Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 08:04 AM EDT

PDB ID	:	9AYQ / pdb_00009ayq
Title	:	SMARCA2 in complex with a pyridine-2-one-based inhibitor
Authors	:	Farrow, N.A.; Cocozaki, A.
Deposited on	:	2024-03-08
Resolution	:	2.90 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:

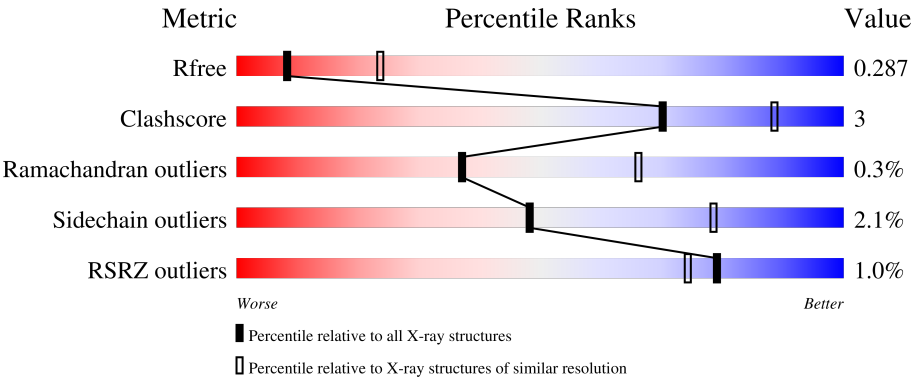
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	693	% 74% 9% 17%
1	B	693	% 74% 9% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9634 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 Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4761	3026	839	867	29			
1	B	576	Total	C	N	O	S	0	0	0
			4761	3030	836	866	29			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	MET	-	initiating methionine	UNP P51531
A	470	SER	-	expression tag	UNP P51531
A	471	TYR	-	expression tag	UNP P51531
A	472	TYR	-	expression tag	UNP P51531
A	473	HIS	-	expression tag	UNP P51531
A	474	HIS	-	expression tag	UNP P51531
A	475	HIS	-	expression tag	UNP P51531
A	476	HIS	-	expression tag	UNP P51531
A	477	HIS	-	expression tag	UNP P51531
A	478	HIS	-	expression tag	UNP P51531
A	479	ASP	-	expression tag	UNP P51531
A	480	TYR	-	expression tag	UNP P51531
A	481	ASP	-	expression tag	UNP P51531
A	482	ILE	-	expression tag	UNP P51531
A	483	PRO	-	expression tag	UNP P51531
A	484	THR	-	expression tag	UNP P51531
A	485	THR	-	expression tag	UNP P51531
A	486	GLU	-	expression tag	UNP P51531
A	487	ASN	-	expression tag	UNP P51531
A	488	LEU	-	expression tag	UNP P51531
A	489	TYR	-	expression tag	UNP P51531
A	490	PHE	-	expression tag	UNP P51531
A	491	GLN	-	expression tag	UNP P51531
A	492	SER	-	expression tag	UNP P51531
A	493	ILE	-	expression tag	UNP P51531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	494	ALA	-	expression tag	UNP P51531
A	694	ALA	-	linker	UNP P51531
A	695	ALA	-	linker	UNP P51531
A	696	SER	-	linker	UNP P51531
A	697	GLY	-	linker	UNP P51531
A	698	GLY	-	linker	UNP P51531
A	699	SER	-	linker	UNP P51531
A	700	GLY	-	linker	UNP P51531
A	1158	SER	-	linker	UNP P51531
A	1159	GLY	-	linker	UNP P51531
A	1160	GLY	-	linker	UNP P51531
A	1161	SER	-	linker	UNP P51531
A	1162	GLY	-	linker	UNP P51531
A	1163	GLY	-	linker	UNP P51531
A	1164	SER	-	linker	UNP P51531
A	1165	GLY	-	linker	UNP P51531
A	1303	ASP	-	expression tag	UNP P51531
A	1304	TYR	-	expression tag	UNP P51531
A	1305	LYS	-	expression tag	UNP P51531
A	1306	ASP	-	expression tag	UNP P51531
A	1307	ASP	-	expression tag	UNP P51531
A	1308	ASP	-	expression tag	UNP P51531
A	1309	ASP	-	expression tag	UNP P51531
A	1310	LYS	-	expression tag	UNP P51531
B	469	MET	-	initiating methionine	UNP P51531
B	470	SER	-	expression tag	UNP P51531
B	471	TYR	-	expression tag	UNP P51531
B	472	TYR	-	expression tag	UNP P51531
B	473	HIS	-	expression tag	UNP P51531
B	474	HIS	-	expression tag	UNP P51531
B	475	HIS	-	expression tag	UNP P51531
B	476	HIS	-	expression tag	UNP P51531
B	477	HIS	-	expression tag	UNP P51531
B	478	HIS	-	expression tag	UNP P51531
B	479	ASP	-	expression tag	UNP P51531
B	480	TYR	-	expression tag	UNP P51531
B	481	ASP	-	expression tag	UNP P51531
B	482	ILE	-	expression tag	UNP P51531
B	483	PRO	-	expression tag	UNP P51531
B	484	THR	-	expression tag	UNP P51531
B	485	THR	-	expression tag	UNP P51531
B	486	GLU	-	expression tag	UNP P51531

