



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 01:18 PM EDT

PDB ID : 2OFW  
Title : Crystal structure of the APSK domain of human PAPSS1 complexed with 2 APS molecules  
Authors : Sekulic, N.; Lavie, A.  
Deposited on : 2007-01-04  
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

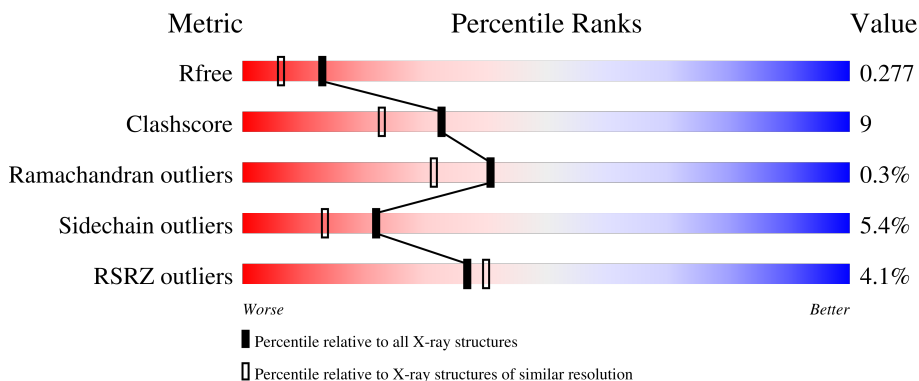
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	 6% 77% 18% .
1	B	208	 4% 72% 18% . 7%
1	C	208	 2% 78% 16% . .
1	D	208	 5% 74% 23% . .
1	E	208	 4% 81% 13% . .

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Mol	Chain	Length	Quality of chain
1	F	208	4% 78% 18% ..
1	G	208	5% 79% 16% ..
1	H	208	2% 76% 15% • 7%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13687 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 APS kinase domain of the PAPS synthetase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1574	979	281	306	8	0	3	0
1	B	193	1497	935	265	289	8	0	0	0
1	C	204	1583	987	282	306	8	0	0	0
1	D	204	1583	987	282	306	8	0	0	0
1	E	203	1562	974	277	303	8	0	0	0
1	F	204	1573	981	278	306	8	5	0	0
1	G	201	1553	971	273	301	8	0	0	0
1	H	193	1492	932	262	290	8	0	0	0

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	-	cloning artifact	UNP O43252
A	21	GLY	-	cloning artifact	UNP O43252
A	22	HIS	-	cloning artifact	UNP O43252
A	?	-	GLU	deletion	UNP O43252
A	?	-	ILE	deletion	UNP O43252
A	?	-	PRO	deletion	UNP O43252
A	?	-	GLY	deletion	UNP O43252
A	?	-	SER	deletion	UNP O43252
A	?	-	LEU	deletion	UNP O43252
A	?	-	CYS	deletion	UNP O43252
A	?	-	LYS	deletion	UNP O43252
A	?	-	LYS	deletion	UNP O43252
A	?	-	VAL	deletion	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP O43252
A	?	-	LEU	deletion	UNP O43252
A	?	-	SER	deletion	UNP O43252
A	?	-	ASN	deletion	UNP O43252
A	?	-	ASN	deletion	UNP O43252
A	?	-	ALA	deletion	UNP O43252
A	?	-	GLN	deletion	UNP O43252
A	?	-	ASN	deletion	UNP O43252
A	?	-	TRP	deletion	UNP O43252
A	?	-	GLY	deletion	UNP O43252
A	?	-	MET	deletion	UNP O43252
A	?	-	GLN	deletion	UNP O43252
A	55	ILE	VAL	conflict	UNP O43252
A	221	ASN	GLN	conflict	UNP O43252
A	226	LEU	VAL	conflict	UNP O43252
B	20	GLN	-	cloning artifact	UNP O43252
B	21	GLY	-	cloning artifact	UNP O43252
B	22	HIS	-	cloning artifact	UNP O43252
B	?	-	GLU	deletion	UNP O43252
B	?	-	ILE	deletion	UNP O43252
B	?	-	PRO	deletion	UNP O43252
B	?	-	GLY	deletion	UNP O43252
B	?	-	SER	deletion	UNP O43252
B	?	-	LEU	deletion	UNP O43252
B	?	-	CYS	deletion	UNP O43252
B	?	-	LYS	deletion	UNP O43252
B	?	-	LYS	deletion	UNP O43252
B	?	-	VAL	deletion	UNP O43252
B	?	-	LYS	deletion	UNP O43252
B	?	-	LEU	deletion	UNP O43252
B	?	-	SER	deletion	UNP O43252
B	?	-	ASN	deletion	UNP O43252
B	?	-	ASN	deletion	UNP O43252
B	?	-	ALA	deletion	UNP O43252
B	?	-	GLN	deletion	UNP O43252
B	?	-	ASN	deletion	UNP O43252
B	?	-	TRP	deletion	UNP O43252
B	?	-	GLY	deletion	UNP O43252
B	?	-	MET	deletion	UNP O43252
B	?	-	GLN	deletion	UNP O43252
B	55	ILE	VAL	conflict	UNP O43252
B	221	ASN	GLN	conflict	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	LEU	VAL	conflict	UNP O43252
C	20	GLN	-	cloning artifact	UNP O43252
C	21	GLY	-	cloning artifact	UNP O43252
C	22	HIS	-	cloning artifact	UNP O43252
C	?	-	GLU	deletion	UNP O43252
C	?	-	ILE	deletion	UNP O43252
C	?	-	PRO	deletion	UNP O43252
C	?	-	GLY	deletion	UNP O43252
C	?	-	SER	deletion	UNP O43252
C	?	-	LEU	deletion	UNP O43252
C	?	-	CYS	deletion	UNP O43252
C	?	-	LYS	deletion	UNP O43252
C	?	-	LYS	deletion	UNP O43252
C	?	-	VAL	deletion	UNP O43252
C	?	-	LYS	deletion	UNP O43252
C	?	-	LEU	deletion	UNP O43252
C	?	-	SER	deletion	UNP O43252
C	?	-	ASN	deletion	UNP O43252
C	?	-	ASN	deletion	UNP O43252
C	?	-	ALA	deletion	UNP O43252
C	?	-	GLN	deletion	UNP O43252
C	?	-	ASN	deletion	UNP O43252
C	?	-	TRP	deletion	UNP O43252
C	?	-	GLY	deletion	UNP O43252
C	?	-	MET	deletion	UNP O43252
C	?	-	GLN	deletion	UNP O43252
C	55	ILE	VAL	conflict	UNP O43252
C	221	ASN	GLN	conflict	UNP O43252
C	226	LEU	VAL	conflict	UNP O43252
D	20	GLN	-	cloning artifact	UNP O43252
D	21	GLY	-	cloning artifact	UNP O43252
D	22	HIS	-	cloning artifact	UNP O43252
D	?	-	GLU	deletion	UNP O43252
D	?	-	ILE	deletion	UNP O43252
D	?	-	PRO	deletion	UNP O43252
D	?	-	GLY	deletion	UNP O43252
D	?	-	SER	deletion	UNP O43252
D	?	-	LEU	deletion	UNP O43252
D	?	-	CYS	deletion	UNP O43252
D	?	-	LYS	deletion	UNP O43252
D	?	-	LYS	deletion	UNP O43252
D	?	-	VAL	deletion	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LYS	deletion	UNP O43252
D	?	-	LEU	deletion	UNP O43252
D	?	-	SER	deletion	UNP O43252
D	?	-	ASN	deletion	UNP O43252
D	?	-	ASN	deletion	UNP O43252
D	?	-	ALA	deletion	UNP O43252
D	?	-	GLN	deletion	UNP O43252
D	?	-	ASN	deletion	UNP O43252
D	?	-	TRP	deletion	UNP O43252
D	?	-	GLY	deletion	UNP O43252
D	?	-	MET	deletion	UNP O43252
D	?	-	GLN	deletion	UNP O43252
D	55	ILE	VAL	conflict	UNP O43252
D	221	ASN	GLN	conflict	UNP O43252
D	226	LEU	VAL	conflict	UNP O43252
E	20	GLN	-	cloning artifact	UNP O43252
E	21	GLY	-	cloning artifact	UNP O43252
E	22	HIS	-	cloning artifact	UNP O43252
E	?	-	GLU	deletion	UNP O43252
E	?	-	ILE	deletion	UNP O43252
E	?	-	PRO	deletion	UNP O43252
E	?	-	GLY	deletion	UNP O43252
E	?	-	SER	deletion	UNP O43252
E	?	-	LEU	deletion	UNP O43252
E	?	-	CYS	deletion	UNP O43252
E	?	-	LYS	deletion	UNP O43252
E	?	-	LYS	deletion	UNP O43252
E	?	-	VAL	deletion	UNP O43252
E	?	-	LYS	deletion	UNP O43252
E	?	-	LEU	deletion	UNP O43252
E	?	-	SER	deletion	UNP O43252
E	?	-	ASN	deletion	UNP O43252
E	?	-	ASN	deletion	UNP O43252
E	?	-	ALA	deletion	UNP O43252
E	?	-	GLN	deletion	UNP O43252
E	?	-	ASN	deletion	UNP O43252
E	?	-	TRP	deletion	UNP O43252
E	?	-	GLY	deletion	UNP O43252
E	?	-	MET	deletion	UNP O43252
E	?	-	GLN	deletion	UNP O43252
E	55	ILE	VAL	conflict	UNP O43252
E	221	ASN	GLN	conflict	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
E	226	LEU	VAL	conflict	UNP O43252
F	20	GLN	-	cloning artifact	UNP O43252
F	21	GLY	-	cloning artifact	UNP O43252
F	22	HIS	-	cloning artifact	UNP O43252
F	?	-	GLU	deletion	UNP O43252
F	?	-	ILE	deletion	UNP O43252
F	?	-	PRO	deletion	UNP O43252
F	?	-	GLY	deletion	UNP O43252
F	?	-	SER	deletion	UNP O43252
F	?	-	LEU	deletion	UNP O43252
F	?	-	CYS	deletion	UNP O43252
F	?	-	LYS	deletion	UNP O43252
F	?	-	LYS	deletion	UNP O43252
F	?	-	VAL	deletion	UNP O43252
F	?	-	LYS	deletion	UNP O43252
F	?	-	LEU	deletion	UNP O43252
F	?	-	SER	deletion	UNP O43252
F	?	-	ASN	deletion	UNP O43252
F	?	-	ASN	deletion	UNP O43252
F	?	-	ALA	deletion	UNP O43252
F	?	-	GLN	deletion	UNP O43252
F	?	-	ASN	deletion	UNP O43252
F	?	-	TRP	deletion	UNP O43252
F	?	-	GLY	deletion	UNP O43252
F	?	-	MET	deletion	UNP O43252
F	?	-	GLN	deletion	UNP O43252
F	55	ILE	VAL	conflict	UNP O43252
F	221	ASN	GLN	conflict	UNP O43252
F	226	LEU	VAL	conflict	UNP O43252
G	20	GLN	-	cloning artifact	UNP O43252
G	21	GLY	-	cloning artifact	UNP O43252
G	22	HIS	-	cloning artifact	UNP O43252
G	?	-	GLU	deletion	UNP O43252
G	?	-	ILE	deletion	UNP O43252
G	?	-	PRO	deletion	UNP O43252
G	?	-	GLY	deletion	UNP O43252
G	?	-	SER	deletion	UNP O43252
G	?	-	LEU	deletion	UNP O43252
G	?	-	CYS	deletion	UNP O43252
G	?	-	LYS	deletion	UNP O43252
G	?	-	LYS	deletion	UNP O43252
G	?	-	VAL	deletion	UNP O43252

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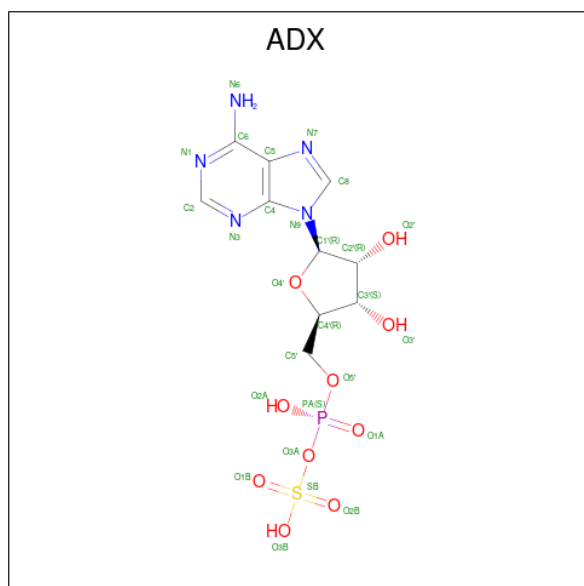
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	deletion	UNP O43252
G	?	-	LEU	deletion	UNP O43252
G	?	-	SER	deletion	UNP O43252
G	?	-	ASN	deletion	UNP O43252
G	?	-	ASN	deletion	UNP O43252
G	?	-	ALA	deletion	UNP O43252
G	?	-	GLN	deletion	UNP O43252
G	?	-	ASN	deletion	UNP O43252
G	?	-	TRP	deletion	UNP O43252
G	?	-	GLY	deletion	UNP O43252
G	?	-	MET	deletion	UNP O43252
G	?	-	GLN	deletion	UNP O43252
G	55	ILE	VAL	conflict	UNP O43252
G	221	ASN	GLN	conflict	UNP O43252
G	226	LEU	VAL	conflict	UNP O43252
H	20	GLN	-	cloning artifact	UNP O43252
H	21	GLY	-	cloning artifact	UNP O43252
H	22	HIS	-	cloning artifact	UNP O43252
H	?	-	GLU	deletion	UNP O43252
H	?	-	ILE	deletion	UNP O43252
H	?	-	PRO	deletion	UNP O43252
H	?	-	GLY	deletion	UNP O43252
H	?	-	SER	deletion	UNP O43252
H	?	-	LEU	deletion	UNP O43252
H	?	-	CYS	deletion	UNP O43252
H	?	-	LYS	deletion	UNP O43252
H	?	-	LYS	deletion	UNP O43252
H	?	-	VAL	deletion	UNP O43252
H	?	-	LYS	deletion	UNP O43252
H	?	-	LEU	deletion	UNP O43252
H	?	-	SER	deletion	UNP O43252
H	?	-	ASN	deletion	UNP O43252
H	?	-	ASN	deletion	UNP O43252
H	?	-	ALA	deletion	UNP O43252
H	?	-	GLN	deletion	UNP O43252
H	?	-	ASN	deletion	UNP O43252
H	?	-	TRP	deletion	UNP O43252
H	?	-	GLY	deletion	UNP O43252
H	?	-	MET	deletion	UNP O43252
H	?	-	GLN	deletion	UNP O43252
H	55	ILE	VAL	conflict	UNP O43252
H	221	ASN	GLN	conflict	UNP O43252

