Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 05:06 AM EDT

PDB ID	:	2GKS
Title	:	Crystal Structure of the Bi-functional ATP Sulfurylase-APS Kinase from Aquifex aeolicus, a Chemolithotrophic Thermophile
Authors	:	Yu, Z.; MacRea, I.J.; Lansdon, E.B.; Segel, I.H.; Fisher, A.J.
Deposited on	:	2006-04-03
Resolution	:	2.31 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:

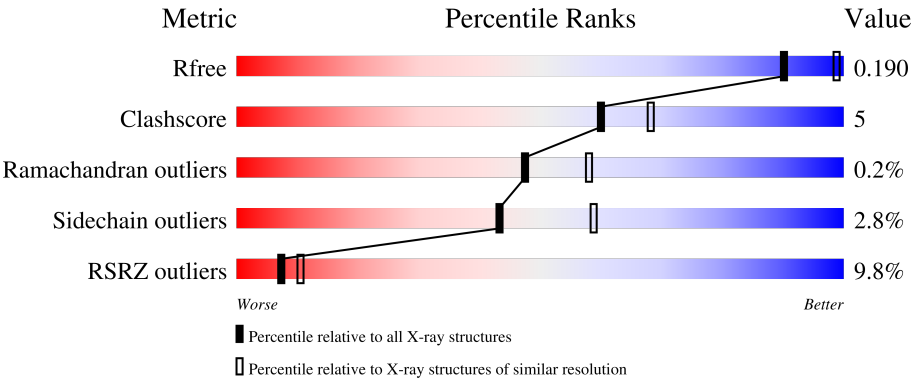
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	546	8% 85% 10%
1	B	546	11% 83% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8853 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.

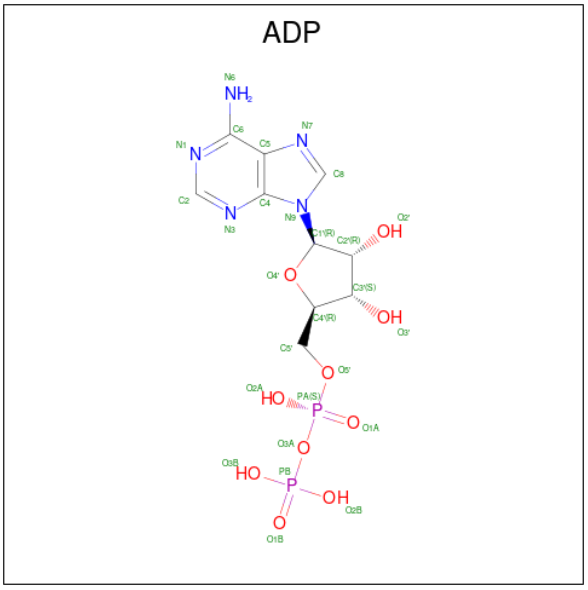
- Molecule 1 is a protein called Bifunctional SAT/APS kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4186	2701	708	759	18			
1	B	529	Total	C	N	O	S	0	0	0
			4260	2750	722	770	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	LYS	SEE REMARK 999	UNP O67174
B	21	GLU	LYS	SEE REMARK 999	UNP O67174

- 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		

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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		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

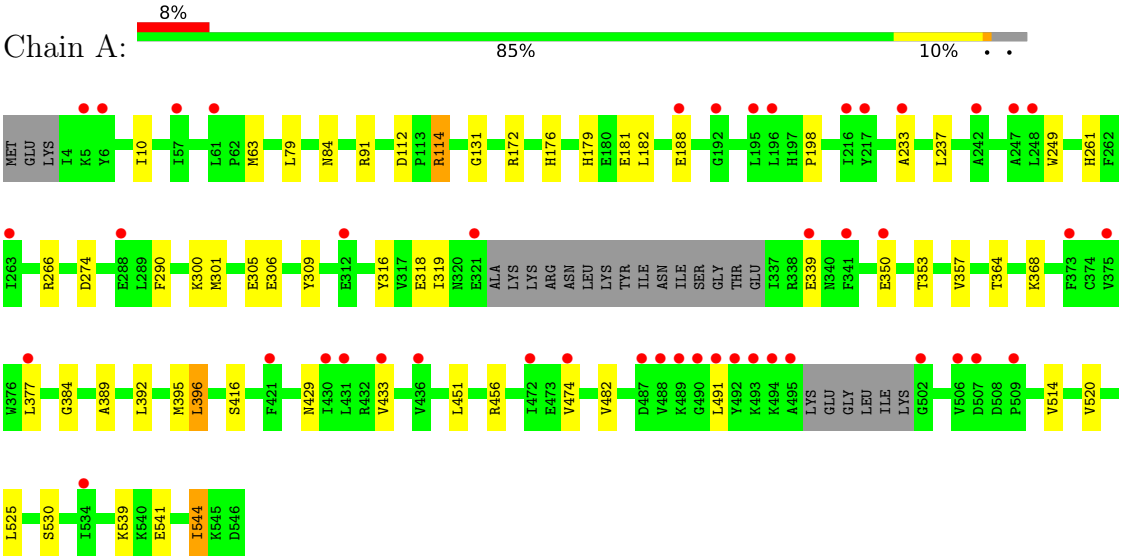
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	159	Total	O	0	0
			159	159		

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.