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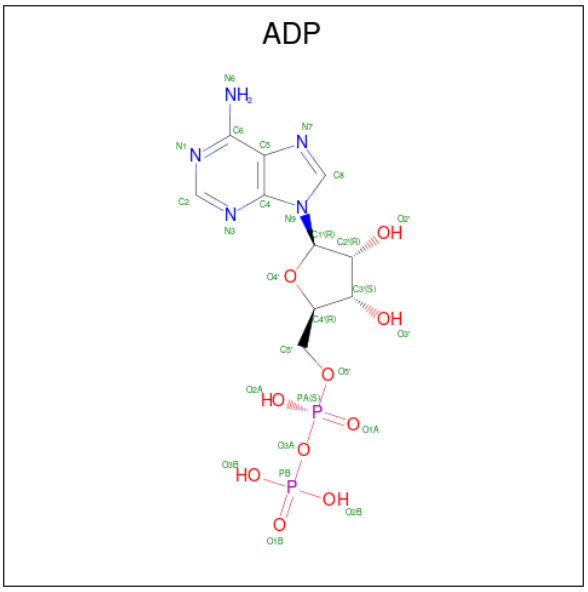
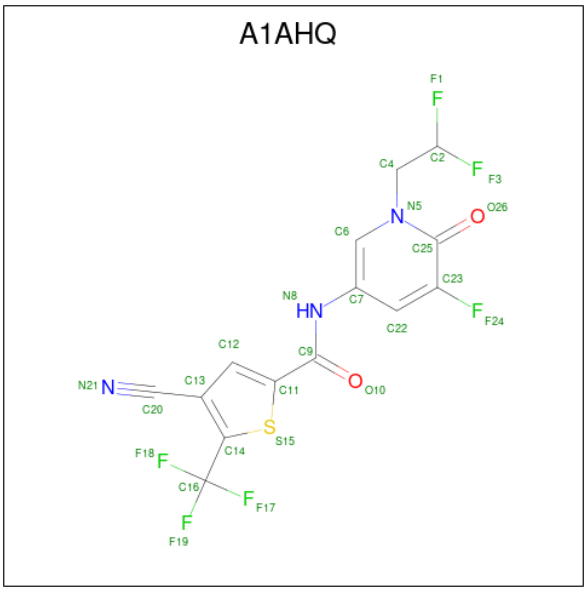
Chain	Residue	Modelled	Actual	Comment	Reference
B	487	ASN	-	expression tag	UNP P51531
B	488	LEU	-	expression tag	UNP P51531
B	489	TYR	-	expression tag	UNP P51531
B	490	PHE	-	expression tag	UNP P51531
B	491	GLN	-	expression tag	UNP P51531
B	492	SER	-	expression tag	UNP P51531
B	493	ILE	-	expression tag	UNP P51531
B	494	ALA	-	expression tag	UNP P51531
B	694	ALA	-	linker	UNP P51531
B	695	ALA	-	linker	UNP P51531
B	696	SER	-	linker	UNP P51531
B	697	GLY	-	linker	UNP P51531
B	698	GLY	-	linker	UNP P51531
B	699	SER	-	linker	UNP P51531
B	700	GLY	-	linker	UNP P51531
B	1158	SER	-	linker	UNP P51531
B	1159	GLY	-	linker	UNP P51531
B	1160	GLY	-	linker	UNP P51531
B	1161	SER	-	linker	UNP P51531
B	1162	GLY	-	linker	UNP P51531
B	1163	GLY	-	linker	UNP P51531
B	1164	SER	-	linker	UNP P51531
B	1165	GLY	-	linker	UNP P51531
B	1303	ASP	-	expression tag	UNP P51531
B	1304	TYR	-	expression tag	UNP P51531
B	1305	LYS	-	expression tag	UNP P51531
B	1306	ASP	-	expression tag	UNP P51531
B	1307	ASP	-	expression tag	UNP P51531
B	1308	ASP	-	expression tag	UNP P51531
B	1309	ASP	-	expression tag	UNP P51531
B	1310	LYS	-	expression tag	UNP P51531

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is 4-cyano-N-[1-(2,2-difluoroethyl)-5-fluoro-6-oxo-1,6-dihydropyridin-3-yl]-5-(trifluoromethyl)thiophene-2-carboxamide (CCD ID: A1AHQ) (formula: $C_{14}H_7F_6N_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			26	14	6	3	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	0	0
			26	14	6	3	2	1		

- Molecule 4 is water.

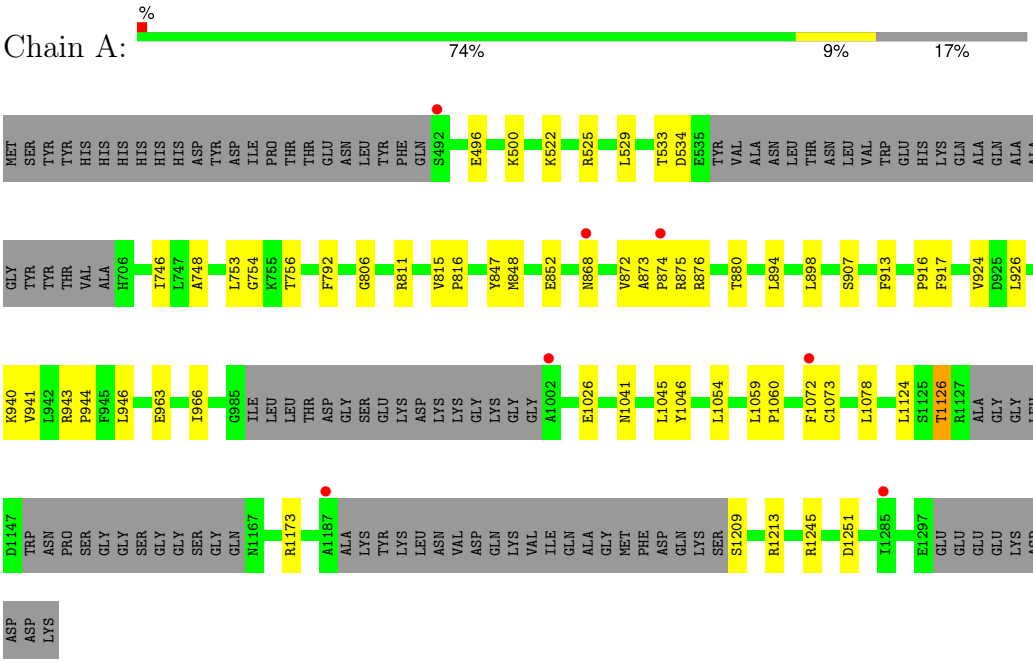
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	2	Total	O	0	0
			2	2		

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.

