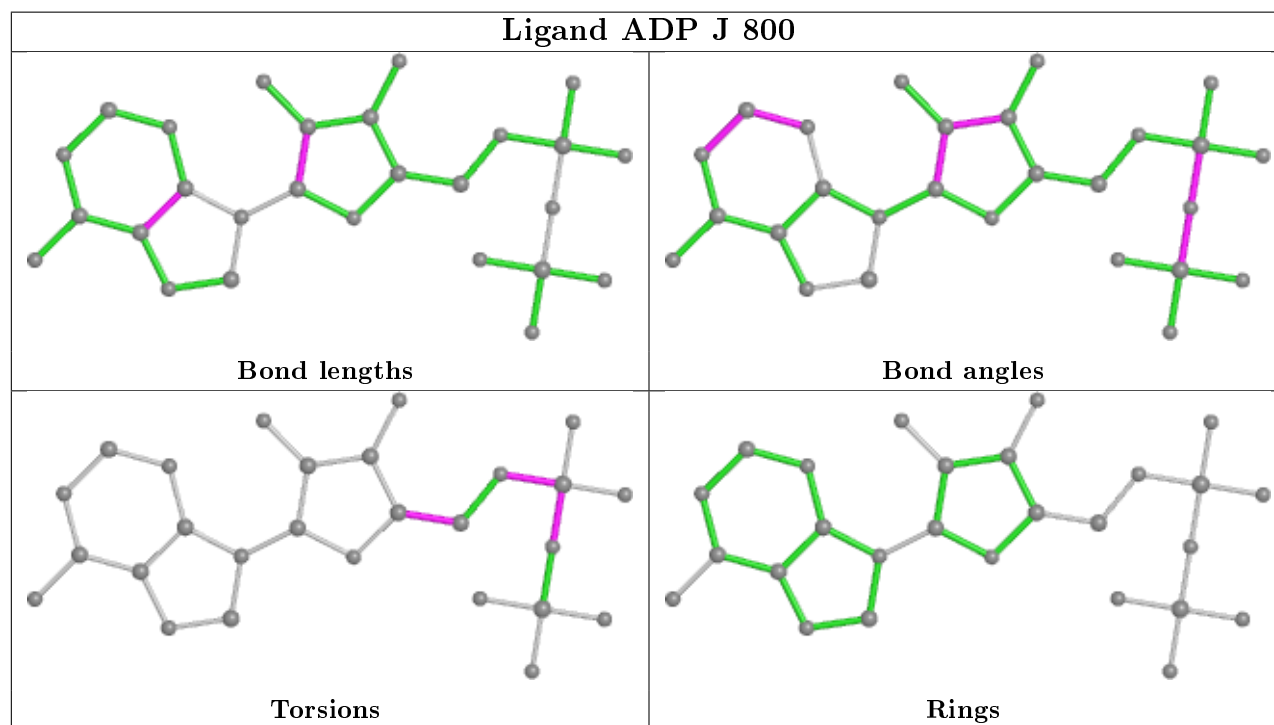
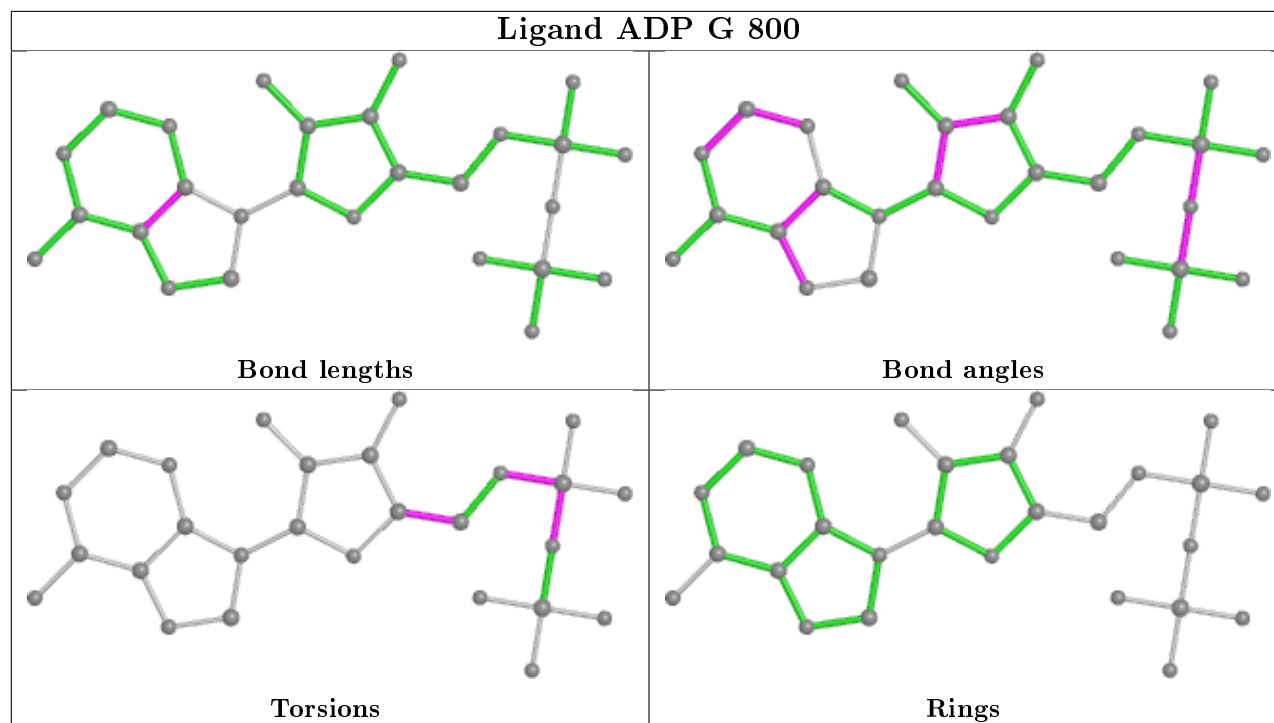
## Ligand ADP L 800