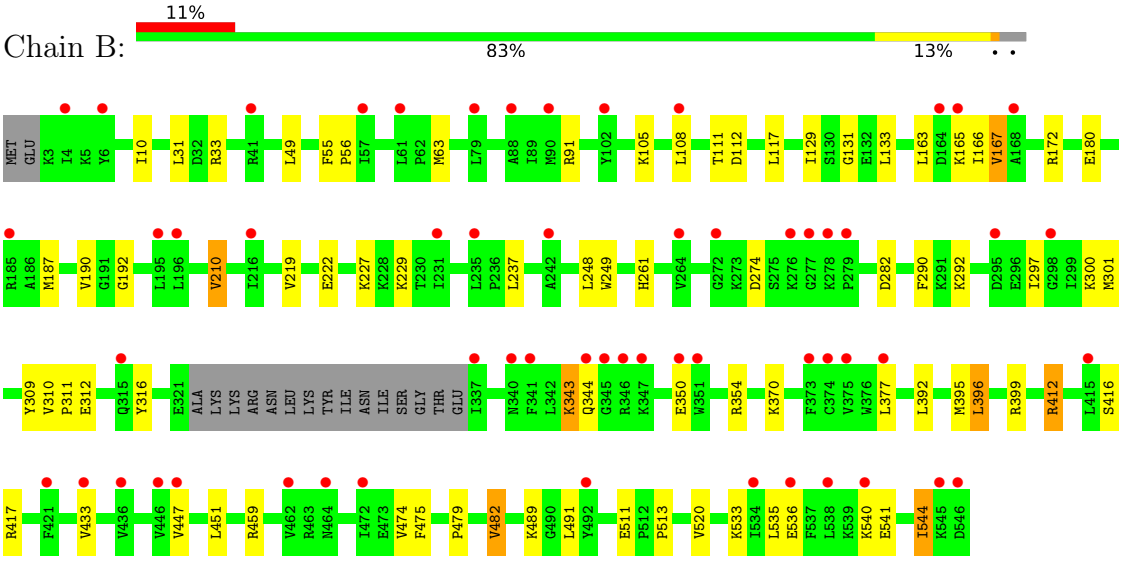
• Molecule 1: Bifunctional SAT/APS kinase

Chain A:



• Molecule 1: Bifunctional SAT/APS kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.23Å 67.28Å 108.73Å 90.00° 105.43° 90.00°	Depositor
Resolution (Å)	19.62 – 2.31 19.62 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.62-2.31) 98.8 (19.62-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.240 0.194 , 0.190	Depositor DCC
R_{free} test set	2542 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8853	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: 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	0.52	4/4281 (0.1%)	0.58	1/5788 (0.0%)
1	B	0.50	1/4357 (0.0%)	0.60	0/5885
All	All	0.51	5/8638 (0.1%)	0.59	1/11673 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	GLU	CD-OE1	10.52	1.37	1.25
1	A	339	GLU	CD-OE2	10.51	1.37	1.25
1	A	350	GLU	CD-OE1	5.57	1.31	1.25
1	A	339	GLU	CG-CD	5.50	1.60	1.51
1	B	292	LYS	CE-NZ	5.21	1.62	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	LEU	CA-CB-CG	5.35	127.60	115.30

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	4186	0	4230	36	0
1	B	4260	0	4328	43	0
2	A	54	0	24	2	0
2	B	54	0	24	0	0
3	A	140	0	0	0	0
3	B	159	0	0	2	0
All	All	8853	0	8606	79	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 5.