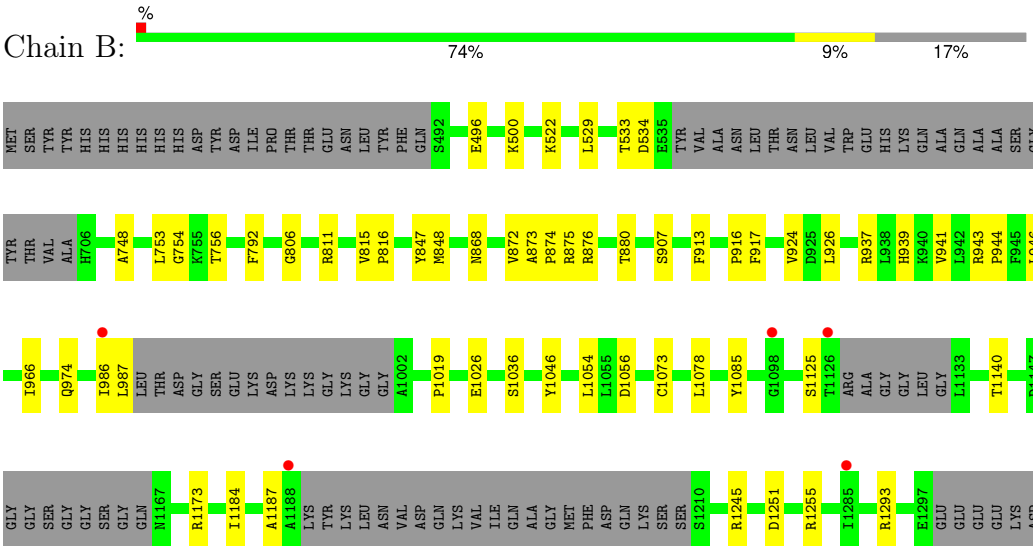
• Molecule 1: Probable global transcription activator SNF2L2

Chain A:



• Molecule 1: Probable global transcription activator SNF2L2

Chain B:




ASP
ASP
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.11Å 63.97Å 126.58Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	47.24 – 2.90 47.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	79.3 (47.24-2.90) 79.3 (47.24-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.287 0.237 , 0.287	Depositor DCC
R_{free} test set	1741 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	66.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9634	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.61% 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: A1AHQ, 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	0.65	0/4846	0.75	0/6521
1	B	0.65	0/4846	0.74	0/6523
All	All	0.65	0/9692	0.74	0/13044

There are no bond length outliers.

There are no bond angle outliers.

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	4761	0	4826	34	0
1	B	4761	0	4832	29	0
2	A	27	0	12	5	0
2	B	27	0	12	3	0
3	A	26	0	0	1	0
3	B	26	0	0	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
All	All	9634	0	9682	64	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 3.

All (64) 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:756:THR:HB	2:A:1401:ADP:O2A	1.72	0.90
1:B:754:GLY:HA2	2:B:1401:ADP:O2A	1.90	0.70
1:B:756:THR:HB	2:B:1401:ADP:O1A	1.92	0.70
1:A:754:GLY:HA2	2:A:1401:ADP:O1A	1.91	0.69
1:A:848:MET:HB2	1:A:873:ALA:CB	2.31	0.60
1:A:754:GLY:CA	2:A:1401:ADP:O1A	2.49	0.60
1:B:848:MET:HB2	1:B:873:ALA:CB	2.31	0.59
1:B:533:THR:HG23	1:B:937:ARG:HD3	1.87	0.56
1:A:875:ARG:NE	1:A:875:ARG:HA	2.23	0.53
1:B:875:ARG:HA	1:B:875:ARG:NE	2.24	0.53
1:B:916:PRO:HG2	1:B:917:PHE:CE1	2.44	0.53
1:A:496:GLU:O	1:A:500:LYS:HB2	2.09	0.53
1:B:806:GLY:O	1:B:811:ARG:NH1	2.43	0.52
1:B:496:GLU:O	1:B:500:LYS:HB2	2.09	0.52
1:A:806:GLY:O	1:A:811:ARG:NH1	2.42	0.51
1:A:916:PRO:HG2	1:A:917:PHE:CE1	2.46	0.51
1:A:1041:ASN:HA	1:A:1045:LEU:CD1	2.42	0.50
1:A:1072:PHE:CE1	1:A:1124:LEU:HD23	2.46	0.49
1:A:1072:PHE:CD1	1:A:1126:THR:HG22	2.47	0.49
1:A:1140:THR:OG1	1:A:1245:ARG:NH2	2.46	0.48
2:A:1401:ADP:O1A	2:A:1401:ADP:O2B	2.31	0.48
1:B:946:LEU:C	1:B:946:LEU:HD23	2.34	0.47
1:B:1140:THR:OG1	1:B:1245:ARG:NH2	2.47	0.47
1:A:946:LEU:C	1:A:946:LEU:HD23	2.34	0.47
1:B:533:THR:OG1	1:B:941:VAL:HG21	2.15	0.47
1:B:1073:CYS:SG	1:B:1078:LEU:HD23	2.55	0.47
1:B:748:ALA:HA	1:B:880:THR:O	2.14	0.47
1:A:748:ALA:HA	1:A:880:THR:O	2.15	0.47
1:A:966:ILE:HG22	1:A:1054:LEU:HD21	1.97	0.47
1:A:852:GLU:OE2	3:A:1402:A1AHQ:N8	2.48	0.46
1:B:963:GLU:OE1	1:B:1173:ARG:NH2	2.47	0.46
1:A:1073:CYS:SG	1:A:1078:LEU:HD23	2.56	0.46
1:B:1184:ILE:O	1:B:1187:ALA:HB3	2.14	0.46
1:B:848:MET:HB2	1:B:873:ALA:HB1	1.96	0.46
1:B:966:ILE:HG22	1:B:1054:LEU:HD21	1.98	0.46
1:A:848:MET:HB2	1:A:873:ALA:HB1	1.96	0.46
1:A:963:GLU:OE1	1:A:1173:ARG:NH2	2.49	0.46
1:B:522:LYS:HD3	1:B:924:VAL:CG1	2.46	0.45
1:A:533:THR:OG1	1:A:941:VAL:HG21	2.17	0.45
1:A:754:GLY:N	2:A:1401:ADP:O1A	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ILE:HD11	1:A:894:LEU:HD11	1.99	0.45
1:A:936:ARG:O	1:A:940:LYS:HG2	2.17	0.44
1:A:872:VAL:HG23	1:A:872:VAL:O	2.16	0.44
1:A:815:VAL:N	1:A:816:PRO:CD	2.80	0.44
1:A:1209:SER:O	1:A:1213:ARG:HG2	2.17	0.44
1:B:754:GLY:CA	2:B:1401:ADP:O2A	2.62	0.44
1:B:815:VAL:N	1:B:816:PRO:CD	2.81	0.44
1:A:534:ASP:OD1	1:A:937:ARG:NH1	2.51	0.44
1:B:534:ASP:OD1	1:B:937:ARG:NH1	2.51	0.44
1:B:943:ARG:N	1:B:944:PRO:CD	2.81	0.43
1:A:868:ASN:HB3	1:A:876:ARG:HH22	1.83	0.43
1:B:868:ASN:HB3	1:B:876:ARG:HH22	1.82	0.43
1:A:943:ARG:N	1:A:944:PRO:CD	2.82	0.43
1:B:872:VAL:O	1:B:872:VAL:HG23	2.19	0.42
1:B:1056:ASP:HA	1:B:1085:TYR:OH	2.20	0.42
1:B:986:ILE:HG13	1:B:987:LEU:HD12	2.00	0.42
1:A:913:PHE:CZ	1:A:926:LEU:HD21	2.54	0.42
1:B:529:LEU:O	1:B:533:THR:HG22	2.19	0.42
1:B:913:PHE:CZ	1:B:926:LEU:HD21	2.55	0.42
1:A:529:LEU:O	1:A:533:THR:HG22	2.20	0.42
1:A:1059:LEU:HB2	1:A:1060:PRO:HD3	2.02	0.41
1:A:746:ILE:HD11	1:A:898:LEU:HD11	2.01	0.41
1:B:974:GLN:HG3	1:B:1019:PRO:HG3	2.03	0.41
1:A:522:LYS:HD3	1:A:924:VAL:CG1	2.51	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	564/693 (81%)	528 (94%)	34 (6%)	2 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	564/693 (81%)	536 (95%)	27 (5%)	1 (0%)	44 73
All	All	1128/1386 (81%)	1064 (94%)	61 (5%)	3 (0%)	37 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1126	THR
1	A	874	PRO
1	B	874	PRO

