Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 12:34 AM EST

PDB ID	:	4GI7
Title	:	Crystal structure of Klebsiella pneumoniae pantothenate kinase in complex with a pantothenate analogue
Authors	:	Li, B.; Tempel, W.; Smil, D.; Bolshan, Y.; Hong, B.S.; Park, H.W.; Structural Genomics Consortium (SGC)
Deposited on	:	2012-08-08
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

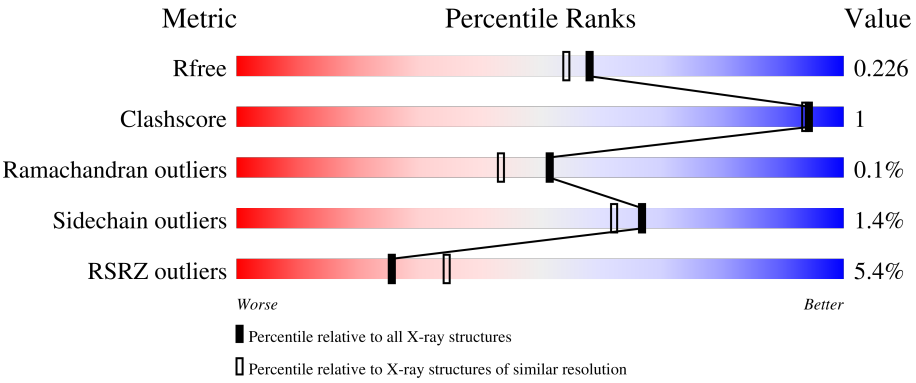
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	7% 89% · 7%
1	B	334	7% 88% · · 7%
1	C	334	4% 87% 5% 7%
1	D	334	2% 88% · 8%

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Mol	Chain	Length	Quality of chain
1	E	334	7% 89% 9%
1	F	334	5% 86% 6% 7%
1	G	334	3% 88% 8%
1	H	334	5% 85% 6% 9%

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	G	1408	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21291 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
1	A	309	Total	C	N	O	S	0	0	0
			2499	1600	431	461	7			
1	C	309	Total	C	N	O	S	0	0	0
			2499	1600	431	461	7			
1	B	309	Total	C	N	O	S	0	1	0
			2502	1602	431	462	7			
1	D	308	Total	C	N	O	S	0	0	0
			2491	1594	430	460	7			
1	E	304	Total	C	N	O	S	0	0	0
			2463	1578	426	453	6			
1	F	309	Total	C	N	O	S	0	0	0
			2499	1600	431	461	7			
1	G	308	Total	C	N	O	S	0	0	0
			2491	1594	430	460	7			
1	H	303	Total	C	N	O	S	0	0	0
			2452	1572	422	452	6			

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
F	990	SER	-	expression tag	UNP B5XYG3
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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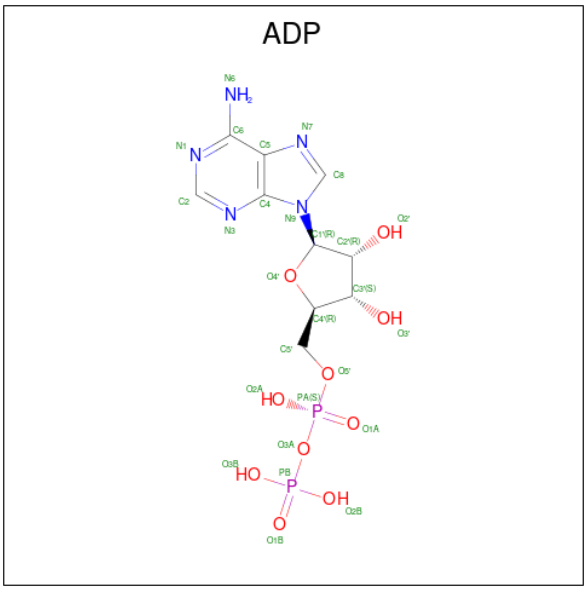
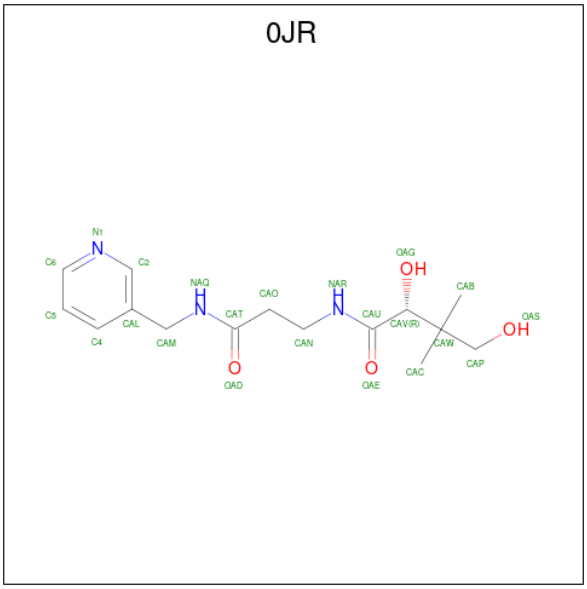
Chain	Residue	Modelled	Actual	Comment	Reference
H	996	LEU	-	expression tag	UNP B5XYG3
H	997	TYR	-	expression tag	UNP B5XYG3
H	998	PHE	-	expression tag	UNP B5XYG3
H	999	GLN	-	expression tag	UNP B5XYG3
H	1000	GLY	-	expression tag	UNP B5XYG3

- 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
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-[(pyridin-3-ylmethyl)amino]propyl}butanamide (three-letter code: 0JR) (formula: $C_{15}H_{23}N_3O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 15 3 4	0	0
3	C	1	Total C N O 22 15 3 4	0	0
3	B	1	Total C N O 22 15 3 4	0	0
3	D	1	Total C N O 22 15 3 4	0	1
3	F	1	Total C N O 22 15 3 4	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total X 4 4	0	0
4	C	7	Total X 7 7	0	0
4	B	5	Total X 5 5	0	0
4	D	8	Total X 8 8	0	0
4	E	3	Total X 3 3	0	0

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

- Molecule 5 is water.

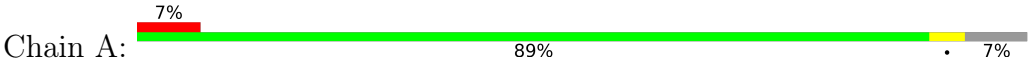
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	C	158	Total O 158 158	0	0
5	B	126	Total O 126 126	0	0
5	D	136	Total O 136 136	0	0
5	E	67	Total O 67 67	0	0
5	F	113	Total O 113 113	0	0
5	G	153	Total O 153 153	0	0
5	H	145	Total O 146 146	0	1

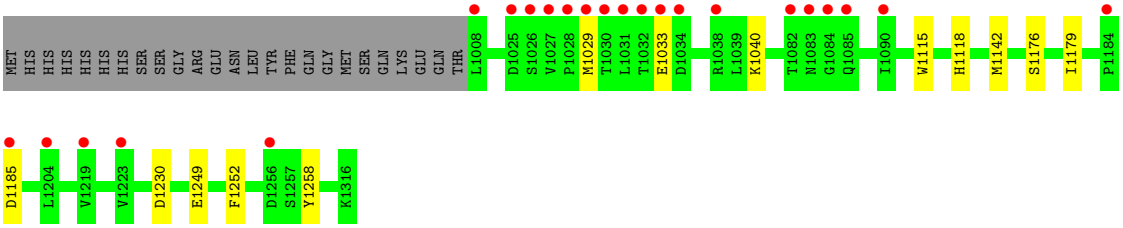
3 Residue-property plots (i)

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

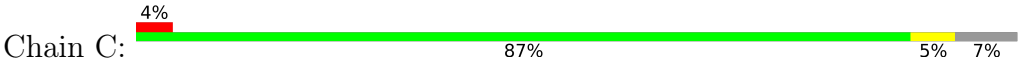
Chain A:

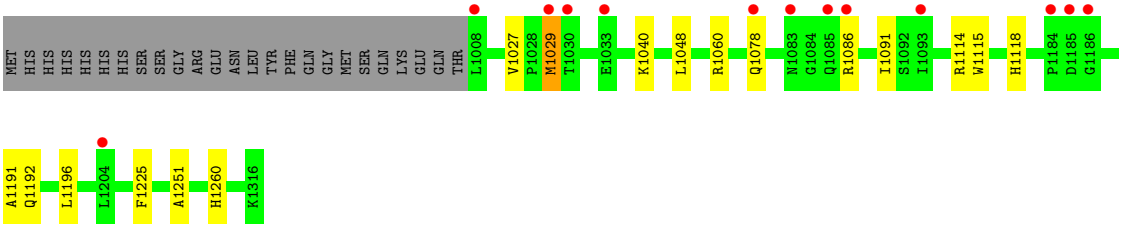




• Molecule 1: Pantothenate kinase

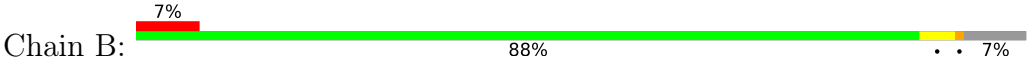
Chain C:

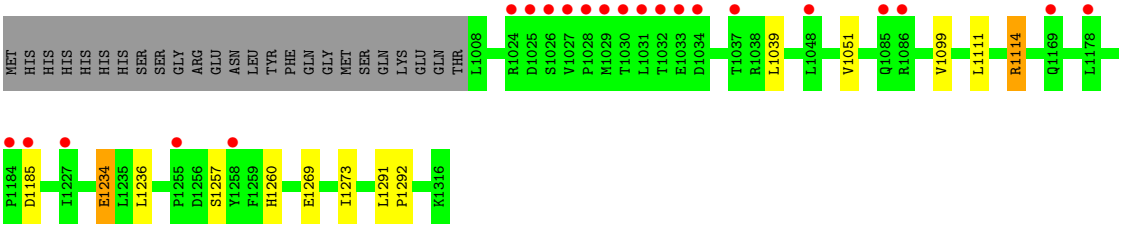




• Molecule 1: Pantothenate kinase

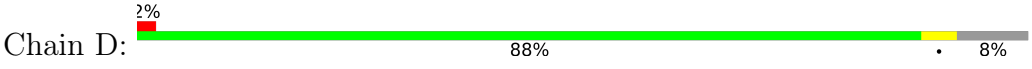
Chain B:

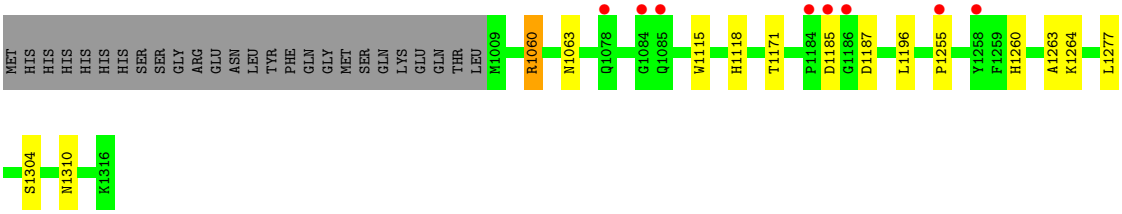




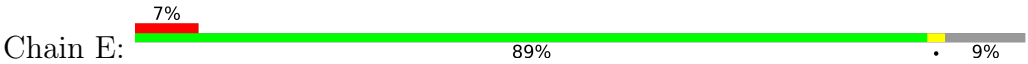
• Molecule 1: Pantothenate kinase

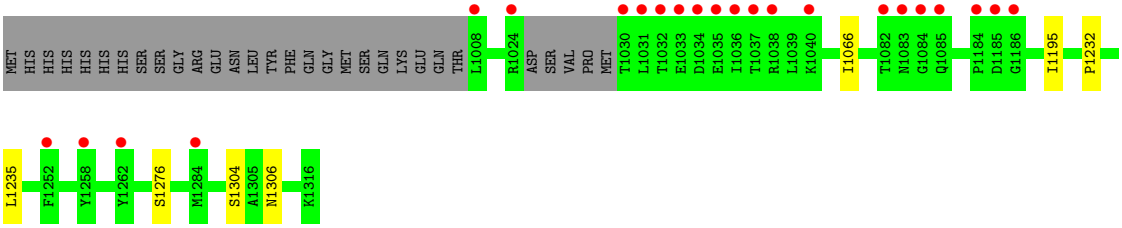
Chain D:



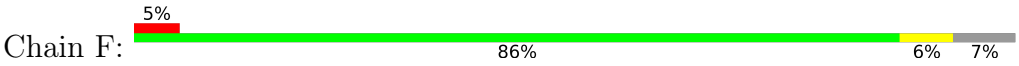


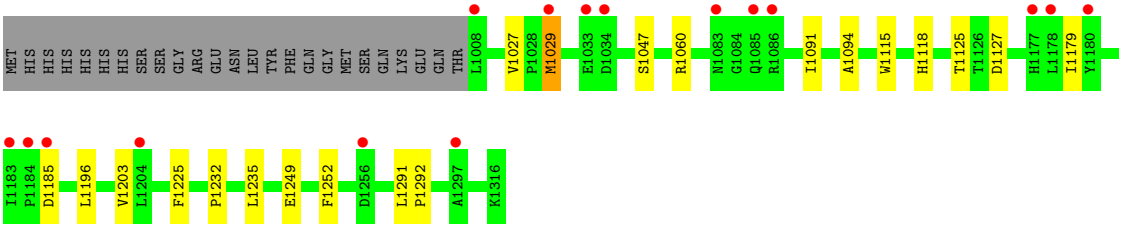
• Molecule 1: Pantothenate kinase



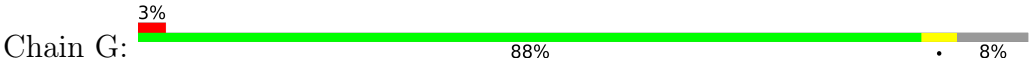


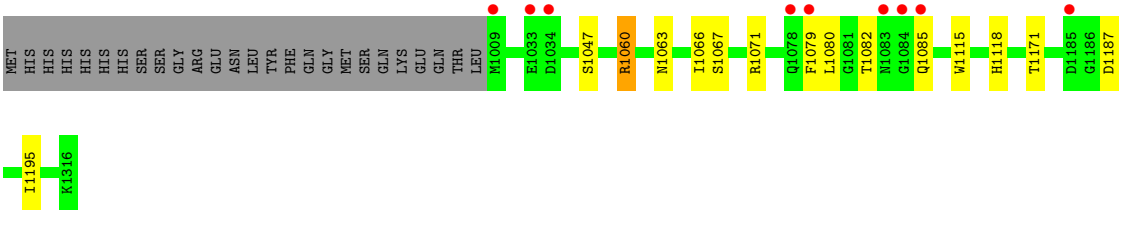
• Molecule 1: Pantothenate kinase



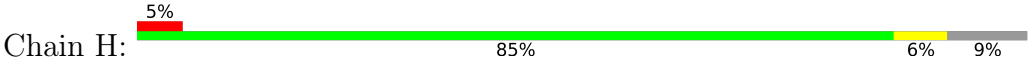


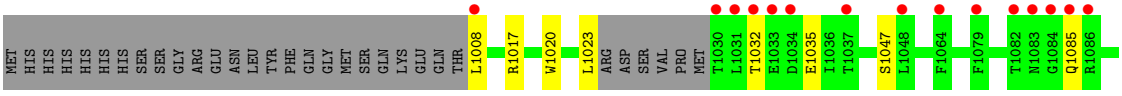
• Molecule 1: Pantothenate kinase

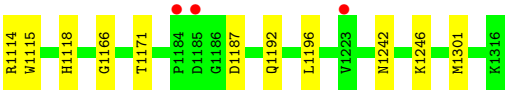




• Molecule 1: Pantothenate kinase






R1114
W1115
H1118
G1166
T1171
P1184
D1185
G1186
D1187
Q1192
L1196
V1223
N1242
K1246
M1301
K1316

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.93Å 130.94Å 193.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.68 – 1.95 39.68 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.68-1.95) 99.8 (39.68-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.220 0.194 , 0.226	Depositor DCC
R_{free} test set	11741 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21291	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 0JR, UNX, 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	0.51	0/2558	0.66	1/3471 (0.0%)
1	B	0.48	0/2564	0.64	0/3479
1	C	0.54	0/2558	0.71	3/3471 (0.1%)
1	D	0.53	0/2550	0.66	0/3460
1	E	0.46	0/2520	0.61	0/3417
1	F	0.52	0/2558	0.68	2/3471 (0.1%)
1	G	0.54	0/2550	0.69	0/3460
1	H	0.52	0/2509	0.66	1/3403 (0.0%)
All	All	0.51	0/20367	0.67	7/27632 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1029	MET	CB-CG-SD	6.19	130.98	112.40
1	A	1230	ASP	CB-CG-OD1	6.11	123.80	118.30
1	F	1029	MET	CB-CA-C	5.70	121.79	110.40
1	C	1029	MET	CB-CG-SD	5.69	129.47	112.40
1	C	1029	MET	CG-SD-CE	5.44	108.90	100.20
1	C	1114	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	H	1301	MET	CA-CB-CG	5.09	121.96	113.30

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	2500	5	0
1	B	2502	0	2506	6	0
1	C	2499	0	2500	9	0
1	D	2491	0	2489	7	0
1	E	2463	0	2465	2	0
1	F	2499	0	2501	10	0
1	G	2491	0	2489	9	0
1	H	2452	0	2452	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	22	0	23	1	0
3	B	22	0	23	0	0
3	C	22	0	23	0	0
3	D	22	0	7	1	0
3	F	22	0	7	0	0
4	A	4	0	0	0	0
4	B	5	0	0	0	0
4	C	7	0	0	0	0
4	D	8	0	0	0	0
4	E	3	0	0	0	0
4	F	7	0	0	0	0
4	G	7	0	0	0	0
4	H	4	0	0	0	0
5	A	125	0	0	1	0
5	B	126	0	0	1	0
5	C	158	0	0	1	0
5	D	136	0	0	0	0
5	E	67	0	0	0	0
5	F	113	0	0	0	0
5	G	153	0	0	0	0
5	H	146	0	0	0	0
All	All	21291	0	20081	54	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 1.

All (54) 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:1060:ARG:HH12	1:D:1063:ASN:HD22	1.35	0.75
1:C:1078:GLN:HG3	5:C:1585:HOH:O	1.96	0.65
1:F:1125:THR:HG22	1:F:1127:ASP:H	1.65	0.61
1:G:1060:ARG:HH12	1:G:1063:ASN:HD22	1.48	0.61
1:G:1079:PHE:CZ	1:H:1023:LEU:HB3	2.37	0.59
1:G:1067:SER:OG	1:G:1071:ARG:NH2	2.36	0.58
1:C:1040:LYS:CE	1:C:1048:LEU:HD11	2.34	0.57
1:H:1020:TRP:O	1:H:1023:LEU:HG	2.04	0.56
1:F:1232:PRO:HD2	1:F:1235:LEU:HD12	1.87	0.56
1:C:1040:LYS:HE3	1:C:1048:LEU:HD11	1.87	0.55
1:G:1115:TRP:HB2	1:G:1118:HIS:CE1	2.43	0.54
1:D:1115:TRP:HB2	1:D:1118:HIS:CE1	2.43	0.54
1:C:1115:TRP:HB2	1:C:1118:HIS:CE1	2.45	0.52
1:H:1115:TRP:HB2	1:H:1118:HIS:CE1	2.45	0.52
1:B:1234:GLU:HG3	5:B:1583:HOH:O	2.11	0.50
1:F:1027:VAL:HG23	1:F:1029:MET:HG3	1.94	0.50
1:A:1142:MET:HB2	5:A:1608:HOH:O	2.11	0.49
1:E:1066:ILE:HD13	1:E:1195:ILE:HD11	1.94	0.49
1:G:1079:PHE:CE1	1:H:1023:LEU:HB3	2.48	0.49
1:H:1085:GLN:HG3	1:H:1166:GLY:O	2.14	0.47
1:F:1115:TRP:HB2	1:F:1118:HIS:CE1	2.49	0.47
1:G:1080:LEU:HD23	1:H:1023:LEU:HD22	1.97	0.47
1:A:1115:TRP:HB2	1:A:1118:HIS:CE1	2.50	0.47
1:H:1171:THR:CG2	1:H:1187:ASP:HB3	2.45	0.46
1:G:1080:LEU:HA	1:H:1023:LEU:HD22	1.97	0.46
1:D:1060:ARG:HH12	1:D:1063:ASN:ND2	2.10	0.45
1:E:1232:PRO:HD2	1:E:1235:LEU:HD12	1.98	0.45
1:B:1111:LEU:O	1:B:1114:ARG:HD2	2.17	0.45
1:D:1171:THR:CG2	1:D:1187:ASP:HB3	2.47	0.45
1:F:1185:ASP:N	1:F:1185:ASP:OD1	2.49	0.45
1:D:1277:LEU:HD13	3:D:1402[A]:0JR:H4	1.98	0.44
1:G:1171:THR:HG23	1:G:1187:ASP:HB3	1.99	0.44
1:A:1258:TYR:HE2	3:A:1402:0JR:C6	2.30	0.43
1:B:1039:LEU:HD13	1:B:1051:VAL:HG11	1.99	0.43
1:A:1249:GLU:HA	1:A:1252:PHE:CE2	2.53	0.43
1:D:1304:SER:HB2	1:D:1310:ASN:ND2	2.34	0.43
1:C:1027:VAL:HG23	1:C:1029:MET:HG3	2.00	0.43
1:F:1094:ALA:HB2	1:F:1203:VAL:HG22	2.00	0.42
1:F:1291:LEU:N	1:F:1292:PRO:CD	2.82	0.42
1:C:1091:ILE:HA	1:C:1225:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1242:ASN:HD21	1:H:1246:LYS:HE3	1.85	0.42
1:B:1269:GLU:O	1:B:1273:ILE:HG12	2.20	0.42
1:C:1251:ALA:HB1	1:C:1260:HIS:HA	2.02	0.41
1:C:1191:ALA:O	1:C:1192:GLN:C	2.58	0.41
1:F:1094:ALA:HB2	1:F:1203:VAL:CG2	2.50	0.41
1:D:1255:PRO:HA	1:D:1260:HIS:CE1	2.55	0.41
1:F:1249:GLU:HA	1:F:1252:PHE:CD2	2.55	0.41
1:B:1099:VAL:HG23	1:B:1236:LEU:HD21	2.03	0.41
1:C:1086:ARG:NH1	1:C:1192:GLN:O	2.51	0.41
1:A:1176:SER:HB3	1:A:1179:ILE:HG12	2.03	0.41
1:B:1291:LEU:N	1:B:1292:PRO:CD	2.83	0.40
1:F:1091:ILE:HA	1:F:1225:PHE:O	2.21	0.40
1:H:1035:GLU:OE1	1:H:1114:ARG:CD	2.69	0.40
1:G:1066:ILE:HD13	1:G:1195:ILE:HD11	2.04	0.40

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%)	302 (98%)	5 (2%)	0	100	100
1	B	308/334 (92%)	300 (97%)	8 (3%)	0	100	100
1	C	307/334 (92%)	301 (98%)	6 (2%)	0	100	100
1	D	306/334 (92%)	300 (98%)	5 (2%)	1 (0%)	41	30
1	E	300/334 (90%)	295 (98%)	5 (2%)	0	100	100
1	F	307/334 (92%)	302 (98%)	5 (2%)	0	100	100
1	G	306/334 (92%)	297 (97%)	8 (3%)	1 (0%)	41	30
1	H	299/334 (90%)	292 (98%)	7 (2%)	0	100	100
All	All	2440/2672 (91%)	2389 (98%)	49 (2%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1263	ALA
1	G	1085	GLN

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%)	274 (99%)	4 (1%)	67	62
1	B	279/301 (93%)	274 (98%)	5 (2%)	59	53
1	C	278/301 (92%)	276 (99%)	2 (1%)	84	82
1	D	277/301 (92%)	273 (99%)	4 (1%)	67	62
1	E	273/301 (91%)	270 (99%)	3 (1%)	73	71
1	F	278/301 (92%)	274 (99%)	4 (1%)	67	62
1	G	277/301 (92%)	274 (99%)	3 (1%)	73	71
1	H	272/301 (90%)	266 (98%)	6 (2%)	52	44
All	All	2212/2408 (92%)	2181 (99%)	31 (1%)	67	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	MET
1	A	1033	GLU
1	A	1040	LYS
1	A	1185	ASP
1	C	1060	ARG
1	C	1196	LEU
1	B	1114	ARG
1	B	1185	ASP
1	B	1234	GLU
1	B	1257	SER
1	B	1260	HIS
1	D	1060	ARG

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Mol	Chain	Res	Type
1	D	1185	ASP
1	D	1196	LEU
1	D	1264	LYS
1	E	1276	SER
1	E	1304	SER
1	E	1306	ASN
1	F	1047	SER
1	F	1060	ARG
1	F	1179	ILE
1	F	1196	LEU
1	G	1047	SER
1	G	1060	ARG
1	G	1082	THR
1	H	1008	LEU
1	H	1017	ARG
1	H	1032	THR
1	H	1047	SER
1	H	1192	GLN
1	H	1196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1073	GLN
1	A	1149	GLN
1	A	1205	GLN
1	C	1014	GLN
1	C	1085	GLN
1	C	1205	GLN
1	C	1311	GLN
1	B	1073	GLN
1	B	1085	GLN
1	B	1311	GLN
1	D	1063	ASN
1	D	1205	GLN
1	D	1260	HIS
1	D	1311	GLN
1	E	1073	GLN
1	E	1205	GLN
1	F	1014	GLN
1	F	1205	GLN
1	F	1311	GLN