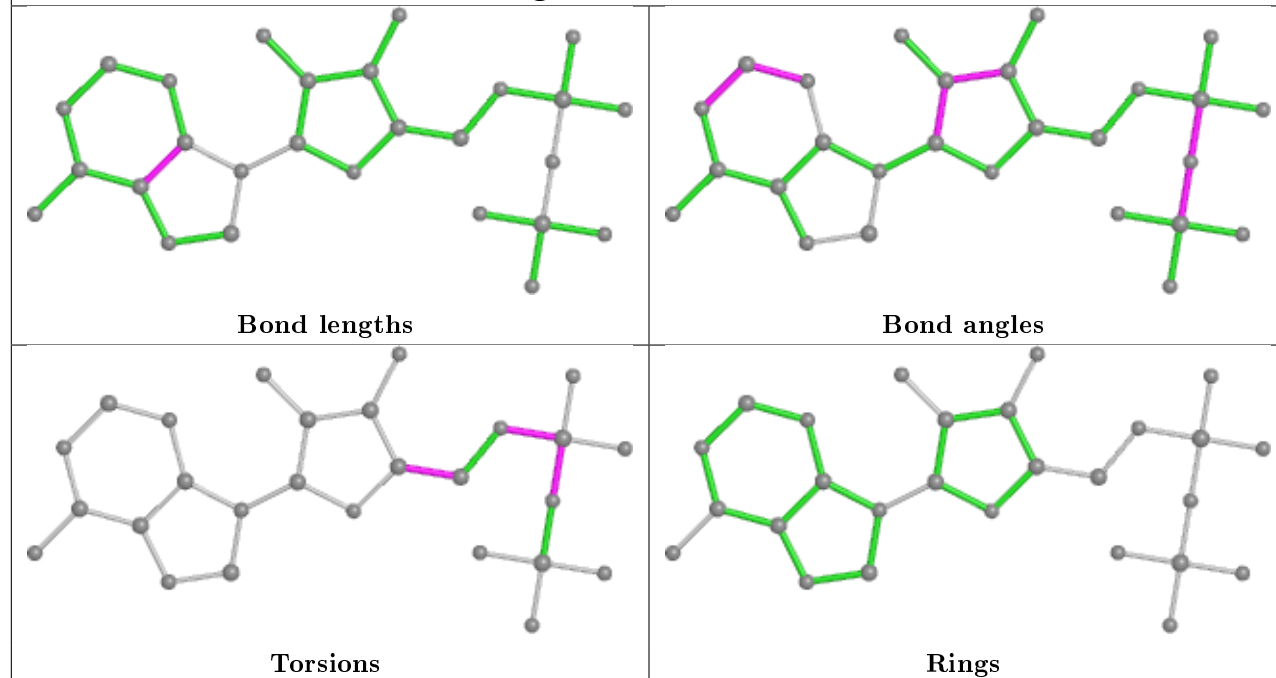
## Ligand ADP B 800



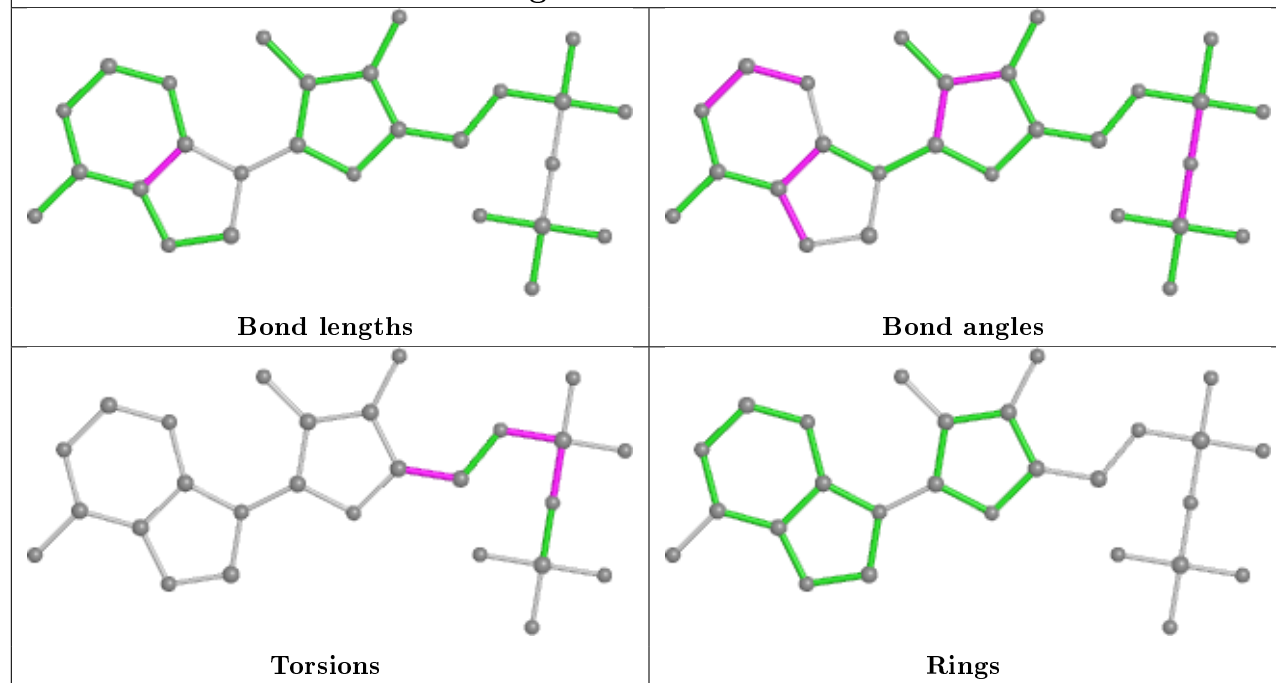




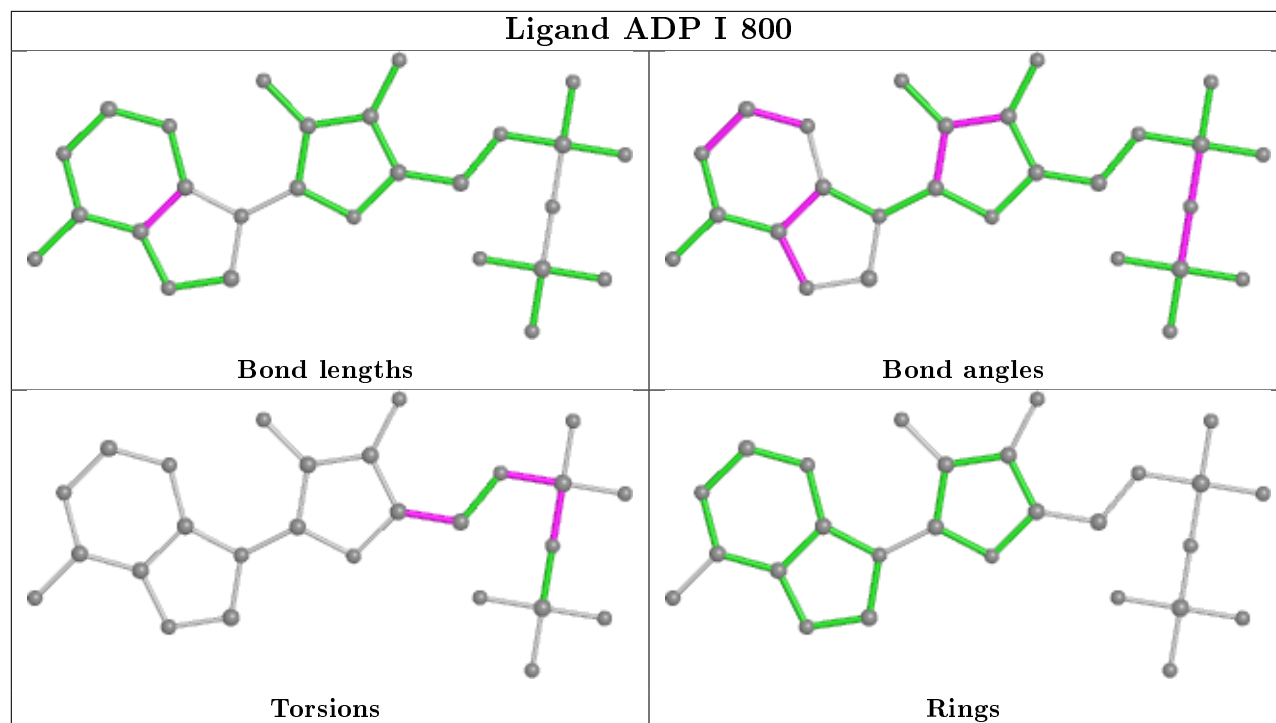
## Ligand ADP E 800



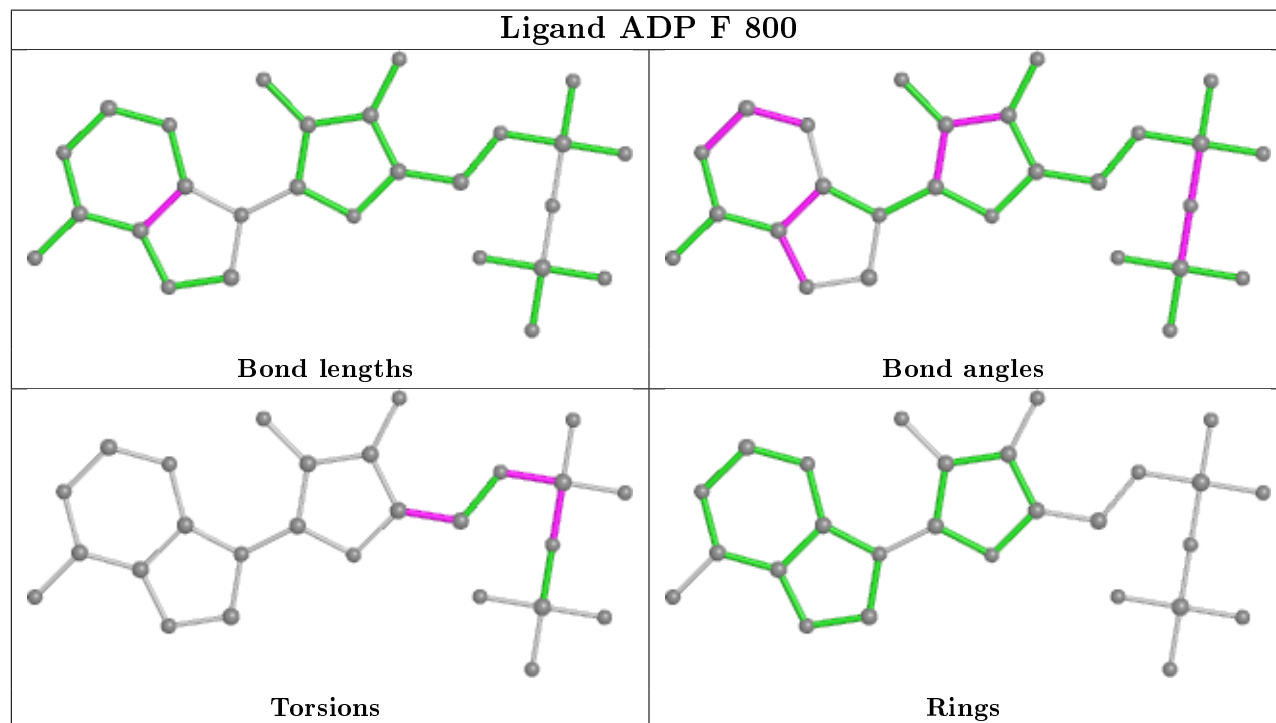
## Ligand ADP K 800

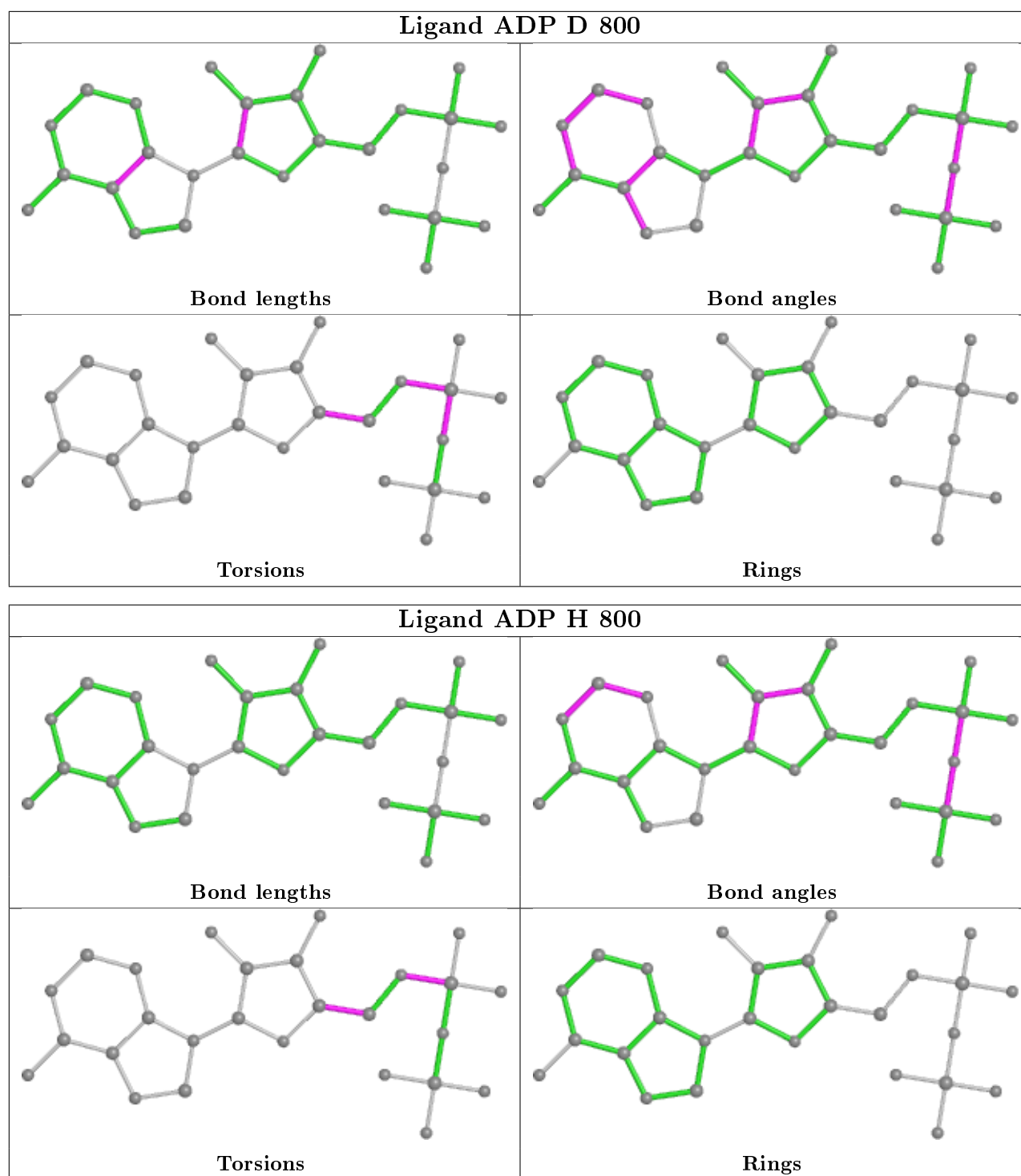


## Ligand ADP I 800



## Ligand ADP F 800





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	438/489 (89%)	0.29	34 (7%) 13 7	71, 120, 172, 275	0
1	B	439/489 (89%)	-0.03	20 (4%) 32 20	57, 92, 153, 208	0
1	C	438/489 (89%)	0.19	31 (7%) 16 9	76, 120, 177, 233	0
1	D	439/489 (89%)	0.24	35 (7%) 12 7	60, 115, 176, 280	0
1	E	439/489 (89%)	0.52	57 (12%) 3 2	66, 132, 211, 261	0
1	F	438/489 (89%)	-0.01	17 (3%) 39 25	60, 95, 169, 215	0