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	523/617 (85%)	514 (98%)	9 (2%)	56 83
1	B	523/617 (85%)	510 (98%)	13 (2%)	42 75
All	All	1046/1234 (85%)	1024 (98%)	22 (2%)	48 78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	ARG
1	A	753	LEU
1	A	792	PHE
1	A	847	TYR
1	A	907	SER
1	A	939	HIS
1	A	1026	GLU
1	A	1046	TYR
1	A	1251	ASP
1	B	753	LEU
1	B	792	PHE
1	B	847	TYR
1	B	907	SER

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Mol	Chain	Res	Type
1	B	939	HIS
1	B	956	SER
1	B	1026	GLU
1	B	1036	SER
1	B	1046	TYR
1	B	1125	SER
1	B	1251	ASP
1	B	1255	ARG
1	B	1293	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	1401	-	24,29,29	0.69	0	29,45,45	0.90	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A1AHQ	A	1402	-	21,27,27	1.46	5 (23%)	20,40,40	2.12	7 (35%)
3	A1AHQ	B	1402	-	21,27,27	1.39	3 (14%)	20,40,40	1.85	5 (25%)
2	ADP	B	1401	-	24,29,29	0.69	0	29,45,45	0.77	1 (3%)

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	A	1401	-	-	5/12/32/32	0/3/3/3
3	A1AHQ	A	1402	-	-	4/16/20/20	0/2/2/2
3	A1AHQ	B	1402	-	-	4/16/20/20	0/2/2/2
2	ADP	B	1401	-	-	1/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	A1AHQ	C25-N5	-2.92	1.35	1.39
3	B	1402	A1AHQ	C25-N5	-2.74	1.35	1.39
3	B	1402	A1AHQ	C22-C23	2.39	1.37	1.35
3	A	1402	A1AHQ	C6-C7	2.30	1.36	1.34
3	A	1402	A1AHQ	F17-C16	2.30	1.41	1.33
3	A	1402	A1AHQ	F19-C16	2.18	1.40	1.33
3	B	1402	A1AHQ	F19-C16	2.12	1.40	1.33
3	A	1402	A1AHQ	F18-C16	2.02	1.40	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	A1AHQ	C11-C9-N8	6.47	123.97	114.03
3	B	1402	A1AHQ	C11-C9-N8	5.30	122.17	114.03
3	A	1402	A1AHQ	C12-C13-C14	2.94	114.85	109.92
3	B	1402	A1AHQ	C4-N5-C6	-2.59	118.14	120.04
3	A	1402	A1AHQ	C6-N5-C25	-2.50	120.85	122.72
3	B	1402	A1AHQ	C12-C13-C14	2.46	114.04	109.92
3	A	1402	A1AHQ	F24-C23-C25	2.39	119.71	115.87
2	B	1401	ADP	C5-C6-N6	2.32	123.84	120.31
3	A	1402	A1AHQ	C7-N8-C9	-2.27	118.51	123.67
2	A	1401	ADP	C5-C6-N6	2.26	123.75	120.31
3	B	1402	A1AHQ	F24-C23-C25	2.24	119.47	115.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	A1AHQ	O26-C25-C23	-2.21	120.40	123.97
2	A	1401	ADP	O3A-PA-O1A	-2.15	104.23	110.70
3	A	1402	A1AHQ	O10-C9-C11	-2.15	116.33	121.08
3	B	1402	A1AHQ	C6-N5-C25	-2.14	121.12	122.72