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Chain	Residue	Modelled	Actual	Comment	Reference
H	226	LEU	VAL	conflict	UNP O43252

- Molecule 2 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>10</sub>PS).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	G	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	G	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
2	H	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	104	Total	O	0	0
			104	104		
4	C	108	Total	O	0	0
			108	108		
4	D	103	Total	O	0	0
			103	103		
4	E	103	Total	O	0	0
			103	103		

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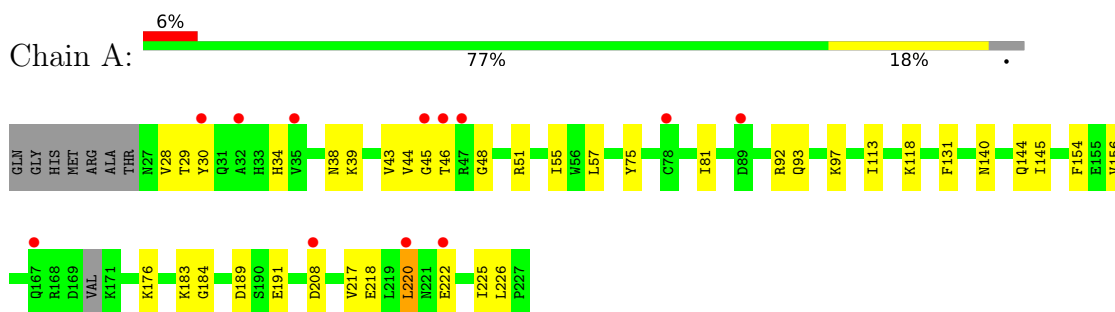
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	F	92	Total O 92 92	0	0
4	G	103	Total O 103 103	0	0
4	H	102	Total O 102 102	0	0

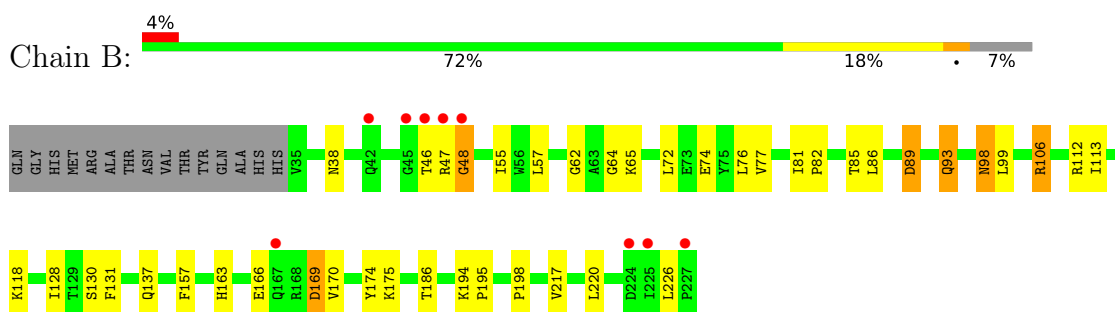
### 3 Residue-property plots [i](#)

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.

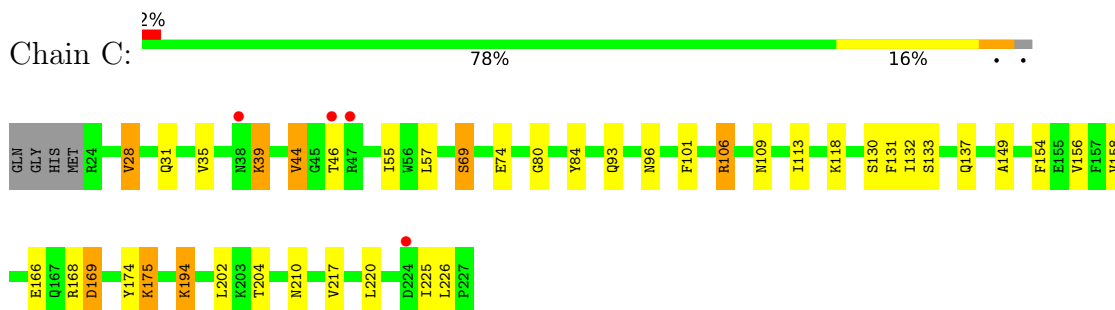
- Molecule 1: APS kinase domain of the PAPS synthetase 1



- Molecule 1: APS kinase domain of the PAPS synthetase 1

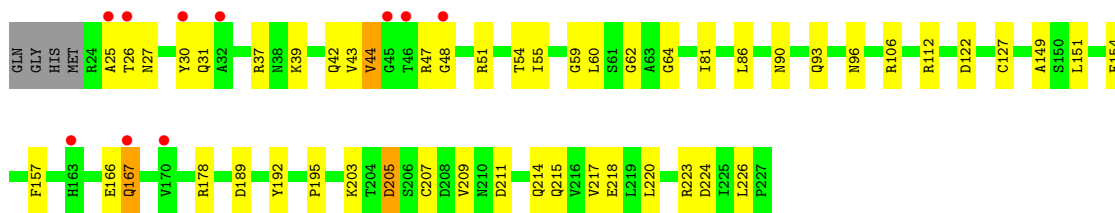


- Molecule 1: APS kinase domain of the PAPS synthetase 1

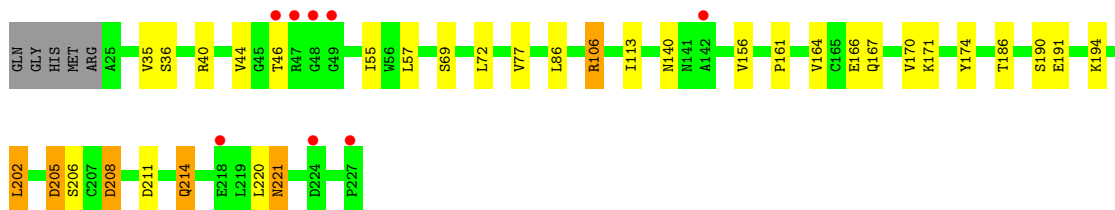
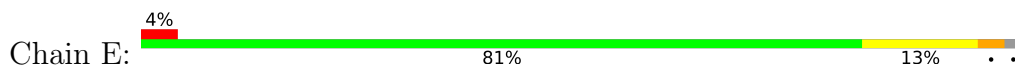


- Molecule 1: APS kinase domain of the PAPS synthetase 1

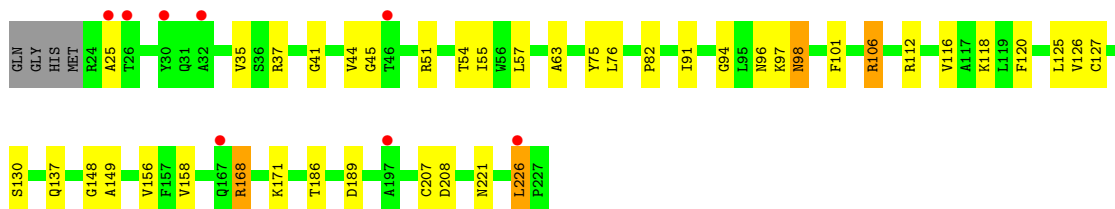
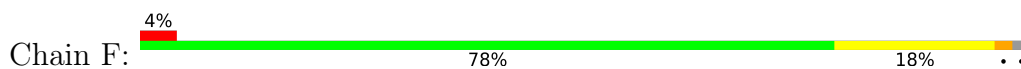




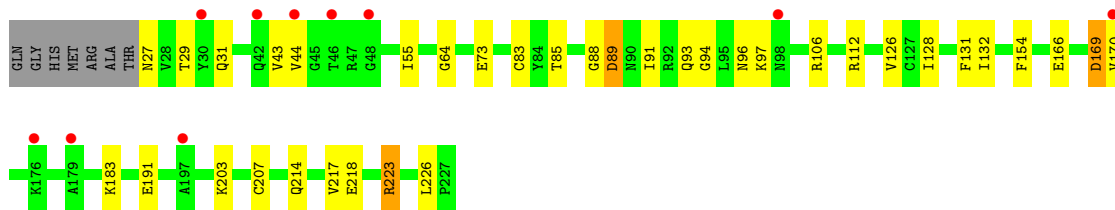
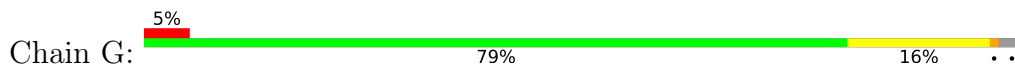
- Molecule 1: APS kinase domain of the PAPS synthetase 1



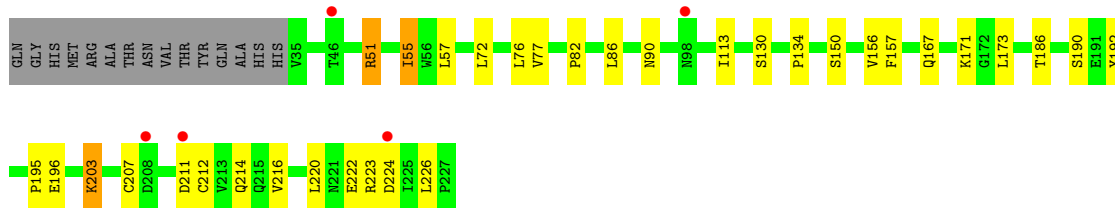
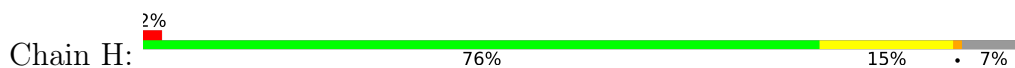
- Molecule 1: APS kinase domain of the PAPS synthetase 1



- Molecule 1: APS kinase domain of the PAPS synthetase 1



- Molecule 1: APS kinase domain of the PAPS synthetase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.19Å 69.03Å 150.61Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 15.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-2.05) 97.4 (15.00-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 2.05Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.217 , 0.282 0.216 , 0.277	Depositor DCC
$R_{free}$ test set	10180 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.90% 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, ADX

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	0.56	0/1601	0.66	0/2165
1	B	0.58	0/1522	0.69	2/2057 (0.1%)
1	C	0.57	0/1611	0.69	2/2179 (0.1%)
1	D	0.58	0/1611	0.65	0/2179
1	E	0.55	0/1590	0.69	2/2153 (0.1%)
1	F	0.55	0/1601	0.68	2/2168 (0.1%)
1	G	0.57	0/1581	0.69	2/2141 (0.1%)
1	H	0.55	0/1517	0.64	0/2050
All	All	0.56	0/12634	0.67	10/17092 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	E	106	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	106	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	F	106	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	106	ARG	NE-CZ-NH1	7.65	124.13	120.30

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	1574	0	1528	25	0
1	B	1497	0	1478	38	0
1	C	1583	0	1550	32	0
1	D	1583	0	1550	44	0
1	E	1562	0	1516	19	0
1	F	1573	0	1528	31	0
1	G	1553	0	1515	27	0
1	H	1492	0	1467	24	0
2	A	54	0	24	0	0
2	B	54	0	24	2	0
2	C	54	0	26	3	0
2	D	54	0	24	3	0
2	E	54	0	25	1	0
2	F	54	0	25	2	0
2	G	54	0	25	3	0
2	H	54	0	25	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	117	0	0	3	1
4	B	104	0	0	5	0
4	C	108	0	0	2	1
4	D	103	0	0	9	0
4	E	103	0	0	2	0
4	F	92	0	0	1	0
4	G	103	0	0	0	0
4	H	102	0	0	1	0
All	All	13687	0	12330	219	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 9.

The worst 5 of 219 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)
4:C:1407:HOH:O	1:D:25:ALA:HB2	1.44	1.14
1:C:31:GLN:H	1:D:90:ASN:HD21	1.15	0.94
1:C:44:VAL:O	1:D:44:VAL:O	1.84	0.94
1:B:175:LYS:HD2	4:B:1234:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ILE:HD11	1:D:220:LEU:HD11	1.63	0.80

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)
4:A:1117:HOH:O	4:C:1392:HOH:O[2_556]	2.16	0.04

## 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	199/208 (96%)	190 (96%)	8 (4%)	1 (0%)	29	18
1	B	191/208 (92%)	185 (97%)	4 (2%)	2 (1%)	15	6
1	C	202/208 (97%)	196 (97%)	5 (2%)	1 (0%)	29	18
1	D	202/208 (97%)	194 (96%)	8 (4%)	0	100	100
1	E	201/208 (97%)	195 (97%)	6 (3%)	0	100	100
1	F	202/208 (97%)	195 (96%)	7 (4%)	0	100	100
1	G	199/208 (96%)	194 (98%)	4 (2%)	1 (0%)	29	18
1	H	191/208 (92%)	184 (96%)	7 (4%)	0	100	100
All	All	1587/1664 (95%)	1533 (97%)	49 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLY
1	B	48	GLY
1	G	169	ASP
1	B	169	ASP

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*Continued from previous page...*

Mol	Chain	Res	Type
1	C	169	ASP

### 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	170/175 (97%)	160 (94%)	10 (6%)	19	11
1	B	163/175 (93%)	154 (94%)	9 (6%)	21	13
1	C	171/175 (98%)	162 (95%)	9 (5%)	22	14
1	D	171/175 (98%)	163 (95%)	8 (5%)	26	18
1	E	167/175 (95%)	155 (93%)	12 (7%)	14	7
1	F	169/175 (97%)	162 (96%)	7 (4%)	30	23
1	G	168/175 (96%)	161 (96%)	7 (4%)	30	22
1	H	162/175 (93%)	152 (94%)	10 (6%)	18	10
All	All	1341/1400 (96%)	1269 (95%)	72 (5%)	22	13

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	183	LYS
1	H	222	GLU
1	G	203	LYS
1	H	150	SER
1	C	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	215	GLN
1	H	90	ASN
1	G	27	ASN
1	G	167	GLN

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Mol	Chain	Res	Type
1	H	167	GLN

