



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 10:00 AM EST

PDB ID : 4F7W
Title : Crystal structure of *Klebsiella pneumoniae* pantothenate kinase in complex with N-pentylpantothenamide
Authors : Li, B.; Tempel, W.; Smil, D.; Bolshan, Y.; Hong, B.S.; Park, H.W.; Structural Genomics Consortium (SGC)
Deposited on : 2012-05-16
Resolution : 2.10 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

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>.

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 : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

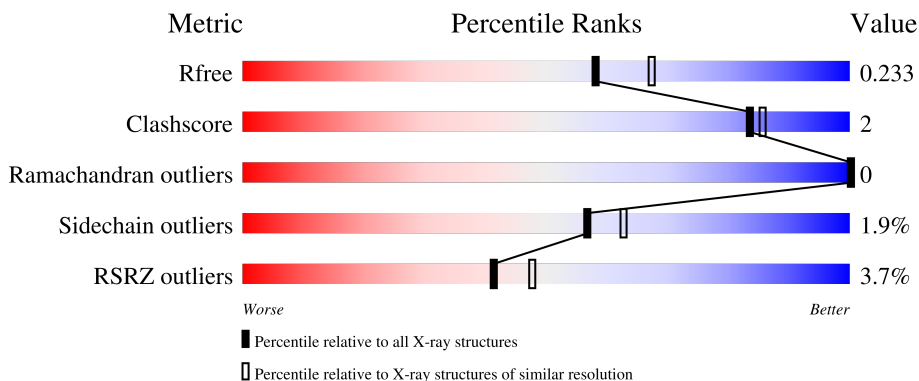
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

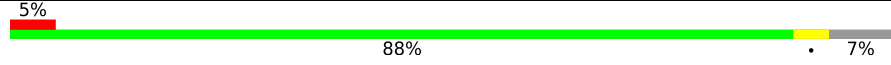
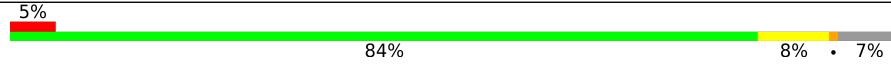
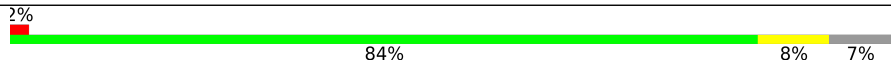

The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	334	 5% 88% 7%
1	B	334	 5% 84% 8% 7%
1	C	334	 2% 84% 8% 7%
1	D	334	 2% 86% 5% 8%

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Mol	Chain	Length	Quality of chain
1	E	334	
1	F	334	
1	G	334	
1	H	334	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	C	1403	-	-	-	X
4	UNX	D	1403	-	-	-	X
4	UNX	D	1406	-	-	-	X
4	UNX	F	1403	-	-	-	X
4	UNX	G	1406	-	-	-	X
4	UNX	G	1407	-	-	-	X
4	UNX	H	1405	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21299 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 Pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2499	1600	431	461	7	0	0	0
1	C	309	2502	1602	431	462	7	0	1	0
1	B	309	2499	1600	431	461	7	0	0	0
1	D	308	2494	1596	430	461	7	0	1	0
1	E	304	2463	1578	426	453	6	0	0	0
1	F	309	2507	1604	433	463	7	0	1	0
1	G	308	2494	1596	430	461	7	0	1	0
1	H	303	2458	1576	422	454	6	0	2	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	expression tag	UNP B5XYG3
A	984	HIS	-	expression tag	UNP B5XYG3
A	985	HIS	-	expression tag	UNP B5XYG3
A	986	HIS	-	expression tag	UNP B5XYG3
A	987	HIS	-	expression tag	UNP B5XYG3
A	988	HIS	-	expression tag	UNP B5XYG3
A	989	HIS	-	expression tag	UNP B5XYG3
A	990	SER	-	expression tag	UNP B5XYG3
A	991	SER	-	expression tag	UNP B5XYG3
A	992	GLY	-	expression tag	UNP B5XYG3
A	993	ARG	-	expression tag	UNP B5XYG3
A	994	GLU	-	expression tag	UNP B5XYG3
A	995	ASN	-	expression tag	UNP B5XYG3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	996	LEU	-	expression tag	UNP B5XYG3
A	997	TYR	-	expression tag	UNP B5XYG3
A	998	PHE	-	expression tag	UNP B5XYG3
A	999	GLN	-	expression tag	UNP B5XYG3
A	1000	GLY	-	expression tag	UNP B5XYG3
C	983	MET	-	expression tag	UNP B5XYG3
C	984	HIS	-	expression tag	UNP B5XYG3
C	985	HIS	-	expression tag	UNP B5XYG3
C	986	HIS	-	expression tag	UNP B5XYG3
C	987	HIS	-	expression tag	UNP B5XYG3
C	988	HIS	-	expression tag	UNP B5XYG3
C	989	HIS	-	expression tag	UNP B5XYG3
C	990	SER	-	expression tag	UNP B5XYG3
C	991	SER	-	expression tag	UNP B5XYG3
C	992	GLY	-	expression tag	UNP B5XYG3
C	993	ARG	-	expression tag	UNP B5XYG3
C	994	GLU	-	expression tag	UNP B5XYG3
C	995	ASN	-	expression tag	UNP B5XYG3
C	996	LEU	-	expression tag	UNP B5XYG3
C	997	TYR	-	expression tag	UNP B5XYG3
C	998	PHE	-	expression tag	UNP B5XYG3
C	999	GLN	-	expression tag	UNP B5XYG3
C	1000	GLY	-	expression tag	UNP B5XYG3
B	983	MET	-	expression tag	UNP B5XYG3
B	984	HIS	-	expression tag	UNP B5XYG3
B	985	HIS	-	expression tag	UNP B5XYG3
B	986	HIS	-	expression tag	UNP B5XYG3
B	987	HIS	-	expression tag	UNP B5XYG3
B	988	HIS	-	expression tag	UNP B5XYG3
B	989	HIS	-	expression tag	UNP B5XYG3
B	990	SER	-	expression tag	UNP B5XYG3
B	991	SER	-	expression tag	UNP B5XYG3
B	992	GLY	-	expression tag	UNP B5XYG3
B	993	ARG	-	expression tag	UNP B5XYG3
B	994	GLU	-	expression tag	UNP B5XYG3
B	995	ASN	-	expression tag	UNP B5XYG3
B	996	LEU	-	expression tag	UNP B5XYG3
B	997	TYR	-	expression tag	UNP B5XYG3
B	998	PHE	-	expression tag	UNP B5XYG3
B	999	GLN	-	expression tag	UNP B5XYG3
B	1000	GLY	-	expression tag	UNP B5XYG3
D	983	MET	-	expression tag	UNP B5XYG3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	984	HIS	-	expression tag	UNP B5XYG3
D	985	HIS	-	expression tag	UNP B5XYG3
D	986	HIS	-	expression tag	UNP B5XYG3
D	987	HIS	-	expression tag	UNP B5XYG3
D	988	HIS	-	expression tag	UNP B5XYG3
D	989	HIS	-	expression tag	UNP B5XYG3
D	990	SER	-	expression tag	UNP B5XYG3
D	991	SER	-	expression tag	UNP B5XYG3
D	992	GLY	-	expression tag	UNP B5XYG3
D	993	ARG	-	expression tag	UNP B5XYG3
D	994	GLU	-	expression tag	UNP B5XYG3
D	995	ASN	-	expression tag	UNP B5XYG3
D	996	LEU	-	expression tag	UNP B5XYG3
D	997	TYR	-	expression tag	UNP B5XYG3
D	998	PHE	-	expression tag	UNP B5XYG3
D	999	GLN	-	expression tag	UNP B5XYG3
D	1000	GLY	-	expression tag	UNP B5XYG3
E	983	MET	-	expression tag	UNP B5XYG3
E	984	HIS	-	expression tag	UNP B5XYG3
E	985	HIS	-	expression tag	UNP B5XYG3
E	986	HIS	-	expression tag	UNP B5XYG3
E	987	HIS	-	expression tag	UNP B5XYG3
E	988	HIS	-	expression tag	UNP B5XYG3
E	989	HIS	-	expression tag	UNP B5XYG3
E	990	SER	-	expression tag	UNP B5XYG3
E	991	SER	-	expression tag	UNP B5XYG3
E	992	GLY	-	expression tag	UNP B5XYG3
E	993	ARG	-	expression tag	UNP B5XYG3
E	994	GLU	-	expression tag	UNP B5XYG3
E	995	ASN	-	expression tag	UNP B5XYG3
E	996	LEU	-	expression tag	UNP B5XYG3
E	997	TYR	-	expression tag	UNP B5XYG3
E	998	PHE	-	expression tag	UNP B5XYG3
E	999	GLN	-	expression tag	UNP B5XYG3
E	1000	GLY	-	expression tag	UNP B5XYG3
F	983	MET	-	expression tag	UNP B5XYG3
F	984	HIS	-	expression tag	UNP B5XYG3
F	985	HIS	-	expression tag	UNP B5XYG3
F	986	HIS	-	expression tag	UNP B5XYG3
F	987	HIS	-	expression tag	UNP B5XYG3
F	988	HIS	-	expression tag	UNP B5XYG3
F	989	HIS	-	expression tag	UNP B5XYG3

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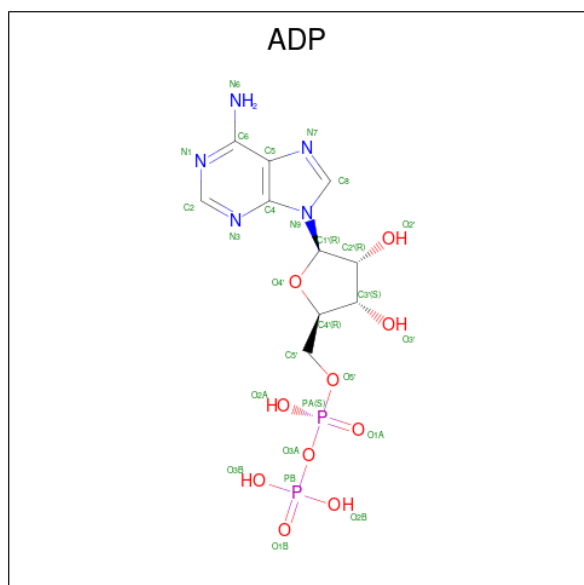
Chain	Residue	Modelled	Actual	Comment	Reference
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F	991	SER	-	expression tag	UNP B5XYG3
F	992	GLY	-	expression tag	UNP B5XYG3
F	993	ARG	-	expression tag	UNP B5XYG3
F	994	GLU	-	expression tag	UNP B5XYG3
F	995	ASN	-	expression tag	UNP B5XYG3
F	996	LEU	-	expression tag	UNP B5XYG3
F	997	TYR	-	expression tag	UNP B5XYG3
F	998	PHE	-	expression tag	UNP B5XYG3
F	999	GLN	-	expression tag	UNP B5XYG3
F	1000	GLY	-	expression tag	UNP B5XYG3
G	983	MET	-	expression tag	UNP B5XYG3
G	984	HIS	-	expression tag	UNP B5XYG3
G	985	HIS	-	expression tag	UNP B5XYG3
G	986	HIS	-	expression tag	UNP B5XYG3
G	987	HIS	-	expression tag	UNP B5XYG3
G	988	HIS	-	expression tag	UNP B5XYG3
G	989	HIS	-	expression tag	UNP B5XYG3
G	990	SER	-	expression tag	UNP B5XYG3
G	991	SER	-	expression tag	UNP B5XYG3
G	992	GLY	-	expression tag	UNP B5XYG3
G	993	ARG	-	expression tag	UNP B5XYG3
G	994	GLU	-	expression tag	UNP B5XYG3
G	995	ASN	-	expression tag	UNP B5XYG3
G	996	LEU	-	expression tag	UNP B5XYG3
G	997	TYR	-	expression tag	UNP B5XYG3
G	998	PHE	-	expression tag	UNP B5XYG3
G	999	GLN	-	expression tag	UNP B5XYG3
G	1000	GLY	-	expression tag	UNP B5XYG3
H	983	MET	-	expression tag	UNP B5XYG3
H	984	HIS	-	expression tag	UNP B5XYG3
H	985	HIS	-	expression tag	UNP B5XYG3
H	986	HIS	-	expression tag	UNP B5XYG3
H	987	HIS	-	expression tag	UNP B5XYG3
H	988	HIS	-	expression tag	UNP B5XYG3
H	989	HIS	-	expression tag	UNP B5XYG3
H	990	SER	-	expression tag	UNP B5XYG3
H	991	SER	-	expression tag	UNP B5XYG3
H	992	GLY	-	expression tag	UNP B5XYG3
H	993	ARG	-	expression tag	UNP B5XYG3
H	994	GLU	-	expression tag	UNP B5XYG3
H	995	ASN	-	expression tag	UNP B5XYG3