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	ADP	C5'-O5'-PA-O1A
2	A	1401	ADP	C5'-O5'-PA-O2A
2	A	1401	ADP	C5'-O5'-PA-O3A
3	A	1402	A1AHQ	F3-C2-C4-N5
3	A	1402	A1AHQ	C6-C7-N8-C9
3	A	1402	A1AHQ	C22-C7-N8-C9
3	B	1402	A1AHQ	F1-C2-C4-N5
3	B	1402	A1AHQ	F3-C2-C4-N5
3	B	1402	A1AHQ	C6-C7-N8-C9
3	A	1402	A1AHQ	F1-C2-C4-N5
2	B	1401	ADP	O4'-C4'-C5'-O5'
2	A	1401	ADP	O4'-C4'-C5'-O5'
2	A	1401	ADP	PA-O3A-PB-O1B
3	B	1402	A1AHQ	C22-C7-N8-C9

There are no ring outliers.

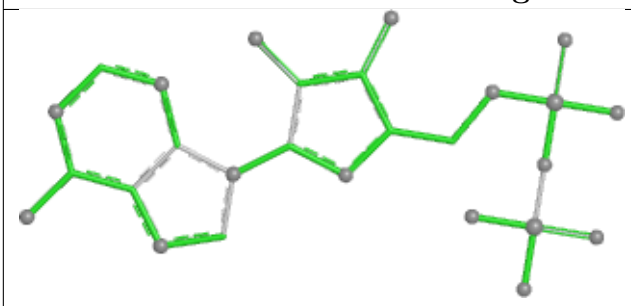
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	ADP	5	0
3	A	1402	A1AHQ	1	0
2	B	1401	ADP	3	0

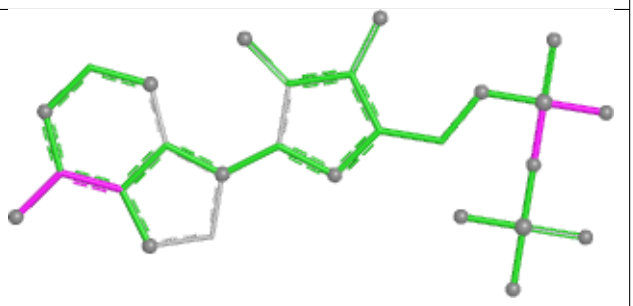
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