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Mol	Chain	Res	Type
1	G	1063	ASN
1	G	1073	GLN
1	G	1078	GLN
1	G	1169	GLN
1	G	1205	GLN
1	H	1063	ASN
1	H	1205	GLN
1	H	1310	ASN
1	H	1311	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 58 ligands modelled in this entry, 45 are unknown - leaving 13 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	ADP	F	1401	-	24,29,29	1.01	1 (4%)	29,45,45	1.06	2 (6%)
2	ADP	E	1401	-	24,29,29	0.93	0	29,45,45	1.34	3 (10%)
2	ADP	C	1401	-	24,29,29	1.02	1 (4%)	29,45,45	1.43	3 (10%)
3	0JR	C	1402	-	20,22,22	1.73	4 (20%)	27,29,29	1.31	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	H	1401	-	24,29,29	1.05	2 (8%)	29,45,45	1.44	3 (10%)
2	ADP	G	1401	-	24,29,29	1.04	3 (12%)	29,45,45	1.51	6 (20%)
3	0JR	B	1402	-	20,22,22	1.59	3 (15%)	27,29,29	1.05	1 (3%)
2	ADP	D	1401	-	24,29,29	1.06	2 (8%)	29,45,45	1.34	4 (13%)
2	ADP	A	1401	-	24,29,29	1.18	1 (4%)	29,45,45	1.28	1 (3%)
2	ADP	B	1401	-	24,29,29	1.06	1 (4%)	29,45,45	1.31	5 (17%)
3	0JR	A	1402	-	20,22,22	1.59	3 (15%)	27,29,29	1.13	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	F	1401	-	-	1/12/32/32	0/3/3/3
2	ADP	E	1401	-	-	1/12/32/32	0/3/3/3
2	ADP	C	1401	-	-	1/12/32/32	0/3/3/3
3	0JR	C	1402	-	-	6/24/24/24	0/1/1/1
2	ADP	H	1401	-	-	1/12/32/32	0/3/3/3
2	ADP	G	1401	-	-	1/12/32/32	0/3/3/3
3	0JR	B	1402	-	-	2/24/24/24	0/1/1/1
2	ADP	D	1401	-	-	2/12/32/32	0/3/3/3
2	ADP	A	1401	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1401	-	-	0/12/32/32	0/3/3/3
3	0JR	A	1402	-	-	2/24/24/24	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	0JR	CAM-CAL	-4.89	1.40	1.51
3	A	1402	0JR	CAM-CAL	-4.87	1.40	1.51
3	C	1402	0JR	C2-N1	4.18	1.43	1.34
3	C	1402	0JR	CAM-CAL	-3.93	1.42	1.51
2	A	1401	ADP	C2-N3	3.25	1.37	1.32
3	A	1402	0JR	C2-N1	3.21	1.41	1.34
3	B	1402	0JR	C2-N1	3.16	1.41	1.34
3	C	1402	0JR	C6-N1	2.83	1.42	1.33
2	B	1401	ADP	C5-C4	2.44	1.47	1.40
3	B	1402	0JR	C6-N1	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1401	ADP	C5-C4	2.33	1.47	1.40
2	D	1401	ADP	C5-C4	2.33	1.47	1.40
2	F	1401	ADP	C5-C4	2.27	1.46	1.40
2	G	1401	ADP	C5-C4	2.22	1.46	1.40
2	D	1401	ADP	C2-N3	2.17	1.35	1.32
2	H	1401	ADP	C5-C4	2.10	1.46	1.40
2	G	1401	ADP	C2-N3	2.08	1.35	1.32
2	G	1401	ADP	C2'-C1'	-2.08	1.50	1.53
2	H	1401	ADP	C2'-C1'	-2.06	1.50	1.53
3	A	1402	0JR	C6-N1	2.03	1.39	1.33
3	C	1402	0JR	CAM-NAQ	2.02	1.49	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1401	ADP	N3-C2-N1	-4.61	121.47	128.68
2	E	1401	ADP	N3-C2-N1	-4.34	121.90	128.68
2	C	1401	ADP	N3-C2-N1	-4.19	122.13	128.68
2	A	1401	ADP	N3-C2-N1	-4.01	122.42	128.68
2	G	1401	ADP	N3-C2-N1	-3.55	123.13	128.68
2	B	1401	ADP	N3-C2-N1	-3.48	123.24	128.68
2	D	1401	ADP	N3-C2-N1	-3.28	123.56	128.68
2	C	1401	ADP	N6-C6-N1	3.22	125.26	118.57
3	C	1402	0JR	CAC-CAW-CAV	3.13	114.25	108.82
3	C	1402	0JR	CAM-NAQ-CAT	2.95	126.93	122.34
2	G	1401	ADP	N6-C6-N1	2.91	124.62	118.57
3	C	1402	0JR	OAS-CAP-CAW	-2.85	107.86	112.96
3	B	1402	0JR	OAS-CAP-CAW	-2.76	108.01	112.96
3	A	1402	0JR	OAS-CAP-CAW	-2.75	108.03	112.96
3	A	1402	0JR	CAB-CAW-CAP	-2.72	103.91	108.90
2	F	1401	ADP	N6-C6-N1	2.54	123.84	118.57
2	C	1401	ADP	C2-N1-C6	2.43	122.92	118.75
2	D	1401	ADP	C2-N1-C6	2.43	122.91	118.75
2	F	1401	ADP	N3-C2-N1	-2.40	124.92	128.68
2	B	1401	ADP	O2B-PB-O3A	-2.40	96.60	104.64
2	G	1401	ADP	O3B-PB-O1B	2.38	120.00	110.68
2	H	1401	ADP	C2-N1-C6	2.35	122.77	118.75
2	G	1401	ADP	O3'-C3'-C4'	-2.28	104.46	111.05
2	G	1401	ADP	C5-C6-N6	-2.25	116.93	120.35
2	H	1401	ADP	O2B-PB-O3A	-2.18	97.34	104.64
2	B	1401	ADP	O3B-PB-O1B	2.17	119.18	110.68
2	D	1401	ADP	N6-C6-N1	2.16	123.06	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1401	ADP	N6-C6-N1	2.16	123.06	118.57
2	D	1401	ADP	O3B-PB-O2B	2.15	115.84	107.64
2	B	1401	ADP	N6-C6-N1	2.12	122.97	118.57
2	G	1401	ADP	O2B-PB-O1B	2.11	118.94	110.68
2	E	1401	ADP	C2-N1-C6	2.09	122.33	118.75
2	B	1401	ADP	O2B-PB-O1B	2.09	118.87	110.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	ADP	PA-O3A-PB-O2B
2	D	1401	ADP	PA-O3A-PB-O2B
2	E	1401	ADP	PA-O3A-PB-O2B
2	G	1401	ADP	PA-O3A-PB-O2B
3	C	1402	0JR	OAS-CAP-CAW-CAV
3	C	1402	0JR	OAS-CAP-CAW-CAB
3	C	1402	0JR	OAS-CAP-CAW-CAC
3	C	1402	0JR	CAL-CAM-NAQ-CAT
2	D	1401	ADP	PA-O3A-PB-O1B
2	C	1401	ADP	PA-O3A-PB-O2B
3	B	1402	0JR	OAS-CAP-CAW-CAB
3	B	1402	0JR	OAS-CAP-CAW-CAC
3	C	1402	0JR	CAN-CAO-CAT-OAD
2	A	1401	ADP	PA-O3A-PB-O1B
3	A	1402	0JR	CAN-CAO-CAT-OAD
2	F	1401	ADP	PA-O3A-PB-O2B
2	H	1401	ADP	PA-O3A-PB-O2B
3	A	1402	0JR	CAN-CAO-CAT-NAQ
3	C	1402	0JR	CAN-CAO-CAT-NAQ

There are no ring outliers.

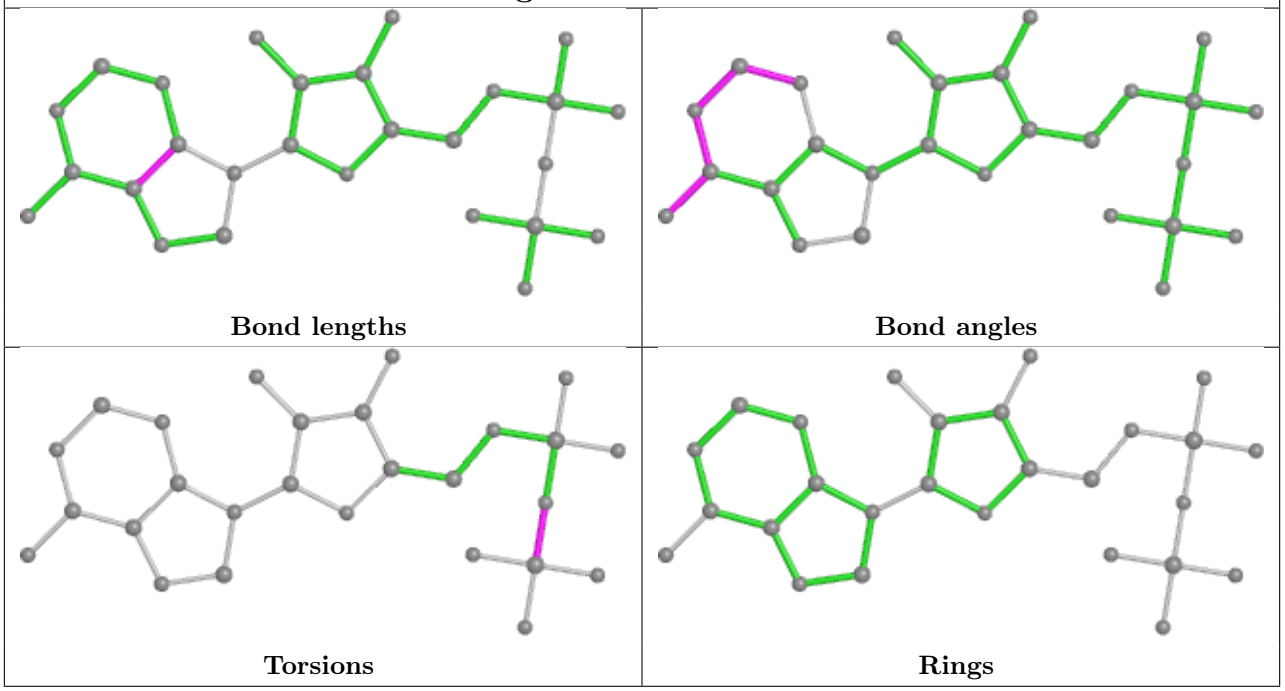
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	0JR	1	0

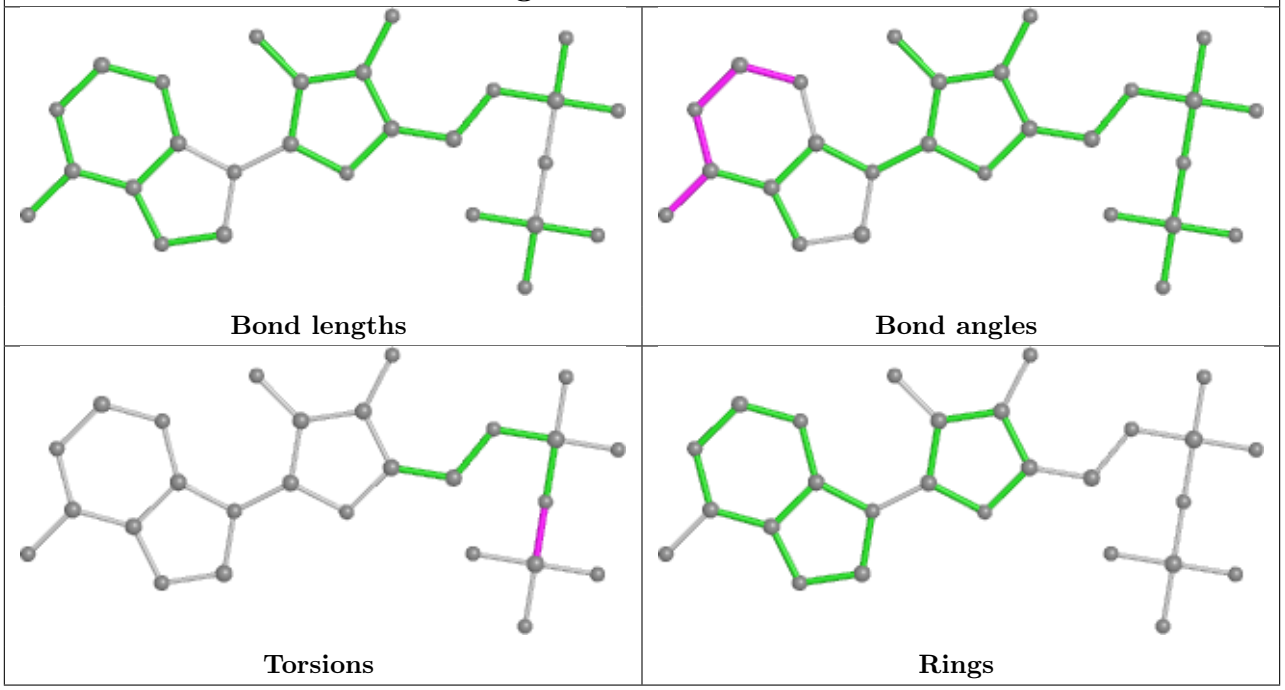
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