All (79) 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:392:LEU:HA	1:A:395:MET:HE2	1.41	0.98
1:B:63:MET:HE3	1:B:129:ILE:HD13	1.45	0.97
1:B:167:VAL:HG22	1:B:190:VAL:HG21	1.64	0.80
1:A:114:ARG:HH21	1:A:114:ARG:HG2	1.49	0.77
1:A:176:HIS:H	1:A:179:HIS:HD2	1.34	0.75
1:B:392:LEU:HA	1:B:395:MET:HE2	1.68	0.75
1:A:114:ARG:HH21	1:A:114:ARG:CG	2.03	0.72
1:B:475:PHE:HB2	1:B:513:PRO:HG2	1.73	0.71
1:B:343:LYS:HG3	1:B:344:GLN:H	1.56	0.70
1:B:63:MET:CE	1:B:129:ILE:HD13	2.22	0.69
1:A:305:GLU:HB2	1:A:318:GLU:HB2	1.75	0.69
1:A:520:VAL:HG11	1:A:530:SER:OG	1.95	0.65
1:B:91:ARG:O	1:B:131:GLY:HA3	2.00	0.62
1:B:399:ARG:HD3	1:B:544:ILE:HG21	1.85	0.59
1:A:318:GLU:H	1:A:318:GLU:CD	2.07	0.59
1:B:105:LYS:HG3	1:B:111:THR:HG23	1.86	0.57
1:A:520:VAL:HG13	1:A:525:LEU:HD12	1.87	0.57
1:B:412:ARG:HA	1:B:416:SER:HB2	1.86	0.55
1:B:417:ARG:HG3	3:B:921:HOH:O	2.07	0.55
1:A:114:ARG:CG	1:A:114:ARG:NH2	2.68	0.54
1:B:210:VAL:HG22	3:B:1019:HOH:O	2.07	0.54
1:A:176:HIS:H	1:A:179:HIS:CD2	2.20	0.53
1:A:520:VAL:HG11	1:A:530:SER:CB	2.39	0.53
1:A:10:ILE:HD13	1:A:63:MET:CE	2.39	0.52
1:B:248:LEU:HD22	1:B:297:ILE:HD11	1.92	0.52
1:B:10:ILE:HD13	1:B:63:MET:CE	2.40	0.52
1:A:377:LEU:HD23	1:A:474:VAL:HB	1.92	0.51
1:B:377:LEU:HD23	1:B:474:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:NH1	1:A:306:GLU:OE2	2.43	0.51
1:B:309:TYR:HB2	1:B:316:TYR:CE2	2.45	0.51
1:B:108:LEU:HD21	1:B:117:LEU:HD23	1.93	0.50
1:A:290:PHE:CD2	1:A:301:MET:HB2	2.47	0.50
1:B:222:GLU:HA	1:B:227:LYS:HE3	1.93	0.49
1:A:539:LYS:HG2	1:A:544:ILE:HG22	1.94	0.49
1:A:305:GLU:CD	1:A:305:GLU:H	2.15	0.49
1:A:433:VAL:HG21	1:A:451:LEU:HD11	1.94	0.49
1:B:187:MET:HE3	1:B:229:LYS:HB3	1.93	0.49
1:A:384:GLY:HA3	2:A:900:ADP:H2	1.78	0.48
1:A:368:LYS:HE2	1:A:541:GLU:O	2.13	0.48
1:B:163:LEU:HD13	1:B:166:ILE:HD11	1.94	0.48
1:B:261:HIS:CD2	1:B:300:LYS:HB3	2.49	0.48
1:B:10:ILE:HD13	1:B:63:MET:HE1	1.96	0.47
1:B:343:LYS:CG	1:B:344:GLN:H	2.24	0.46
1:B:290:PHE:CD2	1:B:301:MET:HB2	2.50	0.46
1:B:312:GLU:H	1:B:312:GLU:CD	2.18	0.46
1:B:533:LYS:HA	1:B:536:GLU:HG2	1.98	0.46
1:A:237:LEU:HD11	1:A:249:TRP:CH2	2.51	0.45
1:B:399:ARG:NH2	1:B:535:LEU:HD21	2.32	0.45
1:B:343:LYS:HG3	1:B:344:GLN:N	2.28	0.45
1:B:167:VAL:CG2	1:B:190:VAL:HG21	2.42	0.45
1:A:10:ILE:HD11	1:A:79:LEU:HD22	1.99	0.45
1:B:540:LYS:NZ	1:B:541:GLU:OE2	2.48	0.44
1:A:198:PRO:HD2	1:A:233:ALA:O	2.17	0.44
1:A:309:TYR:HB2	1:A:316:TYR:CE2	2.52	0.44
1:A:416:SER:HB3	1:A:429:ASN:ND2	2.33	0.43
1:B:310:VAL:HA	1:B:311:PRO:HD2	1.86	0.43
1:A:384:GLY:HA3	2:A:900:ADP:C2	2.53	0.43
1:B:55:PHE:HA	1:B:56:PRO:HD3	1.80	0.43
1:B:180:GLU:OE2	1:B:354:ARG:NH2	2.45	0.43
1:A:112:ASP:OD2	1:A:274:ASP:HB2	2.19	0.43
1:A:63:MET:HE2	1:A:63:MET:HB2	1.75	0.43
1:A:353:THR:HG22	1:A:357:VAL:HB	2.01	0.43
1:B:33:ARG:HA	1:B:133:LEU:HD12	2.00	0.42
1:A:377:LEU:CD1	1:A:389:ALA:HB2	2.50	0.42
1:B:163:LEU:HD13	1:B:166:ILE:CD1	2.50	0.42
1:B:165:LYS:HB2	1:B:192:GLY:HA3	2.01	0.42
1:A:456:ARG:HD2	1:A:514:VAL:HG23	2.02	0.42
1:B:237:LEU:HD11	1:B:249:TRP:CH2	2.55	0.42
1:A:10:ILE:HD13	1:A:63:MET:HE1	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:PRO:HD2	1:B:482:VAL:HG11	2.01	0.41
1:B:459:ARG:NH2	1:B:511:GLU:O	2.37	0.41
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.91	0.41
1:B:112:ASP:OD2	1:B:274:ASP:HB2	2.20	0.41
1:B:31:LEU:HD21	1:B:49:LEU:HD21	2.01	0.41
1:B:392:LEU:HG	1:B:396:LEU:HD22	2.03	0.41
1:A:261:HIS:HA	1:A:300:LYS:O	2.21	0.41
1:A:10:ILE:HD11	1:A:79:LEU:CD2	2.51	0.41
1:A:91:ARG:O	1:A:131:GLY:HA3	2.21	0.40
1:B:433:VAL:HG21	1:B:451:LEU:HD11	2.03	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	516/546 (94%)	505 (98%)	10 (2%)	1 (0%)	47	58
1	B	525/546 (96%)	512 (98%)	12 (2%)	1 (0%)	47	58
All	All	1041/1092 (95%)	1017 (98%)	22 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	LYS
1	A	319	ILE

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	449/480 (94%)	439 (98%)	10 (2%)	52	68
1	B	458/480 (95%)	443 (97%)	15 (3%)	38	52
All	All	907/960 (94%)	882 (97%)	25 (3%)	43	59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	114	ARG
1	A	172	ARG
1	A	181	GLU
1	A	188	GLU
1	A	364	THR
1	A	396	LEU
1	A	482	VAL
1	A	491	LEU
1	A	544	ILE
1	B	167	VAL
1	B	172	ARG
1	B	210	VAL
1	B	219	VAL
1	B	282	ASP
1	B	350	GLU
1	B	370	LYS
1	B	396	LEU
1	B	412	ARG
1	B	447	VAL
1	B	482	VAL
1	B	489	LYS
1	B	491	LEU
1	B	520	VAL
1	B	544	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	179	HIS
1	A	344	GLN
1	A	429	ASN
1	B	137	GLN
1	B	429	ASN