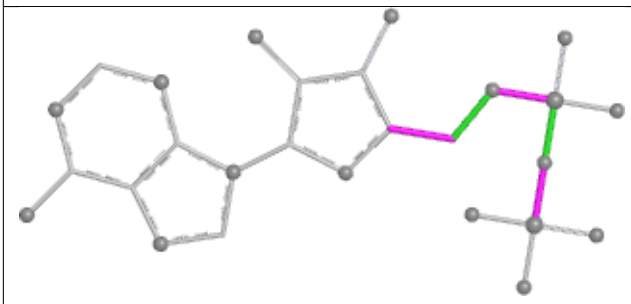
Ligand ADP A 1401



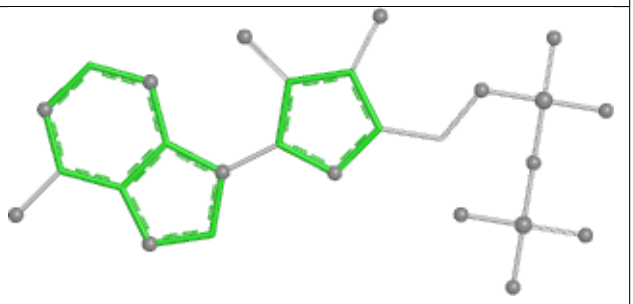
Bond lengths



Bond angles

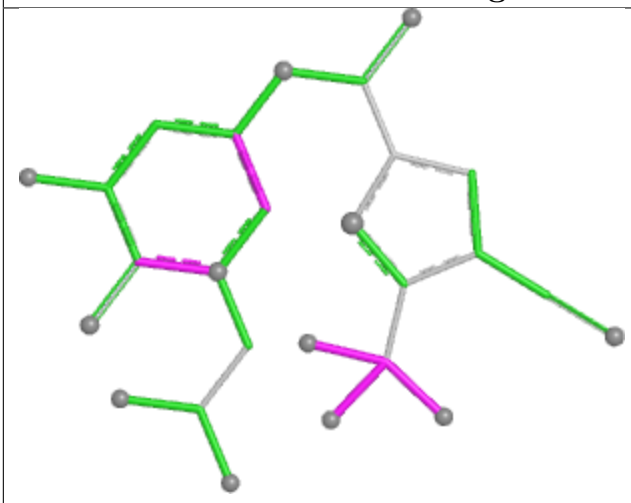


Torsions

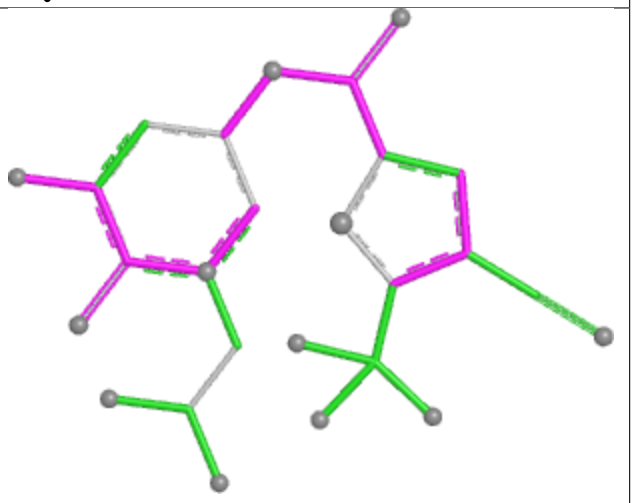


Rings

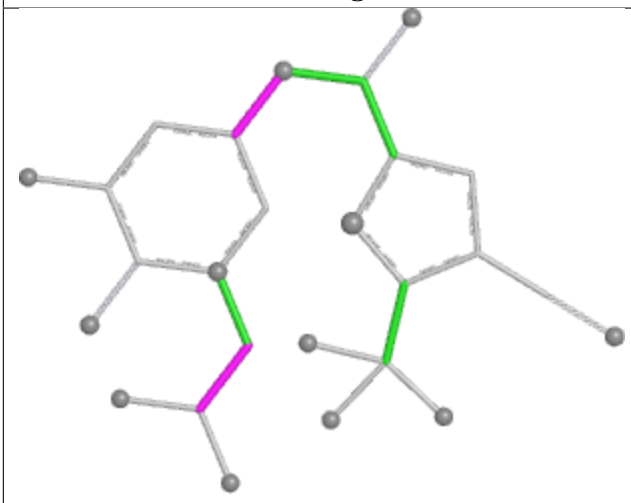
Ligand A1AHQ A 1402



Bond lengths



Bond angles



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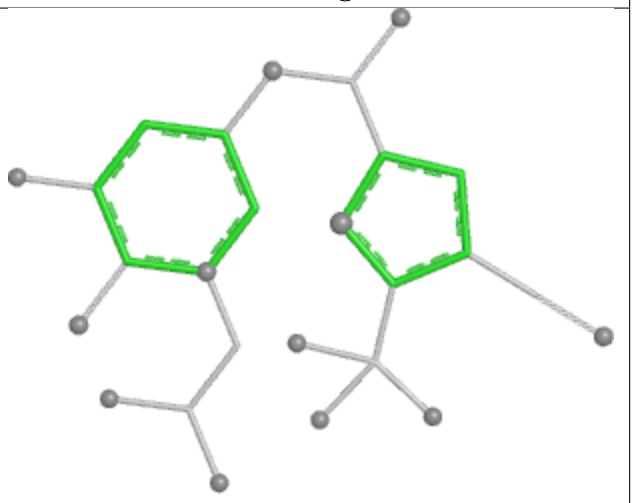
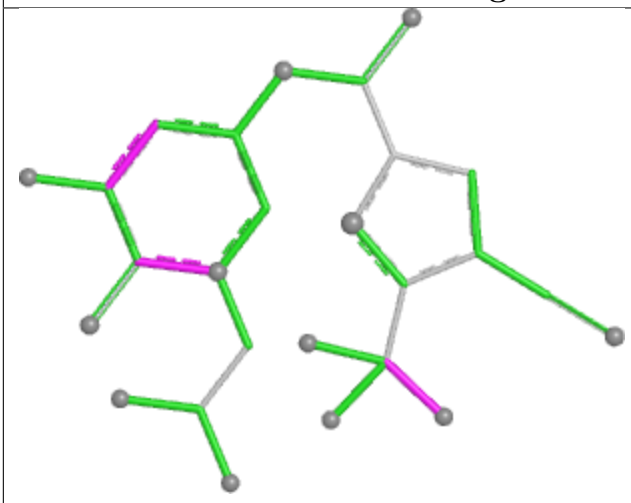
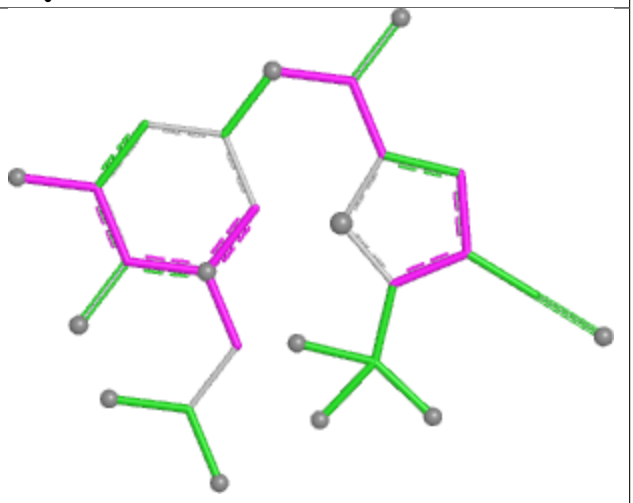