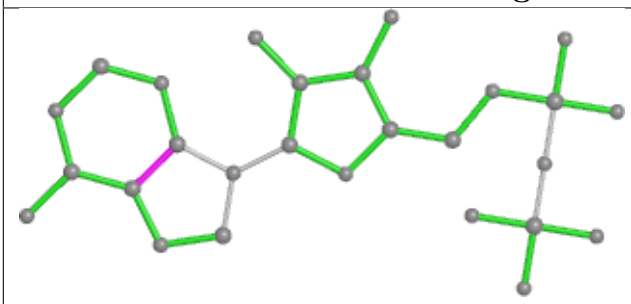
Ligand ADP F 1401



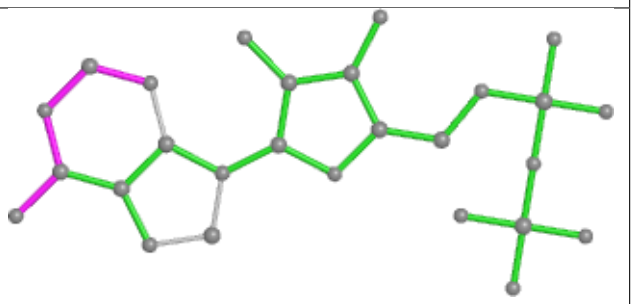
Ligand ADP E 1401



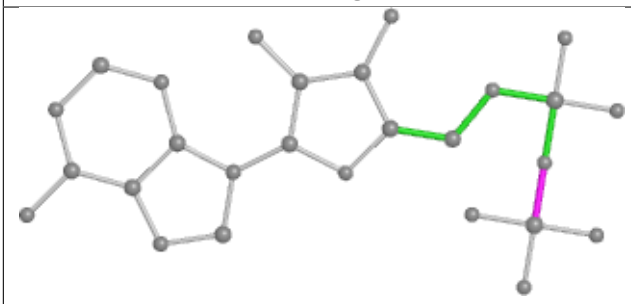
Ligand ADP C 1401



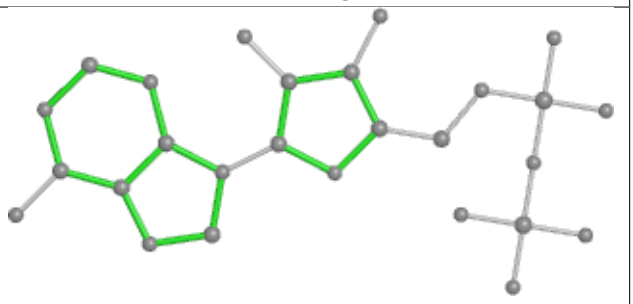
Bond lengths



Bond angles

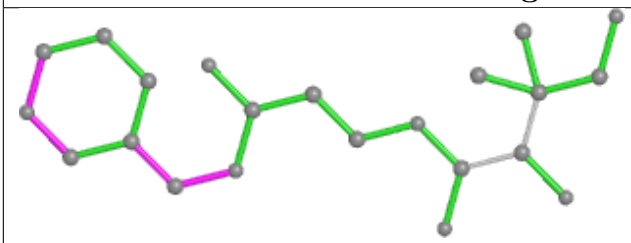


Torsions

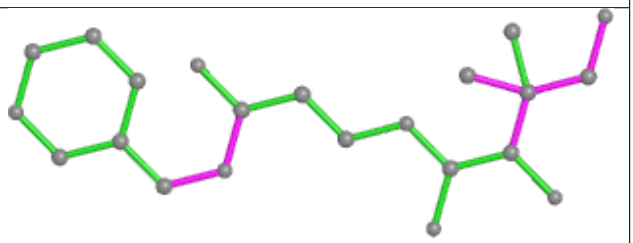


Rings

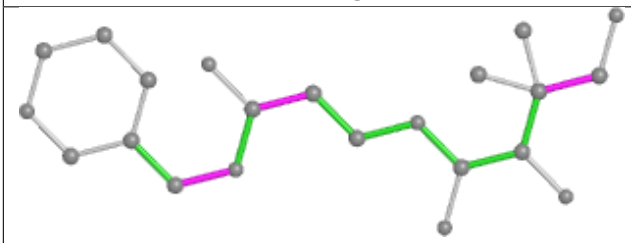
Ligand 0JR C 1402



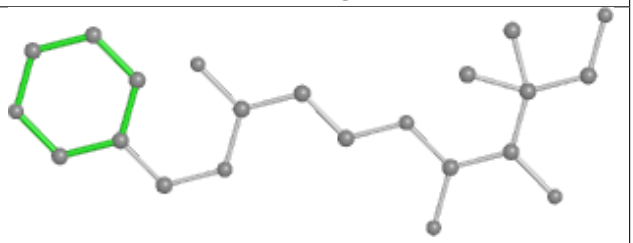
Bond lengths



Bond angles

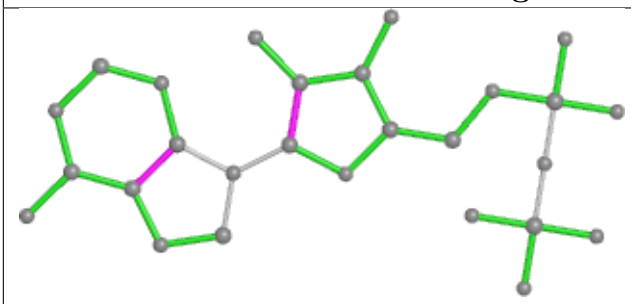


Torsions

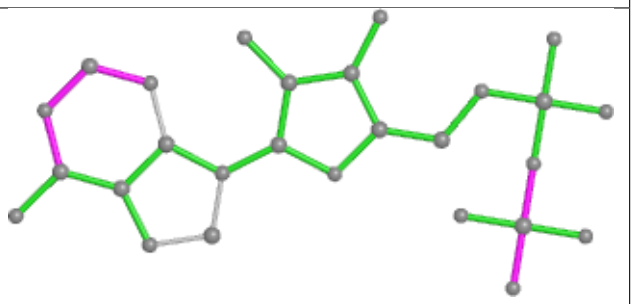


Rings

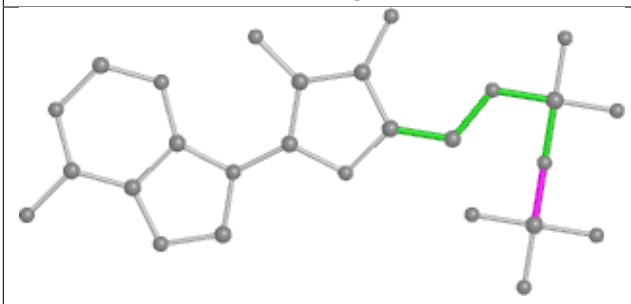
Ligand ADP H 1401



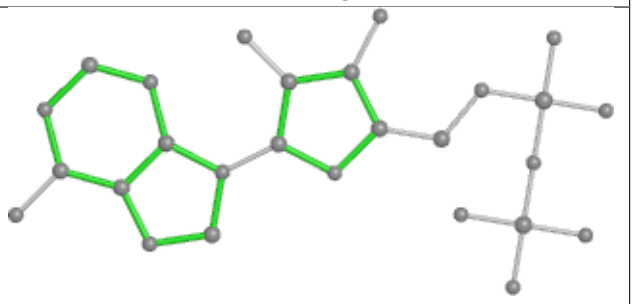
Bond lengths



Bond angles

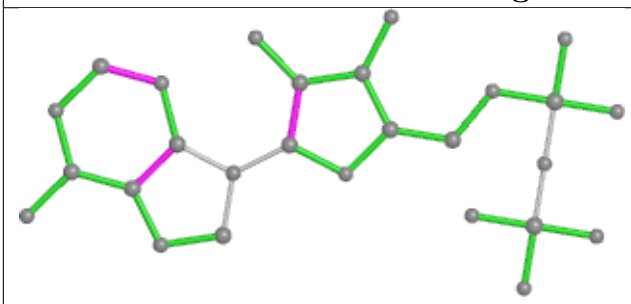


Torsions

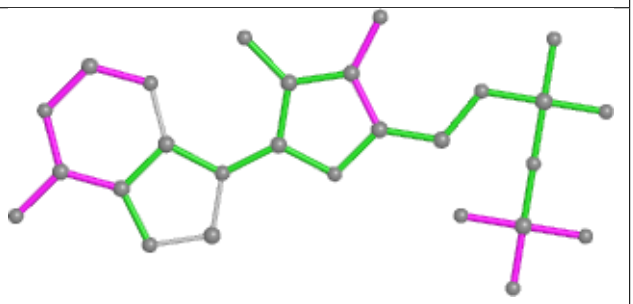


Rings

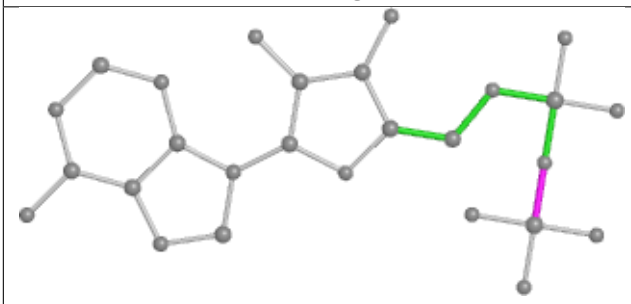
Ligand ADP G 1401



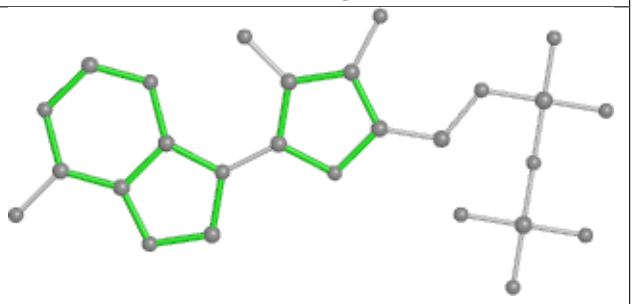
Bond lengths



Bond angles