1	G	437/489 (89%)	0.24	31 (7%) 16 9	60, 111, 169, 221	0
1	H	438/489 (89%)	0.06	20 (4%) 32 20	60, 105, 163, 233	0
1	I	440/489 (89%)	0.24	32 (7%) 15 8	61, 122, 182, 285	0
1	J	445/489 (91%)	-0.01	16 (3%) 42 28	50, 93, 153, 238	0
1	K	438/489 (89%)	0.82	87 (19%) 1 0	64, 142, 208, 239	0
1	L	442/489 (90%)	0.40	46 (10%) 6 4	76, 139, 204, 287	0
All	All	5271/5868 (89%)	0.25	426 (8%) 12 6	50, 115, 188, 287	0

The worst 5 of 426 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	279	ALA	9.2
1	I	432	LEU	8.3
1	D	433	GLU	7.7
1	E	279	ALA	7.7
1	E	432	LEU	7.3

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

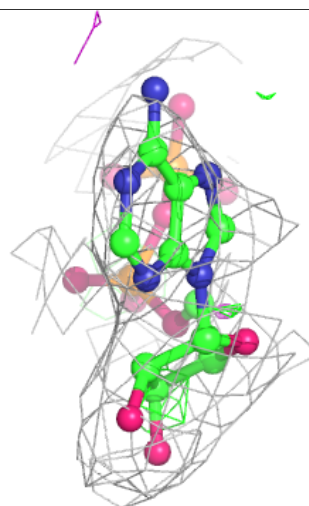
