



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:25 PM UTC

PDB ID : 3DLS / pdb\_00003dls  
Title : Crystal structure of human PAS kinase bound to ADP  
Authors : Antonysamy, S.; Bonanno, J.B.; Romero, R.; Russell, M.; Iizuka, M.; Gheyi, T.; Wasserman, S.R.; Rutter, J.; Sauder, J.M.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-06-29  
Resolution : 2.30 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

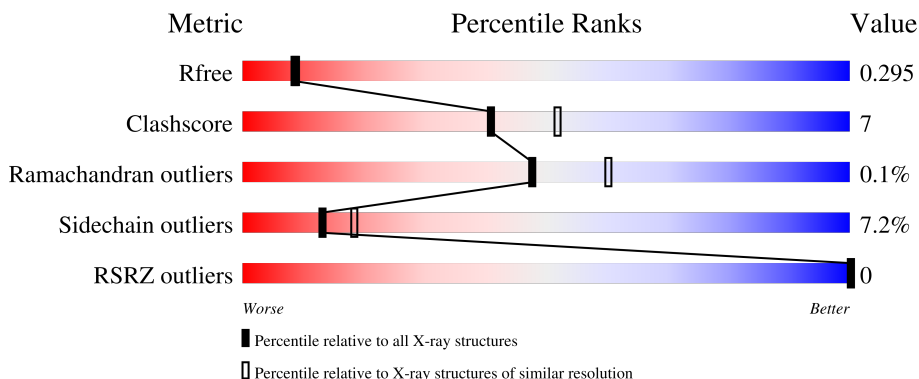
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	335	71% 12% • 15%
1	B	335	66% 16% • 16%
1	C	335	68% 14% • 16%
1	D	335	66% 17% • 15%

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Mol	Chain	Length	Quality of chain
1	E	335	 67% 17% 16%
1	F	335	 70% 12% 16%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13724 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 PAS domain-containing serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2236	1465	350	411	10	0	0	0
1	B	280	2200	1435	353	403	9	0	0	0
1	C	281	2217	1447	355	407	8	0	0	0
1	D	284	2220	1453	351	406	10	0	0	0
1	E	282	2216	1449	353	405	9	0	0	0
1	F	281	2174	1420	345	400	9	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	974	MET	-	expression tag	UNP Q96RG2
A	975	ALA	-	expression tag	UNP Q96RG2
A	976	LEU	-	expression tag	UNP Q96RG2
A	1301	GLU	-	expression tag	UNP Q96RG2
A	1302	GLY	-	expression tag	UNP Q96RG2
A	1303	HIS	-	expression tag	UNP Q96RG2
A	1304	HIS	-	expression tag	UNP Q96RG2
A	1305	HIS	-	expression tag	UNP Q96RG2
A	1306	HIS	-	expression tag	UNP Q96RG2
A	1307	HIS	-	expression tag	UNP Q96RG2
A	1308	HIS	-	expression tag	UNP Q96RG2
B	974	MET	-	expression tag	UNP Q96RG2
B	975	ALA	-	expression tag	UNP Q96RG2
B	976	LEU	-	expression tag	UNP Q96RG2
B	1301	GLU	-	expression tag	UNP Q96RG2
B	1302	GLY	-	expression tag	UNP Q96RG2
B	1303	HIS	-	expression tag	UNP Q96RG2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1304	HIS	-	expression tag	UNP Q96RG2
B	1305	HIS	-	expression tag	UNP Q96RG2
B	1306	HIS	-	expression tag	UNP Q96RG2
B	1307	HIS	-	expression tag	UNP Q96RG2
B	1308	HIS	-	expression tag	UNP Q96RG2
C	974	MET	-	expression tag	UNP Q96RG2
C	975	ALA	-	expression tag	UNP Q96RG2
C	976	LEU	-	expression tag	UNP Q96RG2
C	1301	GLU	-	expression tag	UNP Q96RG2
C	1302	GLY	-	expression tag	UNP Q96RG2
C	1303	HIS	-	expression tag	UNP Q96RG2
C	1304	HIS	-	expression tag	UNP Q96RG2
C	1305	HIS	-	expression tag	UNP Q96RG2
C	1306	HIS	-	expression tag	UNP Q96RG2
C	1307	HIS	-	expression tag	UNP Q96RG2
C	1308	HIS	-	expression tag	UNP Q96RG2
D	974	MET	-	expression tag	UNP Q96RG2
D	975	ALA	-	expression tag	UNP Q96RG2
D	976	LEU	-	expression tag	UNP Q96RG2
D	1301	GLU	-	expression tag	UNP Q96RG2
D	1302	GLY	-	expression tag	UNP Q96RG2
D	1303	HIS	-	expression tag	UNP Q96RG2
D	1304	HIS	-	expression tag	UNP Q96RG2
D	1305	HIS	-	expression tag	UNP Q96RG2
D	1306	HIS	-	expression tag	UNP Q96RG2
D	1307	HIS	-	expression tag	UNP Q96RG2
D	1308	HIS	-	expression tag	UNP Q96RG2
E	974	MET	-	expression tag	UNP Q96RG2
E	975	ALA	-	expression tag	UNP Q96RG2
E	976	LEU	-	expression tag	UNP Q96RG2
E	1301	GLU	-	expression tag	UNP Q96RG2
E	1302	GLY	-	expression tag	UNP Q96RG2
E	1303	HIS	-	expression tag	UNP Q96RG2
E	1304	HIS	-	expression tag	UNP Q96RG2
E	1305	HIS	-	expression tag	UNP Q96RG2
E	1306	HIS	-	expression tag	UNP Q96RG2
E	1307	HIS	-	expression tag	UNP Q96RG2
E	1308	HIS	-	expression tag	UNP Q96RG2
F	974	MET	-	expression tag	UNP Q96RG2
F	975	ALA	-	expression tag	UNP Q96RG2
F	976	LEU	-	expression tag	UNP Q96RG2
F	1301	GLU	-	expression tag	UNP Q96RG2