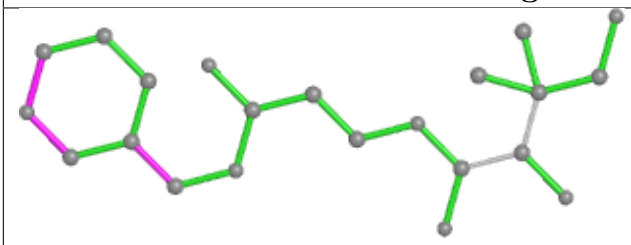


Torsions

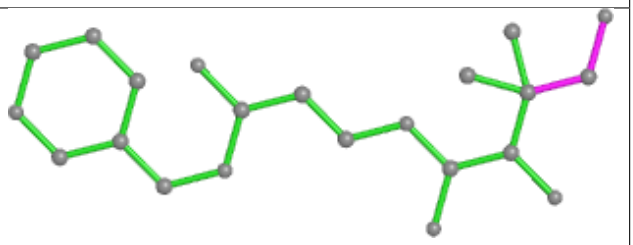


Rings

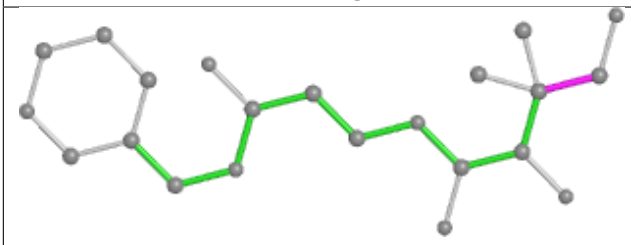
Ligand 0JR B 1402



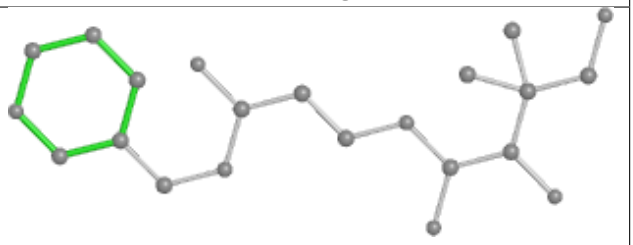
Bond lengths



Bond angles

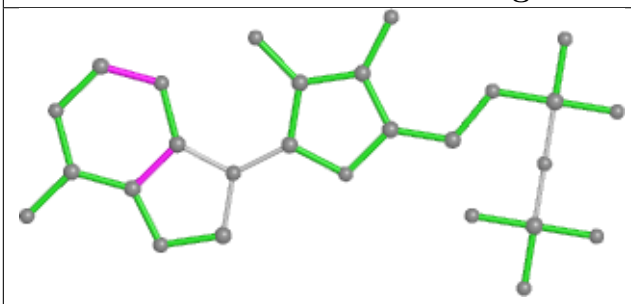


Torsions

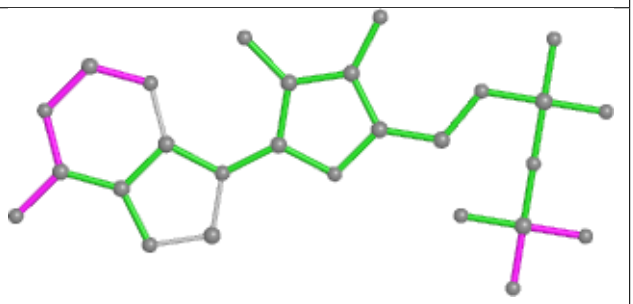


Rings

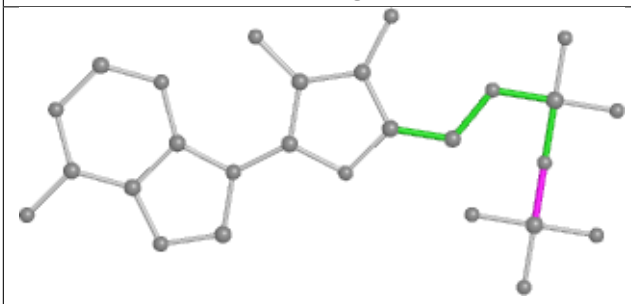
Ligand ADP D 1401



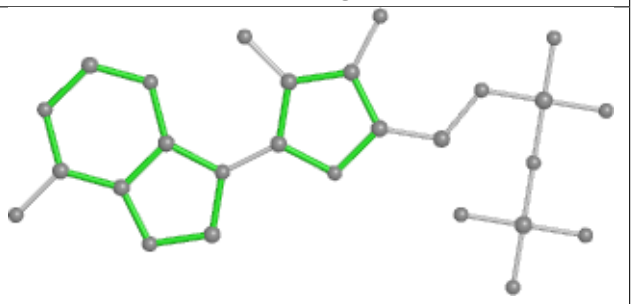
Bond lengths



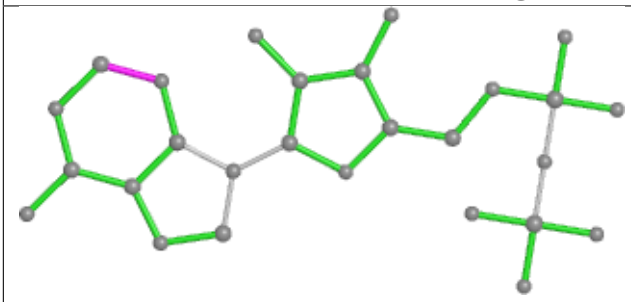
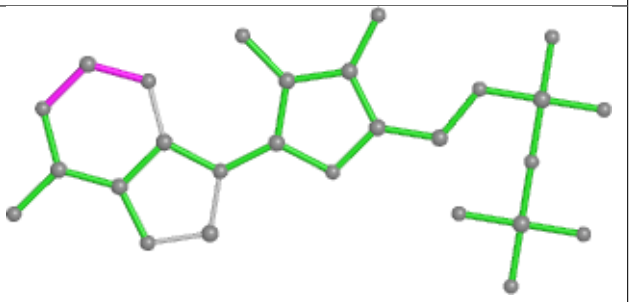
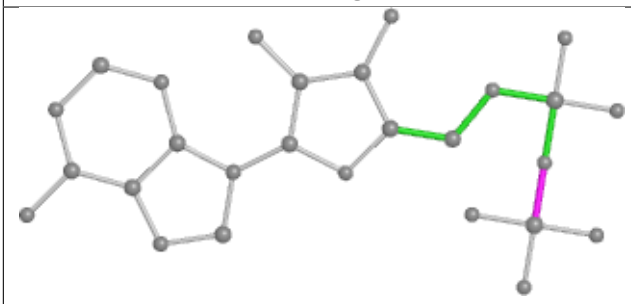
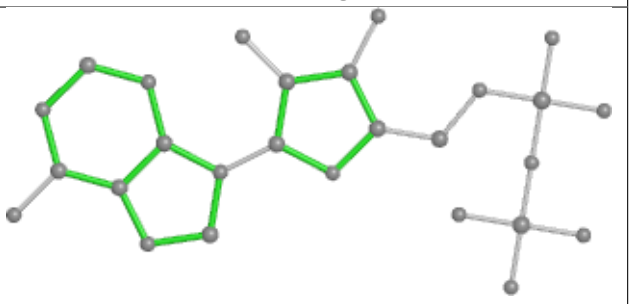
Bond angles

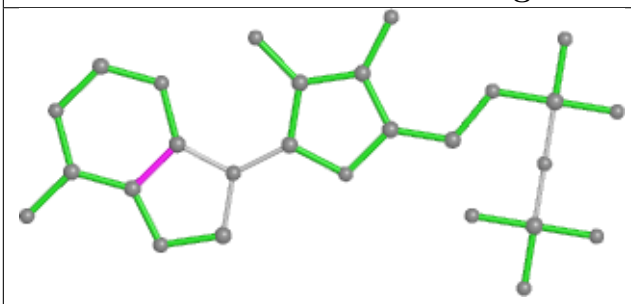
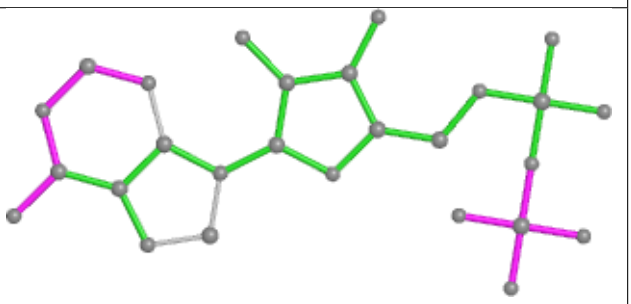
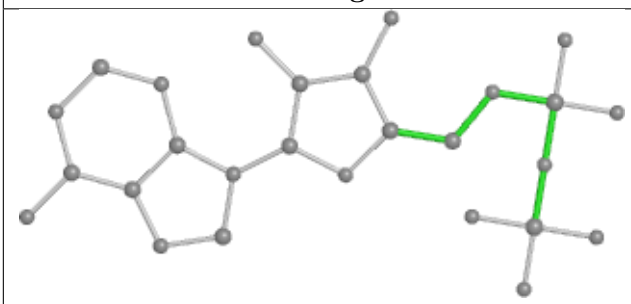
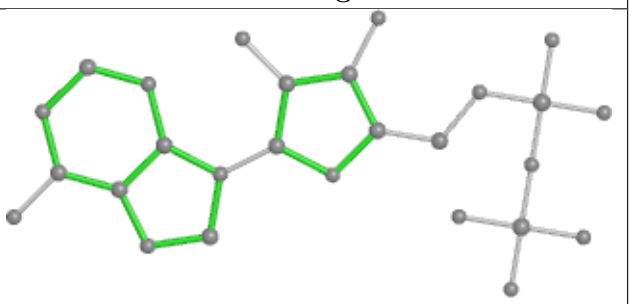


Torsions

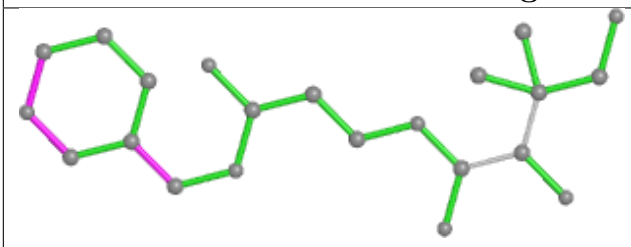


Rings

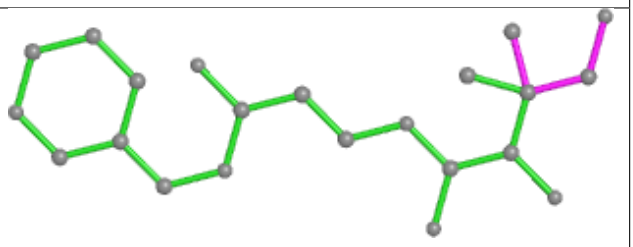
Ligand ADP A 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