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)

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	900	-	24,29,29	1.10	2 (8%)	29,45,45	1.27	3 (10%)
2	ADP	A	902	-	24,29,29	1.09	2 (8%)	29,45,45	1.39	4 (13%)
2	ADP	B	904	-	24,29,29	1.04	2 (8%)	29,45,45	1.31	3 (10%)
2	ADP	B	906	-	24,29,29	1.06	2 (8%)	29,45,45	1.15	2 (6%)

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	900	-	-	2/12/32/32	0/3/3/3
2	ADP	A	902	-	-	0/12/32/32	0/3/3/3
2	ADP	B	904	-	-	1/12/32/32	0/3/3/3
2	ADP	B	906	-	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C5-C4	2.91	1.48	1.40
2	A	902	ADP	C5-C4	2.81	1.48	1.40
2	B	906	ADP	C5-C4	2.69	1.48	1.40
2	B	904	ADP	C5-C4	2.53	1.47	1.40
2	A	900	ADP	C2-N3	2.36	1.35	1.32
2	B	906	ADP	C2-N3	2.30	1.35	1.32
2	A	902	ADP	C2-N3	2.17	1.35	1.32
2	B	904	ADP	O4'-C1'	2.03	1.43	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	ADP	N3-C2-N1	-4.05	122.35	128.68
2	B	904	ADP	N3-C2-N1	-3.77	122.79	128.68
2	B	906	ADP	N3-C2-N1	-3.19	123.70	128.68
2	A	900	ADP	N3-C2-N1	-3.05	123.91	128.68
2	B	906	ADP	C4-C5-N7	-2.64	106.65	109.40
2	A	900	ADP	C4-C5-N7	-2.53	106.77	109.40
2	A	902	ADP	O3A-PB-O1B	-2.46	97.53	111.19
2	A	902	ADP	C4-C5-N7	-2.43	106.87	109.40
2	A	902	ADP	C2-N1-C6	2.41	122.87	118.75
2	B	904	ADP	C2-N1-C6	2.34	122.76	118.75
2	A	900	ADP	O4'-C1'-C2'	-2.33	103.52	106.93
2	B	904	ADP	C4-C5-N7	-2.06	107.25	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	ADP	PA-O3A-PB-O2B
2	B	906	ADP	O4'-C4'-C5'-O5'
2	B	906	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	906	ADP	PB-O3A-PA-O5'
2	A	900	ADP	PA-O3A-PB-O1B
2	B	904	ADP	PA-O3A-PB-O1B
2	B	906	ADP	C5'-O5'-PA-O1A

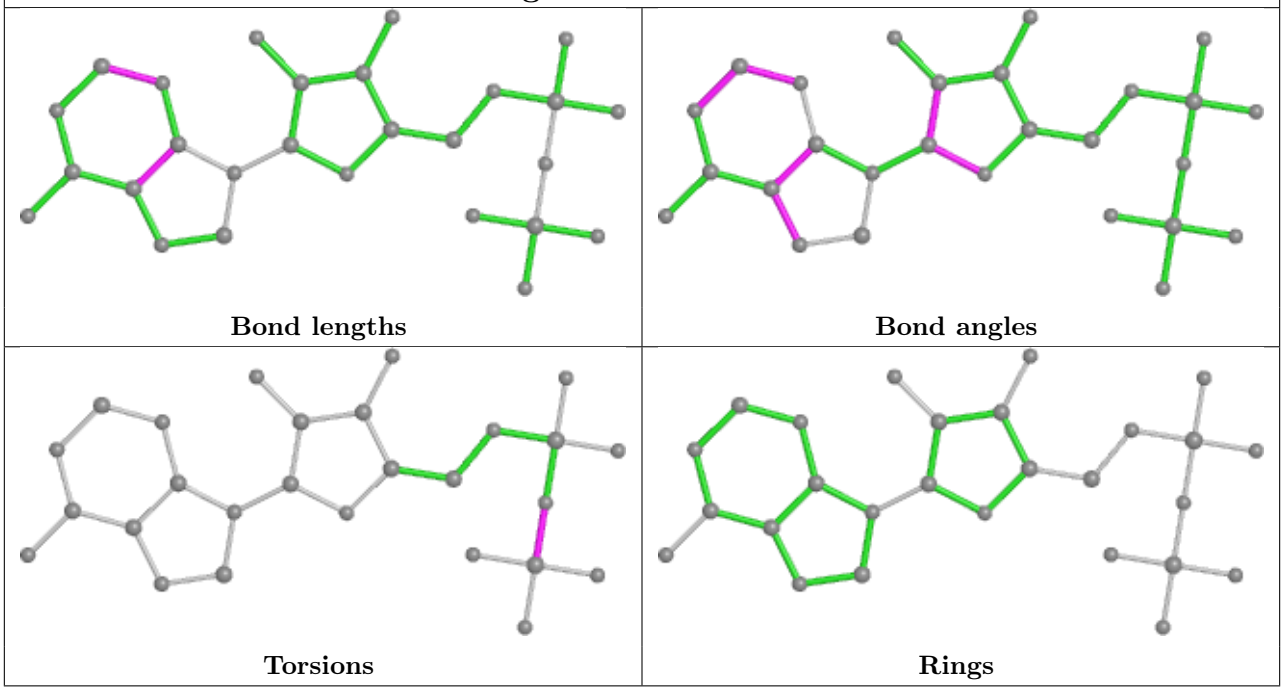
There are no ring outliers.