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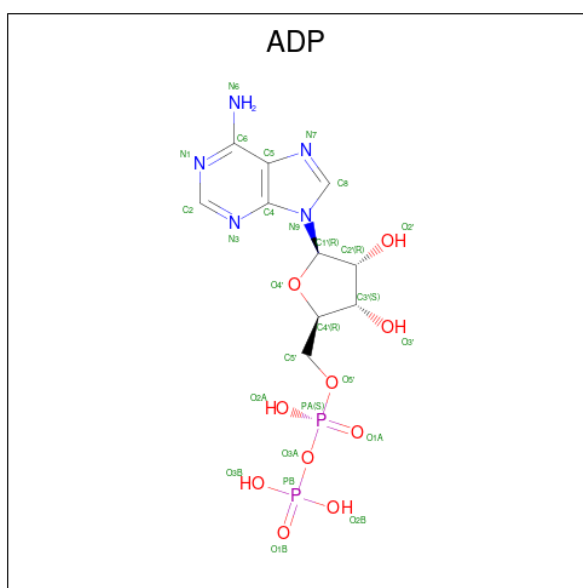
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1302	GLY	-	expression tag	UNP Q96RG2
F	1303	HIS	-	expression tag	UNP Q96RG2
F	1304	HIS	-	expression tag	UNP Q96RG2
F	1305	HIS	-	expression tag	UNP Q96RG2
F	1306	HIS	-	expression tag	UNP Q96RG2
F	1307	HIS	-	expression tag	UNP Q96RG2
F	1308	HIS	-	expression tag	UNP Q96RG2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	57	Total	O	0	0
			57	57		
4	C	47	Total	O	0	0
			47	47		
4	D	48	Total	O	0	0
			48	48		
4	E	39	Total	O	0	0
			39	39		
4	F	34	Total	O	0	0
			34	34		





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.78Å 85.84Å 94.15Å 77.28° 77.50° 60.09°	Depositor
Resolution (Å)	(Not available) – 2.30 91.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 95.9 (91.11-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.29Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.241 , 0.297 0.240 , 0.295	Depositor DCC
$R_{free}$ test set	4846 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.216 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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: MG, 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	0.61	0/2291	0.88	1/3118 (0.0%)
1	B	0.61	0/2252	0.90	1/3062 (0.0%)
1	C	0.59	0/2269	0.87	0/3083
1	D	0.56	0/2274	0.88	1/3094 (0.0%)
1	E	0.57	0/2270	0.86	0/3088
1	F	0.57	0/2226	0.84	0/3033
All	All	0.58	0/13582	0.87	3/18478 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005	LEU	O-C-N	8.04	133.64	123.19
1	A	1125	ILE	CB-CA-C	5.70	119.33	110.83
1	D	1007	SER	CB-CA-C	-5.20	109.60	115.79

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2236	0	2198	26	0
1	B	2200	0	2168	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2217	0	2190	33	0
1	D	2220	0	2178	34	0
1	E	2216	0	2178	31	0
1	F	2174	0	2109	22	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	2	0
3	F	27	0	12	0	0
4	A	55	0	0	1	0
4	B	57	0	0	0	0
4	C	47	0	0	2	0
4	D	48	0	0	0	0
4	E	39	0	0	2	0
4	F	34	0	0	0	0
All	All	13724	0	13093	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 173 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:D:1032:LYS:HZ1	1:D:1074:GLN:HA	1.42	0.83
1:C:1125:ILE:HG23	1:C:1127:ARG:HG3	1.67	0.74
1:A:1240:THR:HG23	1:A:1244:LYS:HD2	1.70	0.73
1:A:1125:ILE:HG23	1:A:1127:ARG:HG3	1.72	0.71
1:E:1094:ILE:HD11	1:E:1196:LEU:HA	1.71	0.71

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/335 (84%)	272 (96%)	11 (4%)	0	100	100
1	B	276/335 (82%)	264 (96%)	12 (4%)	0	100	100
1	C	277/335 (83%)	260 (94%)	17 (6%)	0	100	100
1	D	280/335 (84%)	271 (97%)	9 (3%)	0	100	100
1	E	278/335 (83%)	268 (96%)	9 (3%)	1 (0%)	30	38
1	F	277/335 (83%)	260 (94%)	17 (6%)	0	100	100
All	All	1671/2010 (83%)	1595 (96%)	75 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1009	ALA

### 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	236/291 (81%)	215 (91%)	21 (9%)	9	12
1	B	233/291 (80%)	220 (94%)	13 (6%)	19	28
1	C	235/291 (81%)	221 (94%)	14 (6%)	17	25
1	D	234/291 (80%)	218 (93%)	16 (7%)	14	20
1	E	234/291 (80%)	217 (93%)	17 (7%)	13	18
1	F	226/291 (78%)	207 (92%)	19 (8%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1398/1746 (80%)	1298 (93%)	100 (7%)	13	18