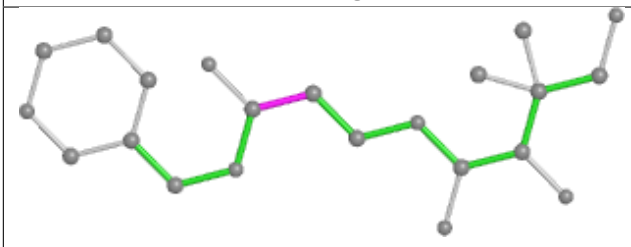
Ligand 0JR A 1402



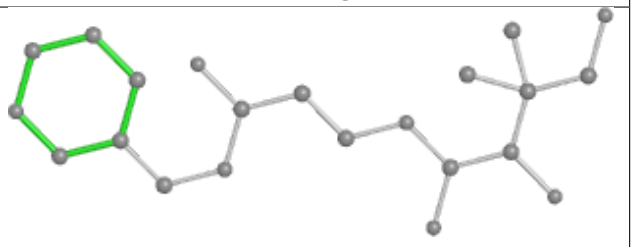
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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%)	0.24	23 (7%)	14	22	17, 28, 63, 110	0
1	B	309/334 (92%)	0.29	22 (7%)	16	24	19, 33, 71, 95	0
1	C	309/334 (92%)	0.12	13 (4%)	36	45	16, 27, 49, 66	0
1	D	308/334 (92%)	0.13	8 (2%)	56	65	16, 28, 54, 71	0
1	E	304/334 (91%)	0.45	23 (7%)	13	21	21, 38, 64, 94	0
1	F	309/334 (92%)	0.16	16 (5%)	27	37	17, 29, 57, 77	0
1	G	308/334 (92%)	0.07	9 (2%)	51	60	17, 27, 48, 86	0
1	H	303/334 (90%)	0.17	18 (5%)	22	30	17, 28, 58, 77	0
All	All	2459/2672 (92%)	0.20	132 (5%)	25	34	16, 29, 60, 110	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1026	SER	8.9
1	A	1027	VAL	8.7
1	B	1026	SER	8.0
1	G	1084	GLY	5.7
1	A	1028	PRO	5.6
1	B	1027	VAL	5.5
1	H	1030	THR	5.5
1	B	1025	ASP	5.3
1	E	1036	ILE	5.0
1	E	1033	GLU	4.9
1	E	1031	LEU	4.8
1	G	1085	GLN	4.7
1	H	1034	ASP	4.6
1	E	1034	ASP	4.5
1	E	1030	THR	4.4
1	H	1032	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	1008	LEU	4.3
1	H	1031	LEU	4.3
1	H	1184	PRO	4.1
1	E	1185	ASP	4.1
1	A	1029	MET	4.0
1	A	1034	ASP	4.0
1	F	1083	ASN	3.9
1	A	1083	ASN	3.8
1	E	1085	GLN	3.8
1	A	1025	ASP	3.8
1	E	1032	THR	3.8
1	A	1085	GLN	3.8
1	C	1185	ASP	3.7
1	D	1184	PRO	3.7
1	B	1255	PRO	3.7
1	H	1037	THR	3.7
1	H	1033	GLU	3.6
1	H	1084	GLY	3.6
1	B	1028	PRO	3.6
1	B	1029	MET	3.6
1	A	1032	THR	3.5
1	G	1079	PHE	3.5
1	B	1185	ASP	3.5
1	D	1186	GLY	3.5
1	E	1037	THR	3.4
1	F	1184	PRO	3.4
1	F	1256	ASP	3.4
1	B	1030	THR	3.4
1	C	1008	LEU	3.3
1	B	1037	THR	3.3
1	F	1178	LEU	3.1
1	H	1185	ASP	3.1
1	A	1084	GLY	3.1
1	D	1084	GLY	3.1
1	A	1033	GLU	3.1
1	B	1085	GLN	3.1
1	H	1085	GLN	3.1
1	A	1008	LEU	3.1
1	G	1009	MET	3.1
1	F	1180	TYR	2.9
1	E	1262	TYR	2.9
1	E	1040	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	1083	ASN	2.9
1	A	1185	ASP	2.9
1	B	1034	ASP	2.9
1	B	1033	GLU	2.8
1	G	1078	GLN	2.8
1	C	1030	THR	2.8
1	G	1033	GLU	2.8
1	A	1030	THR	2.8
1	B	1258	TYR	2.8
1	F	1185	ASP	2.8
1	A	1031	LEU	2.7
1	F	1086	ARG	2.7
1	B	1024	ARG	2.7
1	D	1185	ASP	2.7
1	A	1038	ARG	2.7
1	E	1258	TYR	2.7
1	E	1008	LEU	2.6
1	G	1034	ASP	2.6
1	G	1185	ASP	2.6
1	H	1064	PHE	2.5
1	E	1084	GLY	2.5
1	A	1082	THR	2.5
1	E	1038	ARG	2.5
1	C	1184	PRO	2.5
1	B	1184	PRO	2.5
1	C	1204	LEU	2.5
1	C	1086	ARG	2.5
1	B	1032	THR	2.5
1	F	1034	ASP	2.5
1	E	1035	GLU	2.5
1	F	1177	HIS	2.5
1	A	1256	ASP	2.5
1	E	1252	PHE	2.5
1	F	1008	LEU	2.4
1	C	1083	ASN	2.4
1	A	1184	PRO	2.4
1	E	1284	MET	2.4
1	F	1033	GLU	2.4
1	A	1223	VAL	2.4
1	E	1184	PRO	2.3
1	H	1086	ARG	2.3
1	D	1258	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1078	GLN	2.3
1	A	1219	VAL	2.3
1	C	1093	ILE	2.3
1	C	1033	GLU	2.3
1	H	1048	LEU	2.3
1	D	1085	GLN	2.2
1	F	1085	GLN	2.2
1	F	1029	MET	2.2
1	A	1090	ILE	2.2
1	D	1078	GLN	2.2
1	C	1085	GLN	2.2
1	D	1255	PRO	2.2
1	F	1297	ALA	2.2
1	G	1083	ASN	2.2
1	F	1183	ILE	2.2
1	B	1086	ARG	2.2
1	E	1024	ARG	2.1
1	A	1204	LEU	2.1
1	B	1031	LEU	2.1
1	B	1169	GLN	2.1
1	H	1223	VAL	2.1
1	E	1082	THR	2.1
1	H	1083	ASN	2.1
1	B	1227	ILE	2.1
1	B	1178	LEU	2.1
1	C	1029	MET	2.0
1	C	1186	GLY	2.0
1	B	1048	LEU	2.0
1	H	1082	THR	2.0
1	E	1186	GLY	2.0
1	H	1079	PHE	2.0
1	F	1204	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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^{th} 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	1408	1/1	0.78	0.54	49,49,49,49	0
4	UNX	H	1405	1/1	0.78	0.24	36,36,36,36	0
4	UNX	C	1409	1/1	0.81	0.77	29,29,29,29	0
3	0JR	D	1402[A]	22/22	0.82	0.20	35,44,71,74	0
3	0JR	F	1402[A]	22/22	0.83	0.24	46,52,60,61	0
4	UNX	G	1403	1/1	0.83	0.51	34,34,34,34	0
4	UNX	C	1405	1/1	0.83	0.40	41,41,41,41	0
4	UNX	C	1408	1/1	0.83	0.35	31,31,31,31	0
4	UNX	G	1407	1/1	0.84	0.73	38,38,38,38	0
4	UNX	E	1403	1/1	0.84	0.54	40,40,40,40	0
4	UNX	B	1406	1/1	0.84	0.30	39,39,39,39	0
4	UNX	E	1404	1/1	0.85	0.29	34,34,34,34	0
4	UNX	B	1404	1/1	0.86	0.27	37,37,37,37	0
3	0JR	C	1402	22/22	0.86	0.15	35,39,42,45	0
4	UNX	G	1406	1/1	0.88	0.17	36,36,36,36	0
4	UNX	H	1403	1/1	0.88	0.25	36,36,36,36	0
4	UNX	F	1407	1/1	0.88	0.19	28,28,28,28	0
3	0JR	A	1402	22/22	0.90	0.15	29,34,49,51	0
4	UNX	C	1404	1/1	0.90	0.48	31,31,31,31	0
4	UNX	D	1405	1/1	0.91	0.21	31,31,31,31	0
4	UNX	D	1404	1/1	0.91	0.29	35,35,35,35	0
4	UNX	C	1403	1/1	0.92	0.18	29,29,29,29	0
3	0JR	B	1402	22/22	0.92	0.14	38,42,64,65	0
4	UNX	H	1404	1/1	0.92	0.57	32,32,32,32	0
4	UNX	A	1405	1/1	0.92	0.27	40,40,40,40	0
4	UNX	A	1404	1/1	0.93	0.29	22,22,22,22	0
4	UNX	F	1404	1/1	0.93	0.43	33,33,33,33	0
4	UNX	G	1404	1/1	0.93	0.14	23,23,23,23	0
4	UNX	E	1402	1/1	0.94	0.16	29,29,29,29	0
4	UNX	F	1409	1/1	0.94	0.14	16,16,16,16	0
4	UNX	G	1405	1/1	0.94	0.21	33,33,33,33	0
4	UNX	D	1408	1/1	0.95	0.34	35,35,35,35	0
4	UNX	F	1405	1/1	0.95	0.11	22,22,22,22	0
4	UNX	F	1406	1/1	0.95	0.14	32,32,32,32	0
4	UNX	C	1406	1/1	0.95	0.19	25,25,25,25	0
4	UNX	D	1403	1/1	0.95	0.20	32,32,32,32	0
4	UNX	D	1406	1/1	0.95	0.62	42,42,42,42	0

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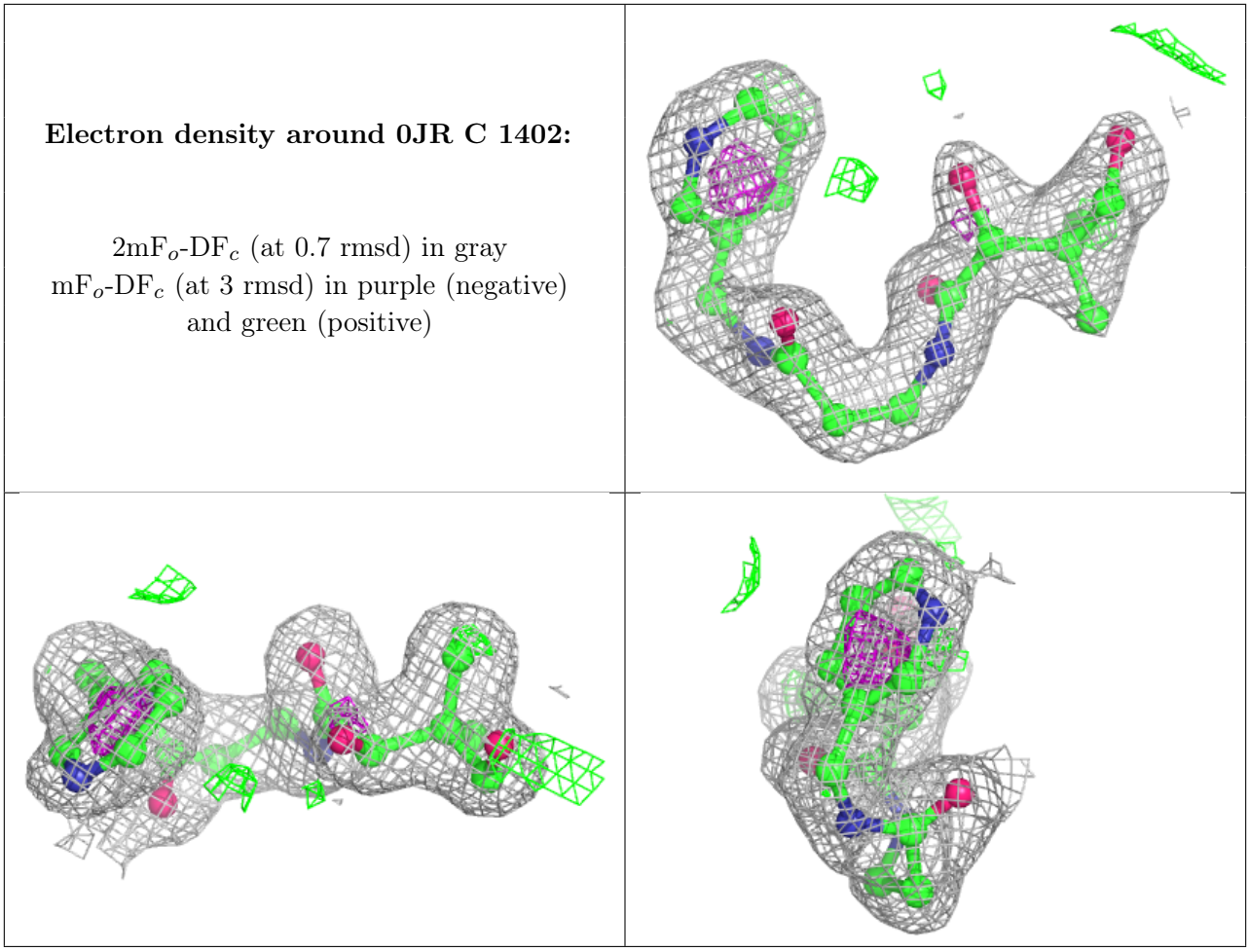
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UNX	F	1403	1/1	0.95	0.20	33,33,33,33	0
4	UNX	B	1405	1/1	0.96	0.30	30,30,30,30	0
4	UNX	D	1410	1/1	0.96	0.30	23,23,23,23	0
4	UNX	G	1402	1/1	0.96	0.25	23,23,23,23	0
4	UNX	D	1407	1/1	0.96	0.11	21,21,21,21	0
4	UNX	A	1406	1/1	0.97	0.24	32,32,32,32	0
2	ADP	E	1401	27/27	0.97	0.07	30,36,43,44	0
4	UNX	C	1407	1/1	0.97	0.14	25,25,25,25	0
4	UNX	F	1408	1/1	0.97	0.13	25,25,25,25	0
4	UNX	A	1403	1/1	0.97	0.15	22,22,22,22	0
2	ADP	D	1401	27/27	0.98	0.09	21,24,28,29	0
4	UNX	B	1403	1/1	0.98	0.17	28,28,28,28	0
4	UNX	H	1402	1/1	0.98	0.13	23,23,23,23	0
2	ADP	B	1401	27/27	0.98	0.08	24,29,35,36	0
4	UNX	D	1409	1/1	0.98	0.19	25,25,25,25	0
2	ADP	H	1401	27/27	0.98	0.09	22,23,27,27	0
4	UNX	B	1407	1/1	0.99	0.18	28,28,28,28	0
2	ADP	A	1401	27/27	0.99	0.08	17,21,25,28	0
2	ADP	F	1401	27/27	0.99	0.08	20,23,24,25	0
2	ADP	G	1401	27/27	0.99	0.07	20,23,27,29	0
2	ADP	C	1401	27/27	0.99	0.09	19,22,25,25	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.

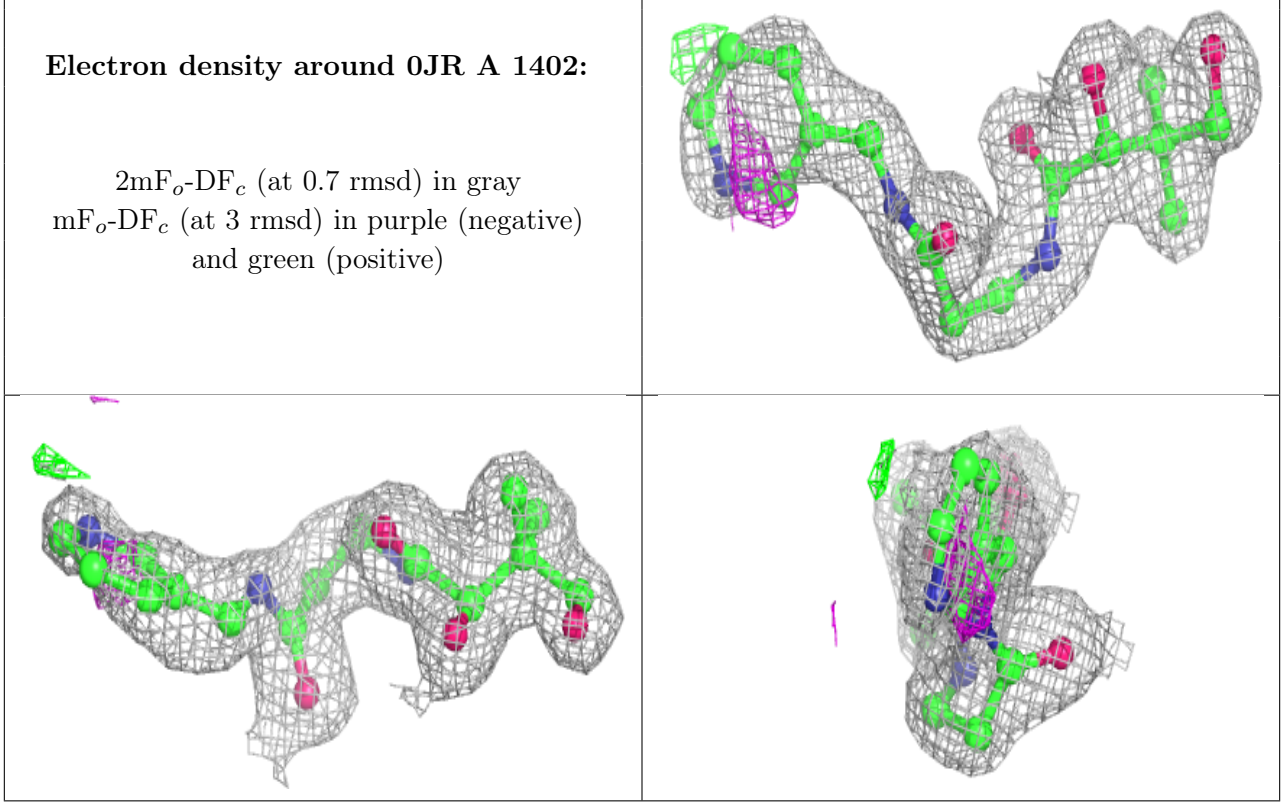
Electron density around 0JR C 1402:

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



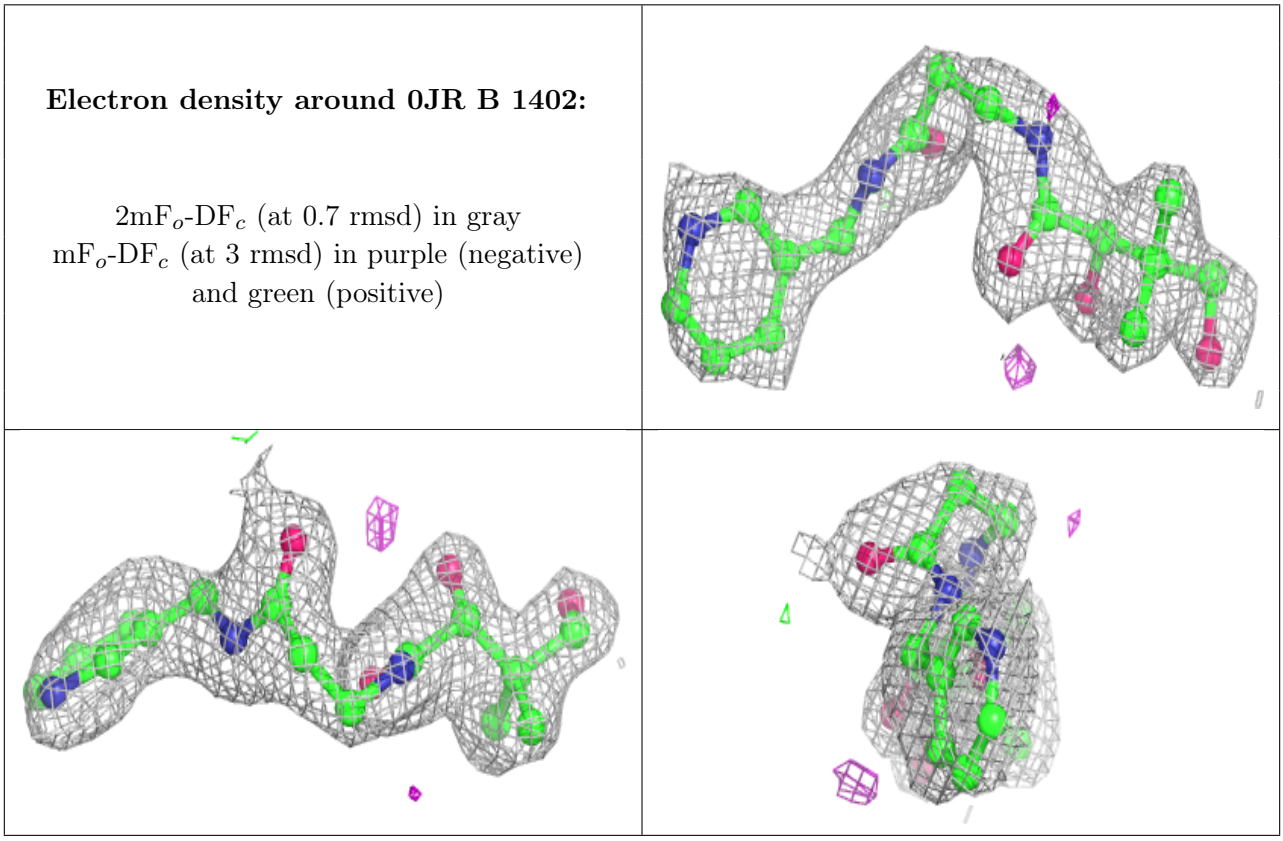
Electron density around 0JR A 1402:

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



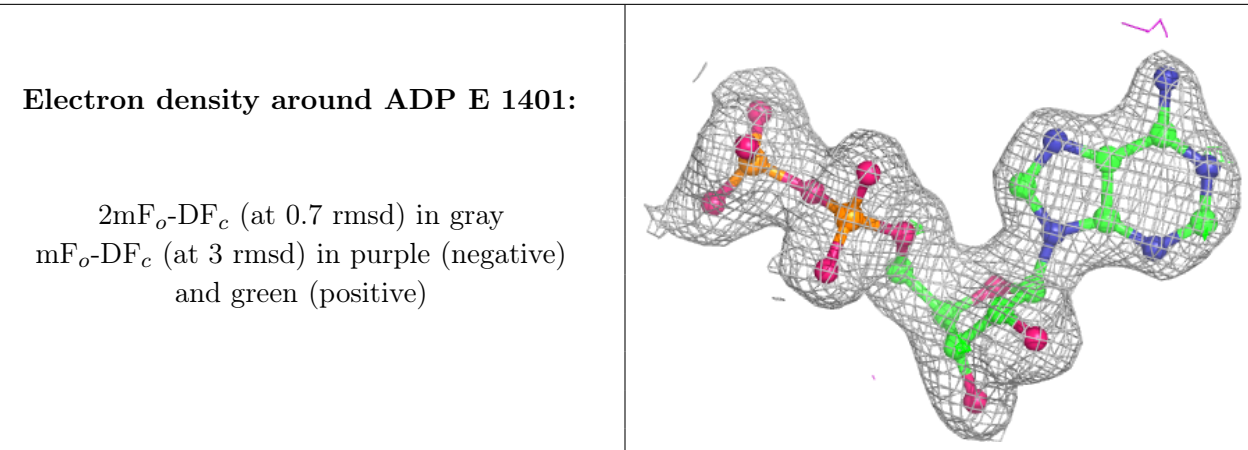
Electron density around 0JR B 1402:

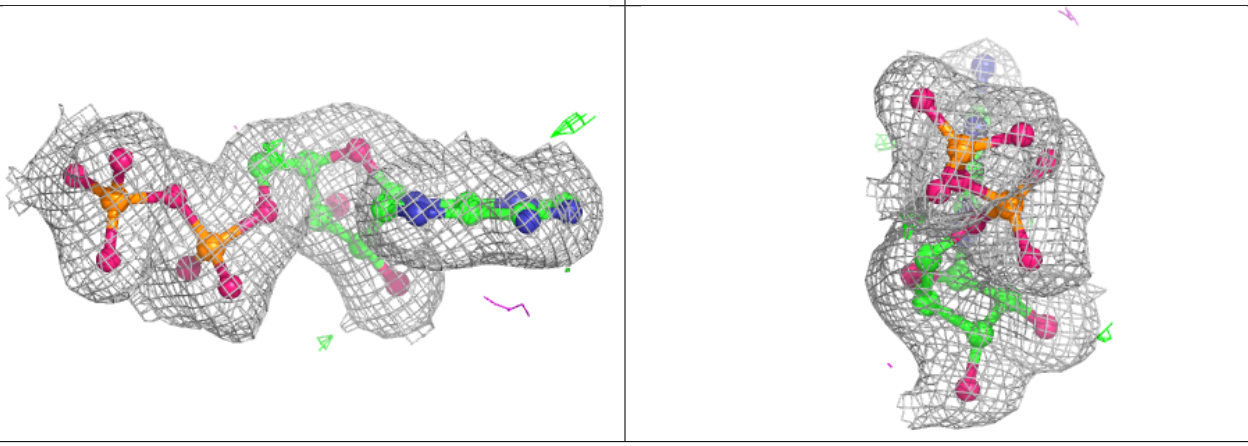
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP E 1401:

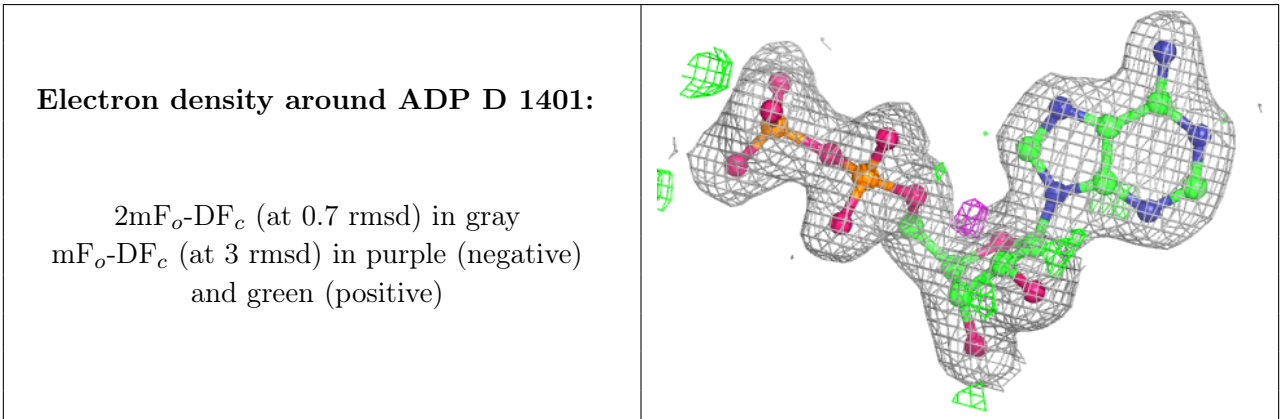
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

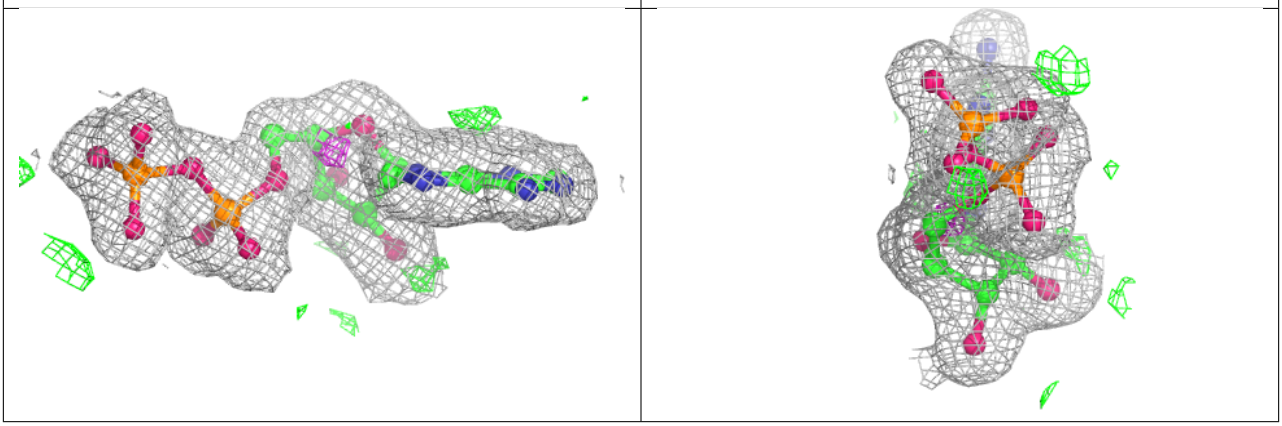




Electron density around ADP D 1401:

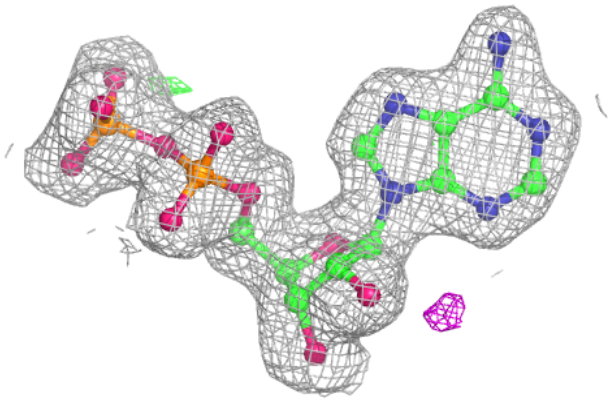
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

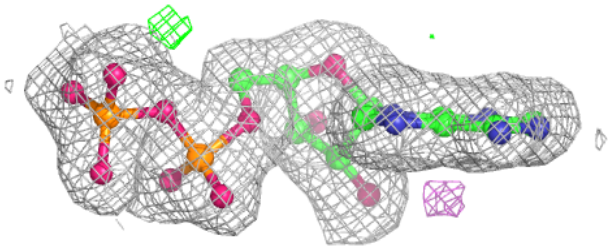


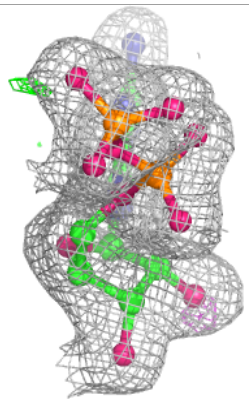


Electron density around ADP B 1401:

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

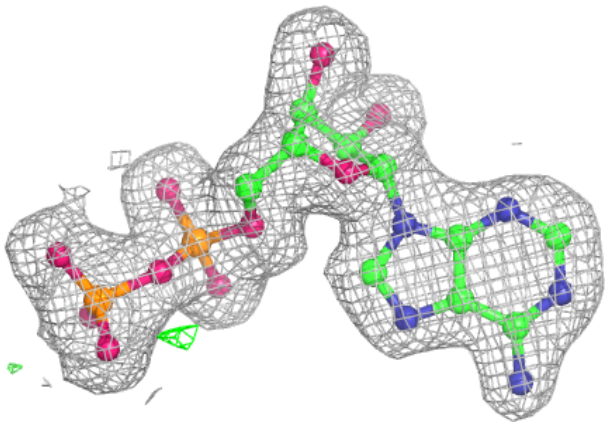


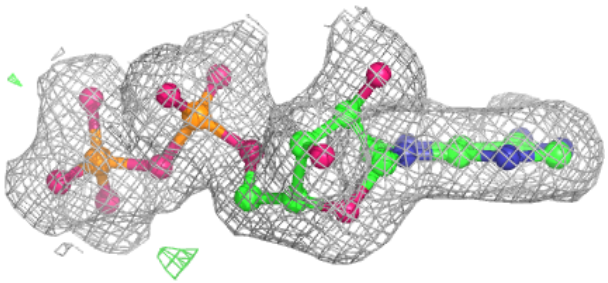


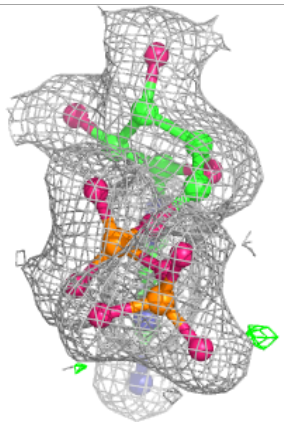


Electron density around ADP H 1401:

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

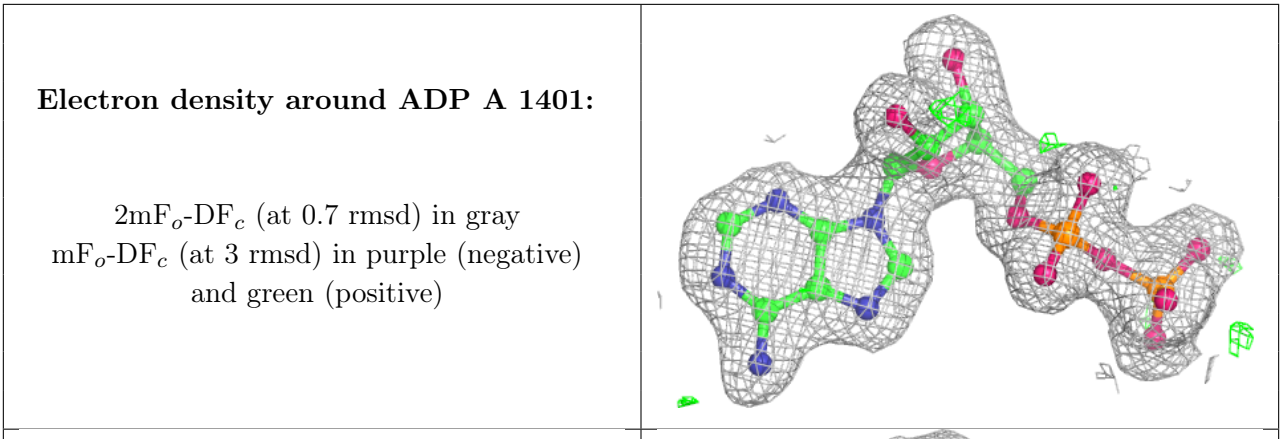






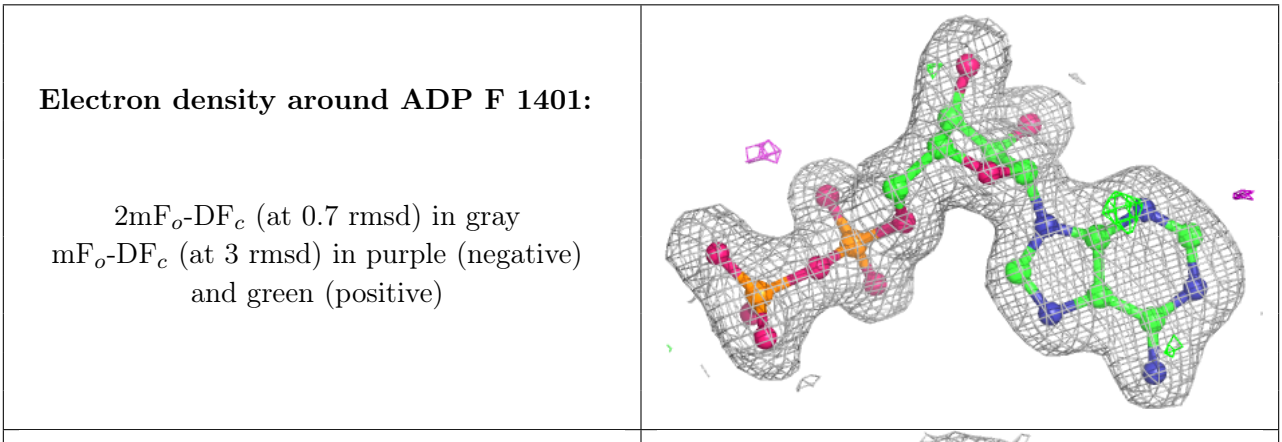
Electron density around ADP A 1401:

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



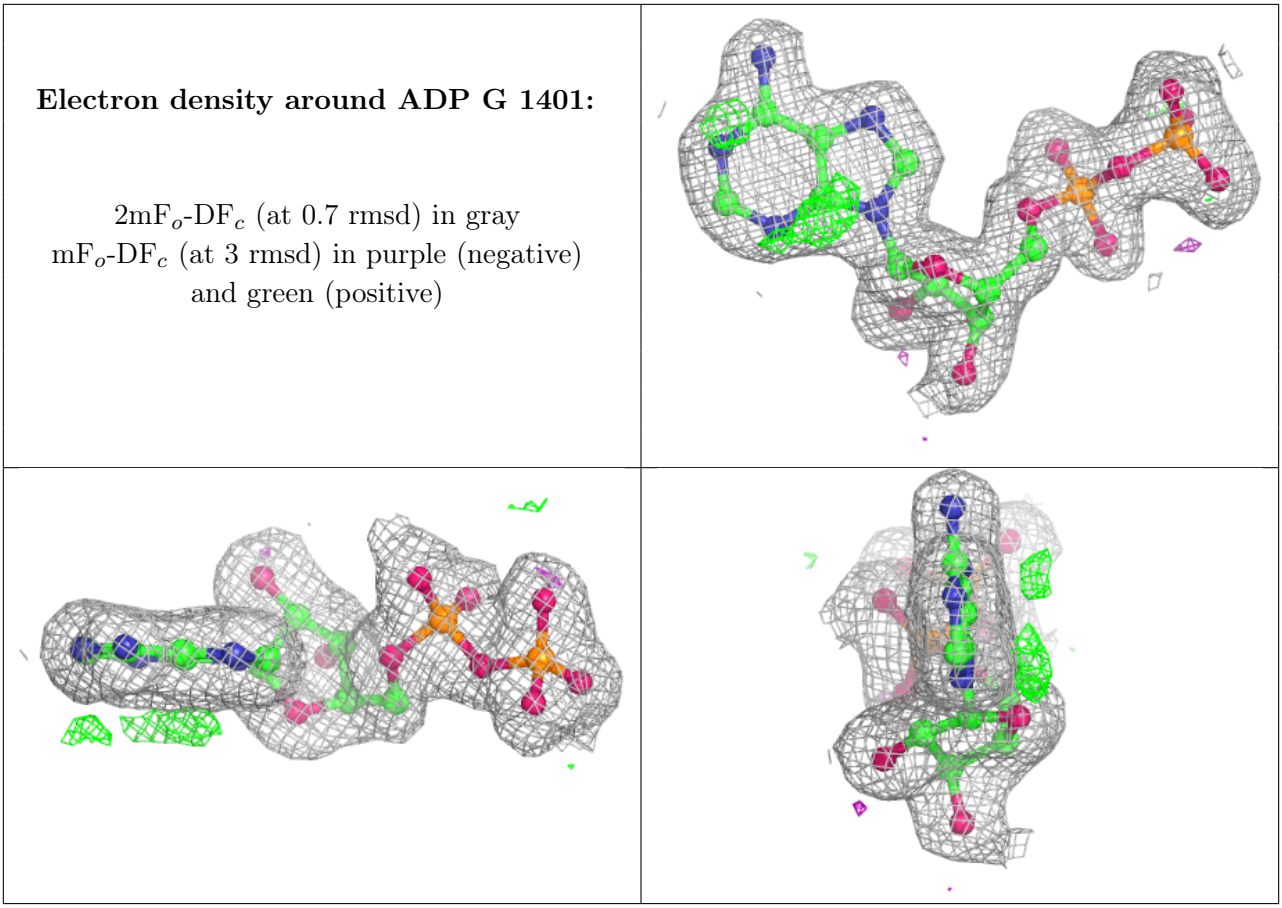
Electron density around ADP F 1401:

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



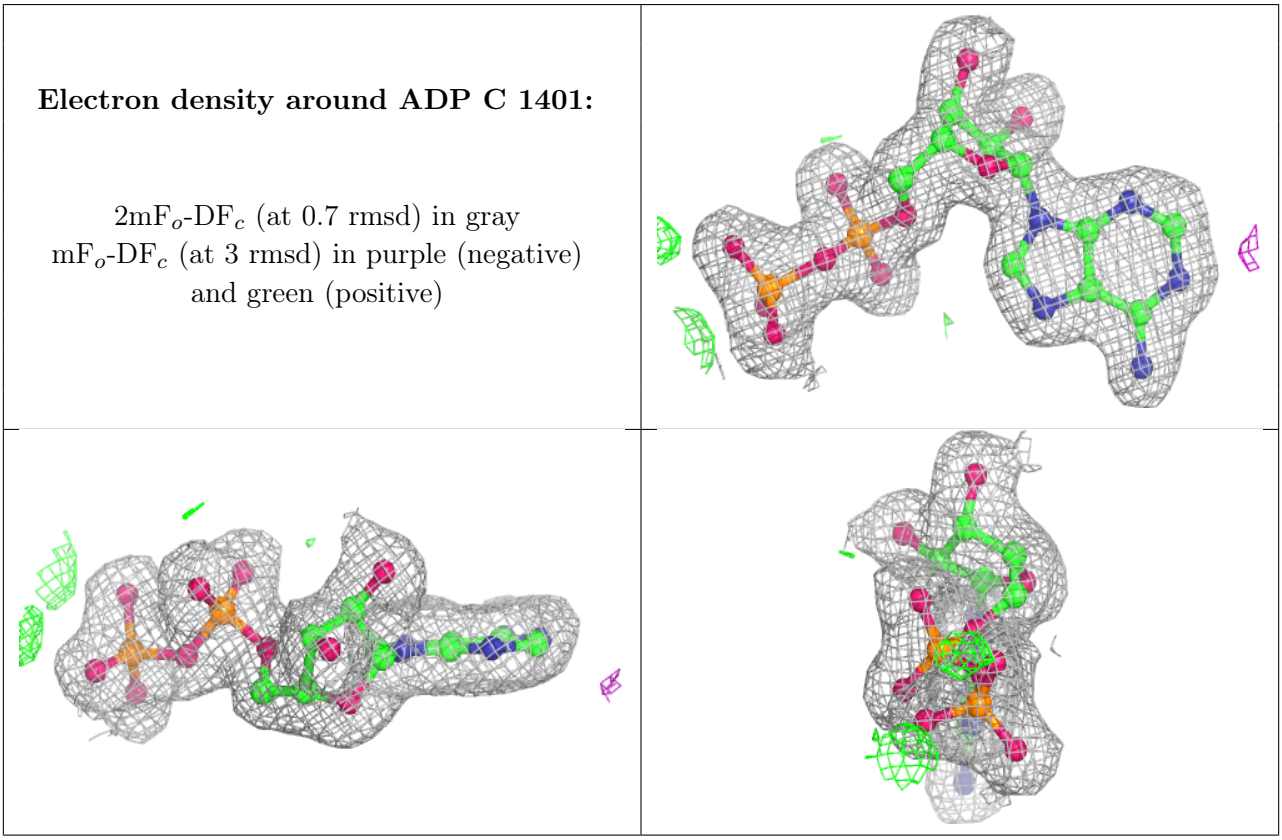
Electron density around ADP G 1401:

$2mF_o$-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 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.