1 monomer is involved in 2 short contacts:

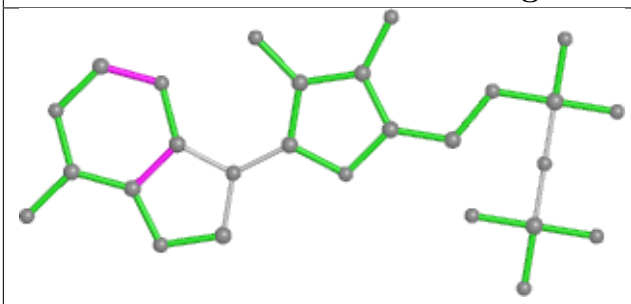
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	ADP	2	0

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

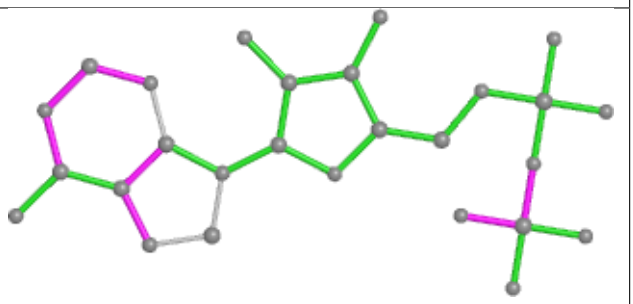
Ligand ADP A 900



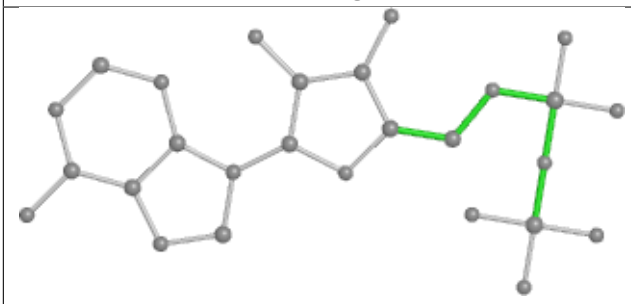
Ligand ADP A 902



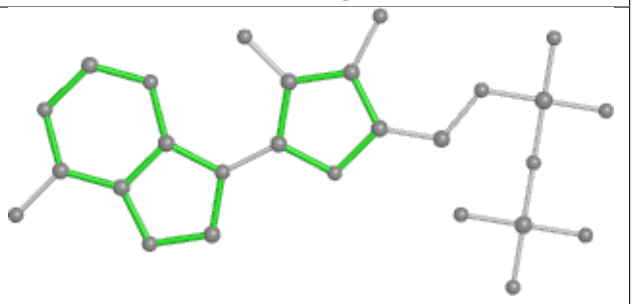
Bond lengths



Bond angles

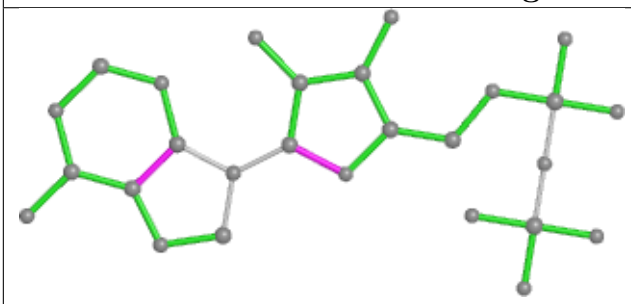


Torsions

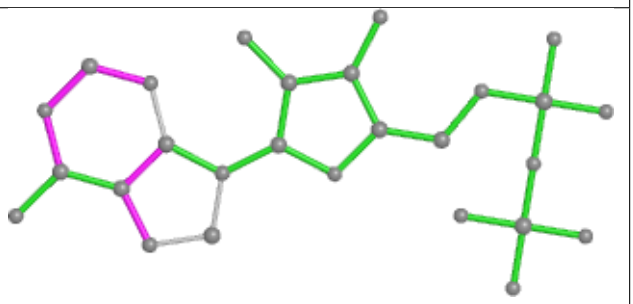


Rings

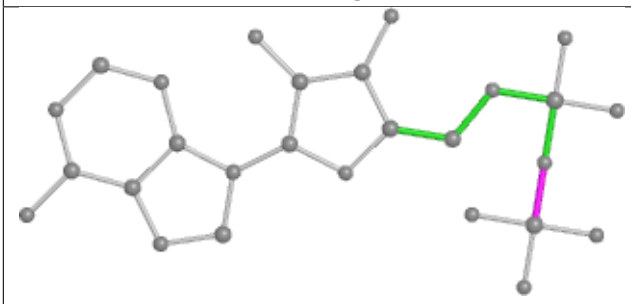
Ligand ADP B 904



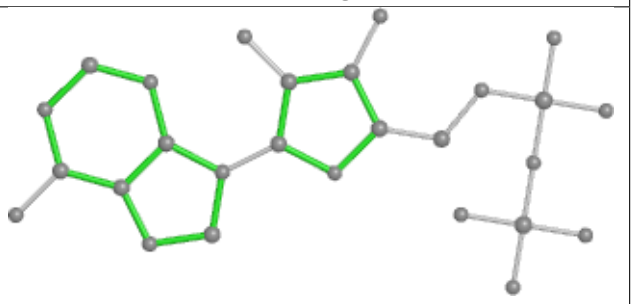
Bond lengths



Bond angles

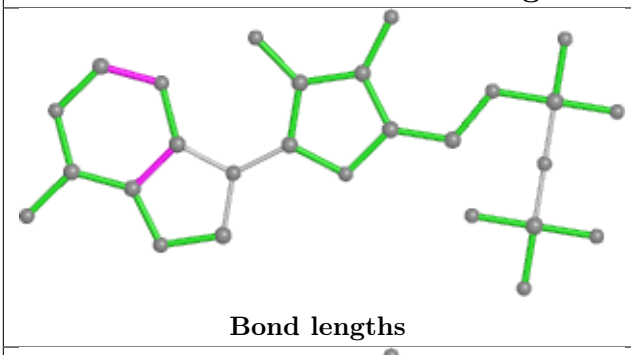


Torsions

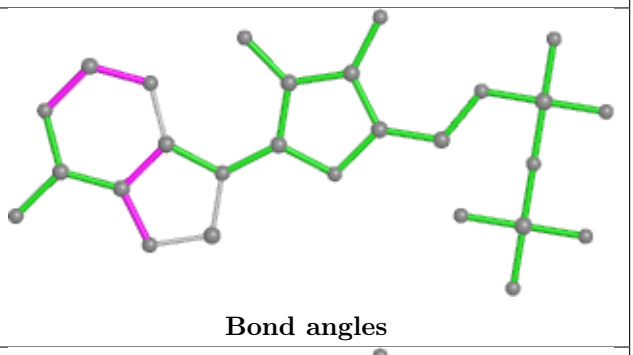


Rings

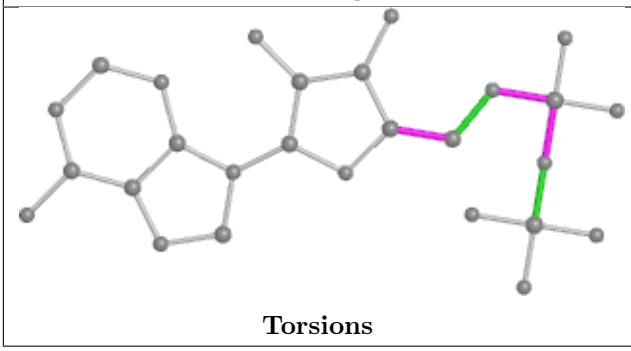
Ligand ADP B 906



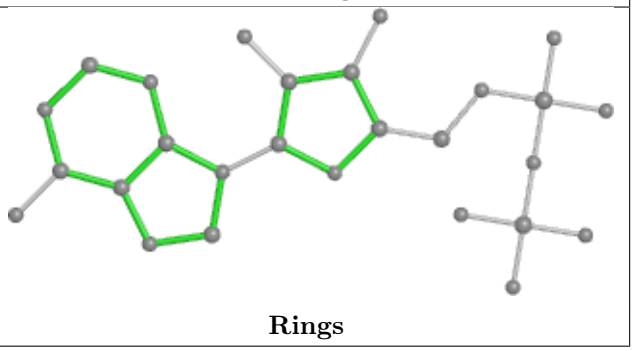
Bond lengths



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	522/546 (95%)	0.61	45 (8%) 10 14	43, 50, 60, 69	0
1	B	529/546 (96%)	0.56	58 (10%) 5 8	37, 50, 57, 68	0
All	All	1051/1092 (96%)	0.58	103 (9%) 7 10	37, 50, 58, 69	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	LEU	6.0
1	A	506	VAL	5.8
1	A	495	ALA	5.5
1	A	488	VAL	5.5
1	B	340	ASN	5.0
1	A	493	LYS	4.8
1	B	346	ARG	4.7
1	A	494	LYS	4.6
1	A	489	LYS	4.6
1	B	546	ASP	4.5
1	B	57	ILE	4.3
1	B	102	TYR	4.3
1	A	6	TYR	4.1
1	A	341	PHE	4.1
1	B	375	VAL	4.1
1	B	347	LYS	4.0
1	A	312	GLU	4.0
1	A	321	GLU	3.9
1	B	545	LYS	3.9
1	A	375	VAL	3.9
1	B	421	PHE	3.9