### 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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADX	G	1700	-	25,29,29	1.13	3 (12%)	26,45,45	1.50	4 (15%)
2	ADX	C	1300	-	25,29,29	1.12	2 (8%)	26,45,45	1.28	3 (11%)
2	ADX	H	1801	3	25,29,29	1.12	3 (12%)	26,45,45	1.23	2 (7%)
2	ADX	E	1501	3	25,29,29	1.14	2 (8%)	26,45,45	1.28	3 (11%)
2	ADX	F	1601	3	25,29,29	1.29	3 (12%)	26,45,45	1.32	4 (15%)
2	ADX	B	1200	-	25,29,29	1.40	2 (8%)	26,45,45	1.62	5 (19%)
2	ADX	A	1100	-	25,29,29	1.47	3 (12%)	26,45,45	1.47	4 (15%)
2	ADX	A	1101	-	25,29,29	1.09	3 (12%)	26,45,45	1.31	3 (11%)
2	ADX	E	1500	-	25,29,29	1.37	3 (12%)	26,45,45	1.43	4 (15%)
2	ADX	H	1800	-	25,29,29	1.17	3 (12%)	26,45,45	1.50	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADX	C	1301	3	25,29,29	1.12	2 (8%)	26,45,45	1.33	3 (11%)
2	ADX	D	1401	3	25,29,29	1.12	3 (12%)	26,45,45	1.26	2 (7%)
2	ADX	G	1701	-	25,29,29	1.16	2 (8%)	26,45,45	1.32	3 (11%)
2	ADX	B	1201	3	25,29,29	1.06	2 (8%)	26,45,45	1.30	3 (11%)
2	ADX	D	1400	-	25,29,29	1.29	1 (4%)	26,45,45	1.53	4 (15%)
2	ADX	F	1600	-	25,29,29	1.64	3 (12%)	26,45,45	1.39	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADX	G	1700	-	-	2/6/32/32	0/3/3/3
2	ADX	C	1300	-	-	2/6/32/32	0/3/3/3
2	ADX	H	1801	3	-	1/6/32/32	0/3/3/3
2	ADX	E	1501	3	-	1/6/32/32	0/3/3/3
2	ADX	F	1601	3	-	2/6/32/32	0/3/3/3
2	ADX	B	1200	-	-	2/6/32/32	0/3/3/3
2	ADX	A	1100	-	-	0/6/32/32	0/3/3/3
2	ADX	A	1101	-	-	5/6/32/32	0/3/3/3
2	ADX	E	1500	-	-	0/6/32/32	0/3/3/3
2	ADX	H	1800	-	-	1/6/32/32	0/3/3/3
2	ADX	C	1301	3	-	1/6/32/32	0/3/3/3
2	ADX	D	1401	3	-	1/6/32/32	0/3/3/3
2	ADX	G	1701	-	-	5/6/32/32	0/3/3/3
2	ADX	B	1201	3	-	1/6/32/32	0/3/3/3
2	ADX	D	1400	-	-	0/6/32/32	0/3/3/3
2	ADX	F	1600	-	-	0/6/32/32	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1600	ADX	PA-O3A	5.92	1.64	1.59
2	D	1400	ADX	PA-O3A	4.90	1.63	1.59
2	A	1100	ADX	PA-O3A	4.88	1.63	1.59
2	B	1200	ADX	PA-O3A	4.20	1.62	1.59
2	F	1601	ADX	PA-O3A	3.70	1.62	1.59

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1400	ADX	N3-C2-N1	-4.54	121.58	128.68
2	B	1200	ADX	C3'-C2'-C1'	4.39	107.59	100.98
2	H	1800	ADX	N3-C2-N1	-4.04	122.37	128.68
2	A	1100	ADX	N3-C2-N1	-3.86	122.65	128.68
2	G	1700	ADX	N3-C2-N1	-3.61	123.04	128.68

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

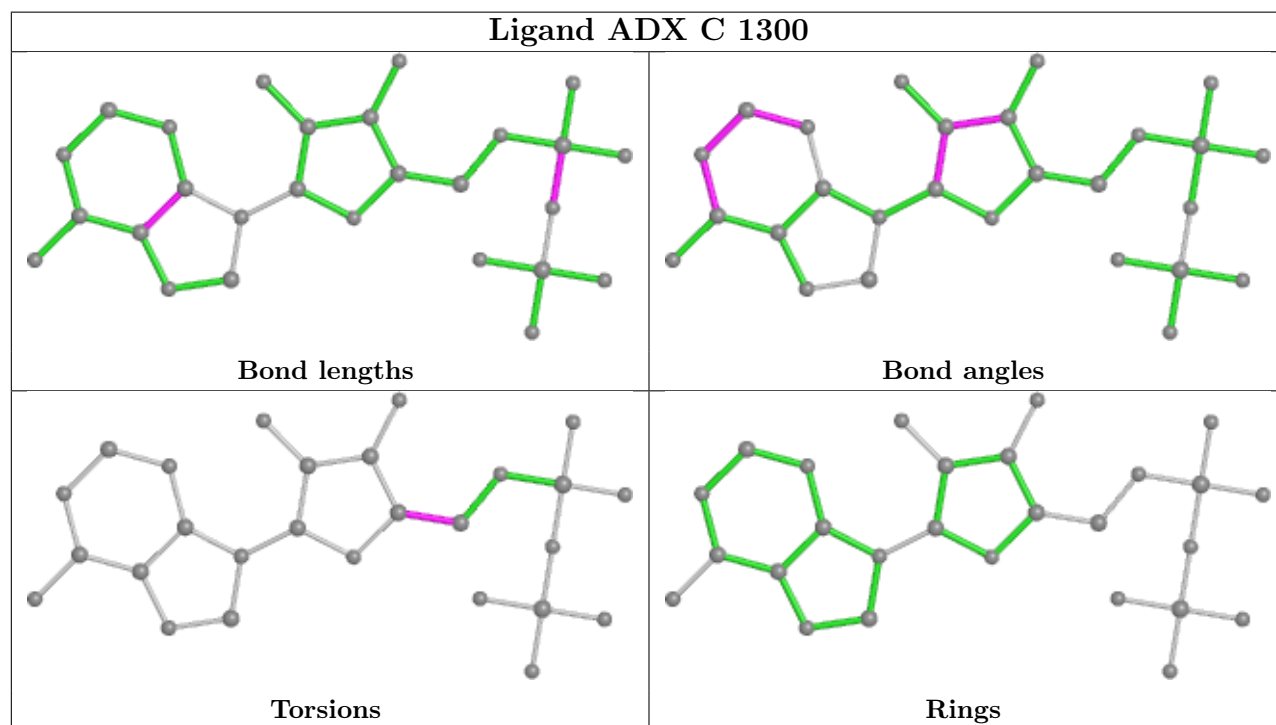
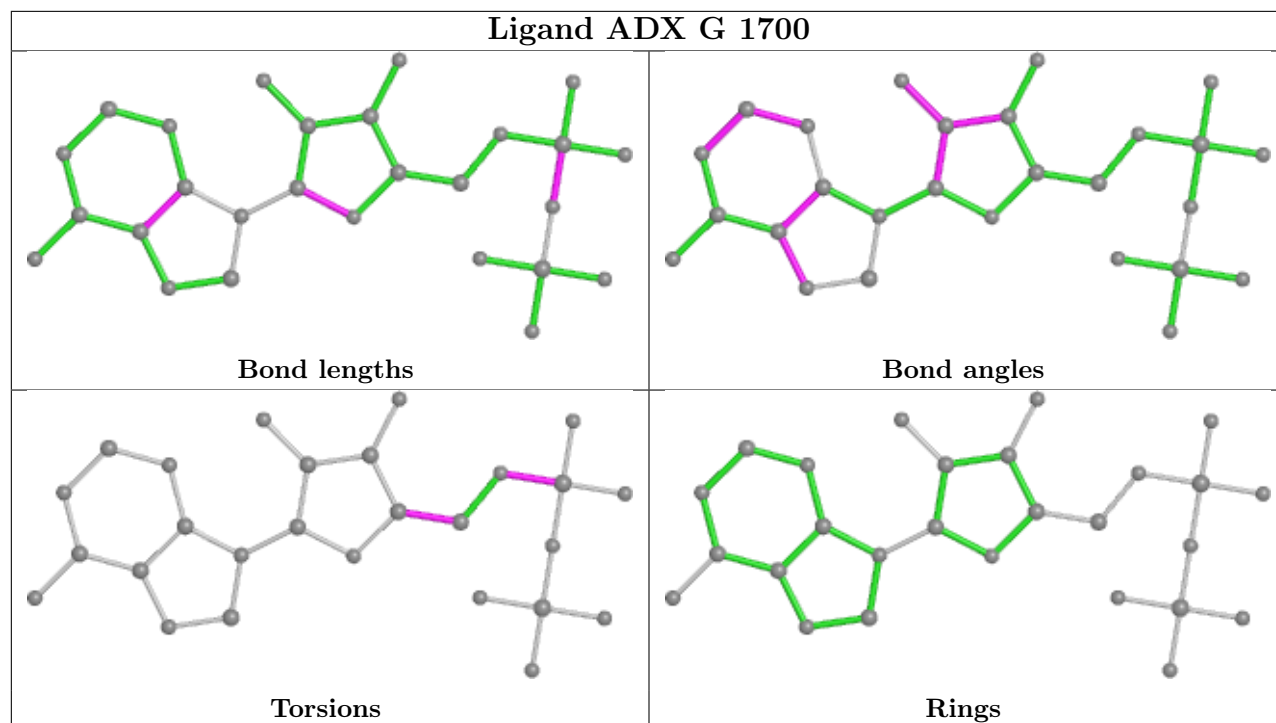
Mol	Chain	Res	Type	Atoms
2	A	1101	ADX	C5'-O5'-PA-O1A
2	A	1101	ADX	O4'-C4'-C5'-O5'
2	G	1701	ADX	C5'-O5'-PA-O1A
2	G	1701	ADX	C5'-O5'-PA-O3A
2	G	1701	ADX	O4'-C4'-C5'-O5'

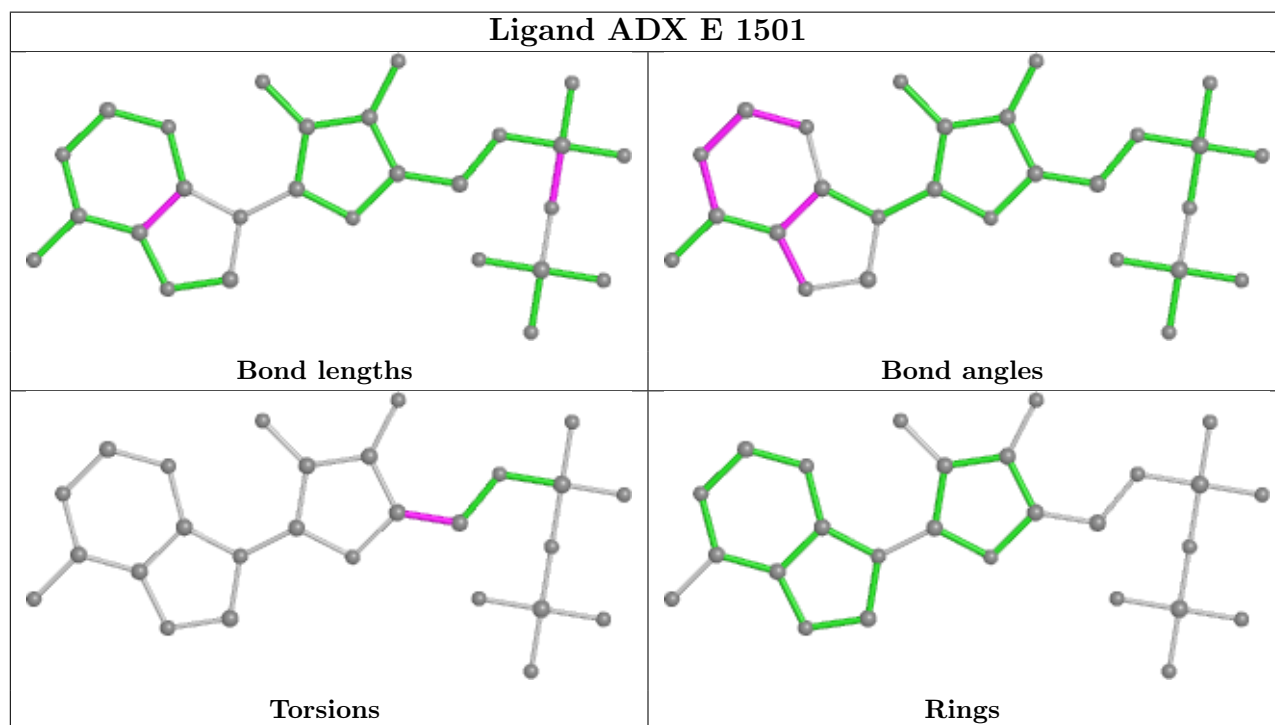
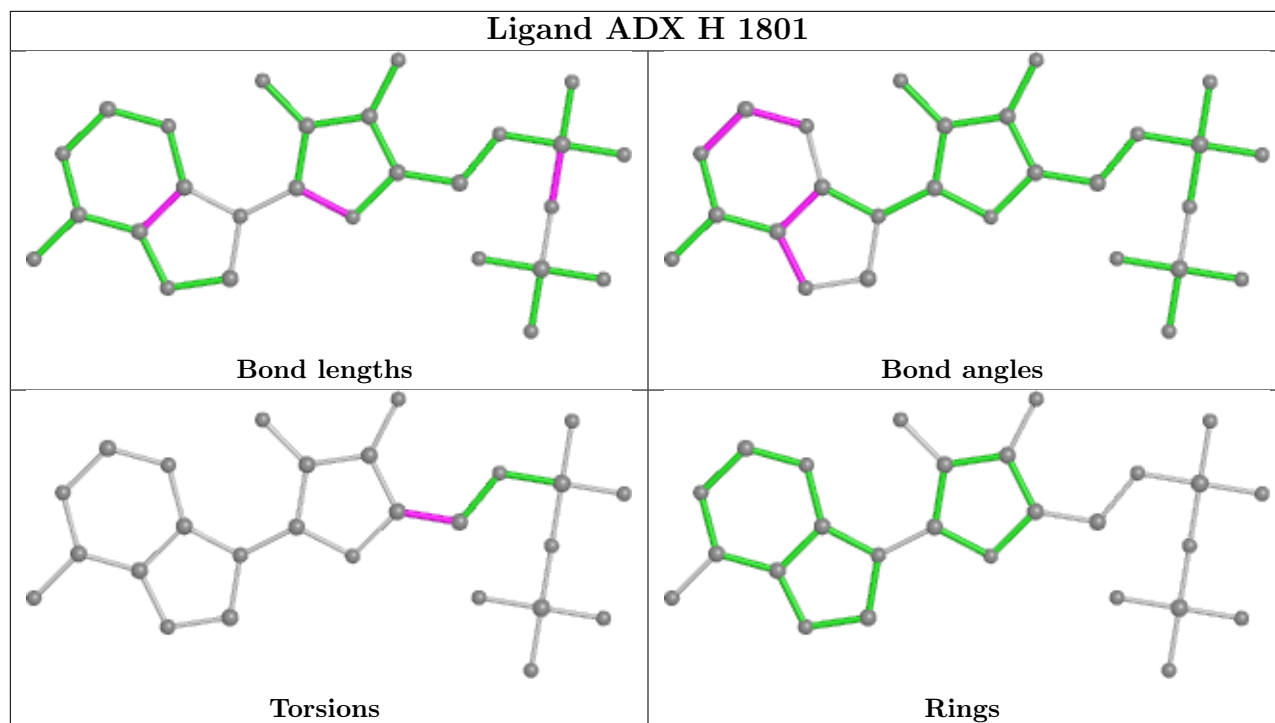
There are no ring outliers.