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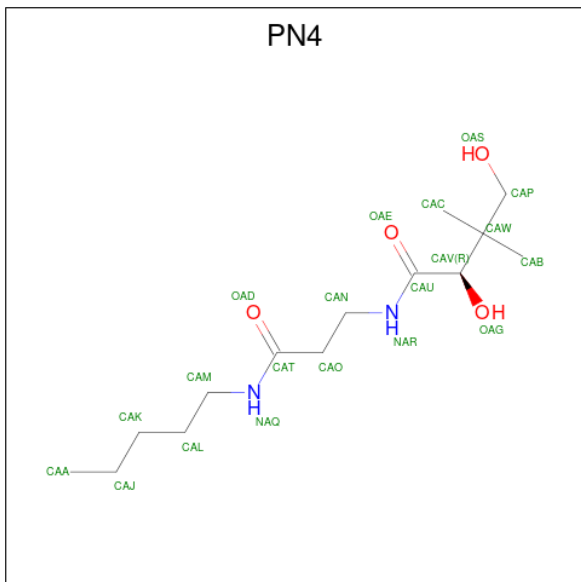
Chain	Residue	Modelled	Actual	Comment	Reference
H	996	LEU	-	expression tag	UNP B5XYG3
H	997	TYR	-	expression tag	UNP B5XYG3
H	998	PHE	-	expression tag	UNP B5XYG3
H	999	GLN	-	expression tag	UNP B5XYG3
H	1000	GLY	-	expression tag	UNP B5XYG3

- 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
			Total	C	N	O	P		
2	A	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	B	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		

- Molecule 3 is (2R)-2,4-dihydroxy-3,3-dimethyl-N-[3-oxo-3-(pentylamino)propyl]butanamide (three-letter code: PN4) (formula: C₁₄H₂₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			20	14	2	4		
3	C	1	Total	C	N	O	0	0
			20	14	2	4		
3	B	1	Total	C	N	O	0	0
			20	14	2	4		
3	D	1	Total	C	N	O	0	0
			20	14	2	4		
3	E	1	Total	C	N	O	0	0
			20	14	2	4		
3	F	1	Total	C	N	O	0	0
			20	14	2	4		
3	G	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	X	0	0
			1	1		
4	C	7	Total	X	0	0
			7	7		
4	B	7	Total	X	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	8	Total X 8 8	0	0
4	F	7	Total X 7 7	0	0
4	G	6	Total X 6 6	0	0
4	H	4	Total X 4 4	0	0

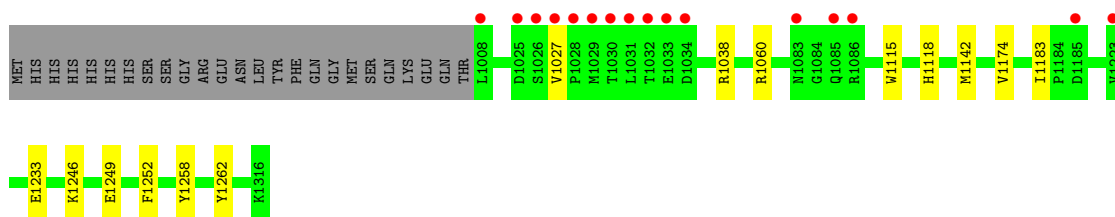
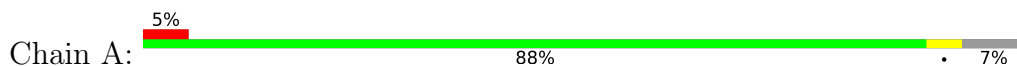
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	C	146	Total O 146 146	0	0
5	B	126	Total O 126 126	0	0
5	D	140	Total O 140 140	0	0
5	E	83	Total O 83 83	0	0
5	F	128	Total O 128 128	0	0
5	G	130	Total O 130 130	0	0
5	H	103	Total O 103 103	0	0

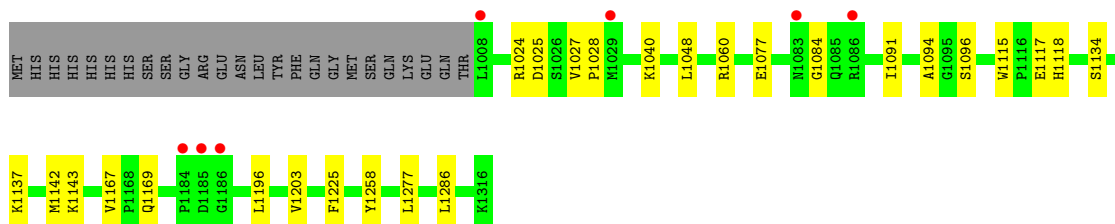
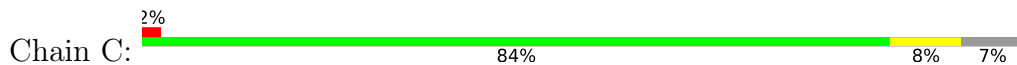
3 Residue-property plots [i](#)

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.

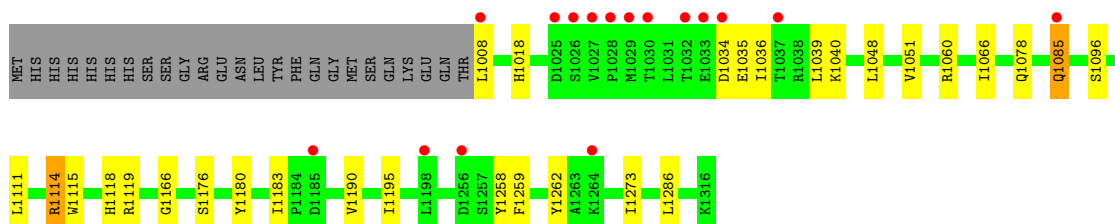
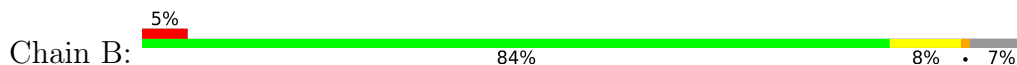
- Molecule 1: Pantothenate kinase



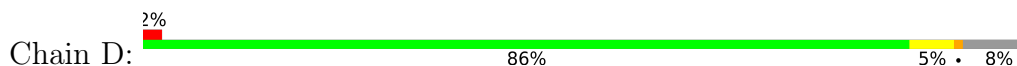
- Molecule 1: Pantothenate kinase

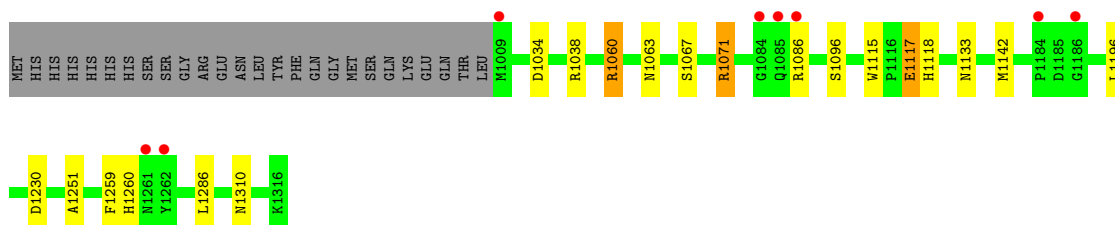


- Molecule 1: Pantothenate kinase

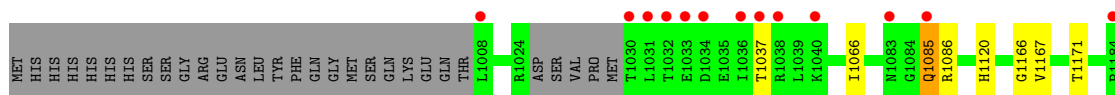
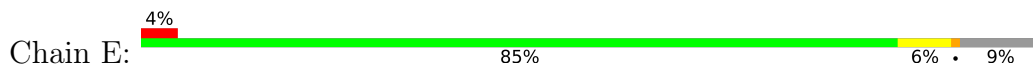


- Molecule 1: Pantothenate kinase

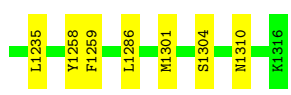
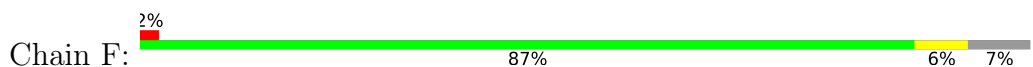




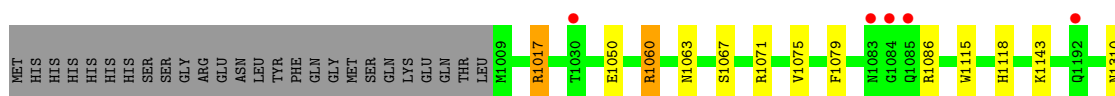
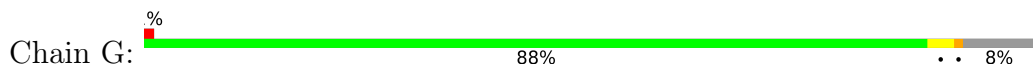
• Molecule 1: Pantothenate kinase



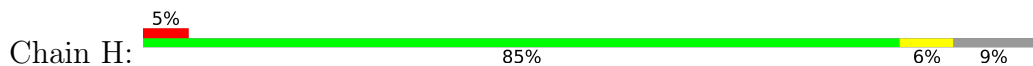
• Molecule 1: Pantothenate kinase

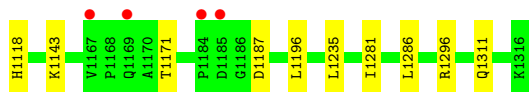


• Molecule 1: Pantothenate kinase



• Molecule 1: Pantothenate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.84Å 130.82Å 192.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 2.10 39.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.65-2.10) 99.9 (39.65-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.185 , 0.226 0.194 , 0.233	Depositor DCC
R_{free} test set	9425 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.090 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21299	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UNX, PN4, 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	0.62	0/2558	0.67	0/3471
1	B	0.63	0/2558	0.68	0/3471
1	C	0.67	1/2564 (0.0%)	0.70	0/3479
1	D	0.67	1/2556 (0.0%)	0.71	3/3468 (0.1%)
1	E	0.61	0/2520	0.66	1/3417 (0.0%)
1	F	0.65	0/2566	0.71	2/3482 (0.1%)
1	G	0.64	0/2556	0.71	1/3468 (0.0%)
1	H	0.63	0/2521	0.68	1/3419 (0.0%)
All	All	0.64	2/20399 (0.0%)	0.69	8/27675 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1117	GLU	CD-OE1	6.08	1.32	1.25
1	C	1117	GLU	CD-OE1	5.79	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1296	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	1230	ASP	CB-CG-OD1	5.61	123.35	118.30
1	E	1230	ASP	CB-CG-OD1	5.50	123.25	118.30
1	F	1301	MET	CA-CB-CG	5.47	122.59	113.30
1	D	1071	ARG	NE-CZ-NH1	5.41	123.01	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	2499	0	2501	13	0
1	B	2499	0	2501	21	0
1	C	2502	0	2506	14	0
1	D	2494	0	2493	12	0
1	E	2463	0	2466	10	0
1	F	2507	0	2506	10	0
1	G	2494	0	2495	8	0
1	H	2458	0	2462	10	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
3	A	20	0	28	5	0
3	B	20	0	28	7	0
3	C	20	0	27	3	0
3	D	20	0	28	0	0
3	E	20	0	28	4	0
3	F	20	0	28	3	0
3	G	20	0	28	0	0
4	A	1	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	8	0	0	0	0
4	F	7	0	0	0	0
4	G	6	0	0	0	0
4	H	4	0	0	0	0
5	A	131	0	0	2	0
5	B	126	0	0	0	0
5	C	146	0	0	0	0
5	D	140	0	0	1	0
5	E	83	0	0	1	0
5	F	128	0	0	2	0
5	G	130	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	103	0	0	0	0
All	All	21299	0	20221	96	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 2.