Rings

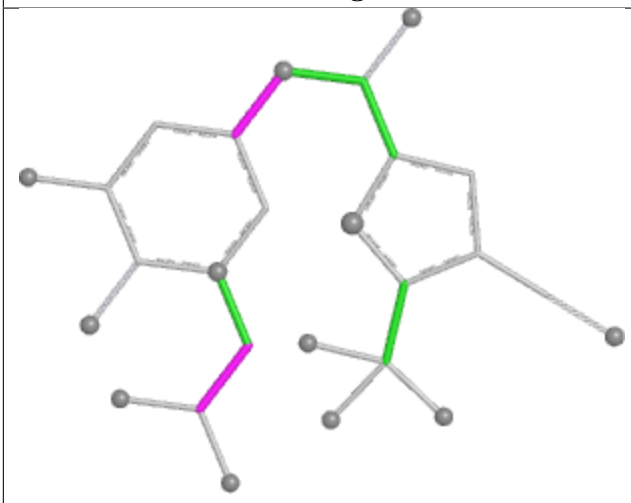
Ligand A1AHQ B 1402



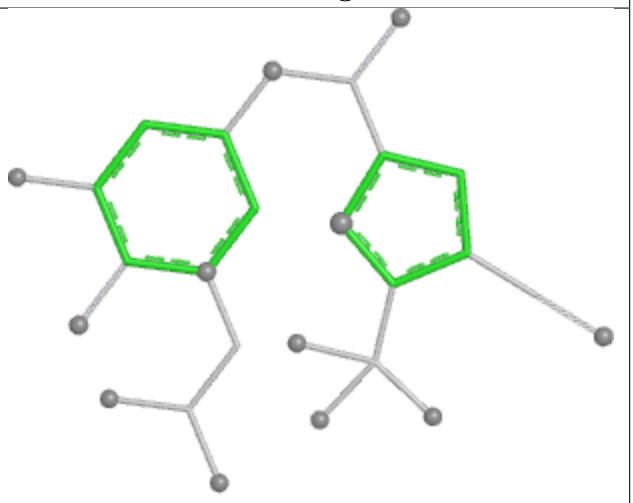
Bond lengths



Bond angles

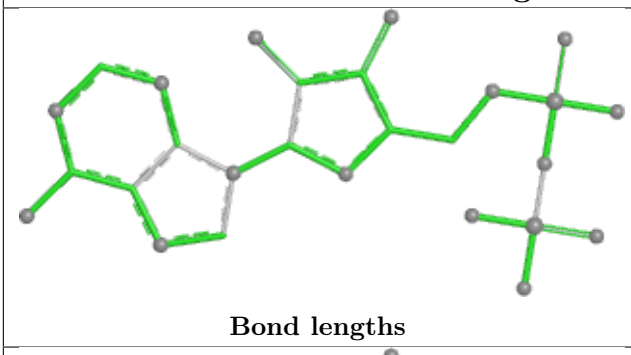


Torsions

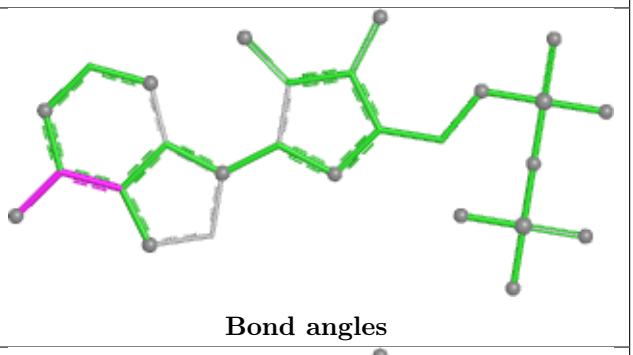


Rings

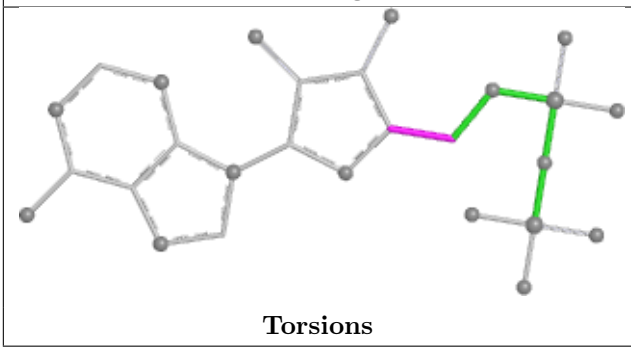
Ligand ADP B 1401



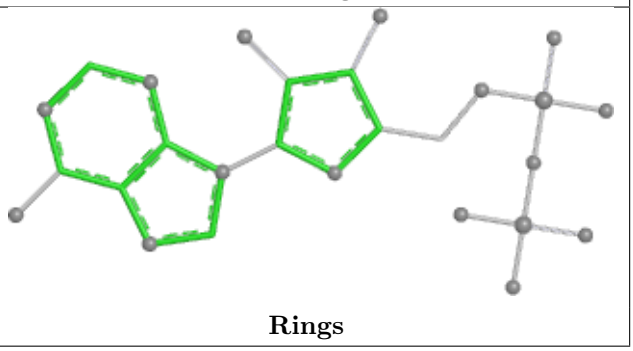
Bond lengths



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	576/693 (83%)	-0.23	7 (1%)	76	71	40, 65, 98, 143	0
1	B	576/693 (83%)	-0.13	5 (0%)	81	76	48, 71, 104, 134	0
All	All	1152/1386 (83%)	-0.18	12 (1%)	79	74	40, 68, 100, 143	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	986	ILE	3.9
1	B	1285	ILE	3.1
1	B	1098	GLY	2.9
1	B	1188	ALA	2.9
1	A	1187	ALA	2.6
1	A	1002	ALA	2.5
1	B	1126	THR	2.5
1	A	874	PRO	2.3
1	A	1072	PHE	2.3
1	A	492	SER	2.2
1	A	868	ASN	2.1
1	A	1285	ILE	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

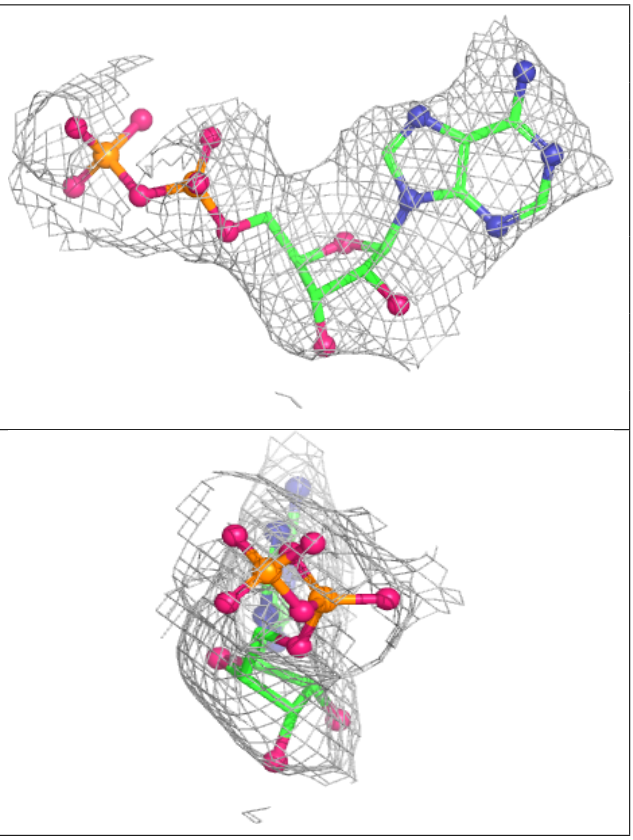
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