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1153	LEU
1	E	1122	LYS
1	F	1245	LEU
1	D	1206	LEU
1	E	1032	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1078	GLN
1	F	1253	GLN
1	F	1256	ASN
1	E	1078	GLN
1	B	1253	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	C	3	2	28,29,29	1.55	5 (17%)	43,45,45	1.74	6 (13%)
3	ADP	F	6	2	28,29,29	1.62	5 (17%)	43,45,45	1.71	7 (16%)
3	ADP	D	4	2	28,29,29	1.52	5 (17%)	43,45,45	1.79	7 (16%)
3	ADP	B	2	2	28,29,29	1.55	5 (17%)	43,45,45	1.92	6 (13%)
3	ADP	A	1	2	28,29,29	1.57	5 (17%)	43,45,45	1.79	8 (18%)
3	ADP	E	5	2	28,29,29	1.60	4 (14%)	43,45,45	1.77	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	3	2	-	4/16/32/32	0/3/3/3
3	ADP	F	6	2	-	0/16/32/32	0/3/3/3
3	ADP	D	4	2	-	0/16/32/32	0/3/3/3
3	ADP	B	2	2	-	1/16/32/32	0/3/3/3
3	ADP	A	1	2	-	1/16/32/32	0/3/3/3
3	ADP	E	5	2	-	0/16/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	ADP	C5-C4	5.21	1.48	1.39
3	E	5	ADP	C5-C4	5.07	1.48	1.39
3	C	3	ADP	C5-C4	4.80	1.47	1.39
3	D	4	ADP	C5-C4	4.77	1.47	1.39
3	A	1	ADP	C5-C4	4.73	1.47	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	ADP	C5-C4-N3	-6.72	117.46	126.72
3	D	4	ADP	C5-C4-N3	-6.18	118.21	126.72
3	F	6	ADP	C5-C4-N3	-5.97	118.50	126.72
3	E	5	ADP	C5-C4-N3	-5.93	118.56	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	ADP	C5-C4-N3	-5.90	118.59	126.72

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

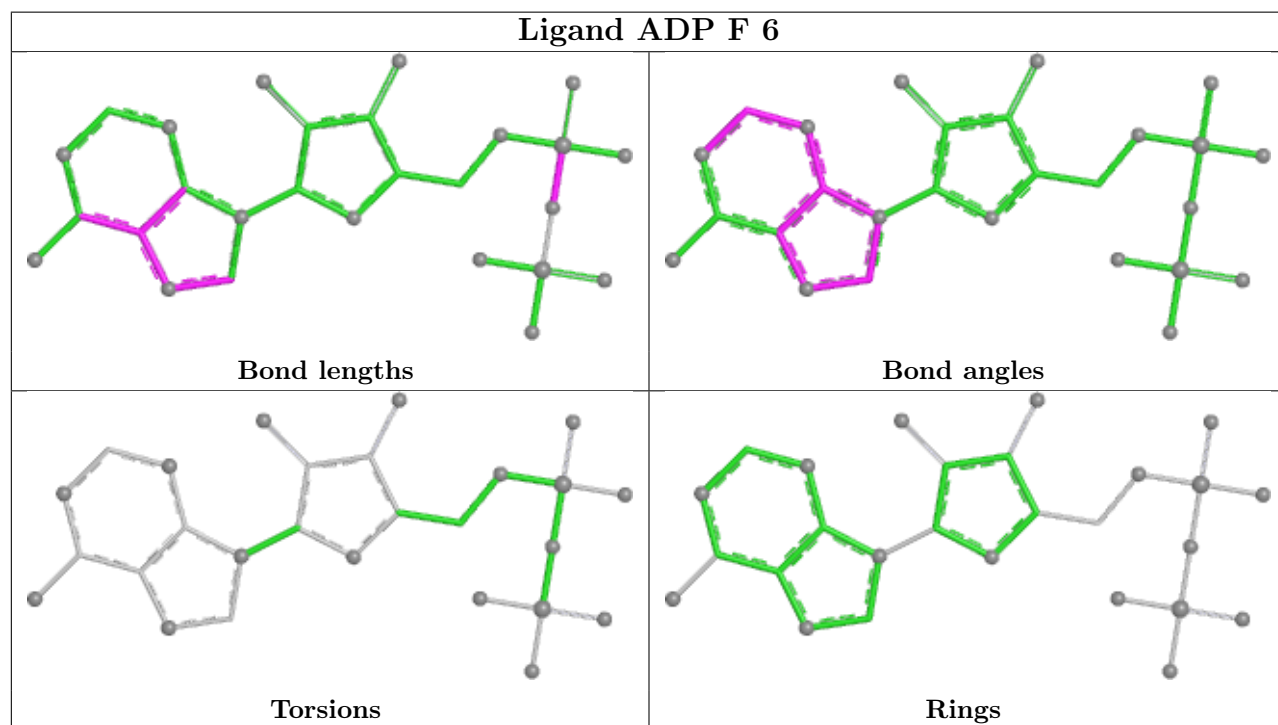
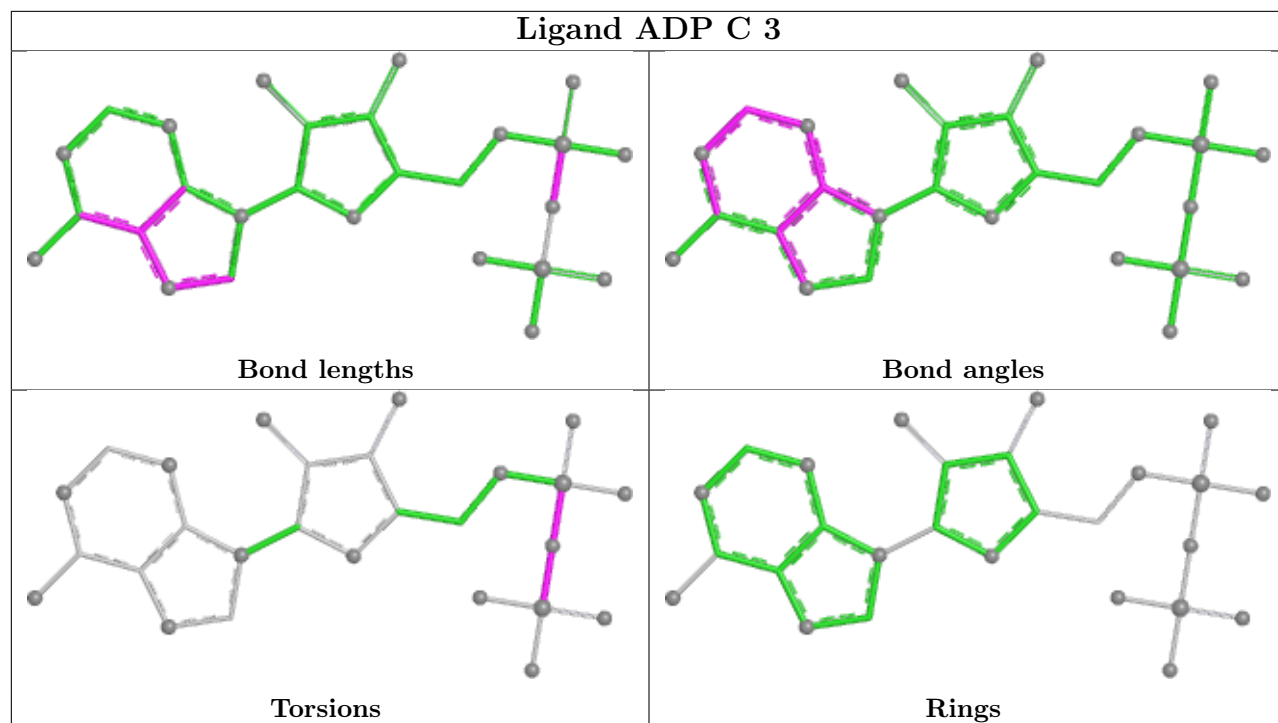
Mol	Chain	Res	Type	Atoms
3	C	3	ADP	PA-O3A-PB-O2B
3	B	2	ADP	PB-O3A-PA-O1A
3	A	1	ADP	PA-O3A-PB-O3B
3	C	3	ADP	PA-O3A-PB-O3B
3	C	3	ADP	PA-O3A-PB-O1B