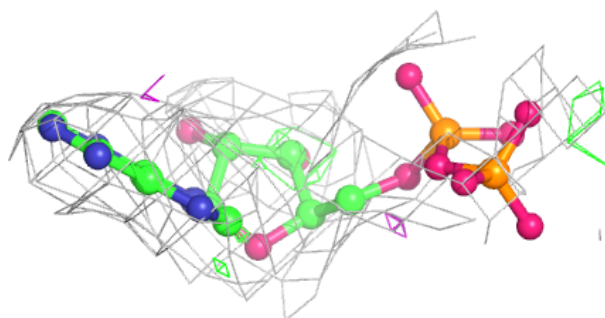
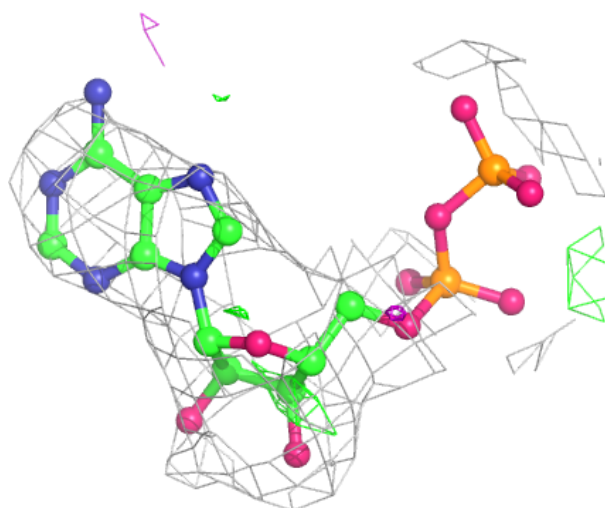
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	ADP	K	800	27/27	0.94	0.18	95,102,110,112	0
2	ADP	L	800	27/27	0.95	0.16	87,90,104,111	0
2	ADP	I	800	27/27	0.95	0.17	78,82,88,90	0
2	ADP	G	800	27/27	0.96	0.16	79,86,95,96	0
2	ADP	E	800	27/27	0.96	0.13	75,83,94,97	0
2	ADP	B	800	27/27	0.96	0.16	71,74,79,84	0
2	ADP	A	800	27/27	0.96	0.15	75,81,95,99	0
2	ADP	D	800	27/27	0.96	0.15	73,76,82,84	0
2	ADP	F	800	27/27	0.97	0.14	76,78,82,83	0
2	ADP	C	800	27/27	0.97	0.14	87,91,101,105	0
2	ADP	H	800	27/27	0.97	0.14	74,77,88,97	0
2	ADP	J	800	27/27	0.98	0.12	59,64,73,73	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.