8 monomers are involved in 14 short contacts:

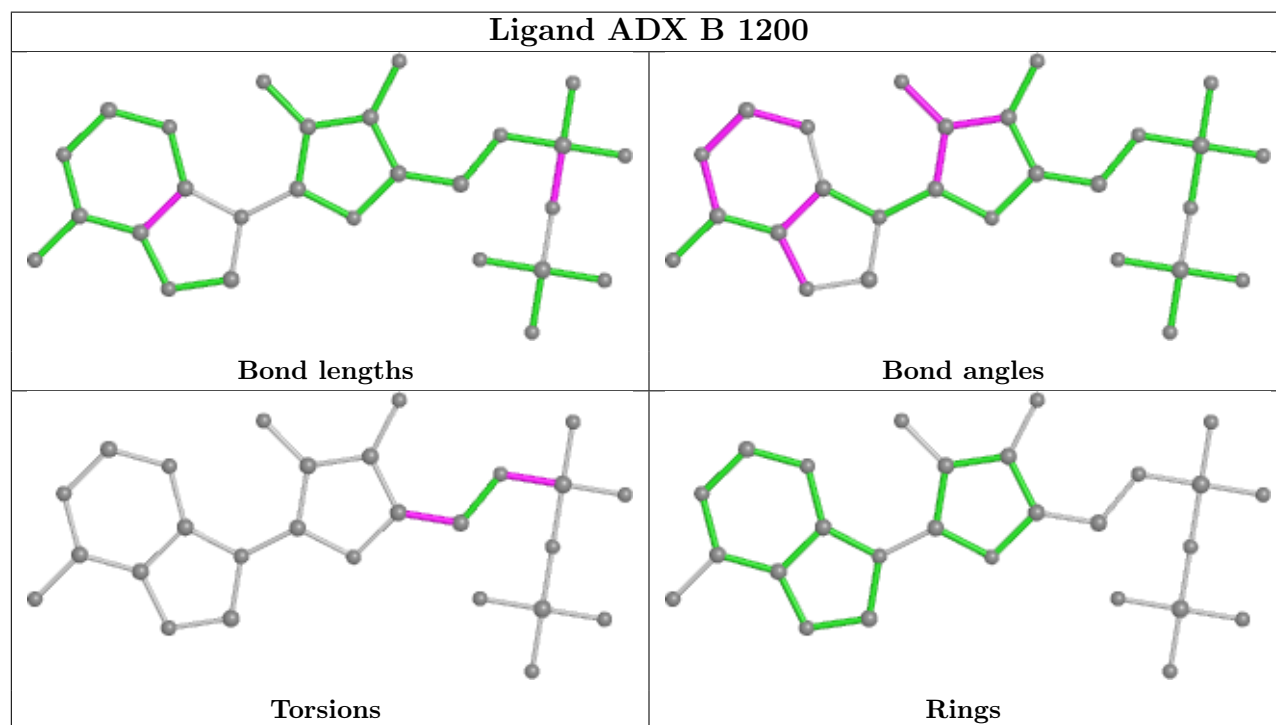
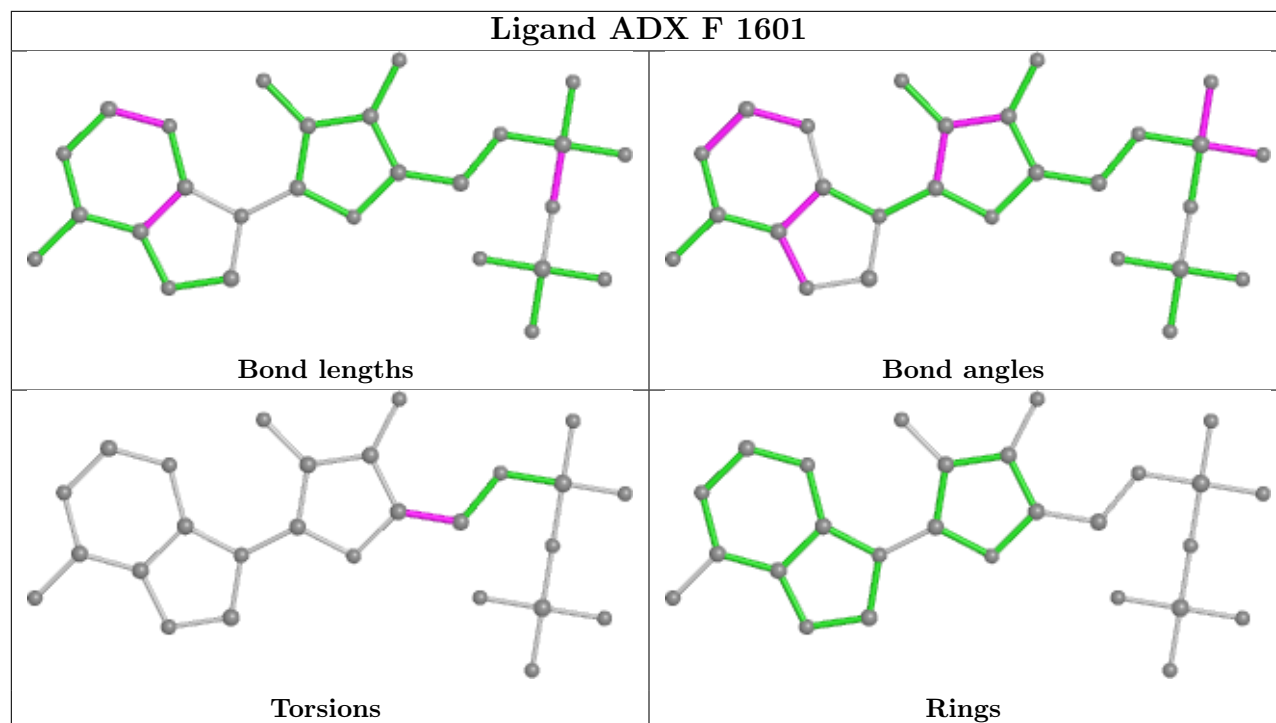
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1700	ADX	1	0
2	C	1300	ADX	1	0
2	F	1601	ADX	2	0
2	E	1500	ADX	1	0
2	C	1301	ADX	2	0
2	D	1401	ADX	3	0
2	G	1701	ADX	2	0
2	B	1201	ADX	2	0

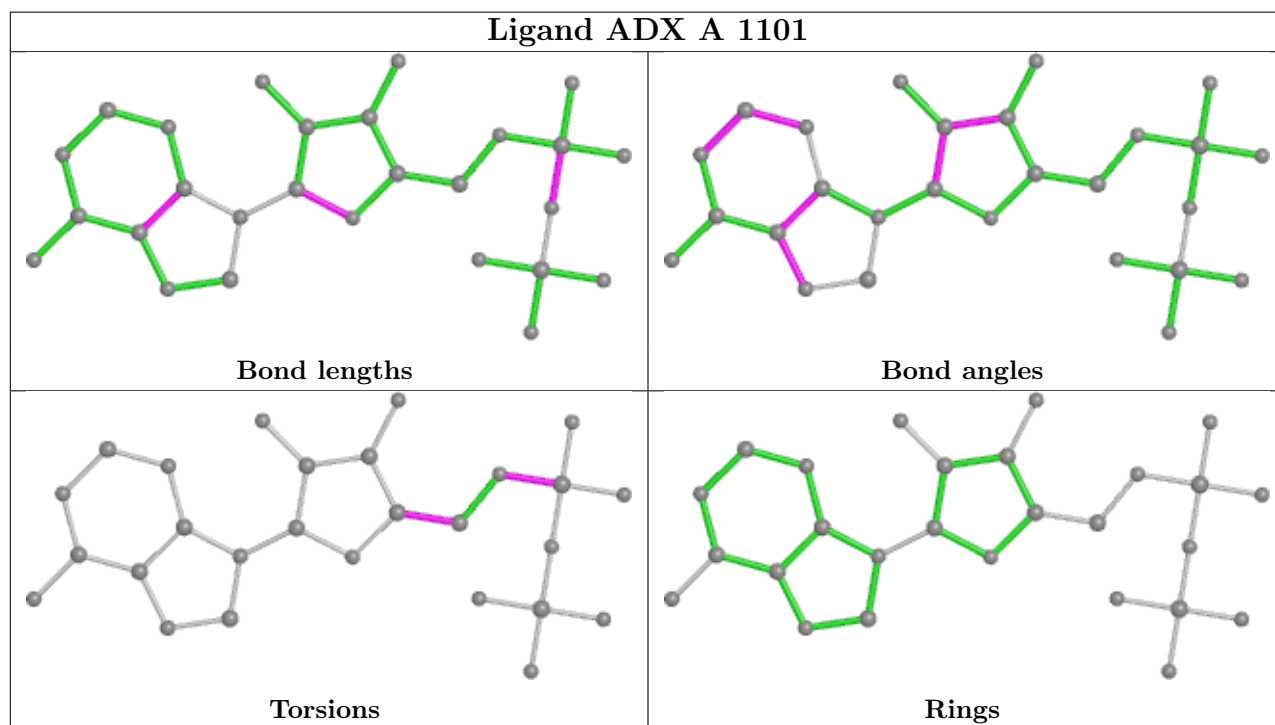
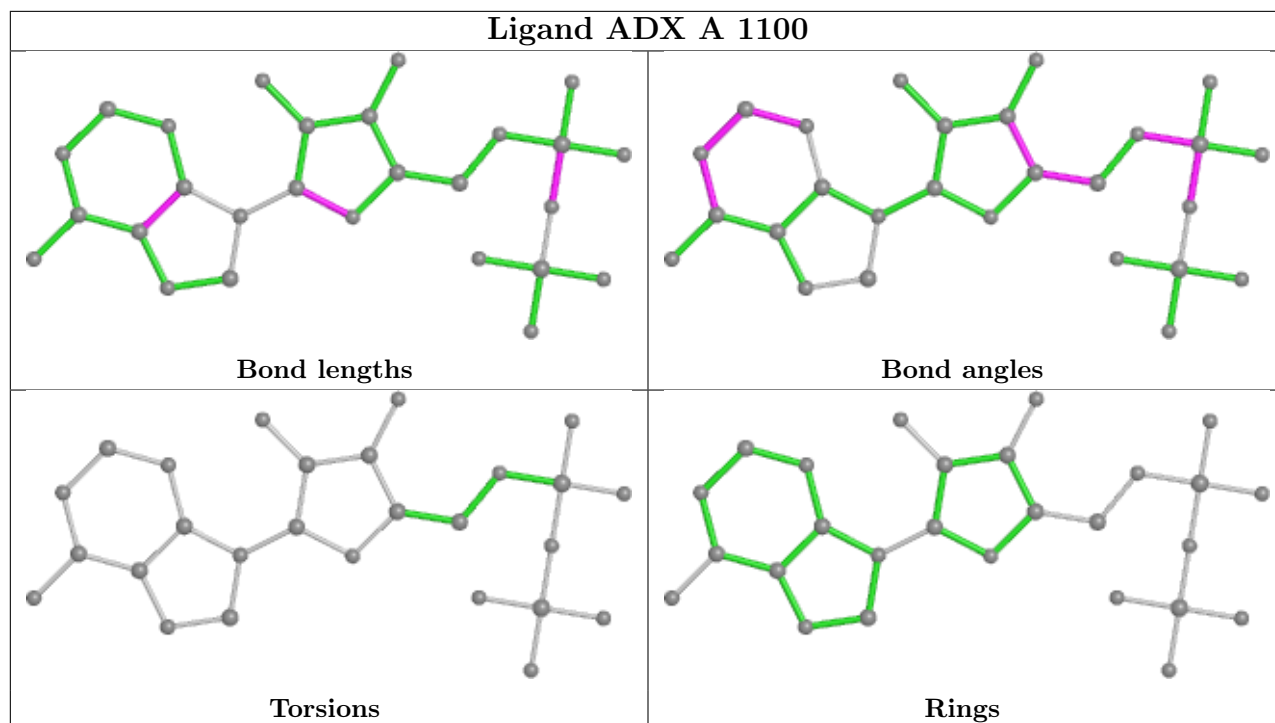
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