The worst 5 of 96 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:TYR:CE1	3:A:1402:PN4:HAA	1.80	1.17
1:C:1258:TYR:HD2	3:C:1402:PN4:HAA	1.18	1.08
1:A:1258:TYR:HE1	3:A:1402:PN4:HAA	1.15	0.99
1:C:1258:TYR:CD2	3:C:1402:PN4:HAA	2.11	0.83
1:D:1133:ASN:HA	1:D:1142:MET:HE1	1.64	0.79

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	307/334 (92%)	300 (98%)	7 (2%)	0	100	100
1	B	307/334 (92%)	302 (98%)	5 (2%)	0	100	100
1	C	308/334 (92%)	300 (97%)	8 (3%)	0	100	100
1	D	307/334 (92%)	299 (97%)	8 (3%)	0	100	100
1	E	300/334 (90%)	294 (98%)	6 (2%)	0	100	100
1	F	308/334 (92%)	304 (99%)	4 (1%)	0	100	100
1	G	307/334 (92%)	300 (98%)	7 (2%)	0	100	100
1	H	301/334 (90%)	289 (96%)	12 (4%)	0	100	100
All	All	2445/2672 (92%)	2388 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/301 (92%)	276 (99%)	2 (1%)	84	88
1	B	278/301 (92%)	270 (97%)	8 (3%)	42	46
1	C	279/301 (93%)	275 (99%)	4 (1%)	67	73
1	D	278/301 (92%)	271 (98%)	7 (2%)	47	52
1	E	273/301 (91%)	265 (97%)	8 (3%)	42	46
1	F	279/301 (93%)	276 (99%)	3 (1%)	73	79
1	G	278/301 (92%)	273 (98%)	5 (2%)	59	65
1	H	274/301 (91%)	269 (98%)	5 (2%)	59	65
All	All	2217/2408 (92%)	2175 (98%)	42 (2%)	57	63

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1276	SER
1	G	1086	ARG
1	F	1030	THR
1	G	1017	ARG
1	H	1031	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1310	ASN
1	H	1069	ASN
1	F	1014	GLN
1	G	1205	GLN
1	E	1019	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 55 ligands modelled in this entry, 40 are unknown - leaving 15 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	PN4	C	1402	-	17,19,19	1.32	1 (5%)	22,24,24	0.88	1 (4%)
2	ADP	F	1401	-	24,29,29	1.01	1 (4%)	29,45,45	1.09	2 (6%)
2	ADP	C	1401	-	24,29,29	0.84	0	29,45,45	1.23	2 (6%)
2	ADP	G	1401	-	24,29,29	1.27	2 (8%)	29,45,45	1.42	5 (17%)
2	ADP	E	1401	-	24,29,29	0.96	2 (8%)	29,45,45	1.39	5 (17%)
3	PN4	F	1402	-	17,19,19	1.49	1 (5%)	22,24,24	0.95	0
2	ADP	H	1401	-	24,29,29	1.14	2 (8%)	29,45,45	1.40	5 (17%)
3	PN4	G	1402	-	17,19,19	1.81	1 (5%)	22,24,24	1.08	1 (4%)
2	ADP	D	1401	-	24,29,29	1.00	1 (4%)	29,45,45	1.26	2 (6%)
2	ADP	B	1401	-	24,29,29	1.09	1 (4%)	29,45,45	1.38	5 (17%)
3	PN4	A	1402	-	17,19,19	0.90	1 (5%)	22,24,24	0.77	0
3	PN4	E	1402	-	17,19,19	0.83	1 (5%)	22,24,24	0.91	1 (4%)
3	PN4	D	1402	-	17,19,19	1.86	1 (5%)	22,24,24	1.03	2 (9%)
2	ADP	A	1401	-	24,29,29	1.16	2 (8%)	29,45,45	1.25	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PN4	B	1402	-	17,19,19	1.66	1 (5%)	22,24,24	0.86	1 (4%)

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	PN4	C	1402	-	-	1/25/25/25	-
2	ADP	F	1401	-	-	1/12/32/32	0/3/3/3
2	ADP	C	1401	-	-	1/12/32/32	0/3/3/3
2	ADP	G	1401	-	-	2/12/32/32	0/3/3/3
2	ADP	E	1401	-	-	0/12/32/32	0/3/3/3
3	PN4	F	1402	-	-	7/25/25/25	-
2	ADP	H	1401	-	-	0/12/32/32	0/3/3/3
3	PN4	G	1402	-	-	1/25/25/25	-
2	ADP	D	1401	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1401	-	-	2/12/32/32	0/3/3/3
3	PN4	A	1402	-	-	4/25/25/25	-
3	PN4	E	1402	-	-	11/25/25/25	-
3	PN4	D	1402	-	-	5/25/25/25	-
2	ADP	A	1401	-	-	1/12/32/32	0/3/3/3
3	PN4	B	1402	-	-	2/25/25/25	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1402	PN4	CAP-CAW	7.14	1.58	1.53
3	G	1402	PN4	CAP-CAW	6.84	1.58	1.53
3	B	1402	PN4	CAP-CAW	6.54	1.57	1.53
3	F	1402	PN4	CAP-CAW	5.40	1.57	1.53
2	G	1401	ADP	O4'-C1'	4.30	1.47	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1401	ADP	N3-C2-N1	-3.91	122.56	128.68
2	H	1401	ADP	N3-C2-N1	-3.70	122.90	128.68
2	A	1401	ADP	N3-C2-N1	-3.69	122.91	128.68
2	G	1401	ADP	N3-C2-N1	-3.67	122.94	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1401	ADP	N3-C2-N1	-3.59	123.07	128.68

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

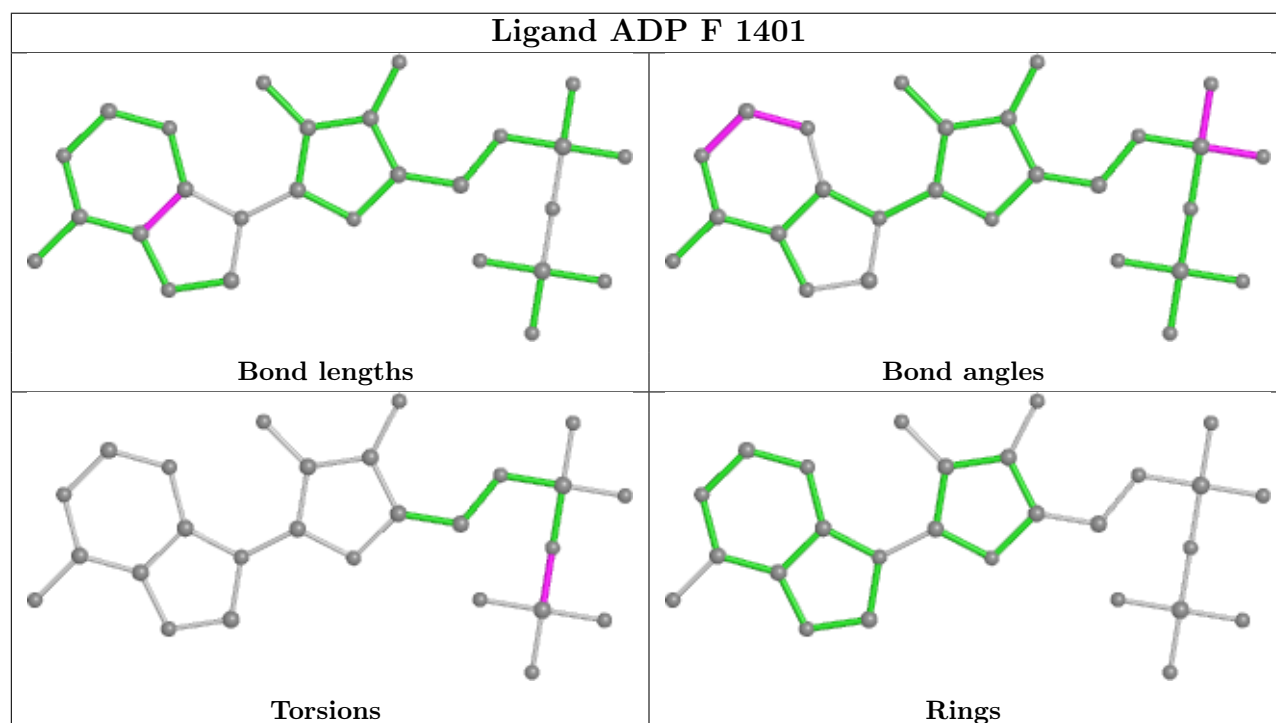
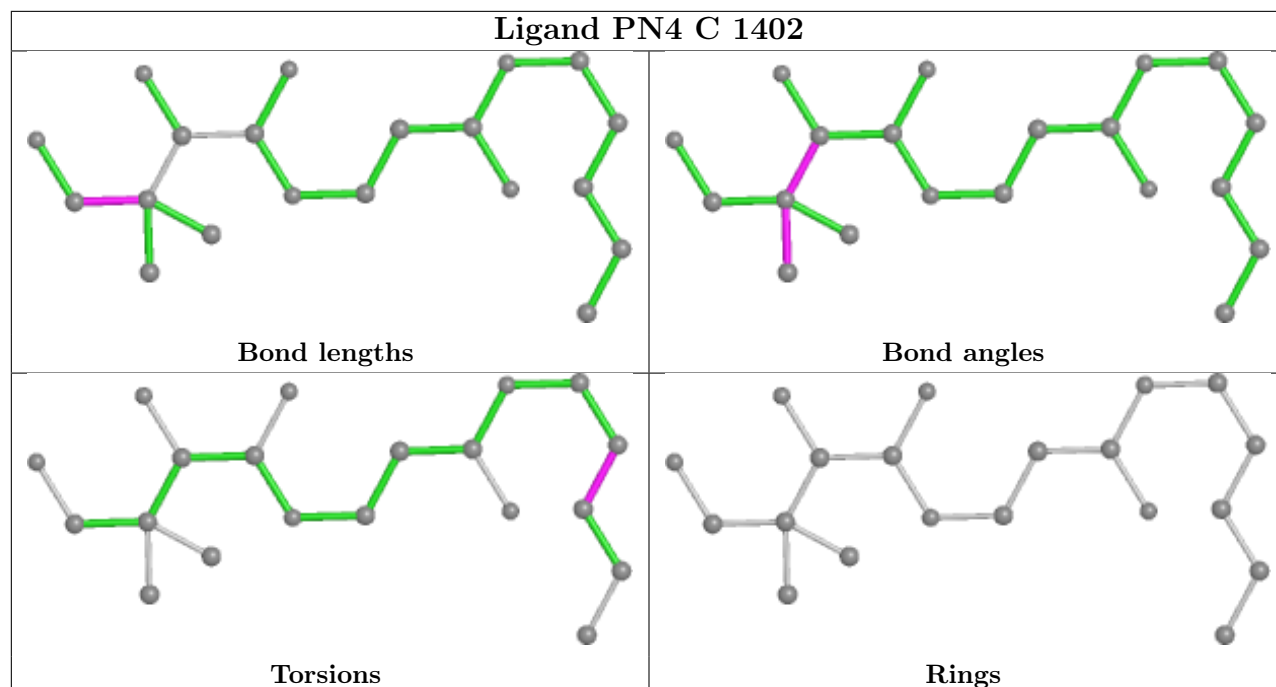
Mol	Chain	Res	Type	Atoms
2	B	1401	ADP	PA-O3A-PB-O2B
2	F	1401	ADP	PA-O3A-PB-O3B
3	D	1402	PN4	OAS-CAP-CAW-CAB
3	E	1402	PN4	OAS-CAP-CAW-CAV
3	E	1402	PN4	OAS-CAP-CAW-CAC

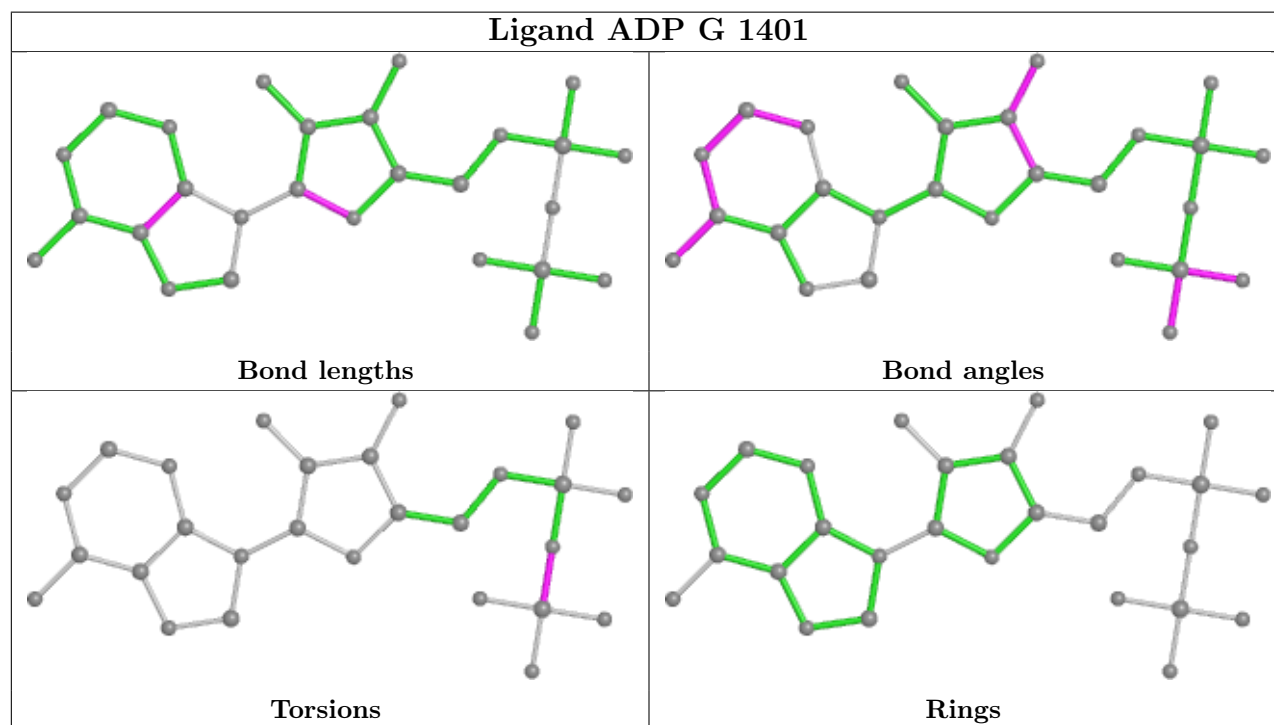
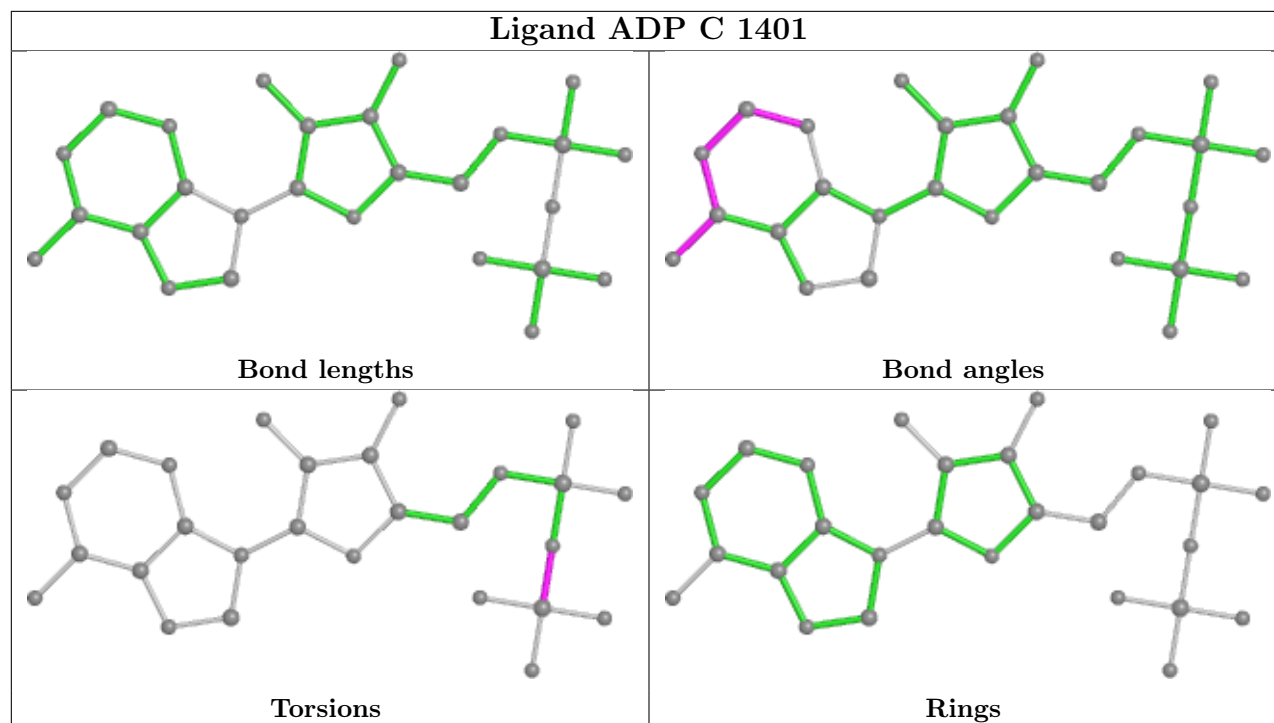
There are no ring outliers.