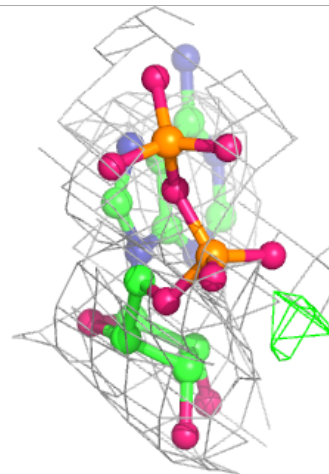
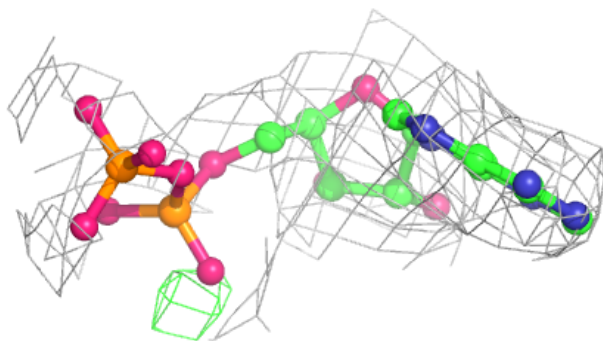
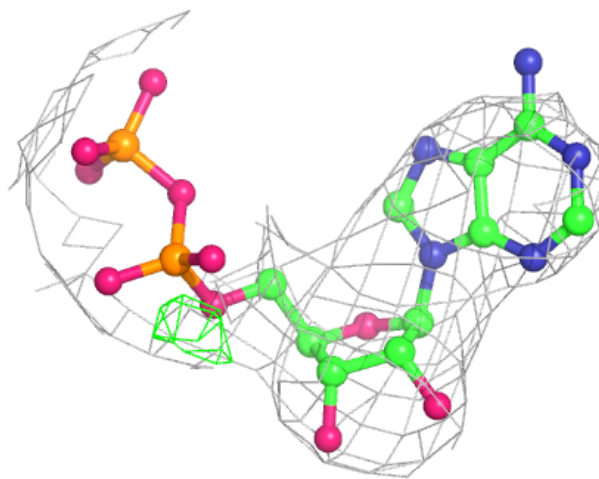
**Electron density around ADP K 800:**

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



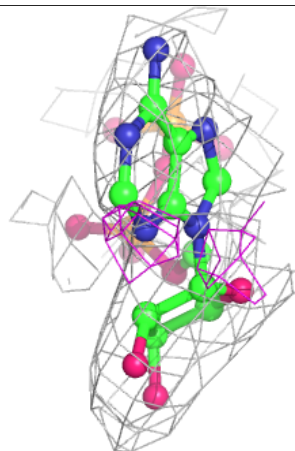
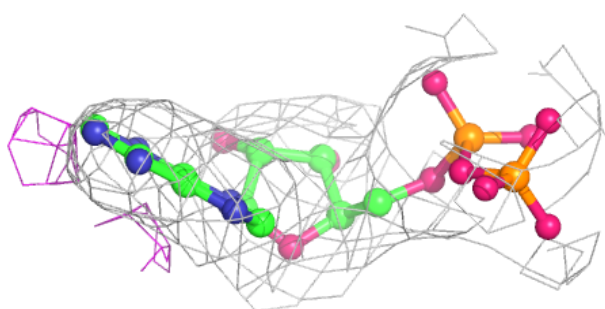
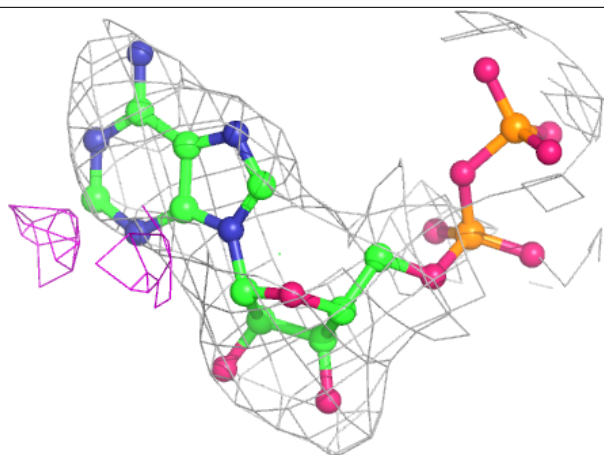
**Electron density around ADP L 800:**