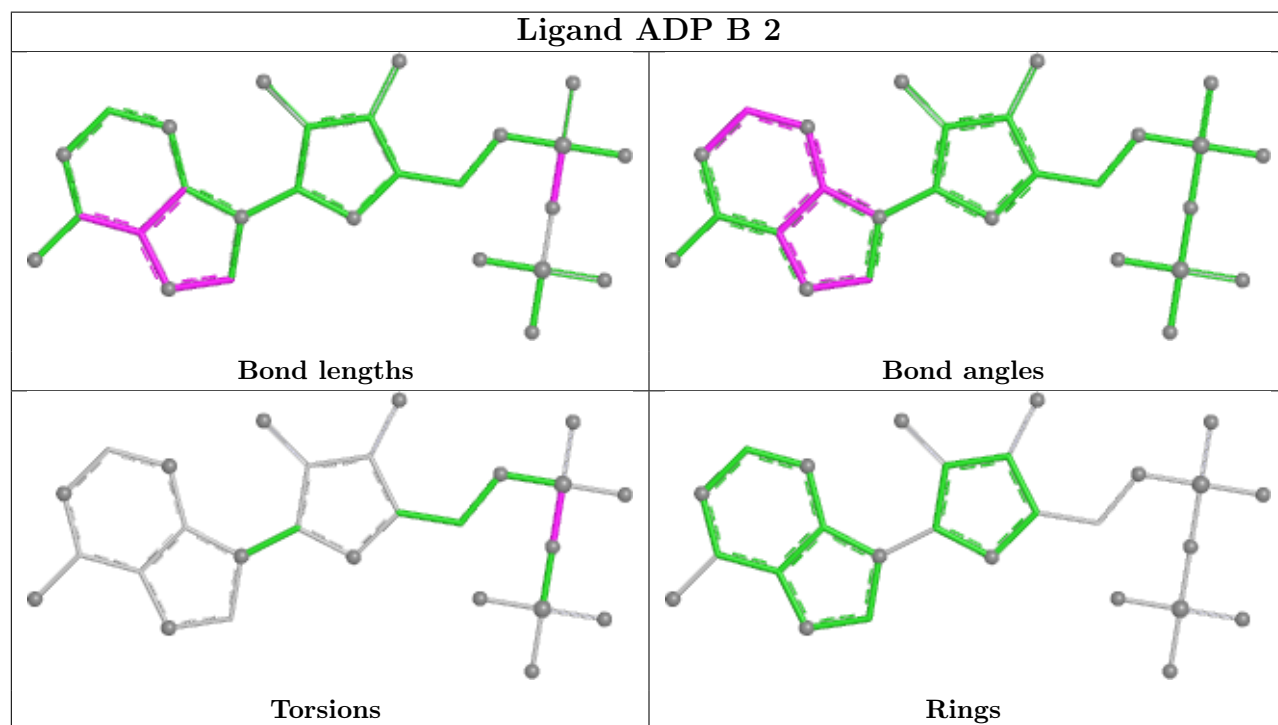
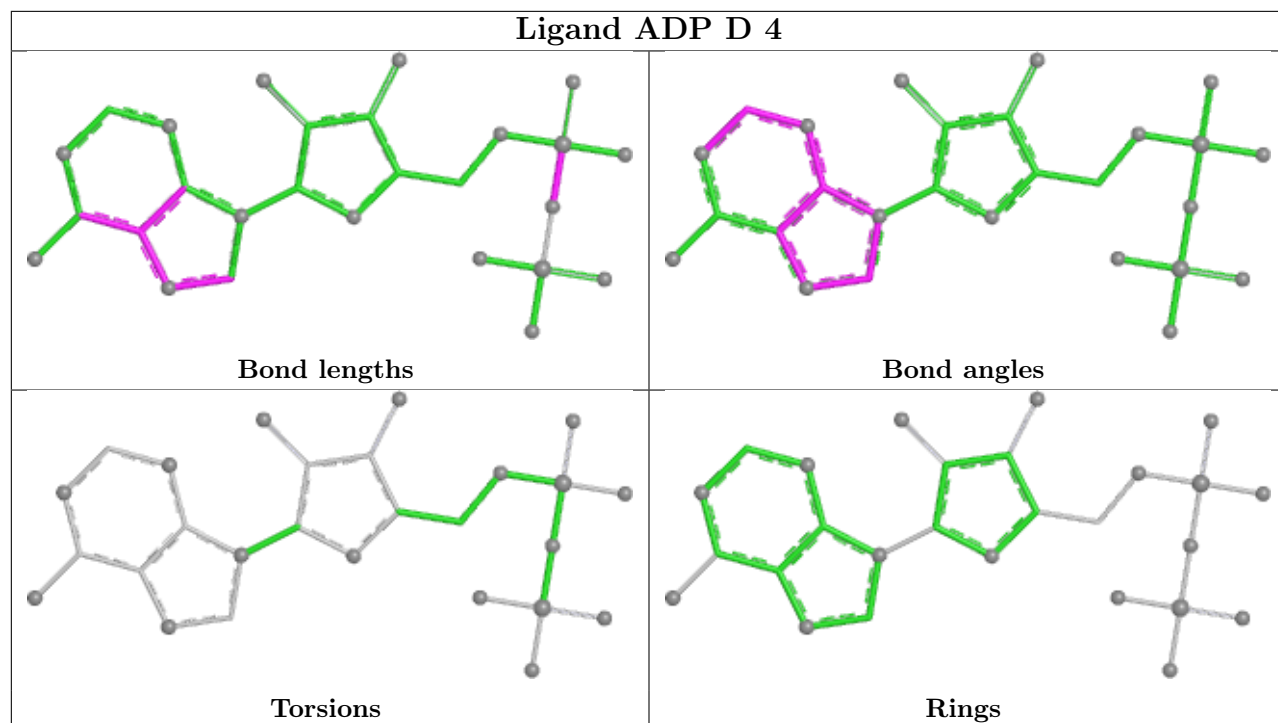
There are no ring outliers.