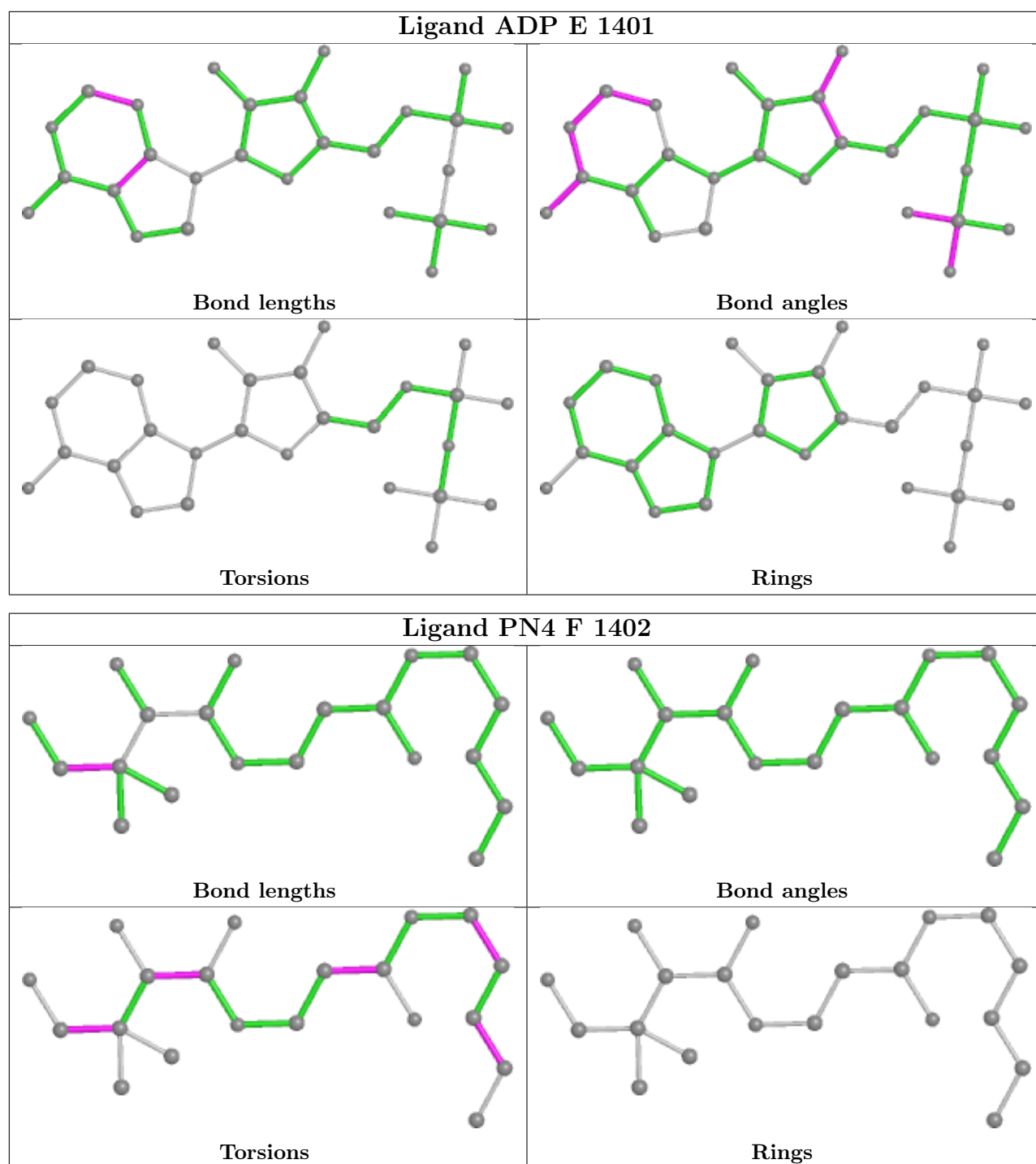
5 monomers are involved in 22 short contacts:

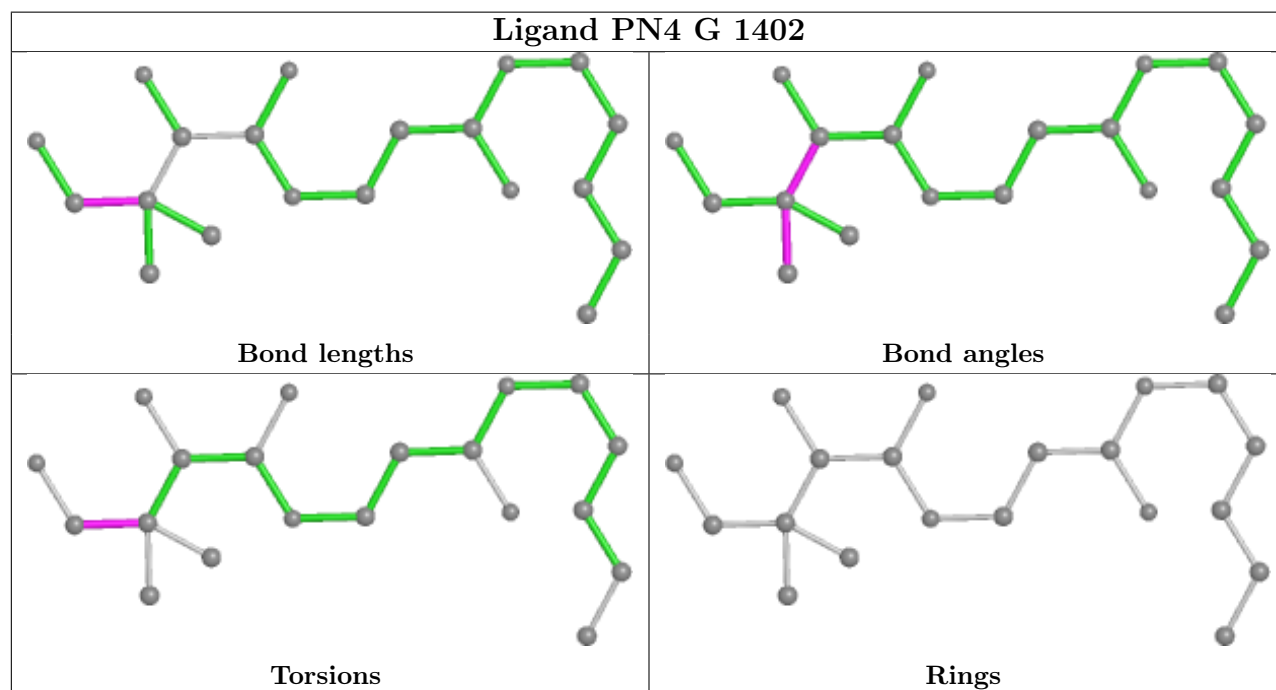
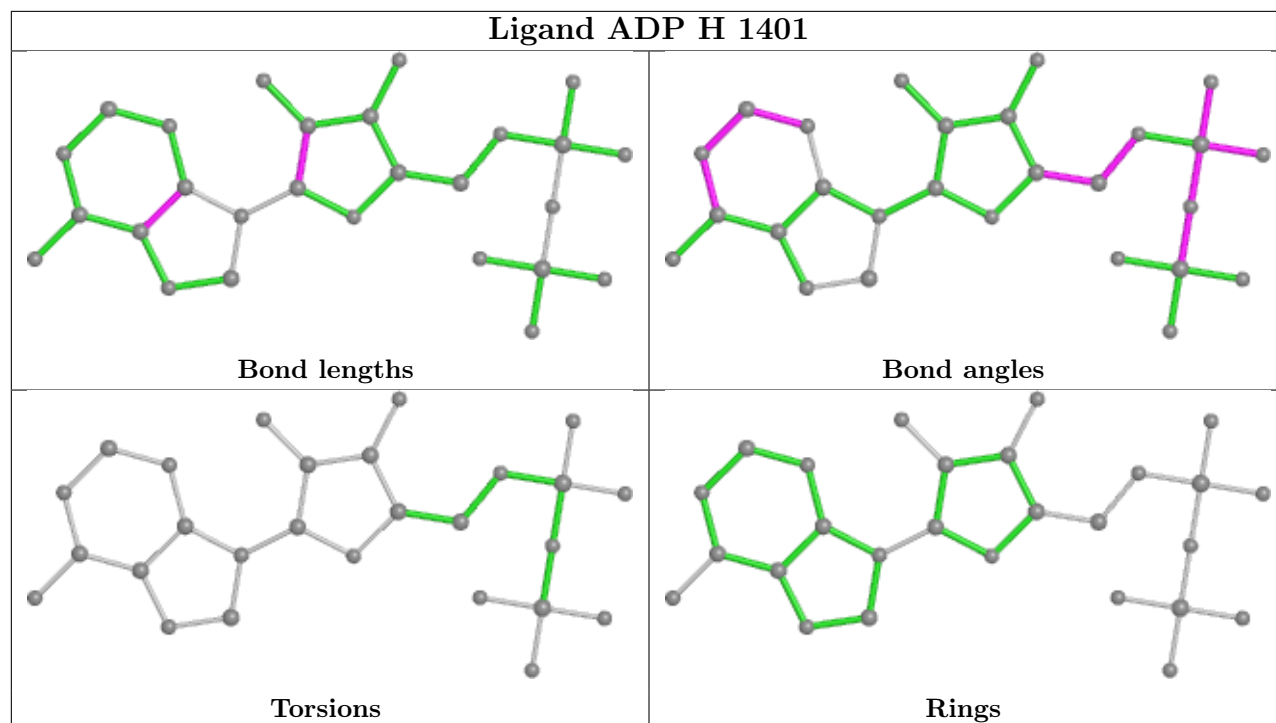
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1402	PN4	3	0
3	F	1402	PN4	3	0
3	A	1402	PN4	5	0
3	E	1402	PN4	4	0
3	B	1402	PN4	7	0