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



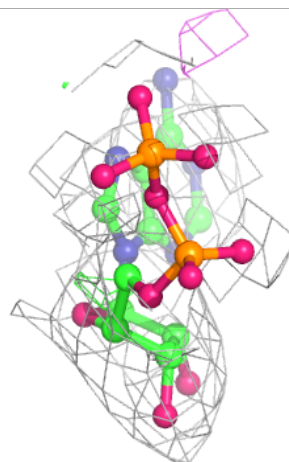
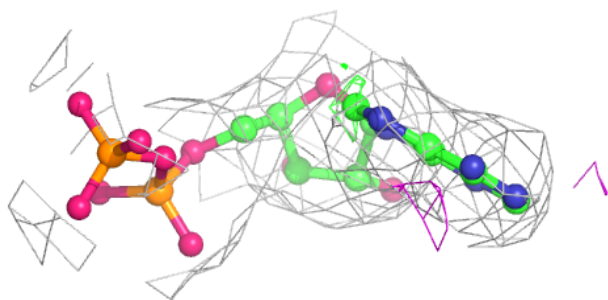
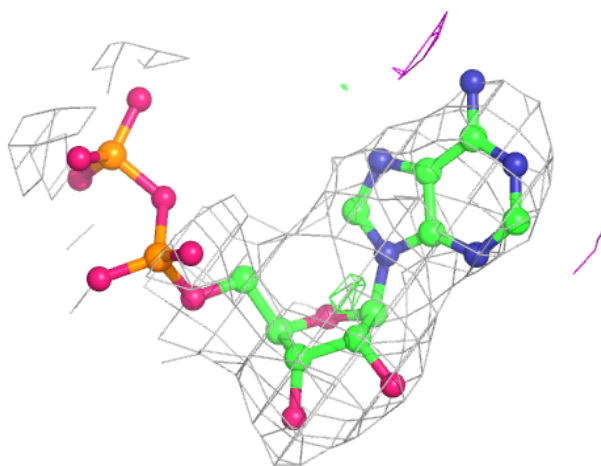
**Electron density around ADP I 800:**

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



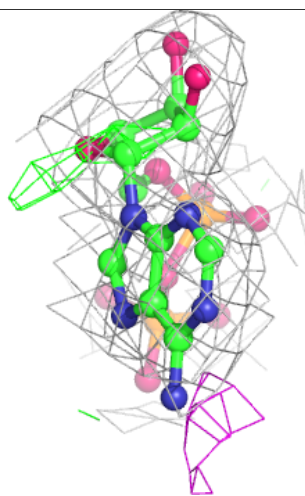
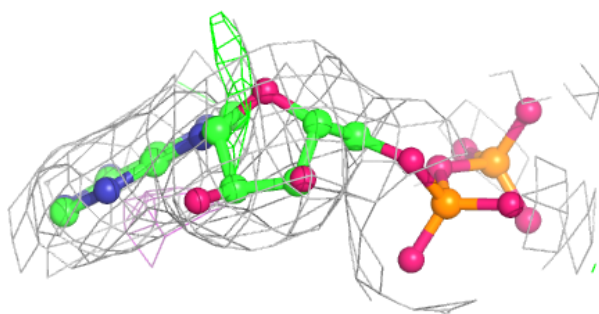
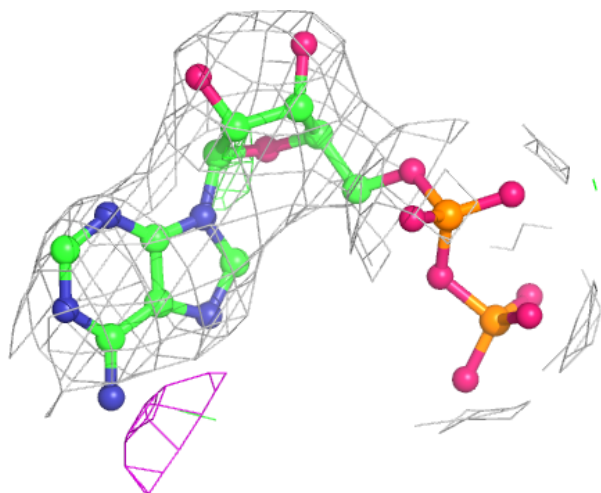
**Electron density around ADP G 800:**

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



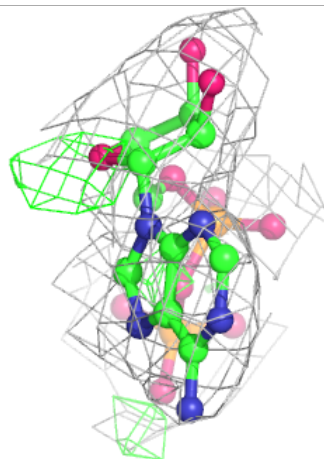
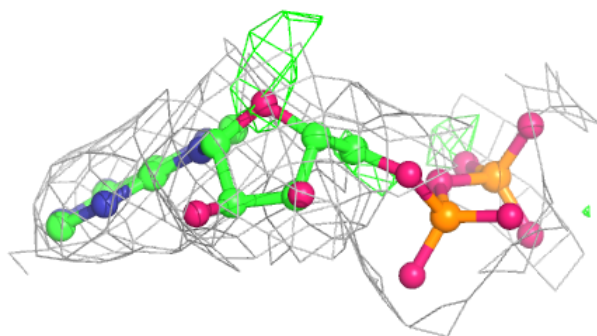
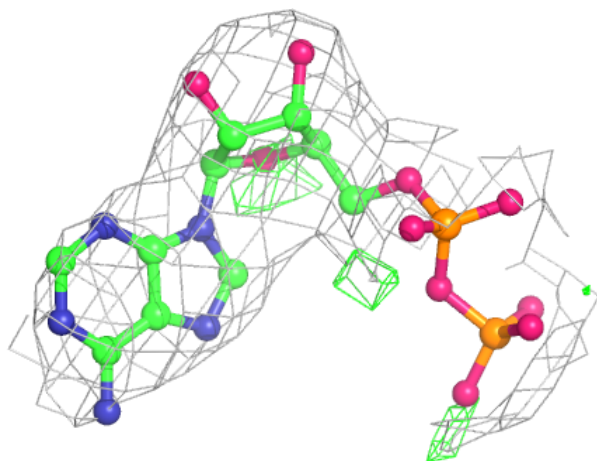
**Electron density around ADP E 800:**