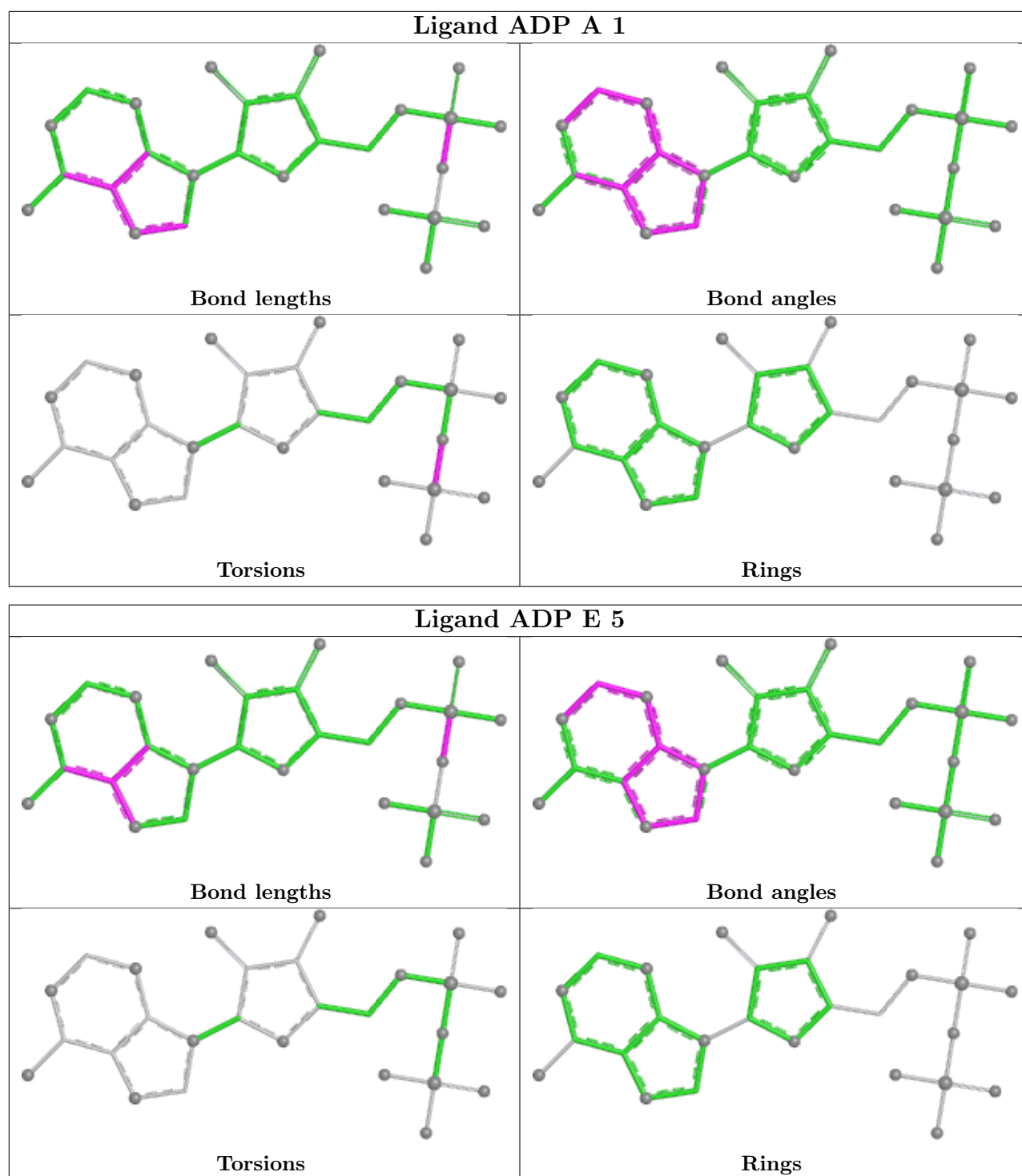
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4	ADP	1	0
3	A	1	ADP	1	0
3	E	5	ADP	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	285/335 (85%)	-1.34	0 100 100	14, 29, 46, 59	0
1	B	280/335 (83%)	-1.29	0 100 100	17, 33, 53, 72	0
1	C	281/335 (83%)	-1.29	0 100 100	17, 32, 54, 72	0
1	D	284/335 (84%)	-1.26	0 100 100	22, 38, 56, 70	0
1	E	282/335 (84%)	-1.24	0 100 100	22, 42, 58, 73	0
1	F	281/335 (83%)	-1.17	0 100 100	26, 46, 67, 76	0
All	All	1693/2010 (84%)	-1.26	0 100 100	14, 37, 59, 76	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