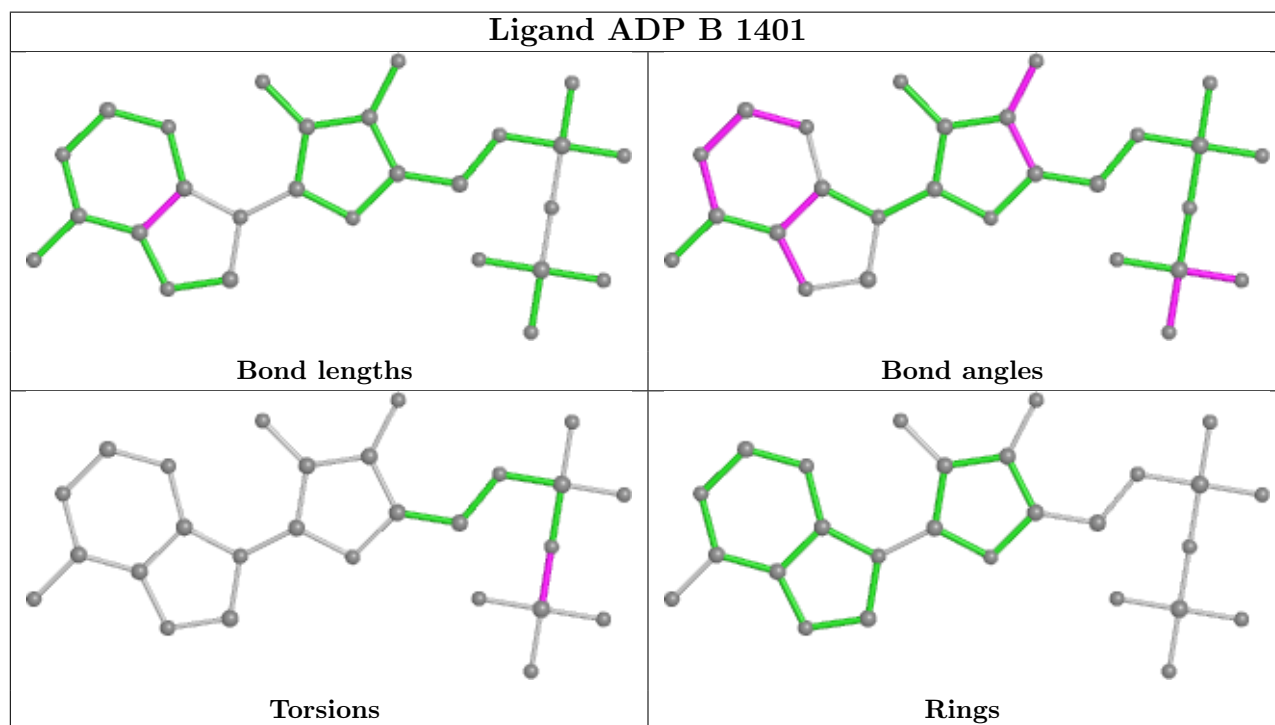
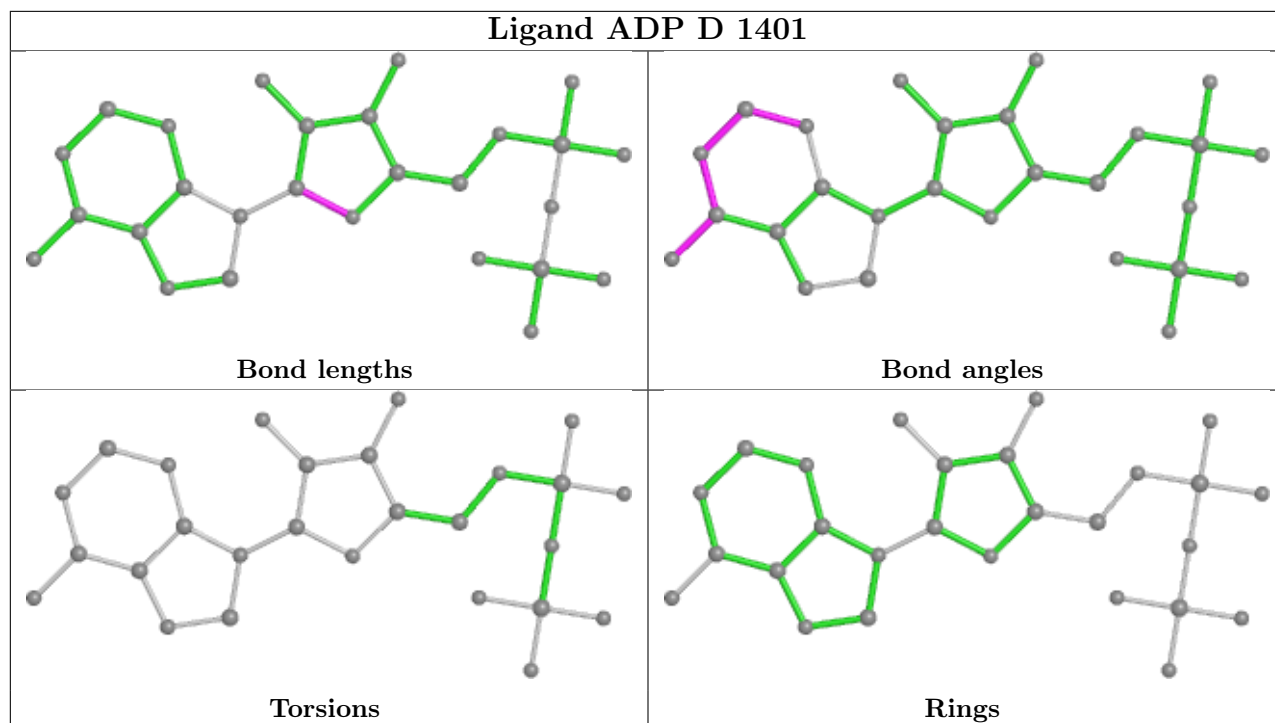
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

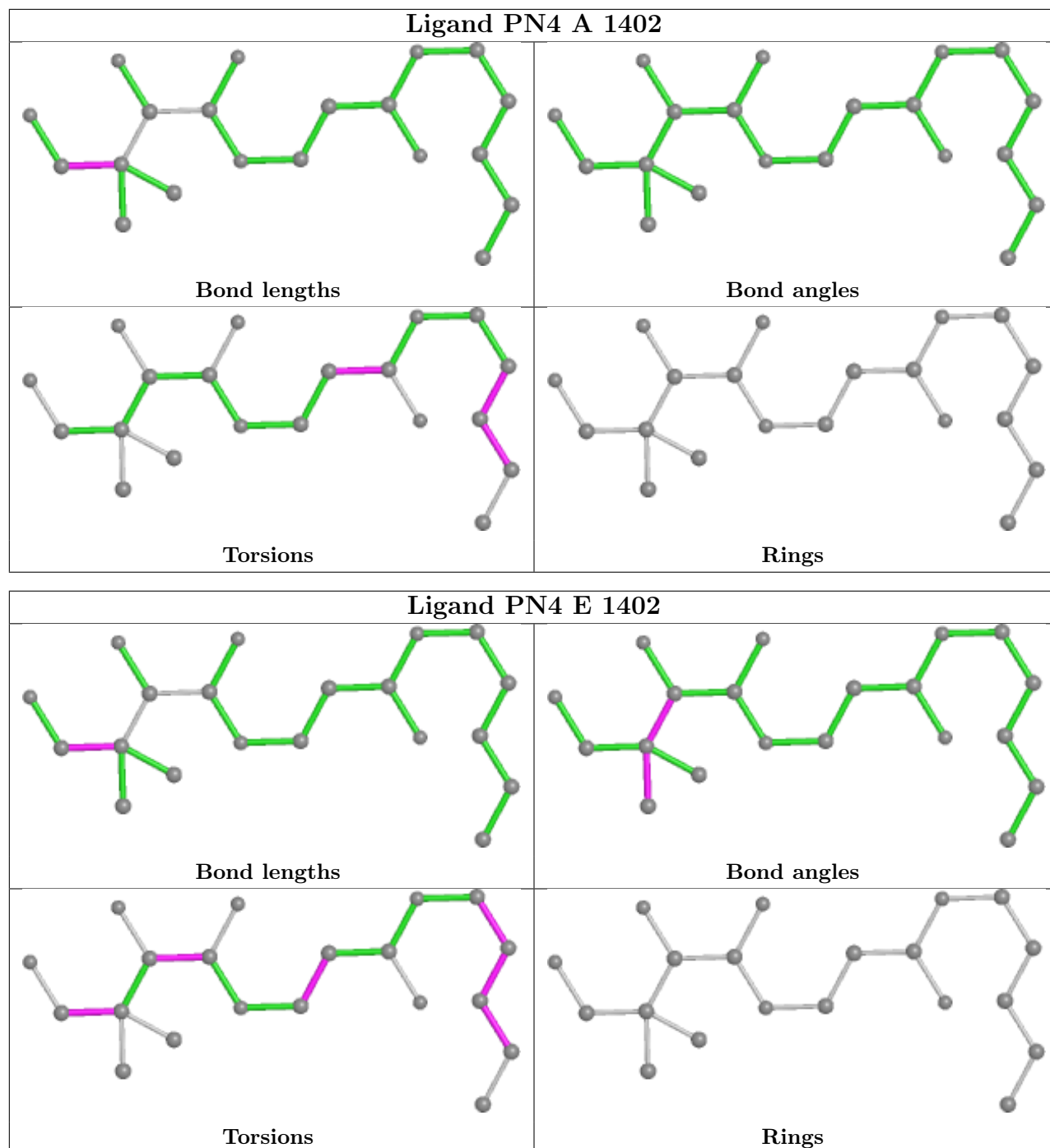


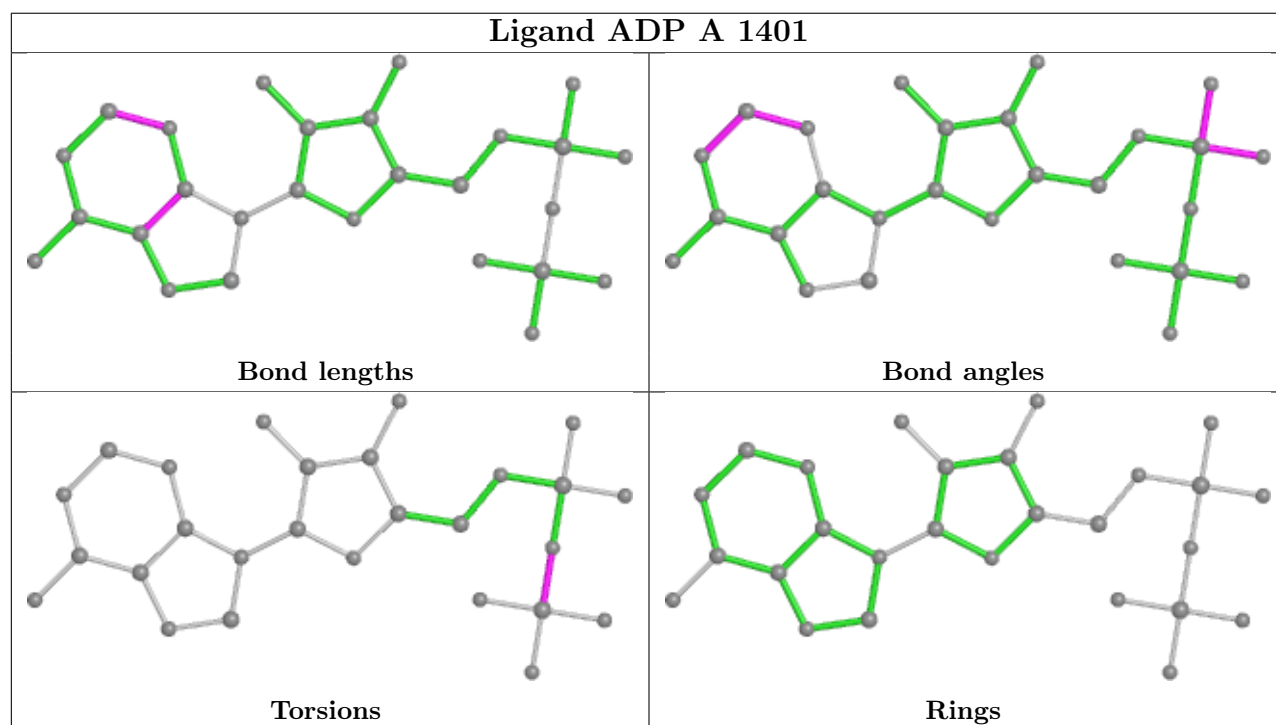
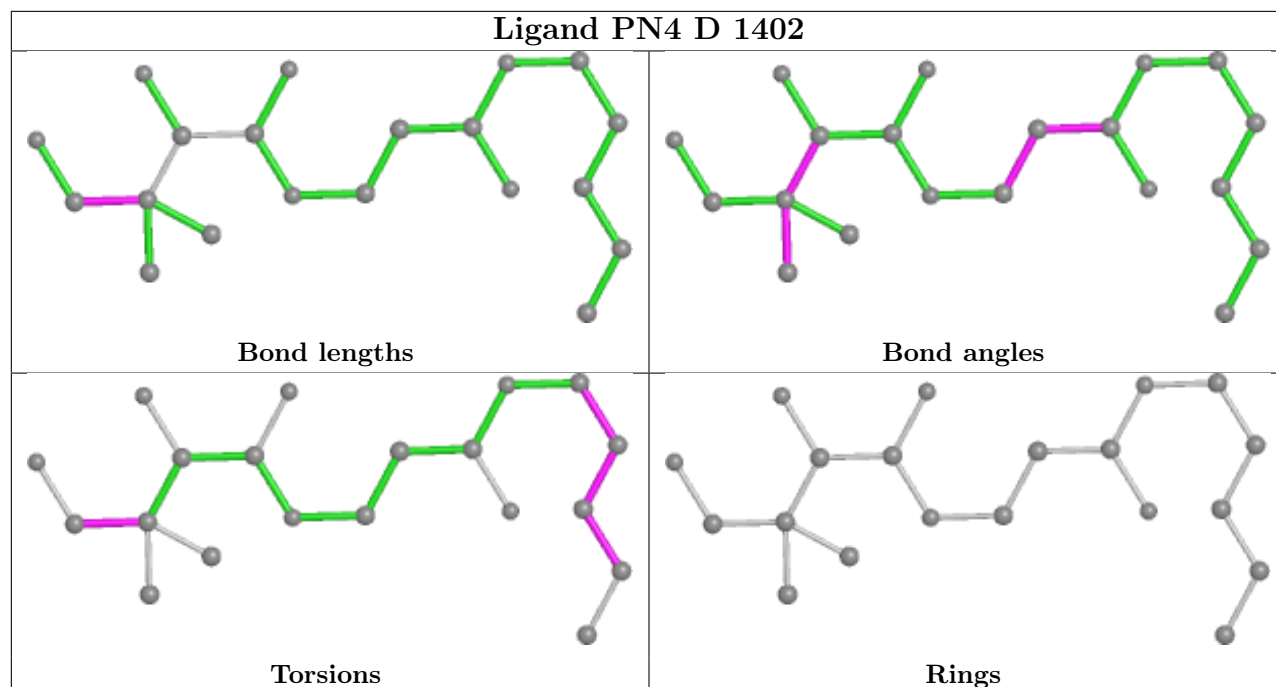