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



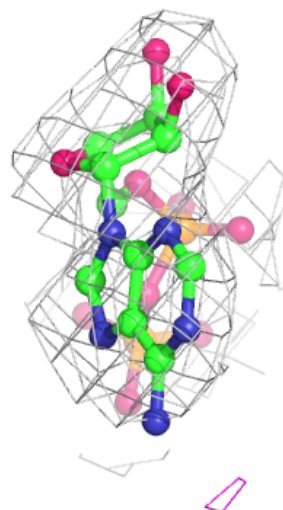
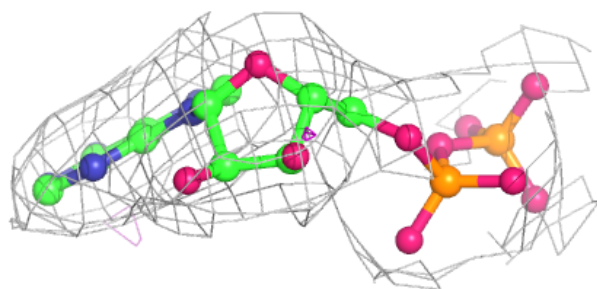
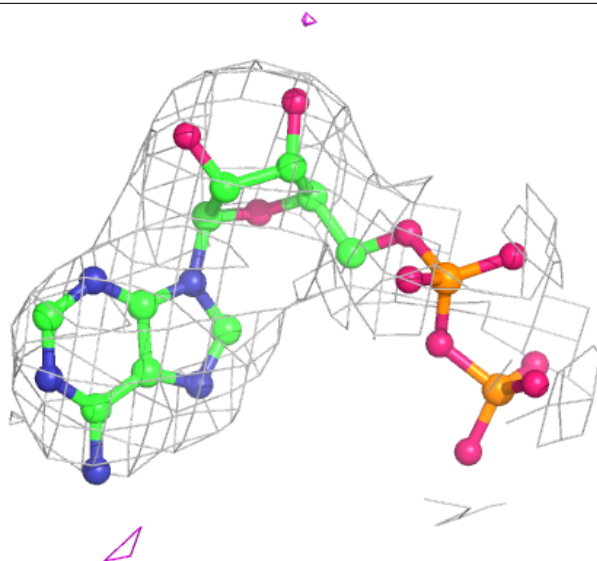
**Electron density around ADP B 800:**

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



**Electron density around ADP A 800:**

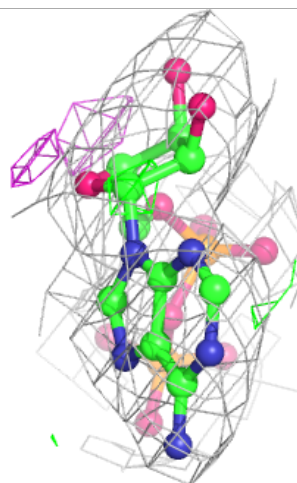
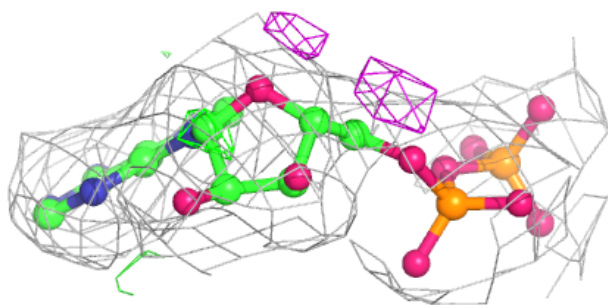
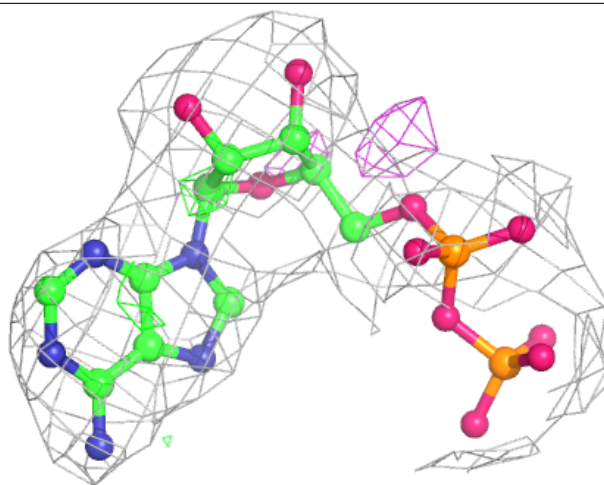
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





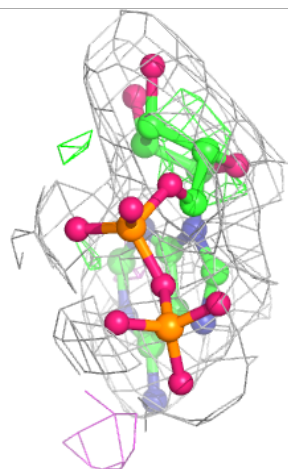
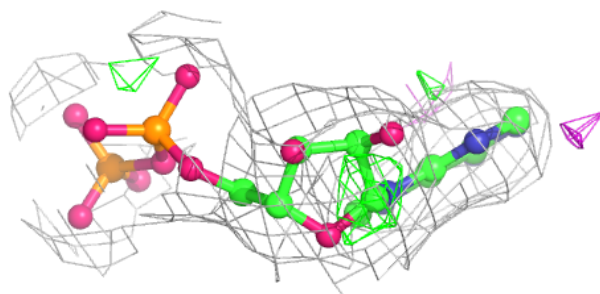
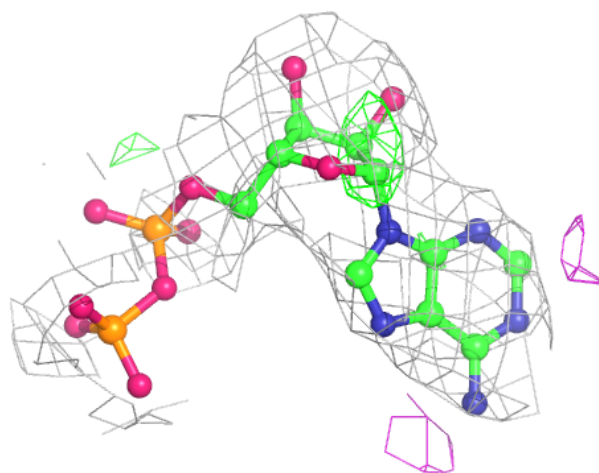
**Electron density around ADP D 800:**