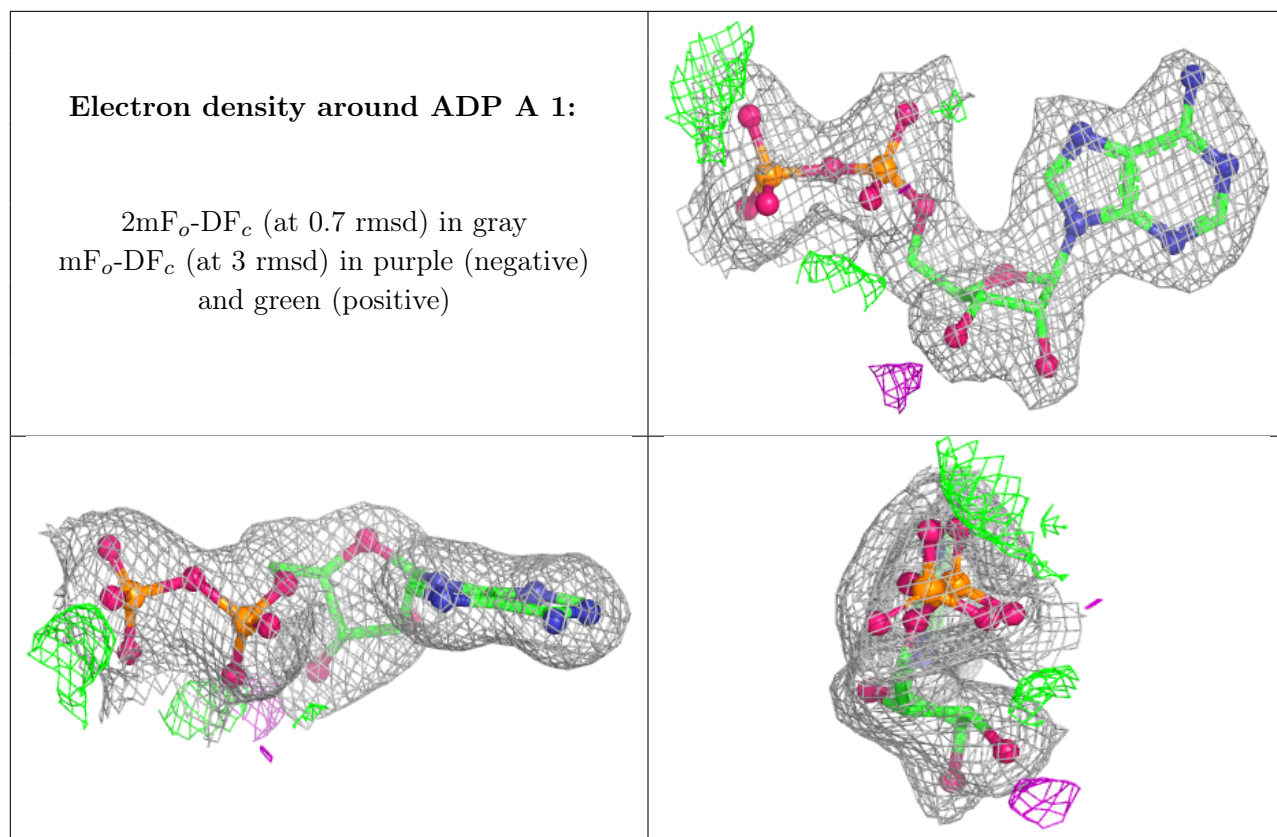
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	10	1/1	0.97	0.05	23,23,23,23	0