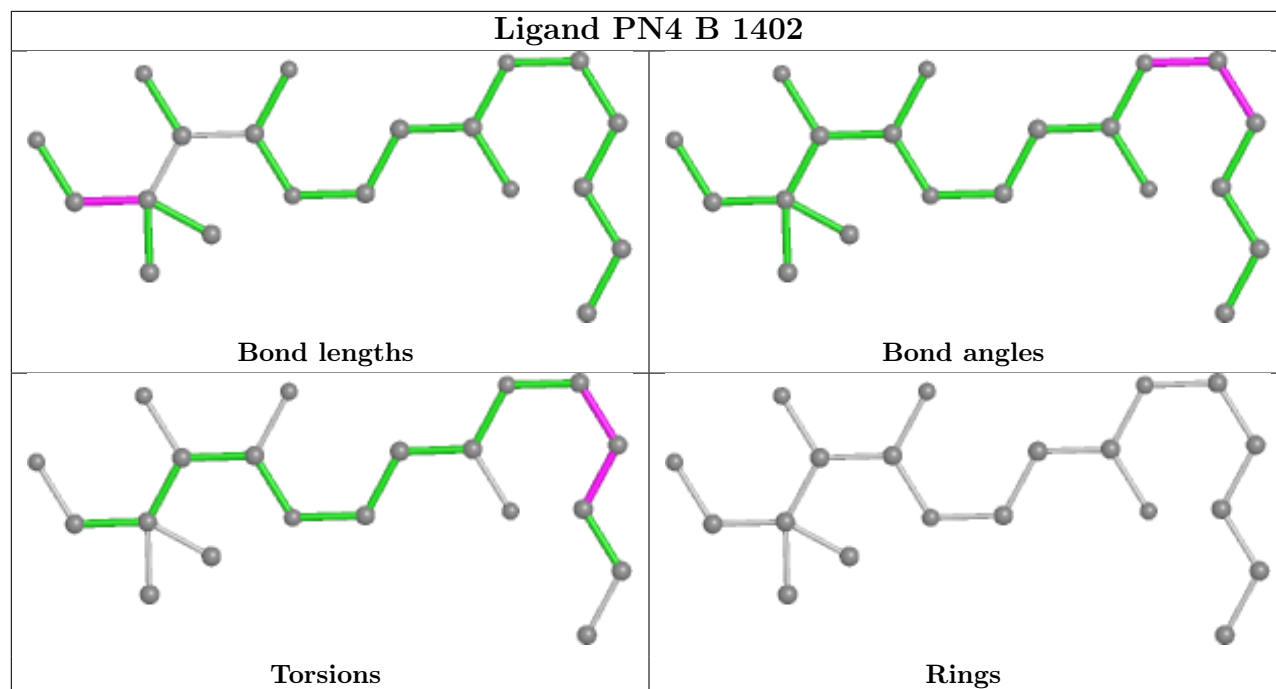












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	309/334 (92%)	-0.07	16 (5%) 27 32	14, 24, 59, 102	0
1	B	309/334 (92%)	-0.03	16 (5%) 27 32	15, 26, 55, 82	0
1	C	309/334 (92%)	-0.17	7 (2%) 60 65	13, 21, 42, 65	0
1	D	308/334 (92%)	-0.23	8 (2%) 56 61	12, 22, 45, 72	0
1	E	304/334 (91%)	0.02	15 (4%) 29 35	16, 29, 57, 84	0
1	F	309/334 (92%)	-0.20	7 (2%) 60 65	12, 23, 45, 72	0
1	G	308/334 (92%)	-0.25	5 (1%) 72 75	14, 23, 44, 69	0
1	H	303/334 (90%)	-0.03	17 (5%) 24 29	14, 26, 58, 70	0
All	All	2459/2672 (92%)	-0.12	91 (3%) 41 48	12, 24, 51, 102	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1026	SER	9.6
1	B	1026	SER	7.1
1	H	1008	LEU	5.1
1	H	1184	PRO	5.0
1	H	1030	THR	4.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
4	UNX	G	1406	1/1	0.61	0.65	26,26,26,26	0
4	UNX	D	1403	1/1	0.64	0.50	18,18,18,18	0
4	UNX	F	1403	1/1	0.66	0.68	23,23,23,23	0
4	UNX	C	1403	1/1	0.66	0.83	25,25,25,25	0
4	UNX	C	1406	1/1	0.68	0.31	31,31,31,31	0
4	UNX	D	1406	1/1	0.69	0.56	35,35,35,35	0
4	UNX	H	1405	1/1	0.69	0.47	32,32,32,32	0
4	UNX	G	1407	1/1	0.80	0.50	23,23,23,23	0
4	UNX	B	1405	1/1	0.80	0.15	31,31,31,31	0
4	UNX	F	1405	1/1	0.81	0.55	26,26,26,26	0
4	UNX	G	1404	1/1	0.82	0.25	31,31,31,31	0
4	UNX	C	1405	1/1	0.83	0.44	29,29,29,29	0
4	UNX	F	1407	1/1	0.83	0.45	29,29,29,29	0
4	UNX	D	1404	1/1	0.83	0.60	28,28,28,28	0
4	UNX	B	1403	1/1	0.84	0.50	21,21,21,21	0
4	UNX	H	1402	1/1	0.86	0.52	24,24,24,24	0
4	UNX	D	1405	1/1	0.87	0.09	27,27,27,27	0
4	UNX	B	1404	1/1	0.87	0.22	20,20,20,20	0
3	PN4	E	1402	20/20	0.88	0.20	42,50,58,67	0
4	UNX	F	1406	1/1	0.89	0.20	24,24,24,24	0
3	PN4	C	1402	20/20	0.91	0.14	26,29,40,42	0
4	UNX	C	1407	1/1	0.92	0.21	30,30,30,30	0
3	PN4	F	1402	20/20	0.92	0.14	24,26,46,49	0
4	UNX	D	1409	1/1	0.92	0.17	23,23,23,23	0
4	UNX	C	1404	1/1	0.92	0.64	29,29,29,29	0
4	UNX	G	1403	1/1	0.93	0.47	28,28,28,28	0
4	UNX	F	1404	1/1	0.94	0.69	28,28,28,28	0
4	UNX	C	1409	1/1	0.94	0.13	21,21,21,21	0
4	UNX	D	1407	1/1	0.94	0.10	12,12,12,12	0
3	PN4	D	1402	20/20	0.94	0.10	21,24,40,41	0
4	UNX	H	1403	1/1	0.94	0.60	30,30,30,30	0
4	UNX	B	1409	1/1	0.94	0.28	24,24,24,24	0
3	PN4	B	1402	20/20	0.95	0.12	24,26,50,50	0
4	UNX	G	1405	1/1	0.96	0.22	19,19,19,19	0
3	PN4	G	1402	20/20	0.96	0.09	22,24,35,35	0
4	UNX	H	1404	1/1	0.96	0.11	25,25,25,25	0
3	PN4	A	1402	20/20	0.96	0.11	20,23,35,35	0

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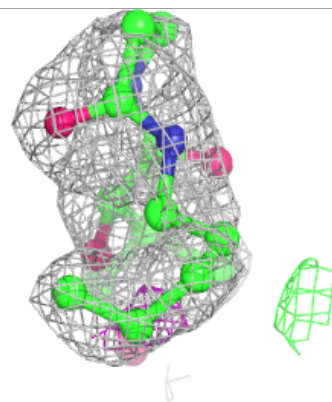
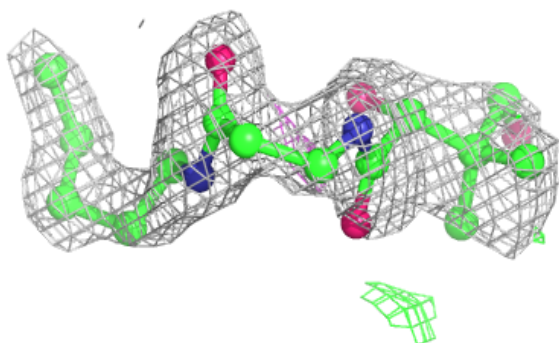
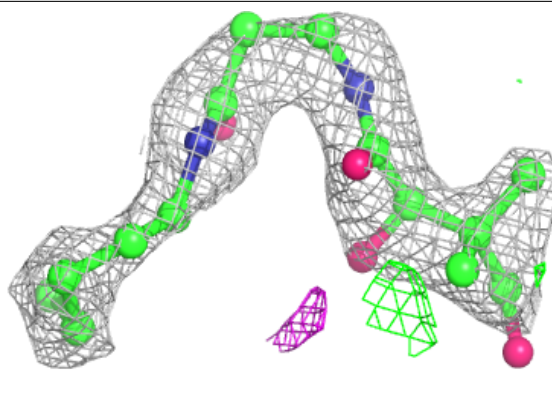
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	UNX	F	1409	1/1	0.97	0.18	25,25,25,25	0
4	UNX	G	1408	1/1	0.97	0.14	19,19,19,19	0
4	UNX	B	1407	1/1	0.97	0.14	18,18,18,18	0
4	UNX	D	1408	1/1	0.97	0.15	21,21,21,21	0
4	UNX	C	1408	1/1	0.97	0.20	25,25,25,25	0
4	UNX	B	1406	1/1	0.97	0.14	20,20,20,20	0
2	ADP	G	1401	27/27	0.98	0.08	14,18,21,21	0
2	ADP	B	1401	27/27	0.98	0.08	18,21,25,28	0
4	UNX	B	1408	1/1	0.98	0.22	29,29,29,29	0
4	UNX	D	1410	1/1	0.98	0.20	17,17,17,17	0
2	ADP	E	1401	27/27	0.98	0.08	19,26,33,33	0
2	ADP	A	1401	27/27	0.99	0.07	16,18,22,23	0
2	ADP	H	1401	27/27	0.99	0.07	19,21,26,27	0
4	UNX	F	1408	1/1	0.99	0.12	18,18,18,18	0
2	ADP	D	1401	27/27	0.99	0.08	12,17,20,21	0
2	ADP	C	1401	27/27	0.99	0.09	15,17,17,18	0
4	UNX	A	1403	1/1	0.99	0.12	21,21,21,21	0
2	ADP	F	1401	27/27	0.99	0.07	13,16,18,18	0

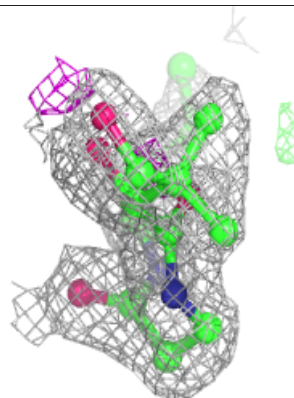
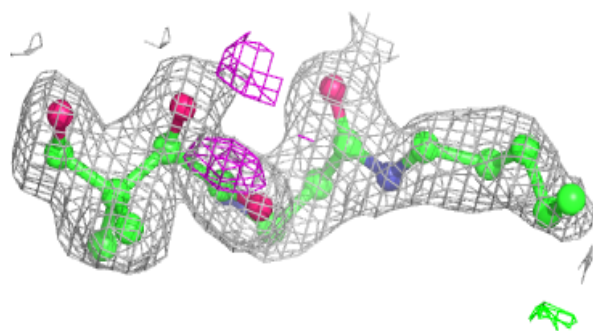
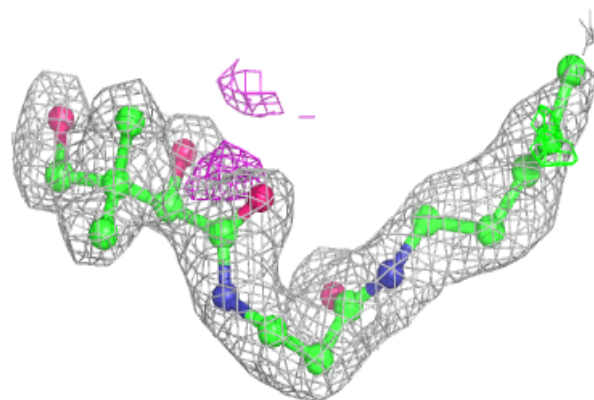
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PN4 E 1402:

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

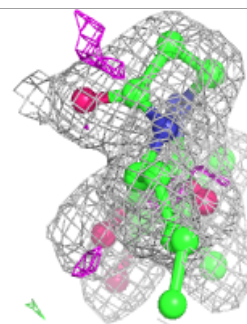
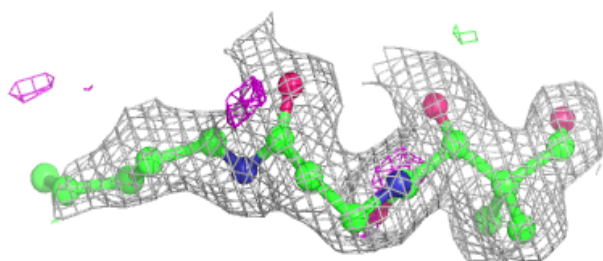
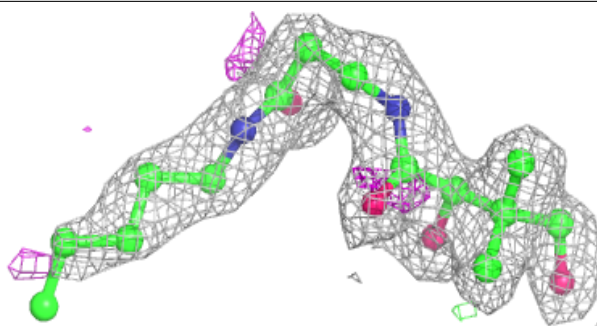
**Electron density around PN4 C 1402:**

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

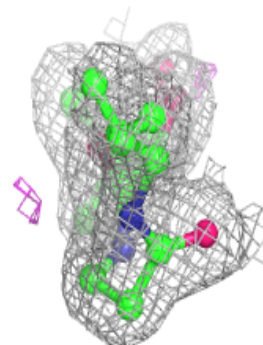
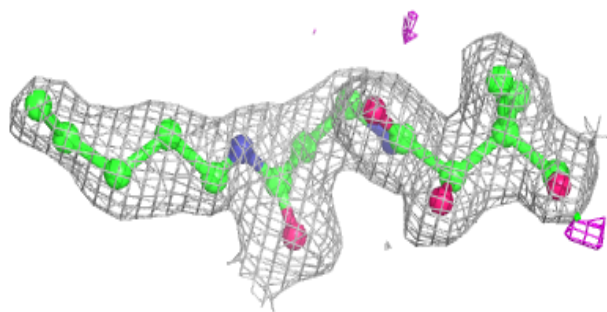
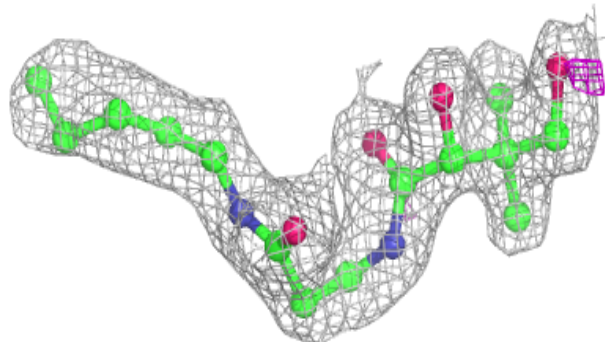


Electron density around PN4 F 1402:

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

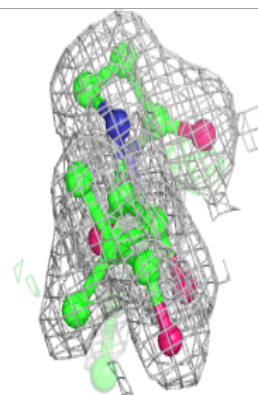
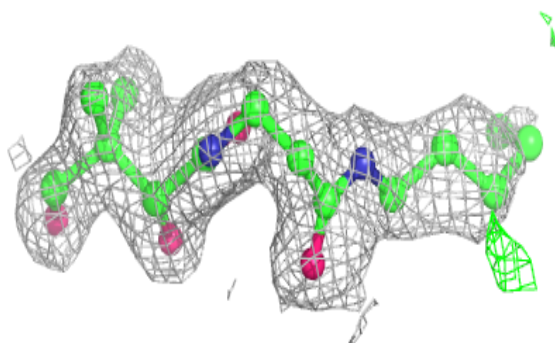
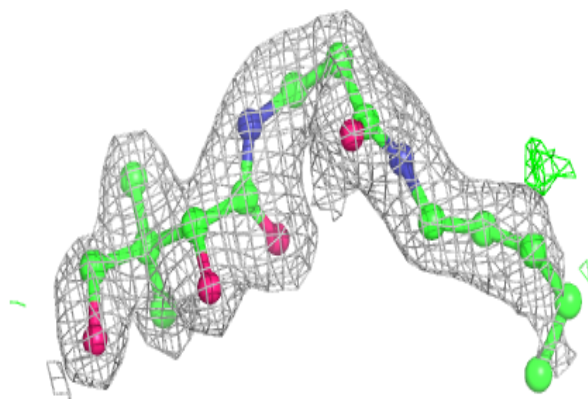
**Electron density around PN4 D 1402:**

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

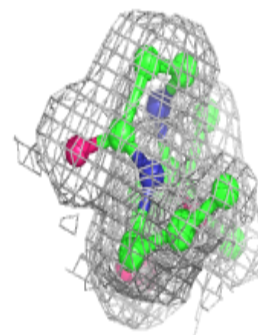
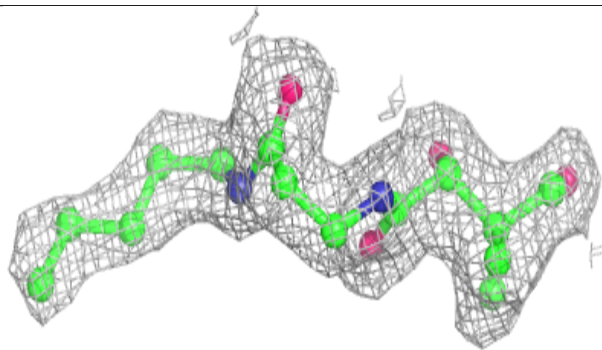
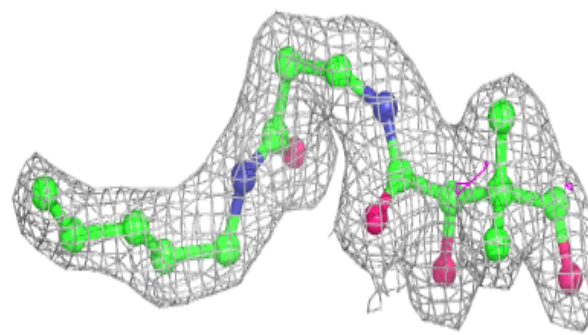


Electron density around PN4 B 1402:

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

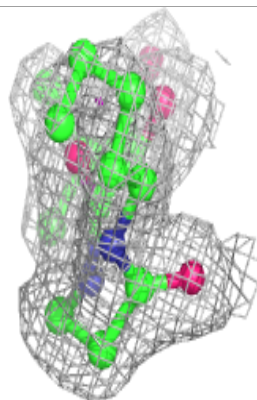
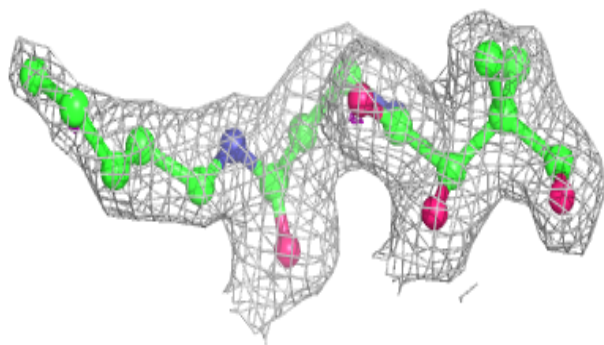
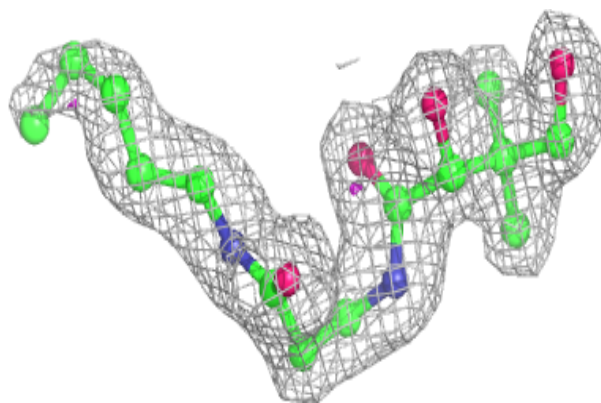
**Electron density around PN4 G 1402:**

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

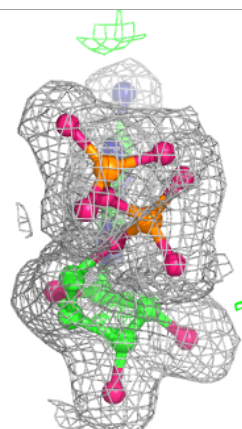
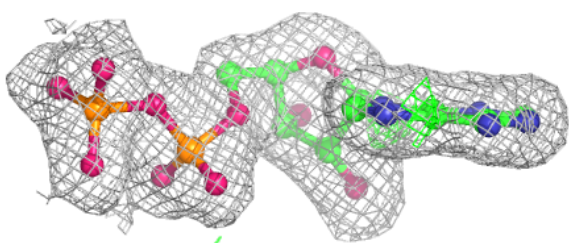
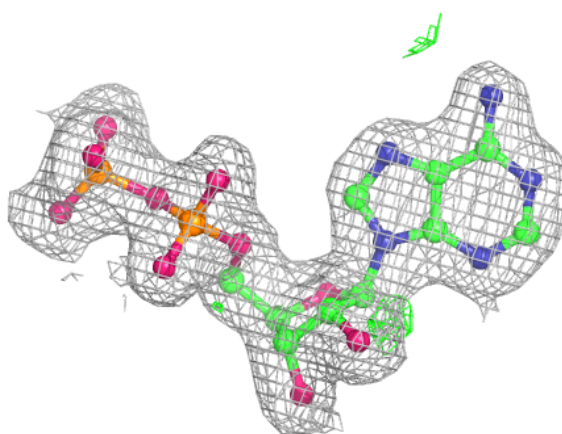


Electron density around PN4 A 1402:

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

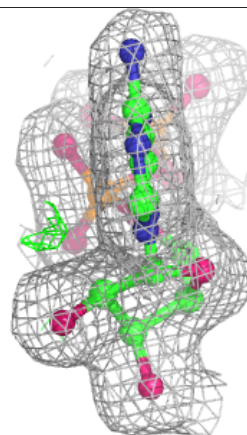
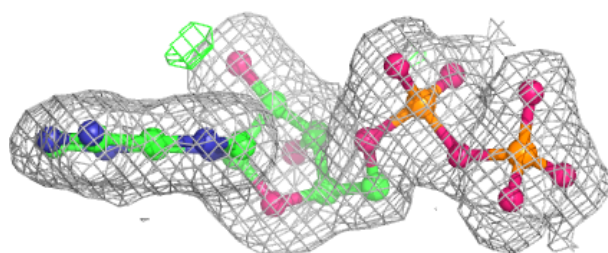
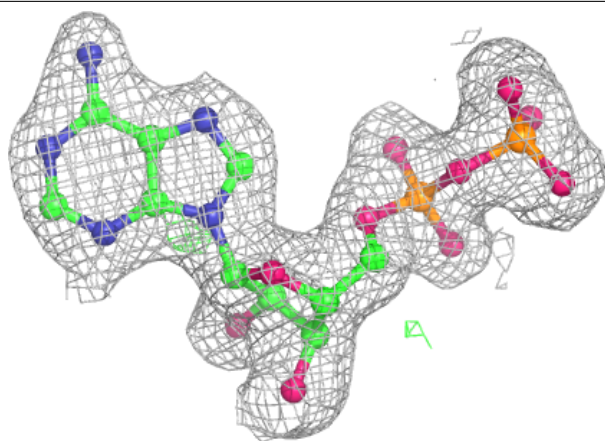
**Electron density around ADP G 1401:**