1	B	195	LEU	3.8
1	A	492	TYR	3.5
1	B	373	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	344	GLN	3.4
1	A	216	ILE	3.4
1	B	536	GLU	3.3
1	A	196	LEU	3.3
1	A	487	ASP	3.3
1	A	472	ILE	3.3
1	B	337	ILE	3.3
1	B	41	ARG	3.3
1	A	421	PHE	3.2
1	A	5	LYS	3.1
1	B	415	LEU	3.1
1	B	242	ALA	3.1
1	A	433	VAL	3.1
1	A	195	LEU	3.0
1	B	79	LEU	2.9
1	B	447	VAL	2.9
1	B	278	LYS	2.9
1	B	165	LYS	2.8
1	B	534	ILE	2.8
1	B	277	GLY	2.8
1	B	374	CYS	2.8
1	A	474	VAL	2.8
1	A	507	ASP	2.8
1	B	492	TYR	2.8
1	A	192	GLY	2.7
1	B	538	LEU	2.7
1	B	345	GLY	2.7
1	A	248	LEU	2.7
1	A	57	ILE	2.6
1	A	502	GLY	2.6
1	A	373	PHE	2.6
1	B	540	LYS	2.6
1	B	472	ILE	2.5
1	A	242	ALA	2.5
1	B	4	ILE	2.5
1	B	351	TRP	2.5
1	A	247	ALA	2.5
1	B	168	ALA	2.5
1	B	196	LEU	2.5
1	B	377	LEU	2.5
1	B	61	LEU	2.5
1	B	295	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	298	GLY	2.4
1	B	108	LEU	2.4
1	A	288	GLU	2.4
1	A	509	PRO	2.4
1	B	464	ASN	2.4
1	A	263	ILE	2.4
1	B	436	VAL	2.4
1	B	279	PRO	2.3
1	B	264	VAL	2.3
1	B	6	TYR	2.3
1	B	272	GLY	2.3
1	B	446	VAL	2.3
1	A	339	GLU	2.2
1	A	430	ILE	2.2
1	A	233	ALA	2.2
1	A	350	GLU	2.2
1	B	235	LEU	2.2
1	A	61	LEU	2.2
1	B	185	ARG	2.2
1	A	490	GLY	2.2
1	A	188	GLU	2.2
1	B	90	MET	2.2
1	B	341	PHE	2.1
1	B	164	ASP	2.1
1	B	276	LYS	2.1
1	B	350	GLU	2.1
1	B	315	GLN	2.1
1	A	431	LEU	2.1
1	B	433	VAL	2.1
1	A	436	VAL	2.1
1	B	462	VAL	2.1
1	B	216	ILE	2.0
1	B	231	ILE	2.0
1	B	88	ALA	2.0
1	A	217	TYR	2.0
1	A	377	LEU	2.0
1	A	534	ILE	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)