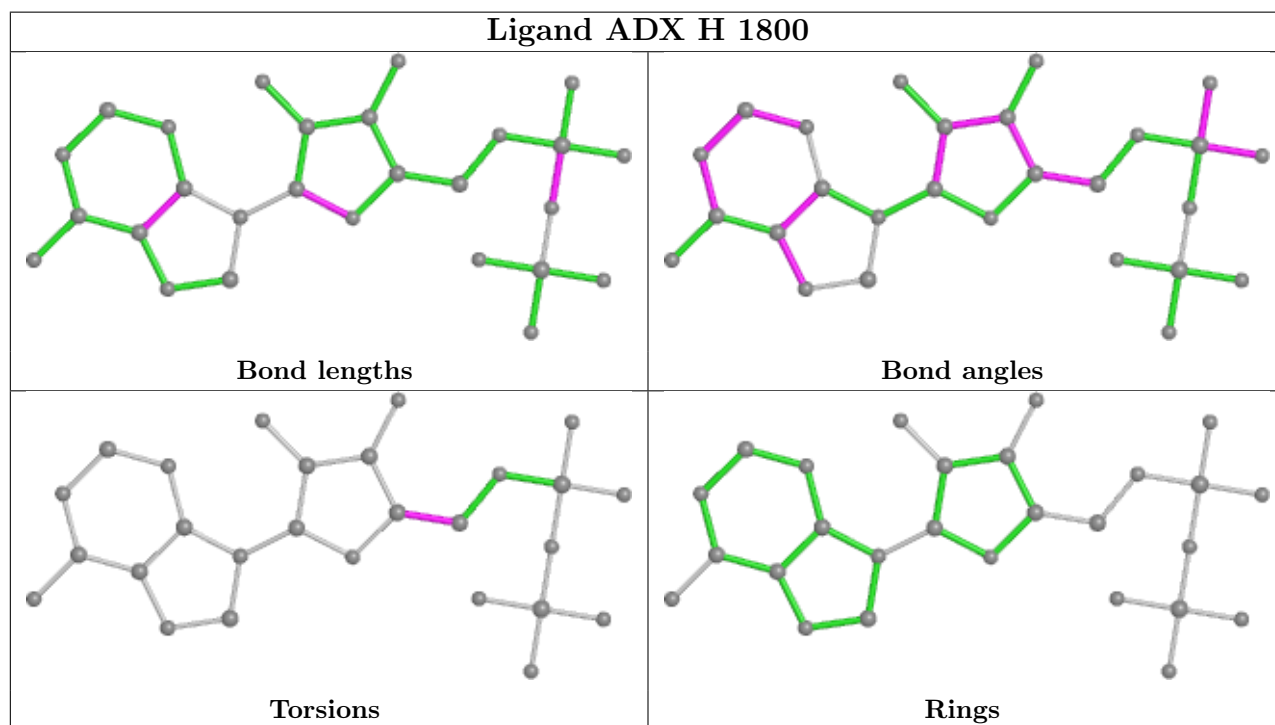
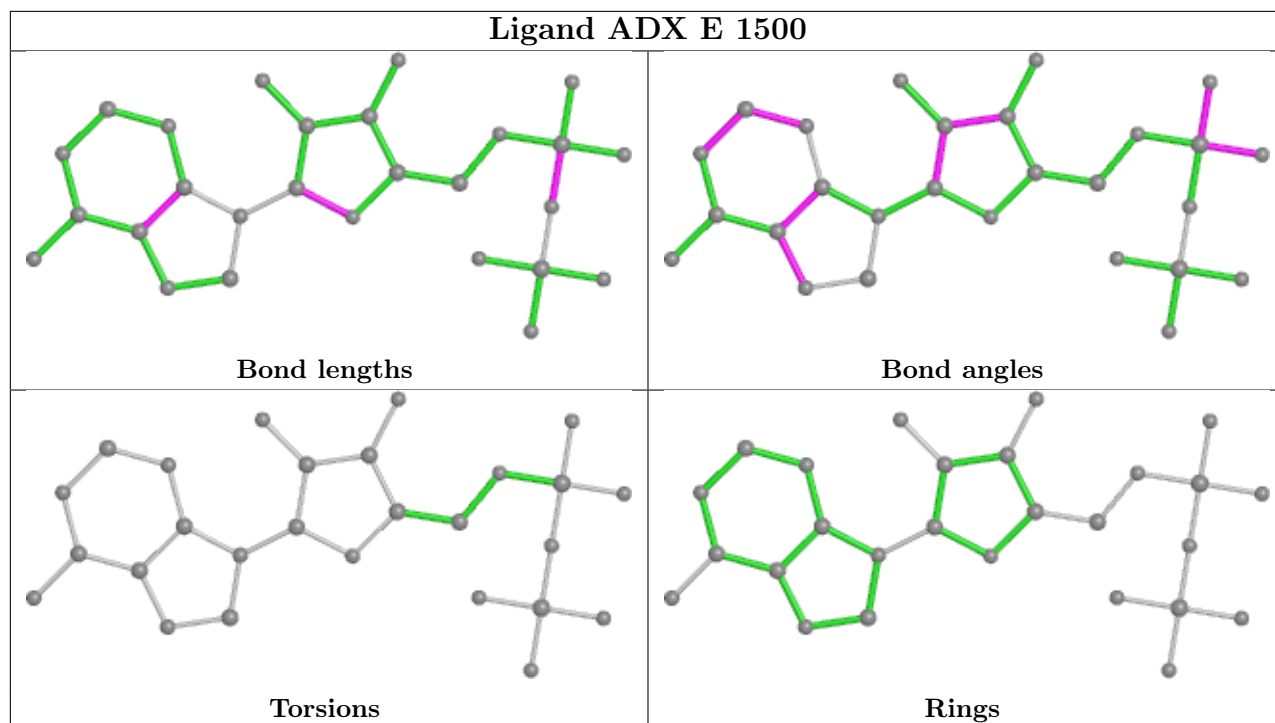


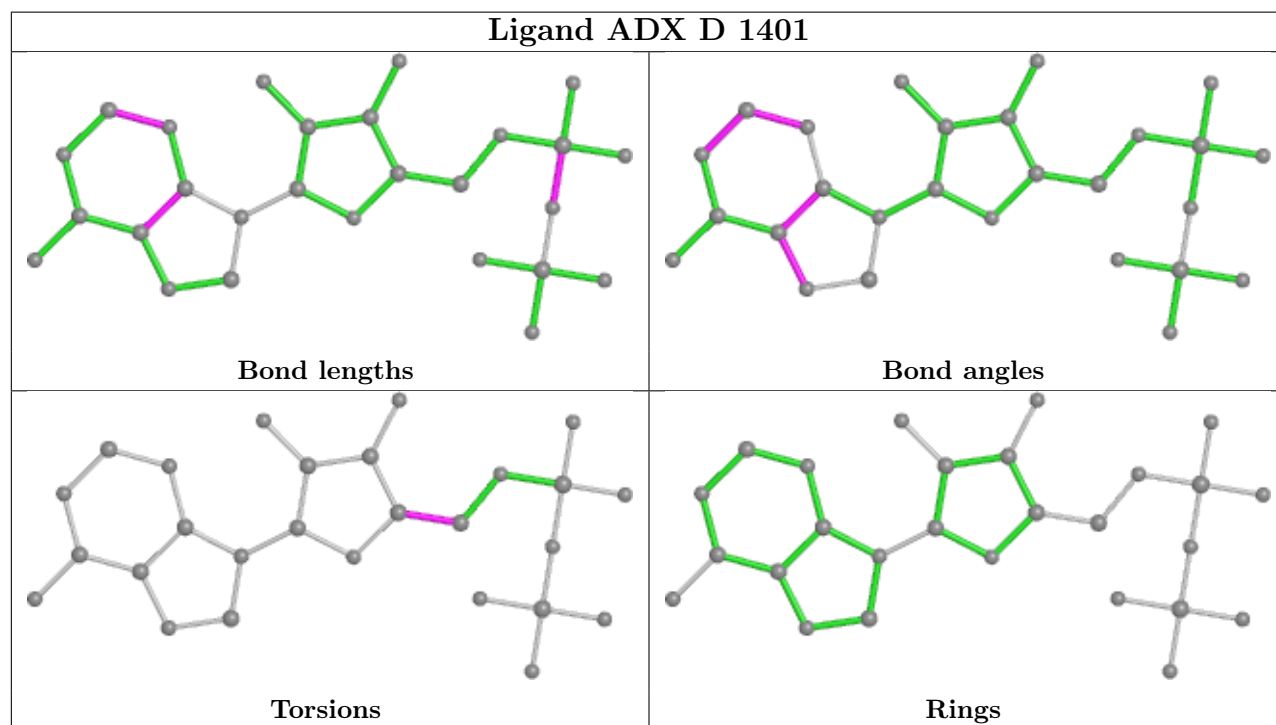
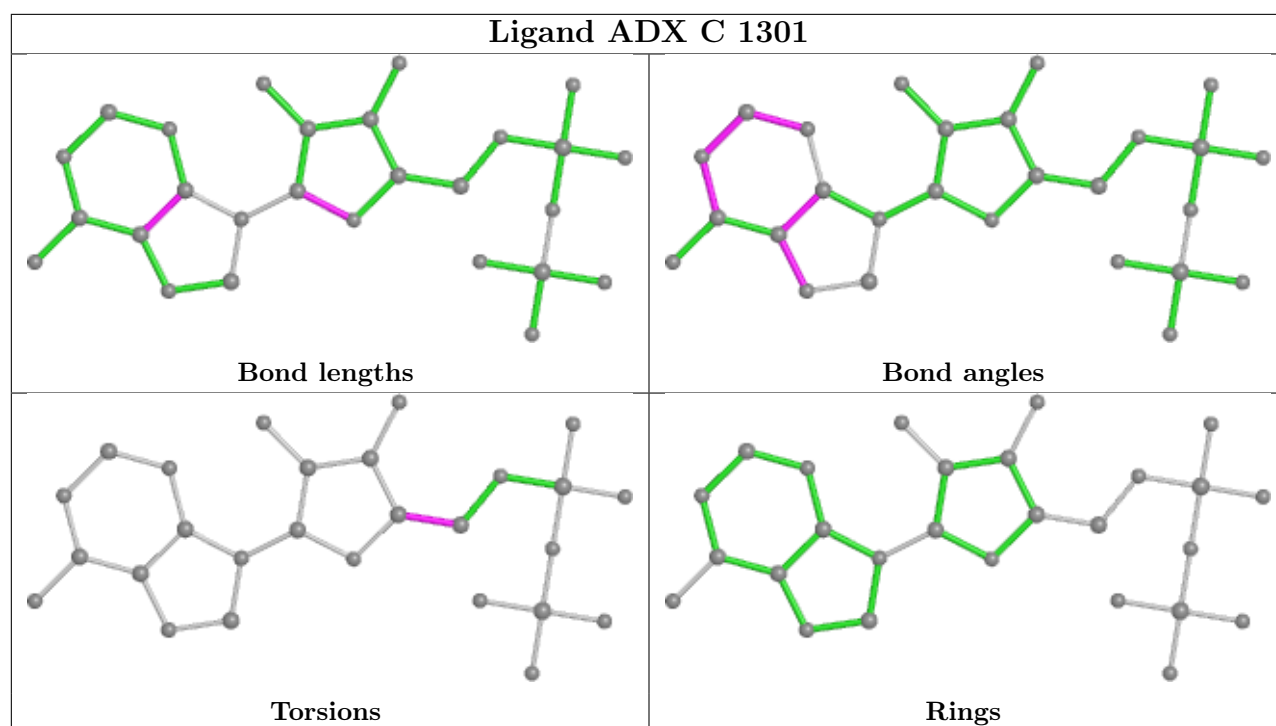


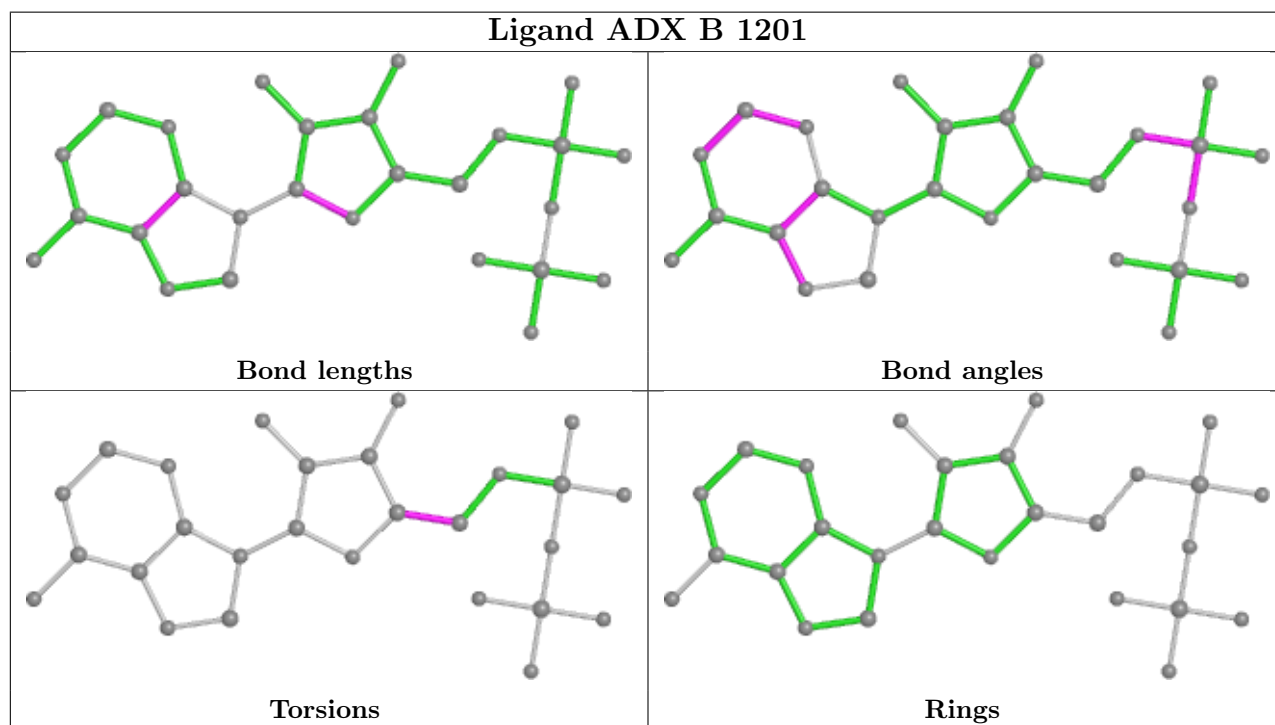
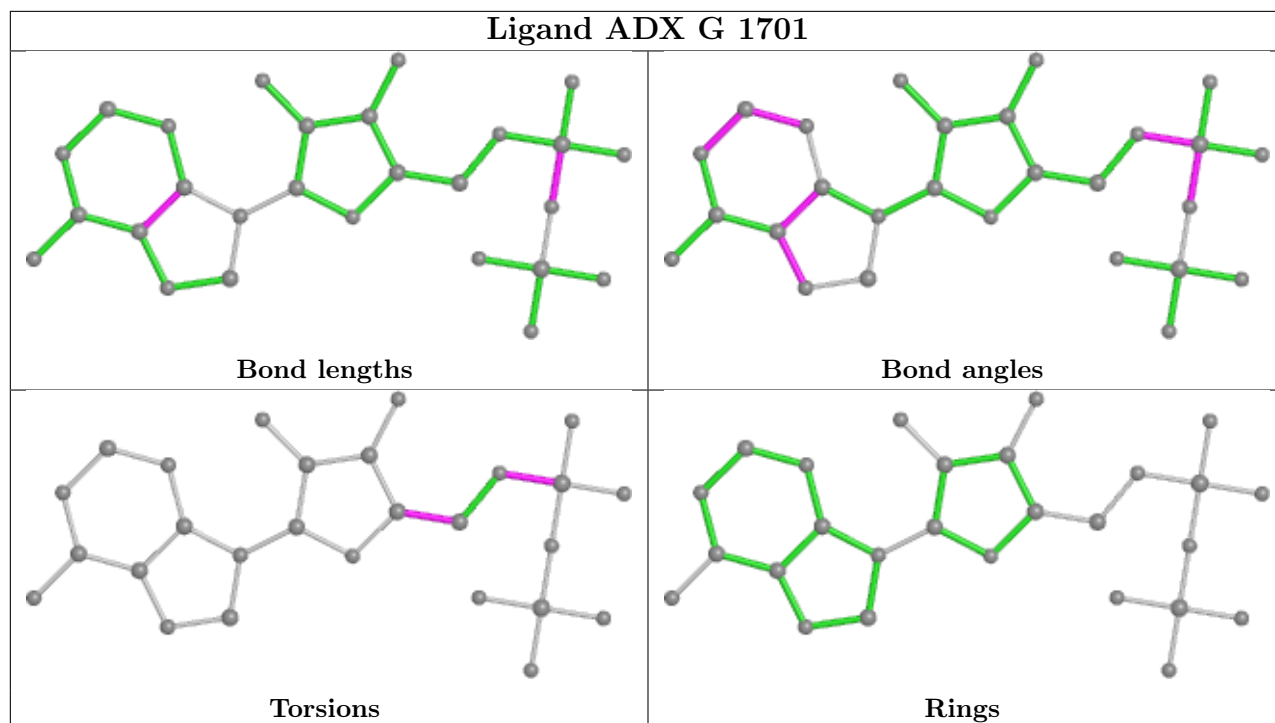