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



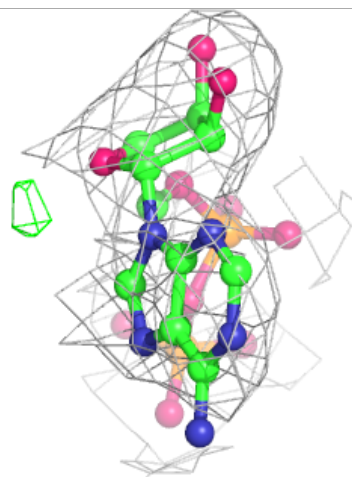
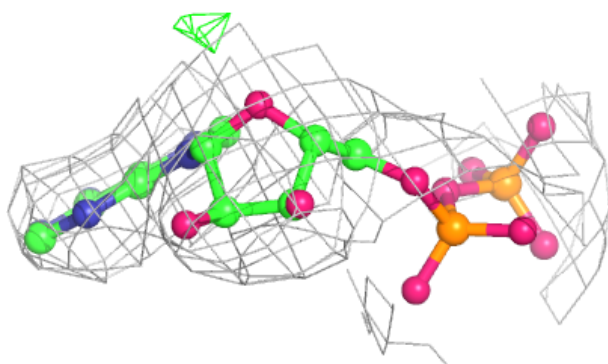
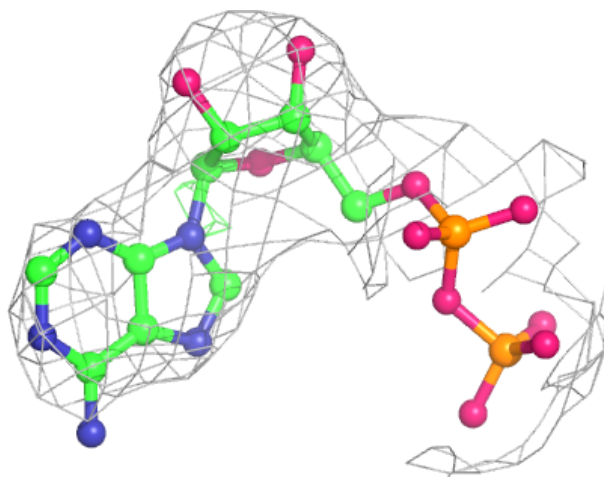
**Electron density around ADP F 800:**

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



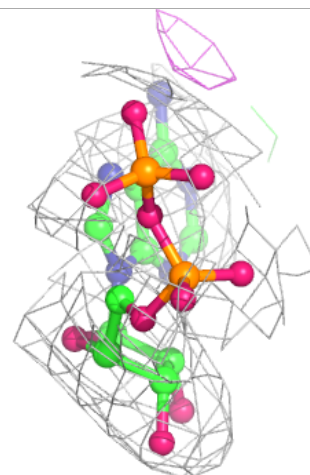
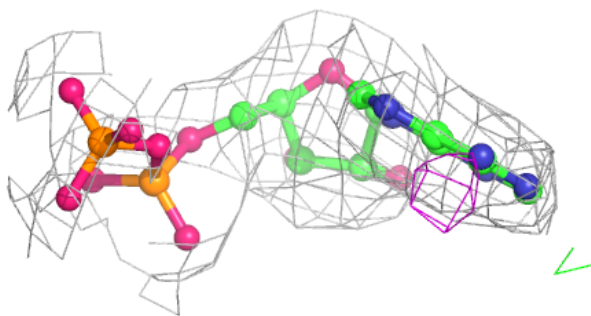
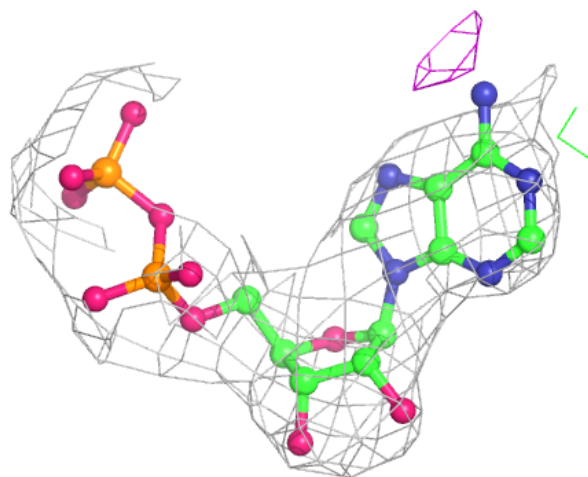
**Electron density around ADP C 800:**

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



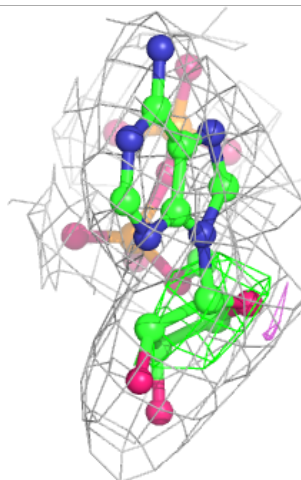
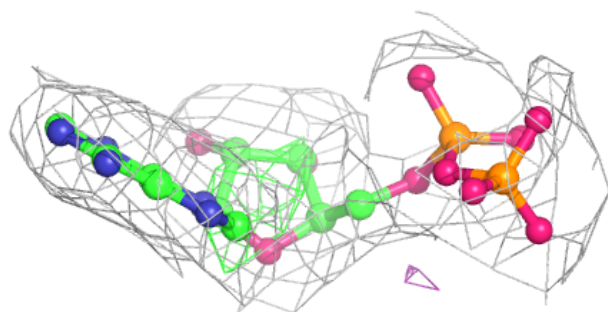
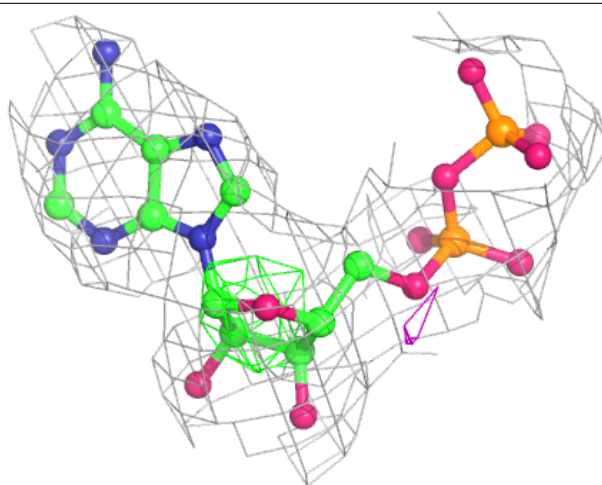
**Electron density around ADP H 800:**

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



**Electron density around ADP J 800:**

$2mF_o-DF_c$  (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.