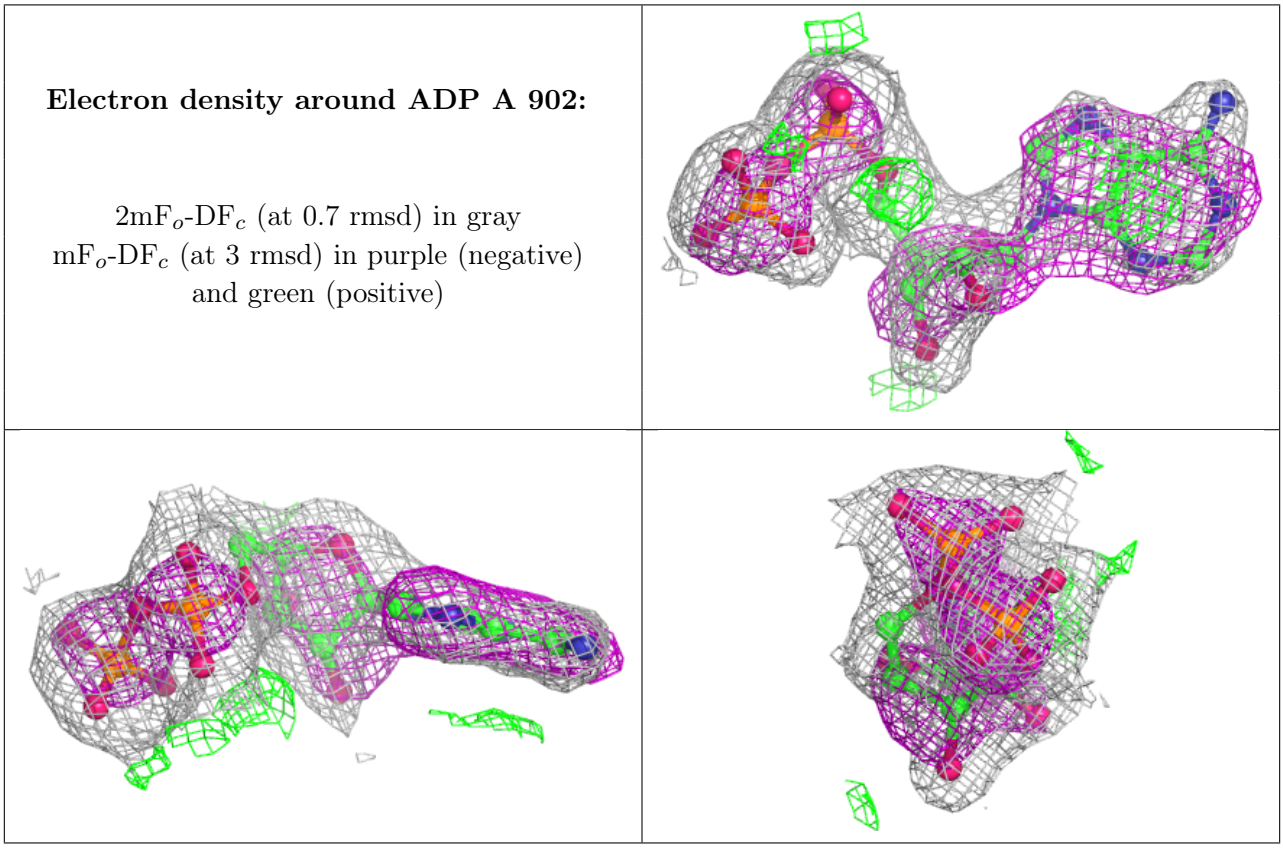
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ADP	A	902	27/27	0.95	0.23	50,56,62,62	0
2	ADP	B	906	27/27	0.95	0.19	54,58,62,62	0
2	ADP	A	900	27/27	0.96	0.15	57,66,66,67	0
2	ADP	B	904	27/27	0.97	0.13	37,49,52,52	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.