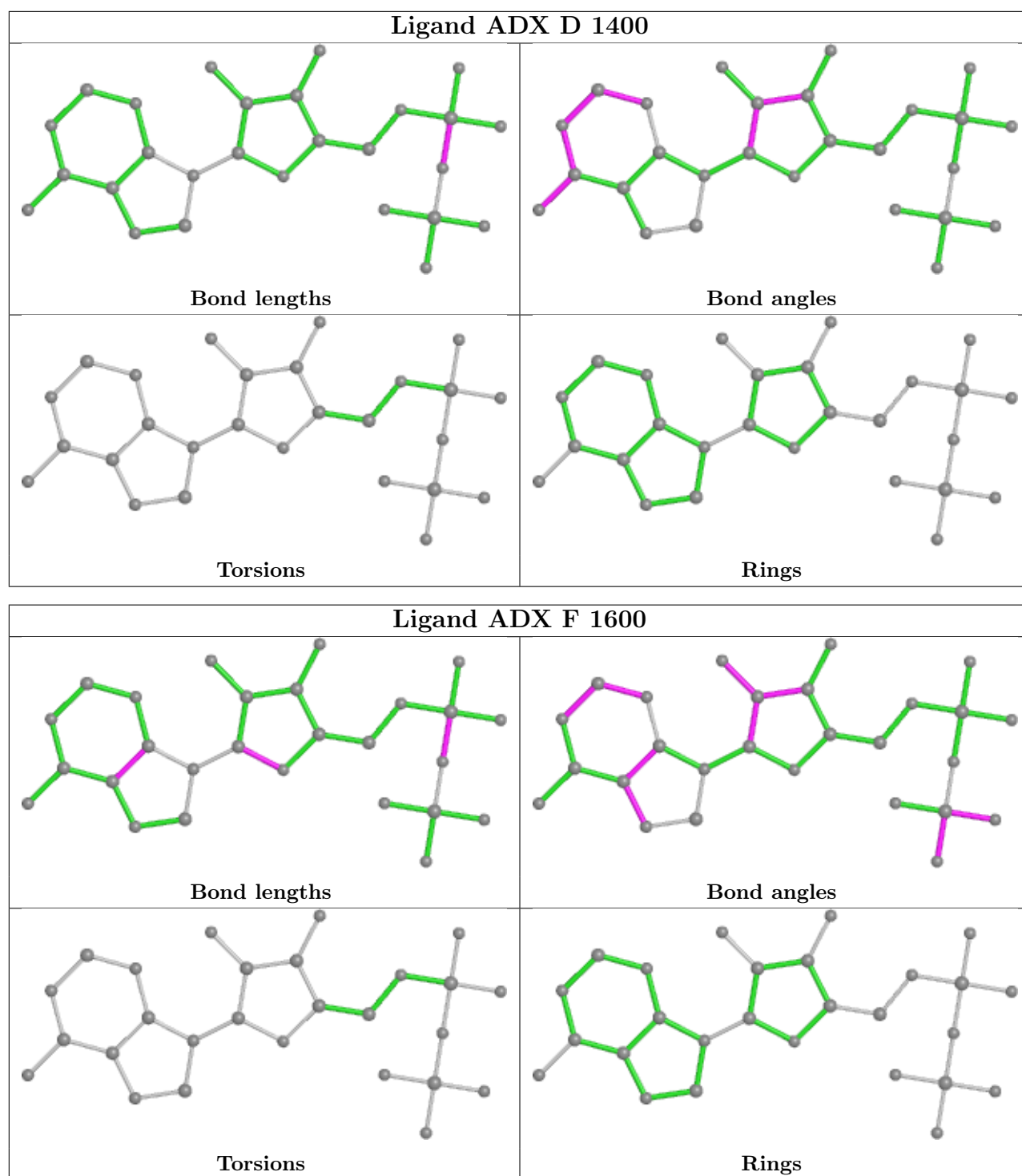












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	200/208 (96%)	0.24	12 (6%) 21 23	13, 26, 44, 47	0
1	B	193/208 (92%)	0.09	9 (4%) 31 33	14, 25, 43, 52	0
1	C	204/208 (98%)	-0.02	4 (1%) 65 69	13, 24, 40, 45	0
1	D	204/208 (98%)	0.16	10 (4%) 29 31	13, 26, 44, 54	0
1	E	203/208 (97%)	0.06	8 (3%) 39 42	15, 28, 42, 50	0
1	F	204/208 (98%)	0.04	8 (3%) 39 42	15, 26, 45, 49	1 (0%)
1	G	201/208 (96%)	0.32	10 (4%) 28 31	14, 29, 45, 47	0
1	H	193/208 (92%)	0.15	5 (2%) 56 60	15, 27, 43, 47	0
All	All	1602/1664 (96%)	0.13	66 (4%) 37 40	13, 26, 44, 54	1 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	TYR	5.7
1	H	46	THR	5.5
1	G	46	THR	5.4
1	G	30	TYR	5.4
1	F	30	TYR	5.2

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

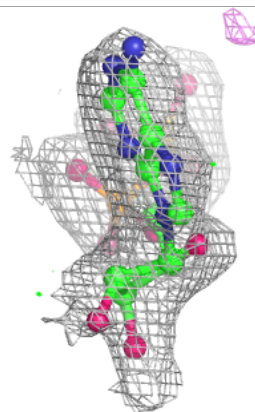
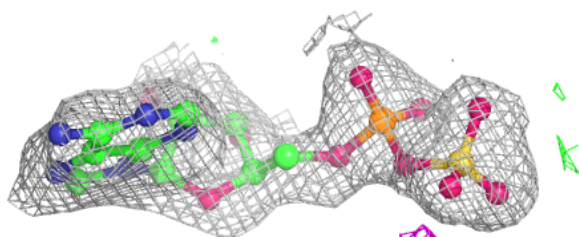
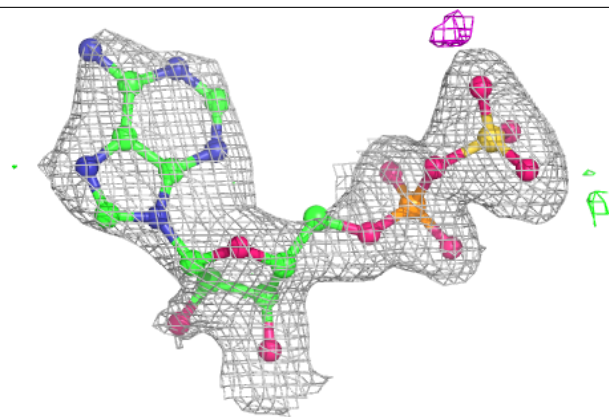
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	ADX	A	1101	27/27	0.94	0.13	24,43,44,45	0
2	ADX	C	1301	27/27	0.94	0.12	13,29,30,31	0
2	ADX	D	1401	27/27	0.95	0.13	21,38,39,40	0
2	ADX	G	1701	27/27	0.95	0.11	20,40,42,43	0
2	ADX	H	1801	27/27	0.95	0.12	21,33,36,36	0
2	ADX	F	1601	27/27	0.96	0.13	19,36,39,39	0
3	MG	E	1005	1/1	0.96	0.18	27,27,27,27	0
2	ADX	H	1800	27/27	0.97	0.10	18,19,23,25	0
2	ADX	B	1201	27/27	0.97	0.09	21,27,29,32	0
2	ADX	E	1501	27/27	0.97	0.10	20,35,37,38	0
3	MG	H	1008	1/1	0.97	0.11	20,20,20,20	0
2	ADX	B	1200	27/27	0.98	0.10	12,19,23,26	0
2	ADX	G	1700	27/27	0.98	0.09	15,22,26,28	0
2	ADX	D	1400	27/27	0.98	0.10	12,17,20,24	0
2	ADX	A	1100	27/27	0.98	0.09	13,22,26,27	0
2	ADX	E	1500	27/27	0.98	0.10	14,16,19,22	0
3	MG	B	1002	1/1	0.98	0.06	18,18,18,18	0
2	ADX	C	1300	27/27	0.98	0.09	12,17,23,26	0
2	ADX	F	1600	27/27	0.98	0.09	12,18,19,22	0
3	MG	C	1003	1/1	0.99	0.08	18,18,18,18	0
3	MG	D	1004	1/1	0.99	0.04	15,15,15,15	0
3	MG	F	1006	1/1	1.00	0.06	19,19,19,19	0

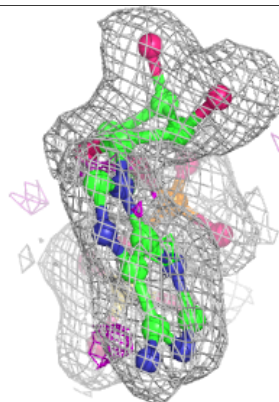
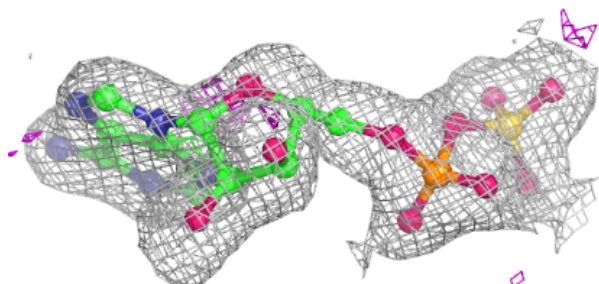
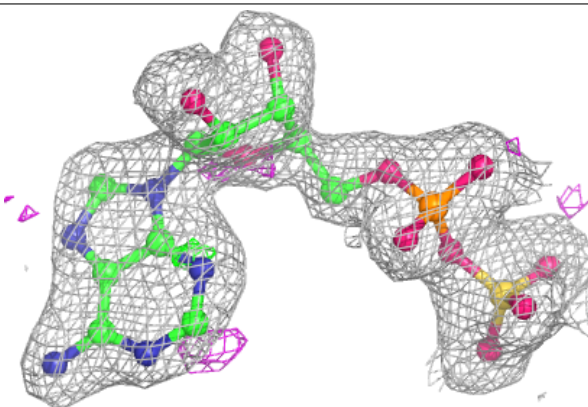
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADX A 1101:**

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

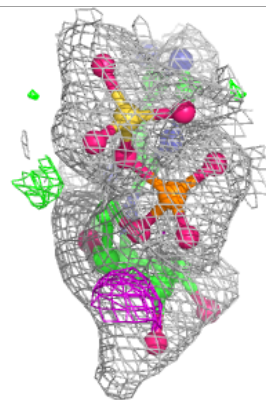
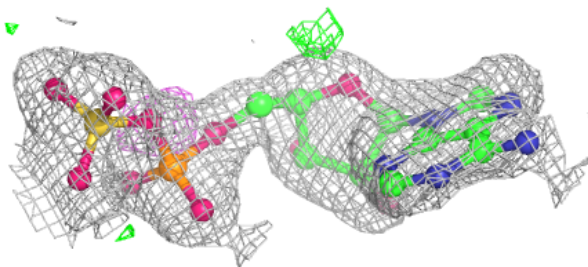
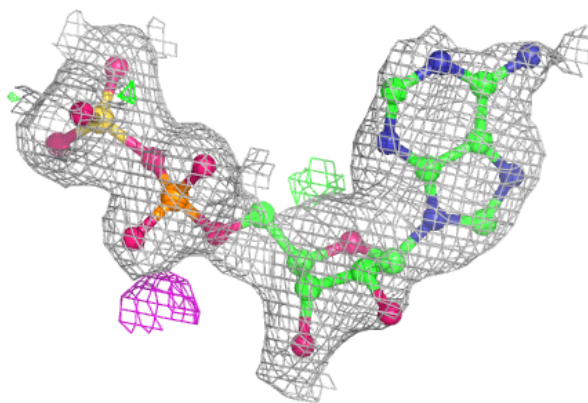
**Electron density around ADX C 1301:**

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

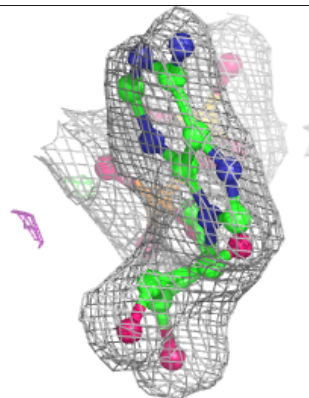
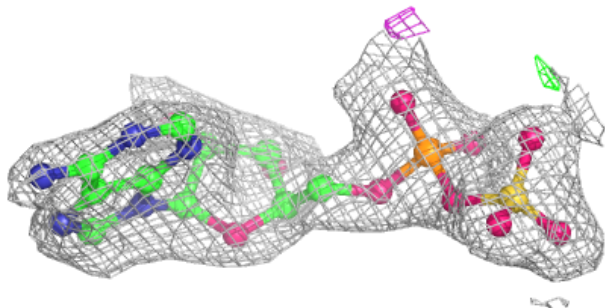
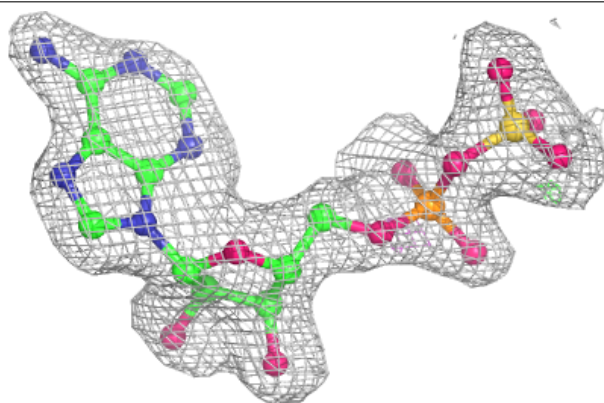