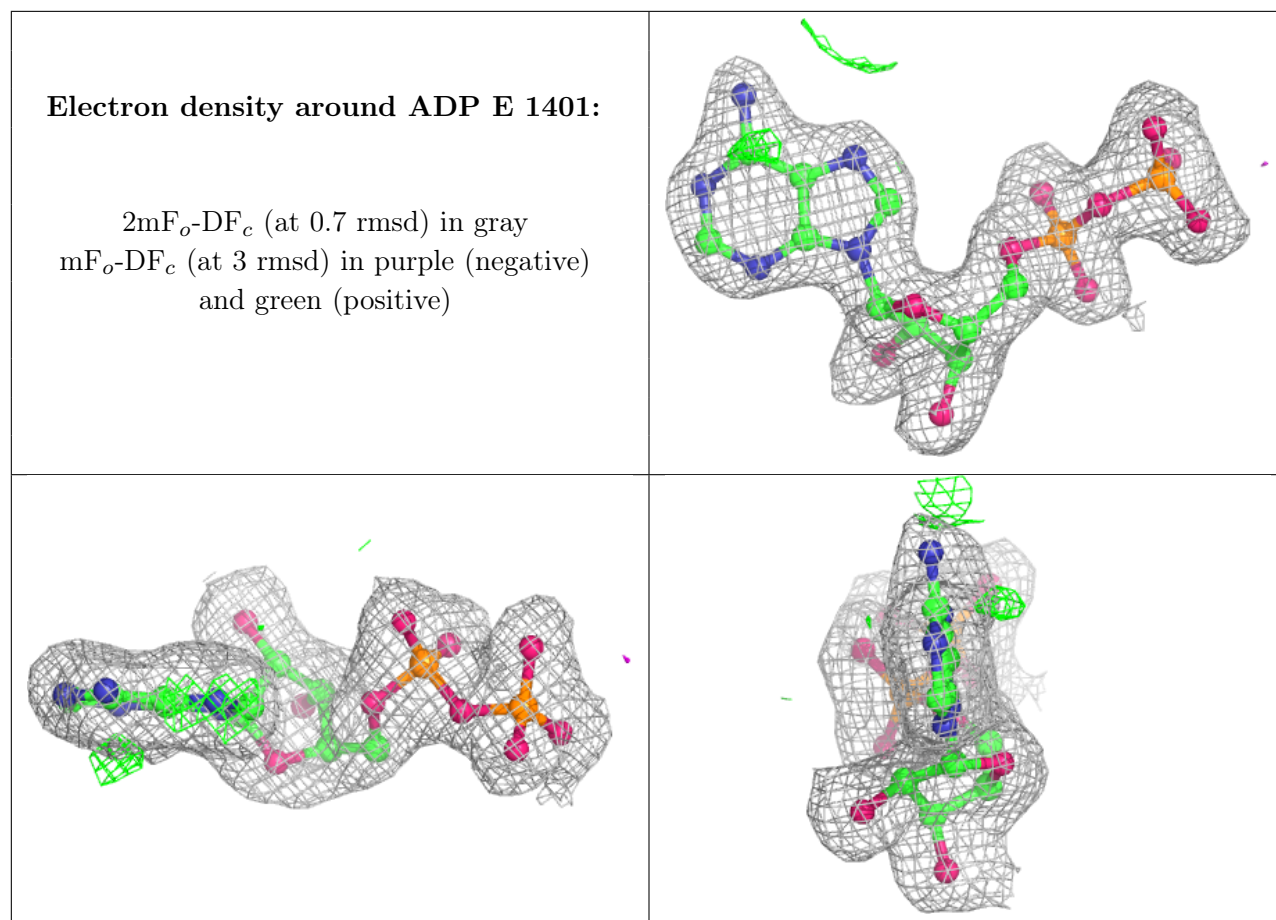
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 1401:

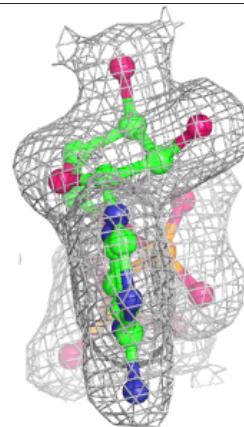
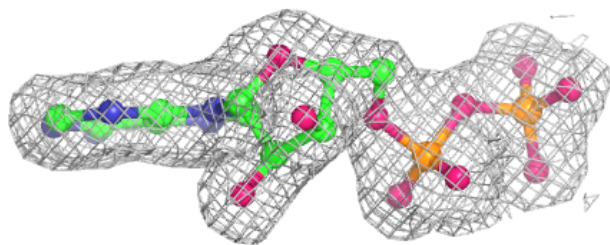
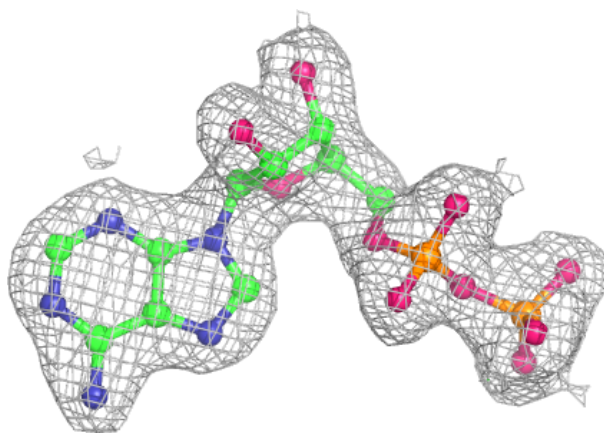
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





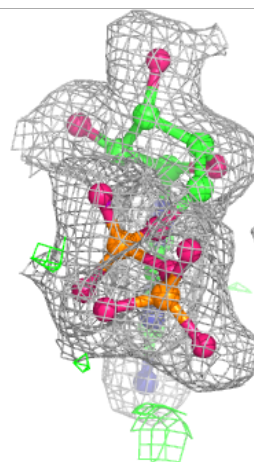
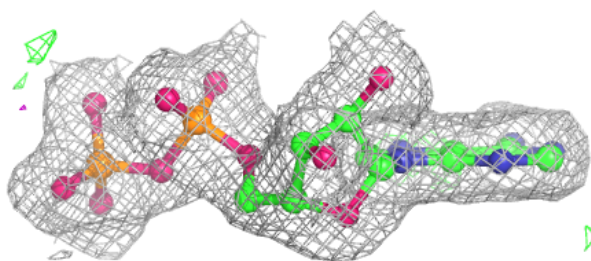
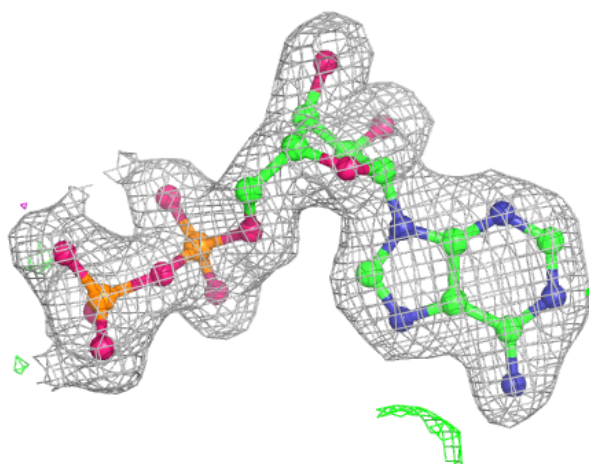
Electron density around ADP A 1401:

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



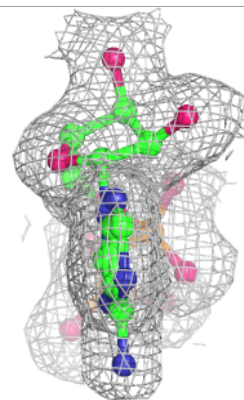
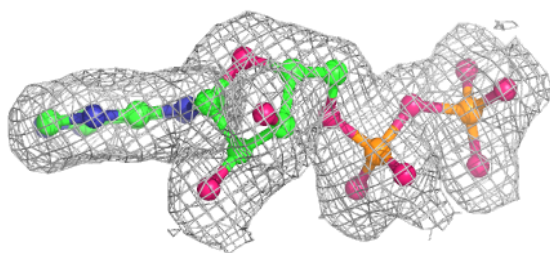
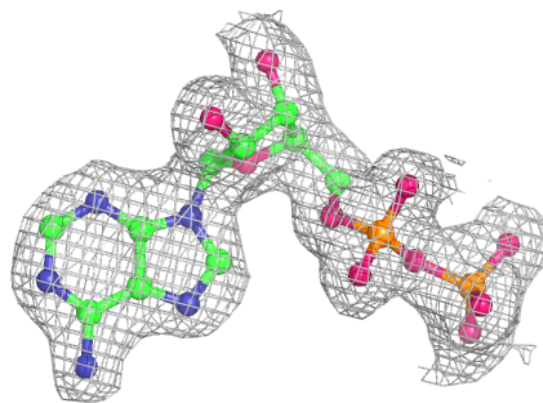
Electron density around ADP H 1401:

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

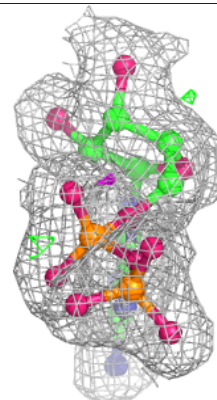
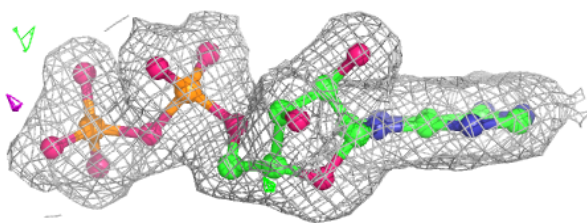
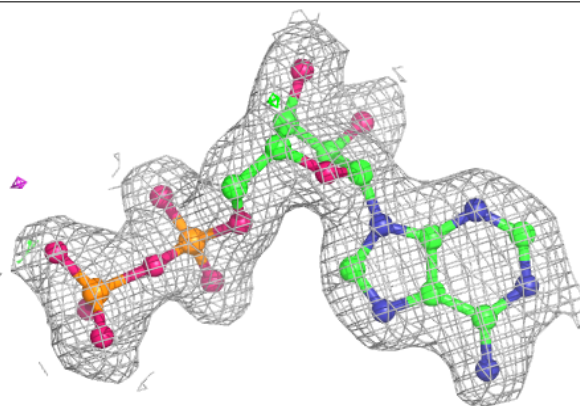


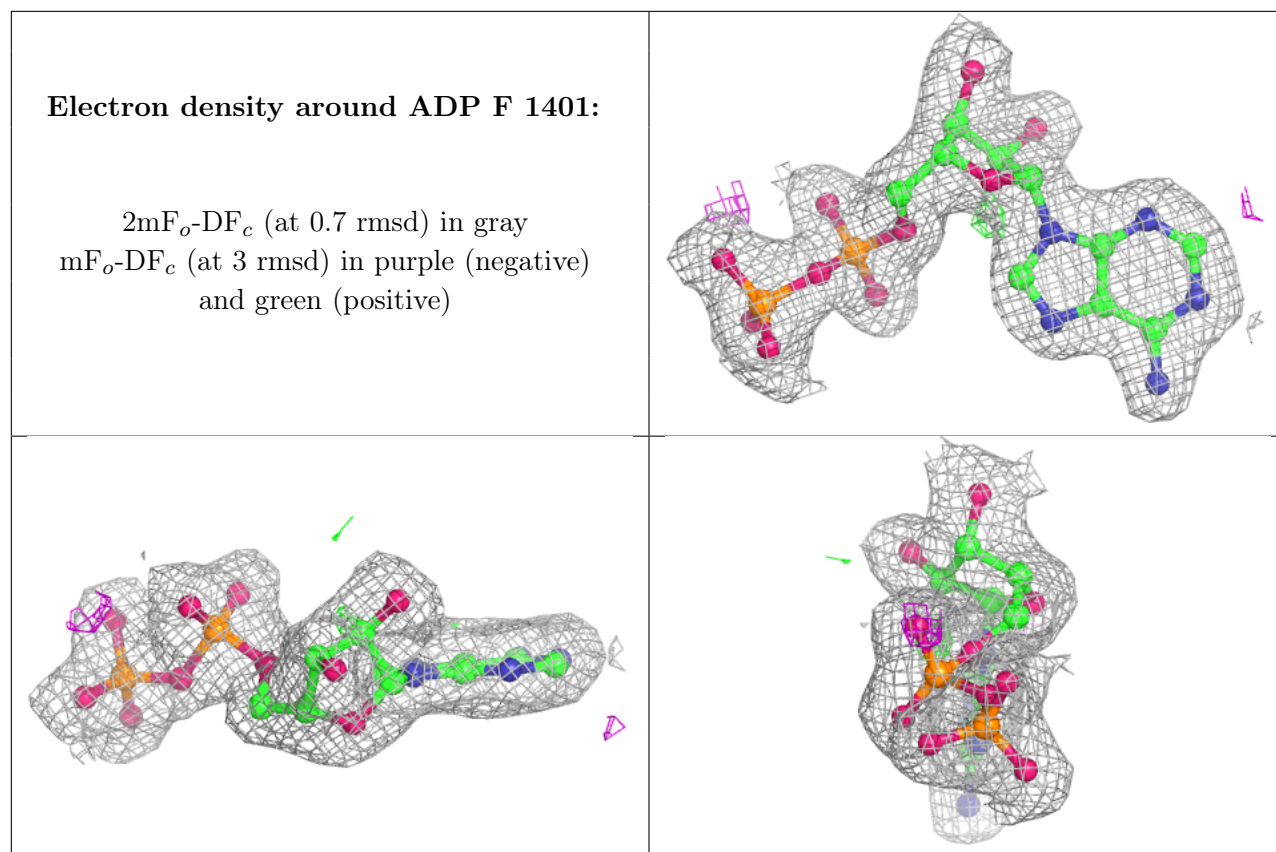
Electron density around ADP D 1401:

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

**Electron density around ADP C 1401:**

$2mF_o-DF_c$ (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.