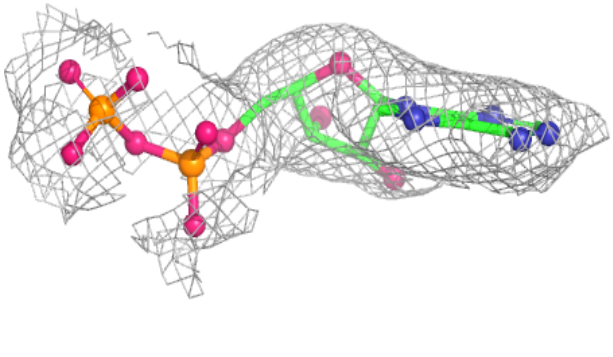
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	1401	27/27	0.96	0.06	50,56,64,66	0
2	ADP	B	1401	27/27	0.96	0.06	51,58,67,68	0
3	A1AHQ	B	1402	26/26	0.96	0.06	54,67,86,93	0
3	A1AHQ	A	1402	26/26	0.97	0.06	43,54,64,75	0

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

Electron density around ADP A 1401:

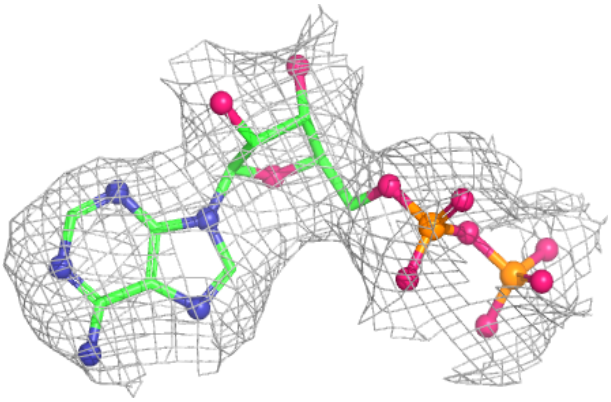
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

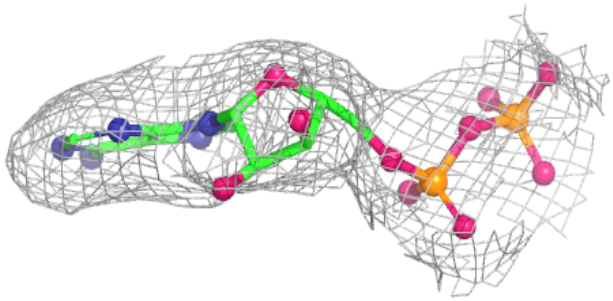


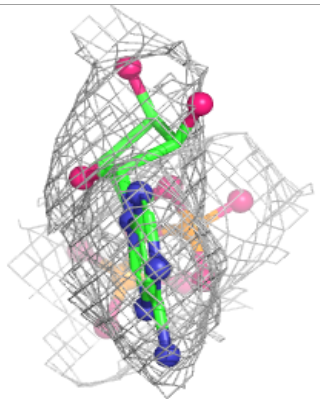


Electron density around ADP B 1401:

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

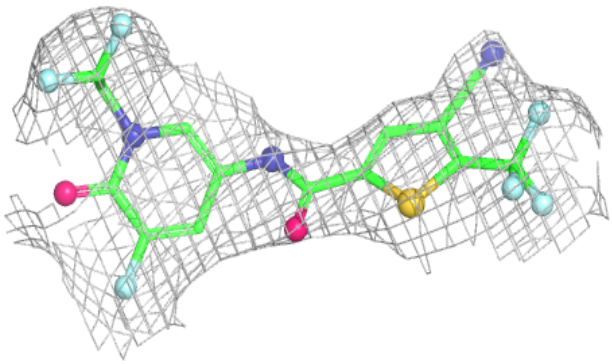


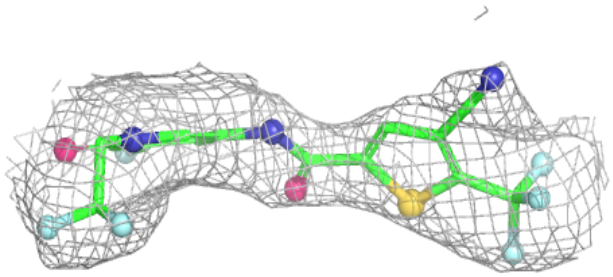


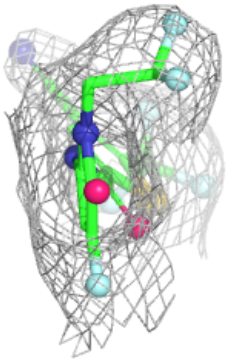


Electron density around A1AHQ B 1402:

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

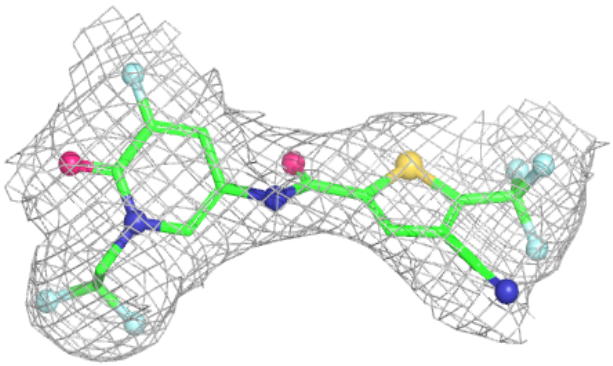


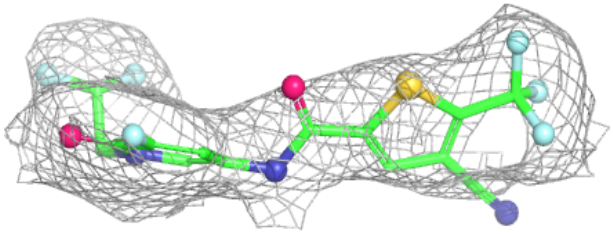


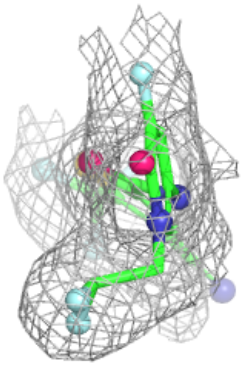


Electron density around A1AHQ A 1402:

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







6.5 Other polymers

There are no such residues in this entry.