**Electron density around ADX D 1401:**

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

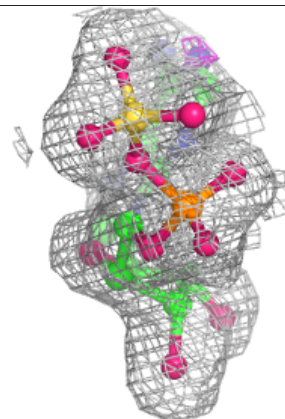
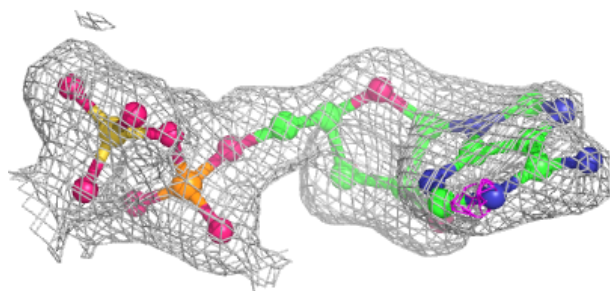
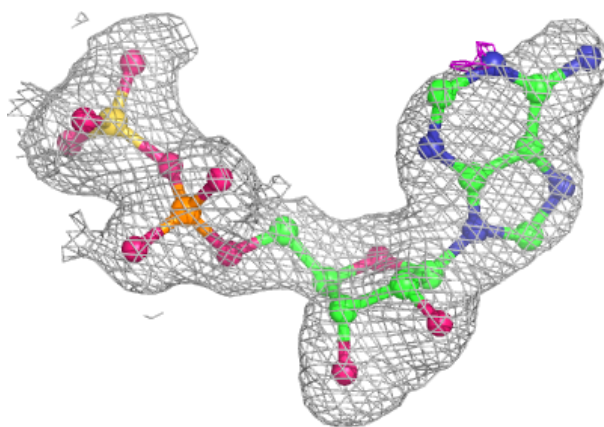
**Electron density around ADX G 1701:**

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



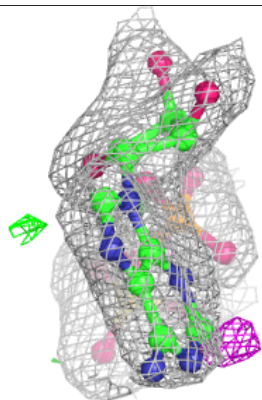
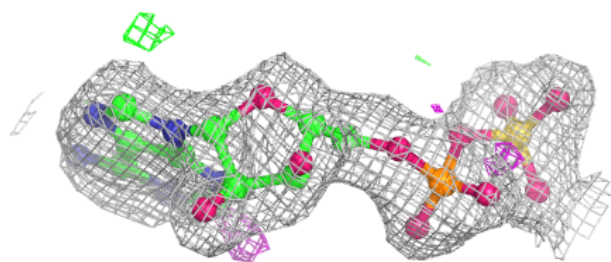
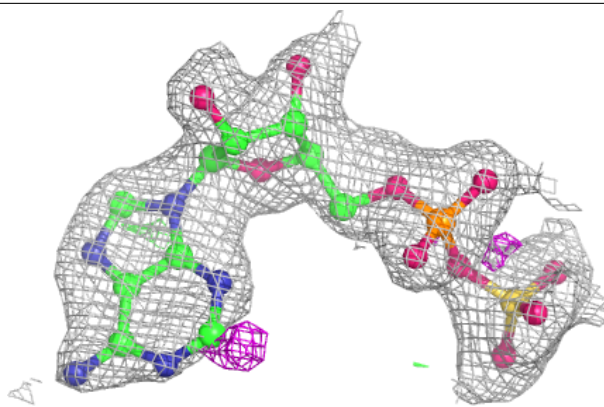
**Electron density around ADX H 1801:**

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



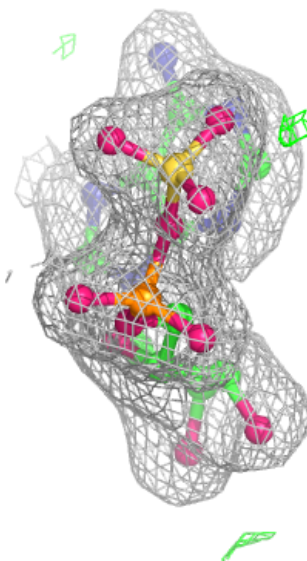
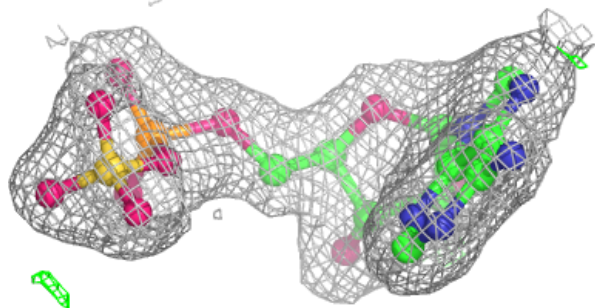
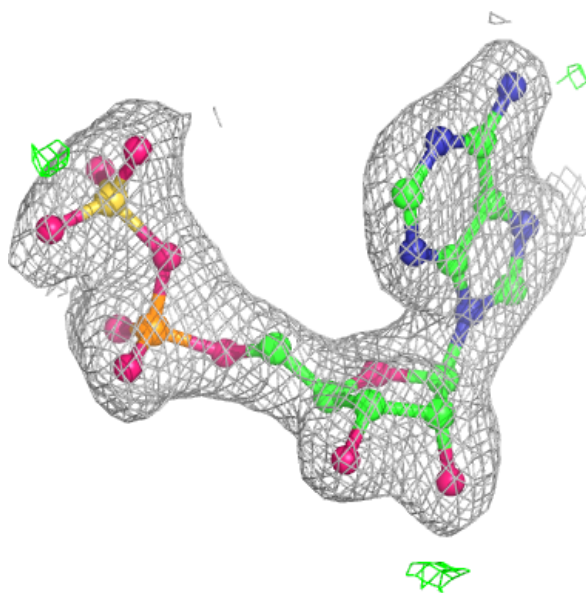
**Electron density around ADX F 1601:**

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



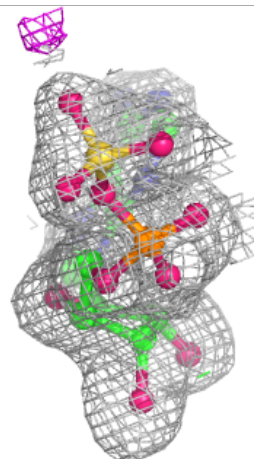
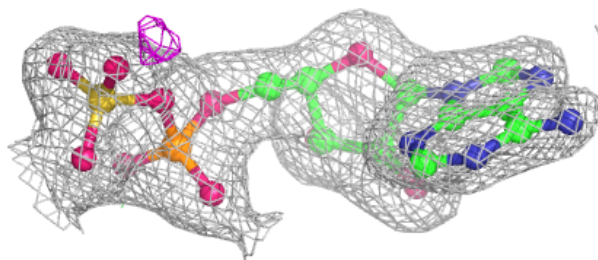
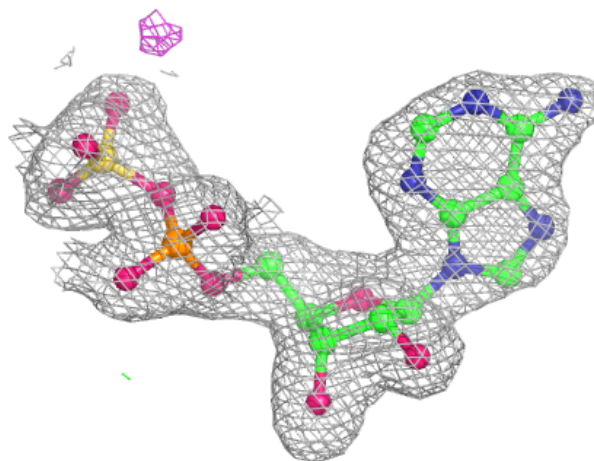
**Electron density around ADX H 1800:**

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



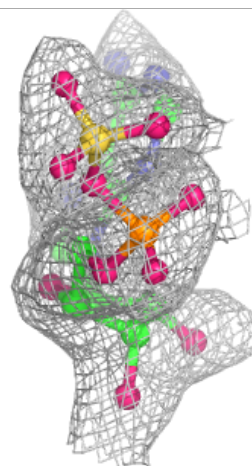
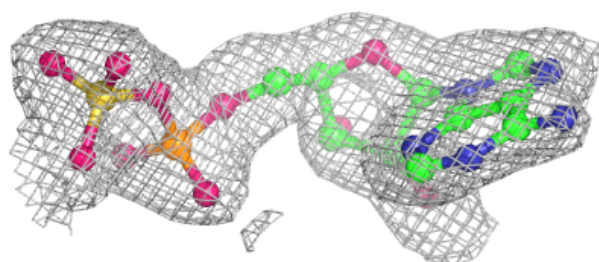
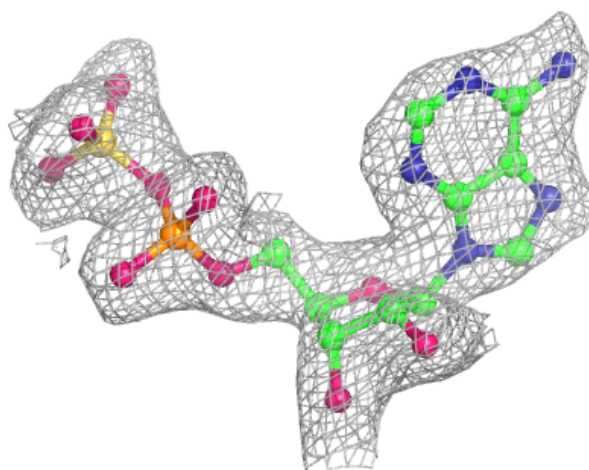
**Electron density around ADX B 1201:**

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



**Electron density around ADX E 1501:**

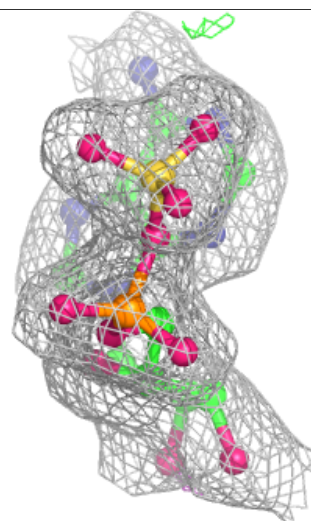
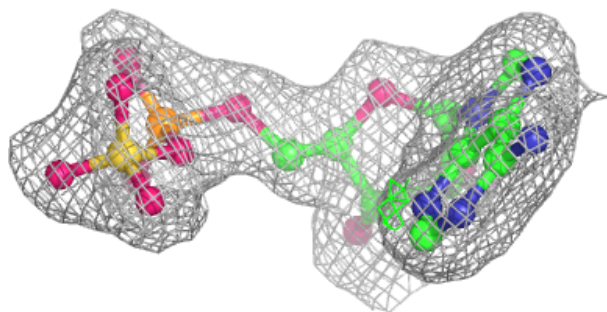
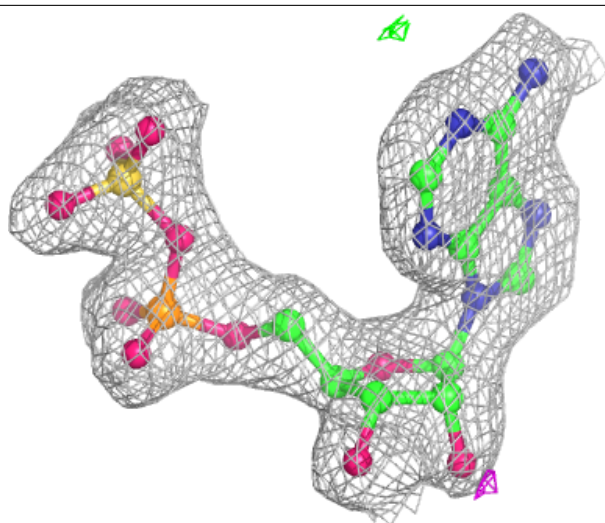
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





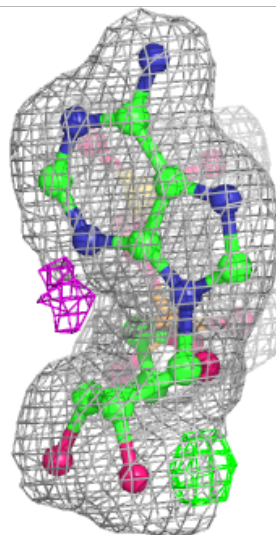
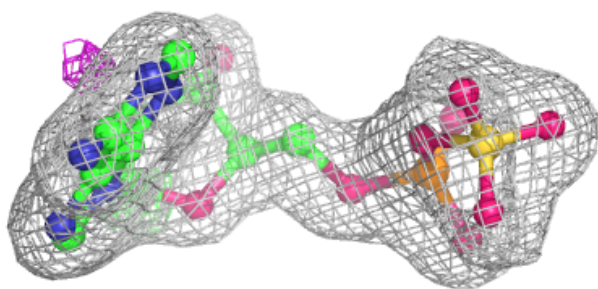
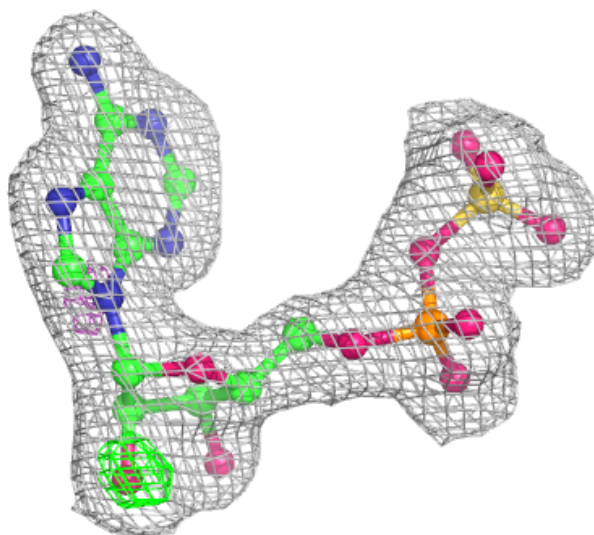
**Electron density around ADX B 1200:**