*Continued on next page...*

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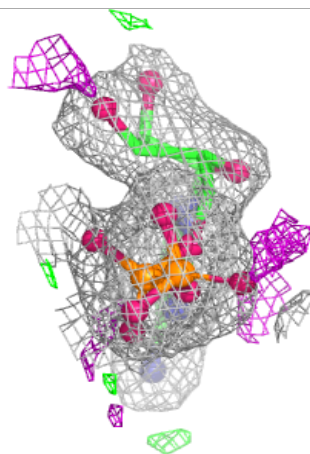
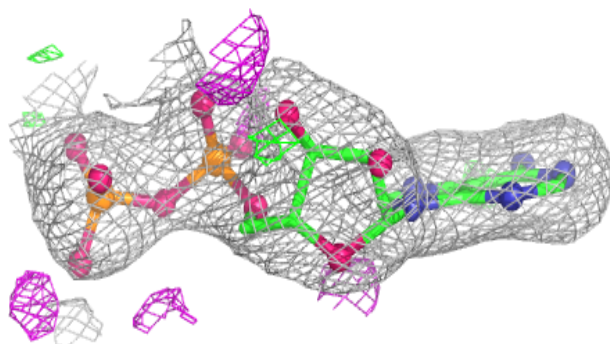
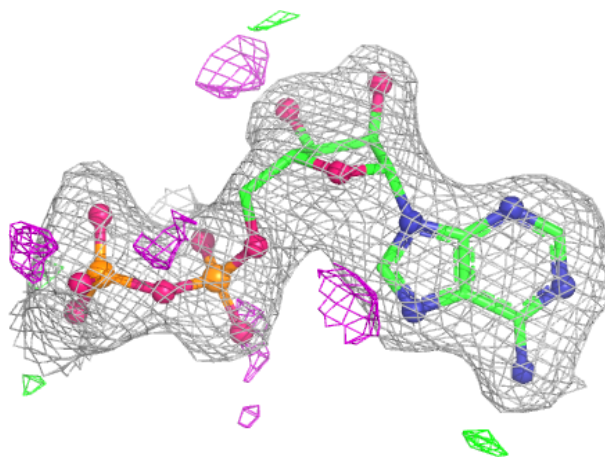
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	21	1/1	0.97	0.06	30,30,30,30	0
2	MG	A	25	1/1	0.98	0.04	22,22,22,22	0
2	MG	A	8	1/1	0.98	0.08	28,28,28,28	0
2	MG	B	19	1/1	0.98	0.06	33,33,33,33	0
2	MG	A	20	1/1	0.98	0.06	24,24,24,24	0
2	MG	D	14	1/1	0.98	0.08	33,33,33,33	0
2	MG	E	16	1/1	0.98	0.06	36,36,36,36	0
2	MG	F	18	1/1	0.98	0.06	31,31,31,31	0
2	MG	A	7	1/1	0.99	0.02	10,10,10,10	0
2	MG	C	22	1/1	0.99	0.02	35,35,35,35	0
2	MG	D	13	1/1	0.99	0.02	14,14,14,14	0
2	MG	B	24	1/1	0.99	0.03	26,26,26,26	0
2	MG	D	23	1/1	0.99	0.02	31,31,31,31	0
2	MG	E	15	1/1	0.99	0.04	24,24,24,24	0
2	MG	C	11	1/1	0.99	0.04	13,13,13,13	0
2	MG	F	17	1/1	0.99	0.04	25,25,25,25	0
2	MG	C	12	1/1	0.99	0.11	35,35,35,35	0
3	ADP	A	1	27/27	0.99	0.03	13,20,33,36	0
3	ADP	B	2	27/27	0.99	0.03	12,23,34,41	0
3	ADP	D	4	27/27	0.99	0.03	22,32,37,43	0
3	ADP	E	5	27/27	0.99	0.04	27,36,52,53	0
2	MG	B	9	1/1	1.00	0.02	15,15,15,15	0
3	ADP	C	3	27/27	1.00	0.03	17,21,30,36	0
3	ADP	F	6	27/27	1.00	0.03	34,40,45,46	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.



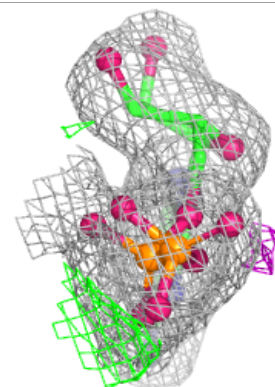
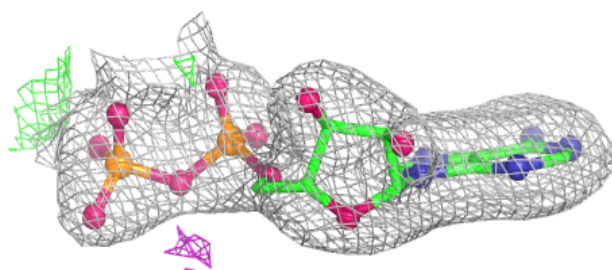
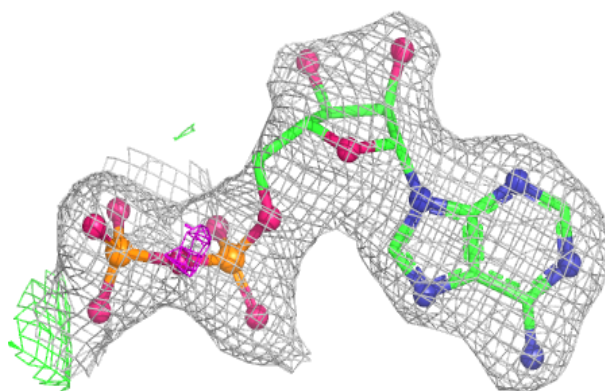
**Electron density around ADP B 2:**