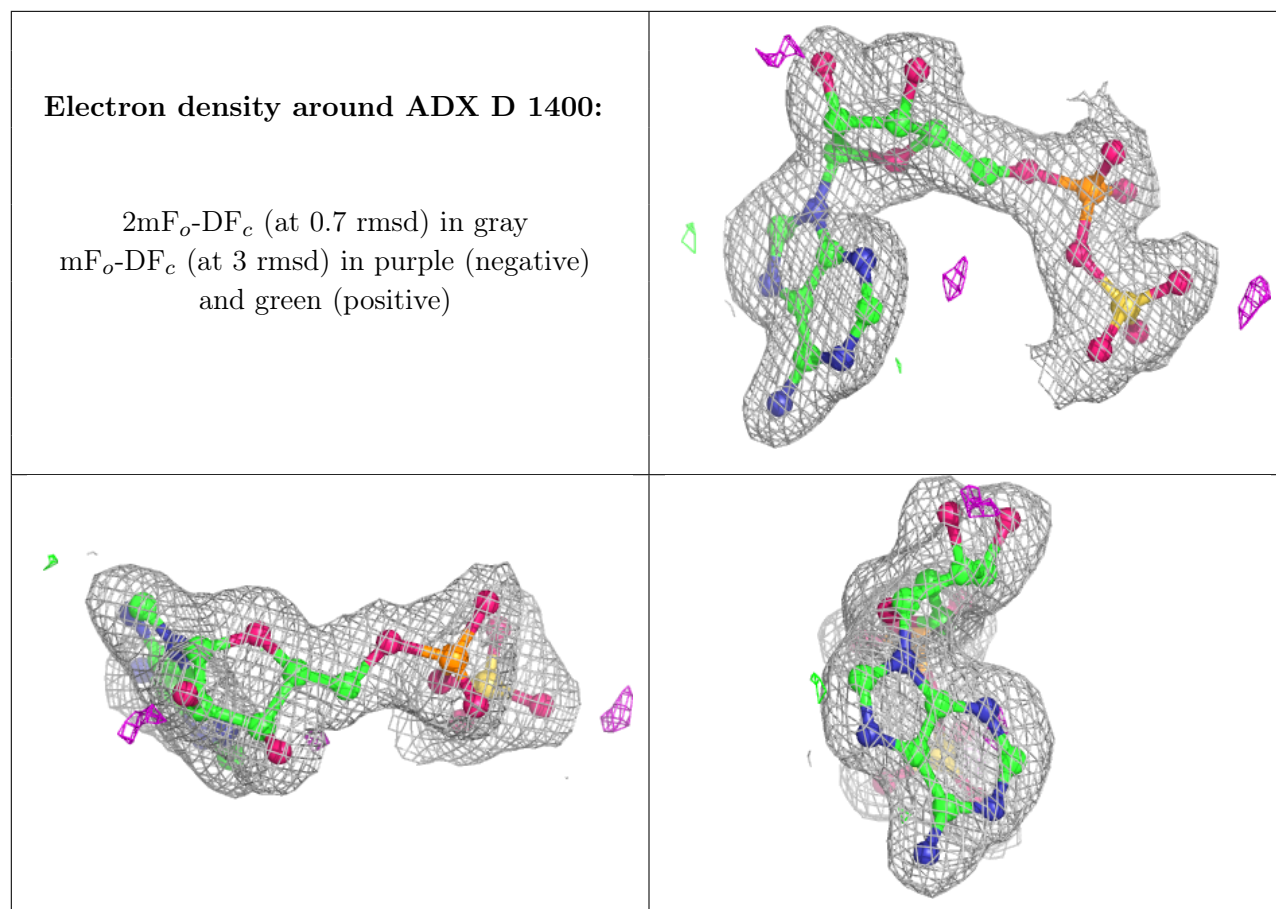
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADX G 1700:**

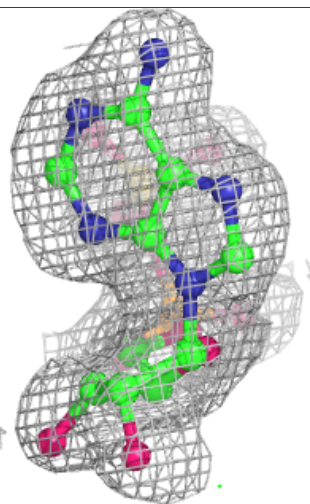
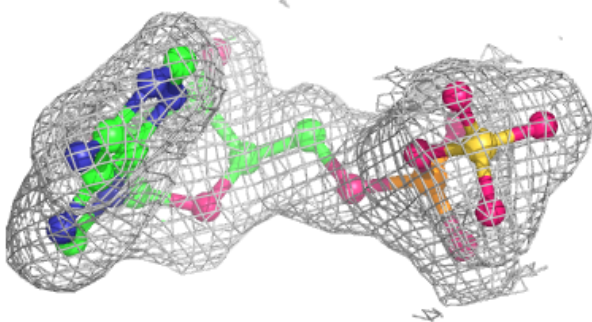
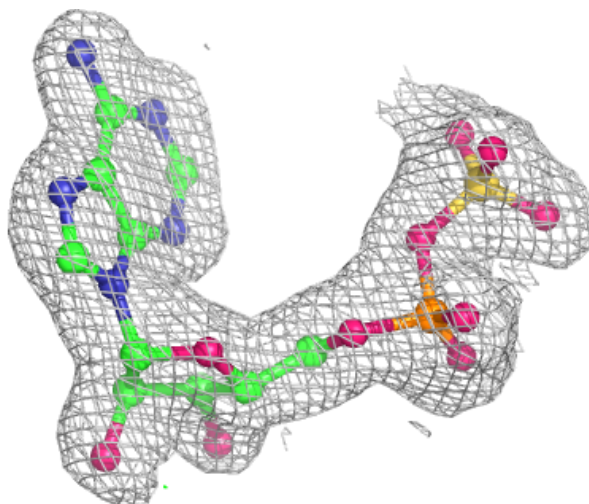
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





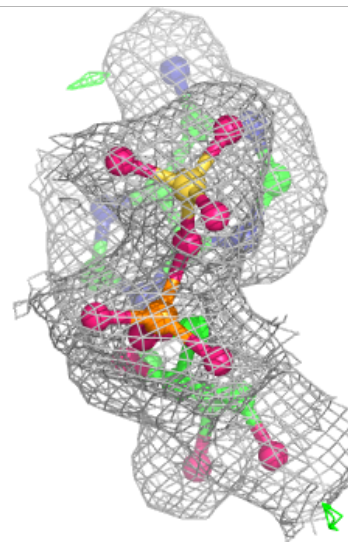
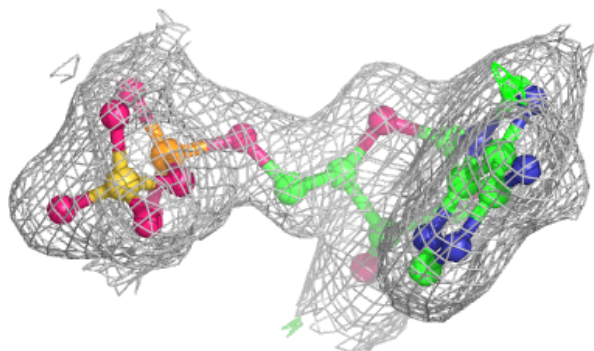
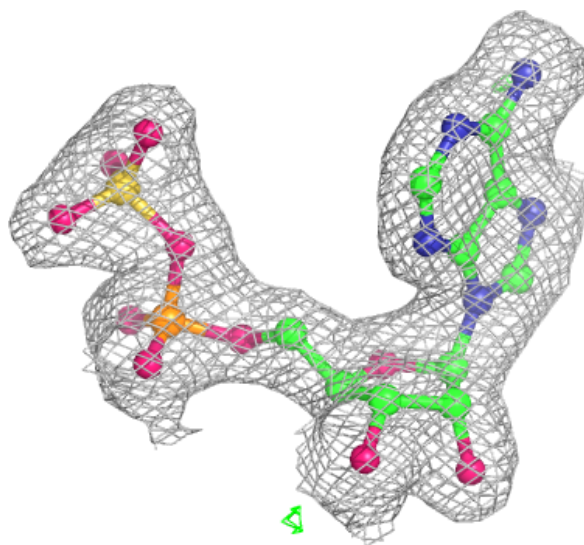
**Electron density around ADX A 1100:**

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



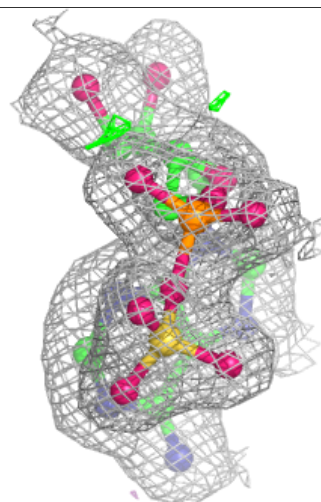
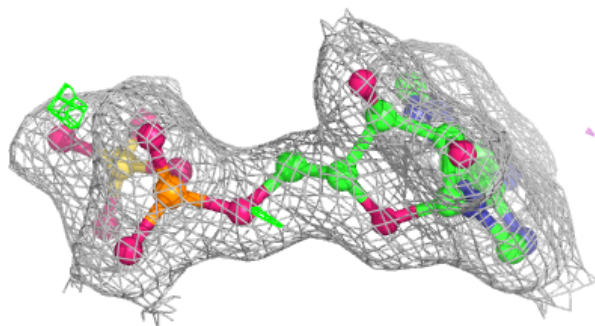
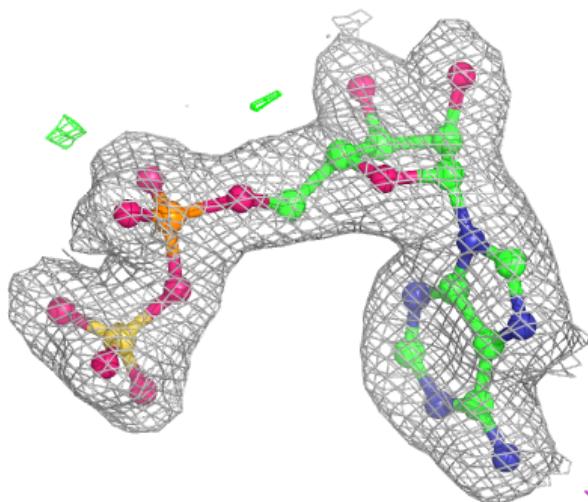
**Electron density around ADX E 1500:**

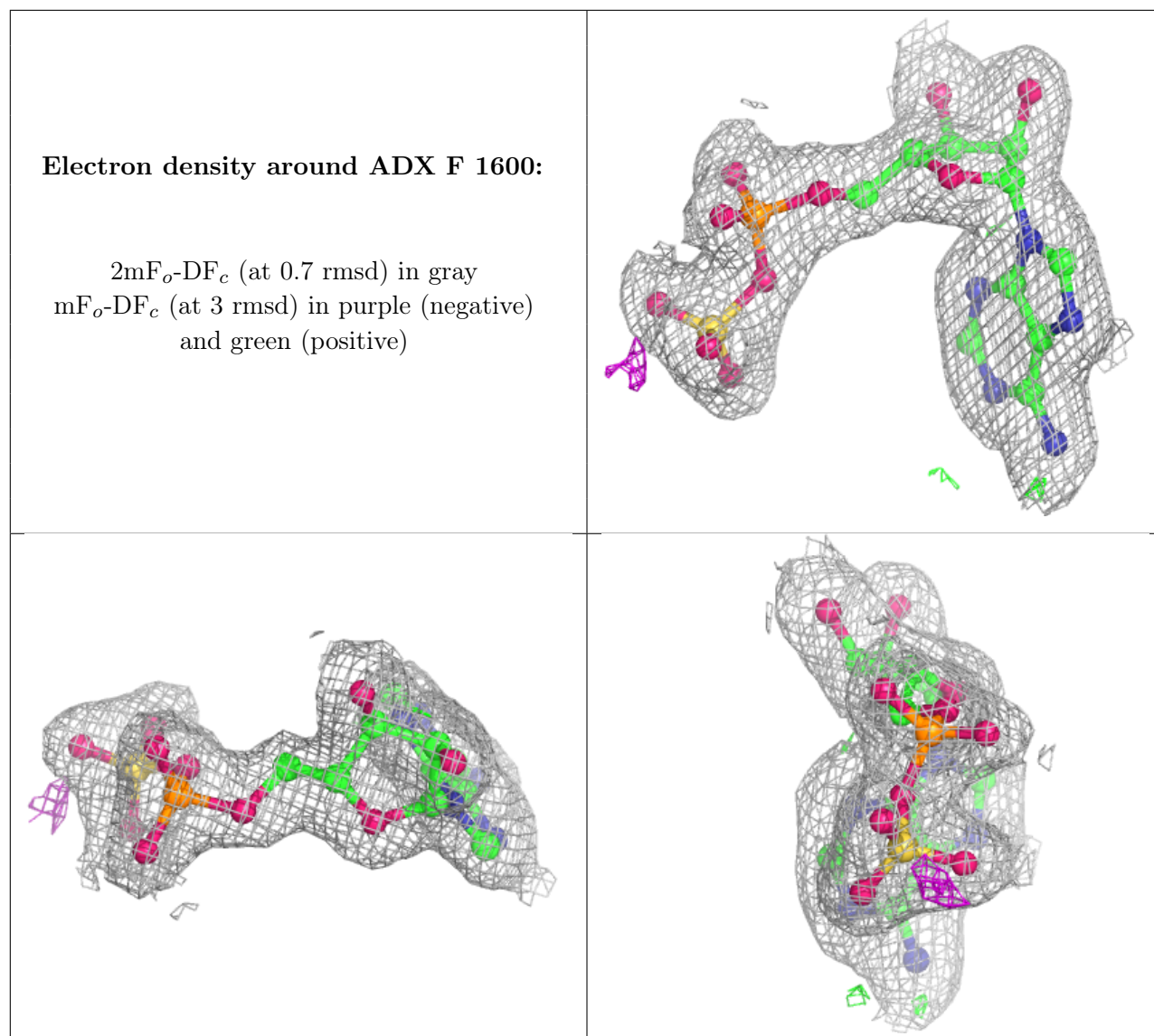
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADX C 1300:**

$2mF_o-DF_c$  (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.