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

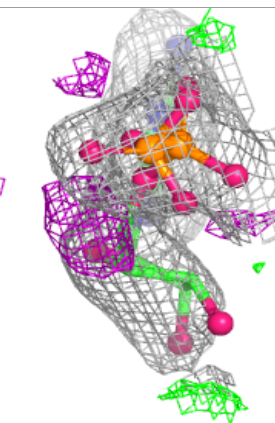
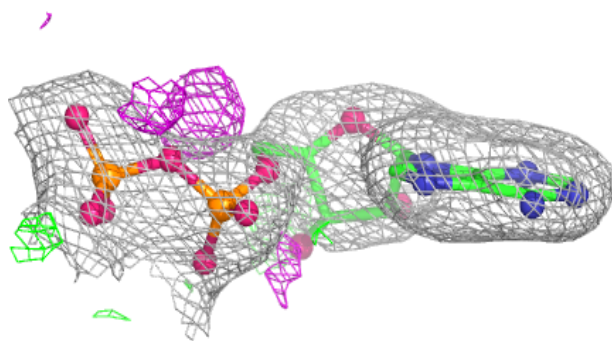
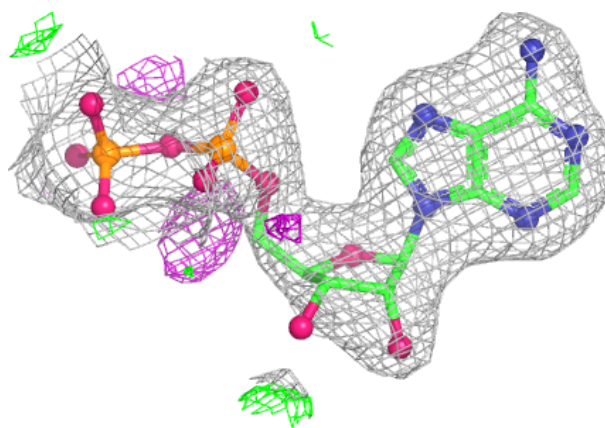


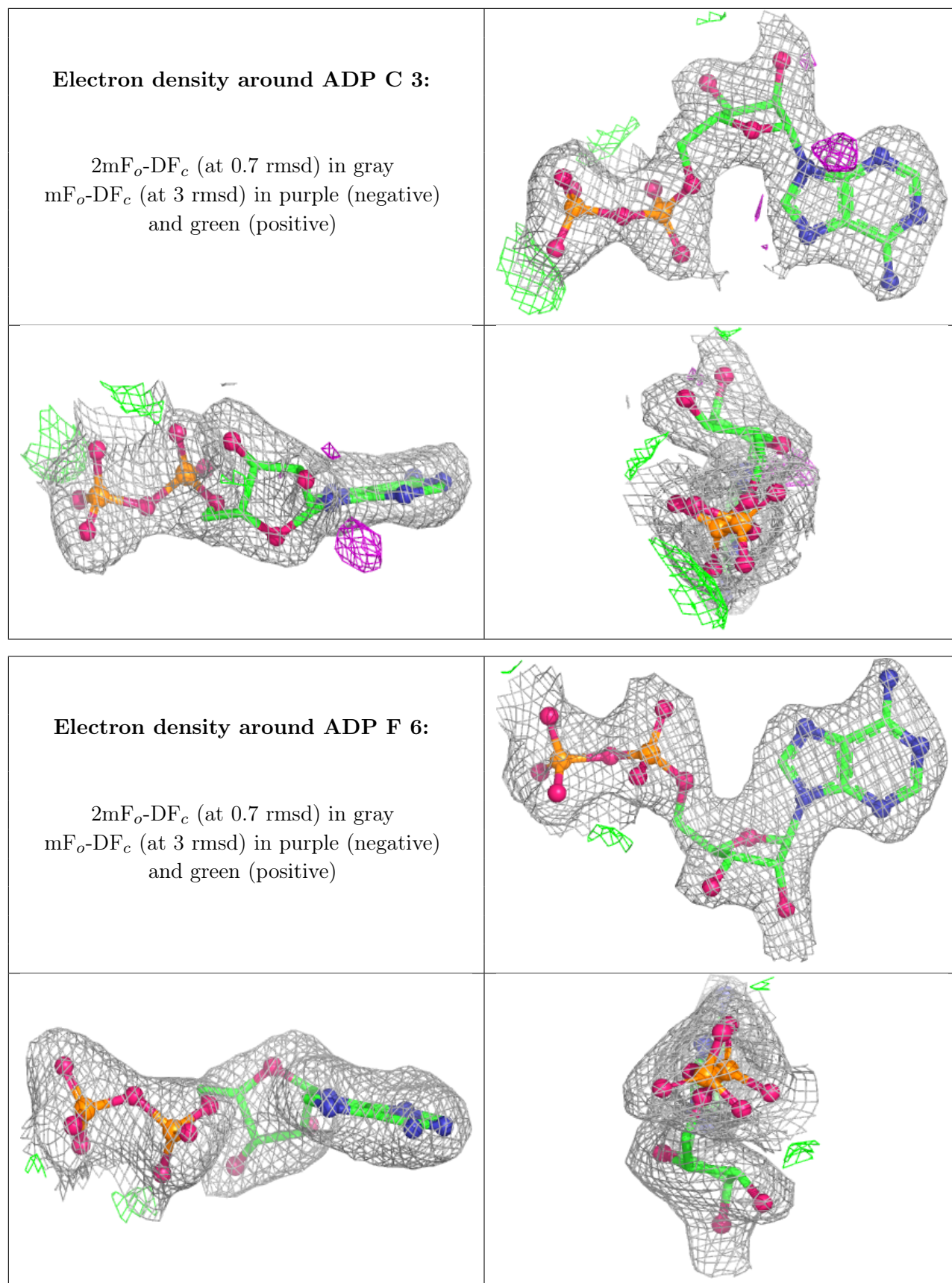
**Electron density around ADP D 4:**

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

**Electron density around ADP E 5:**

$2mF_o-DF_c$  (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.