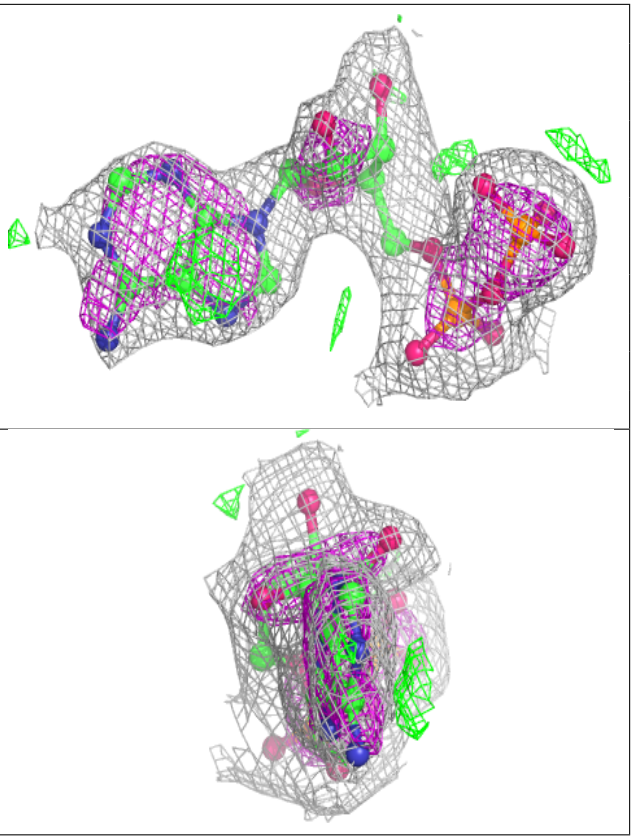
Electron density around ADP A 902:

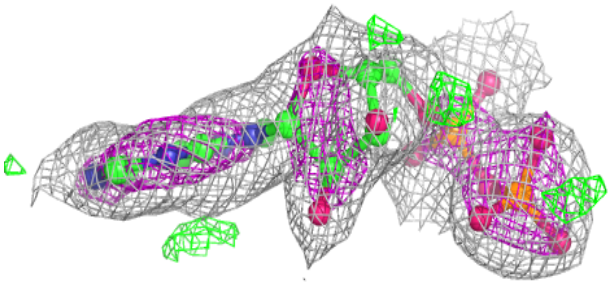
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP B 906:

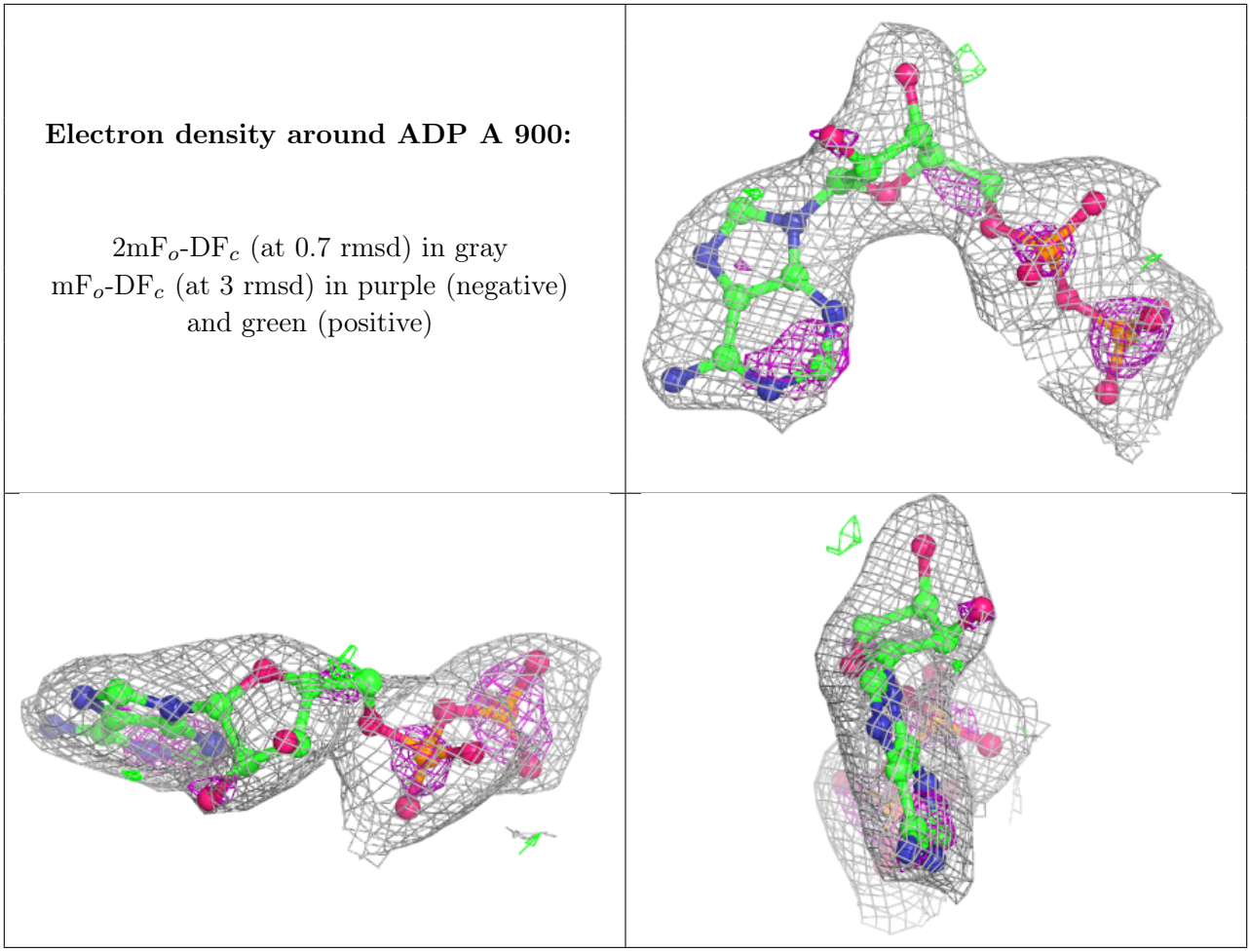
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





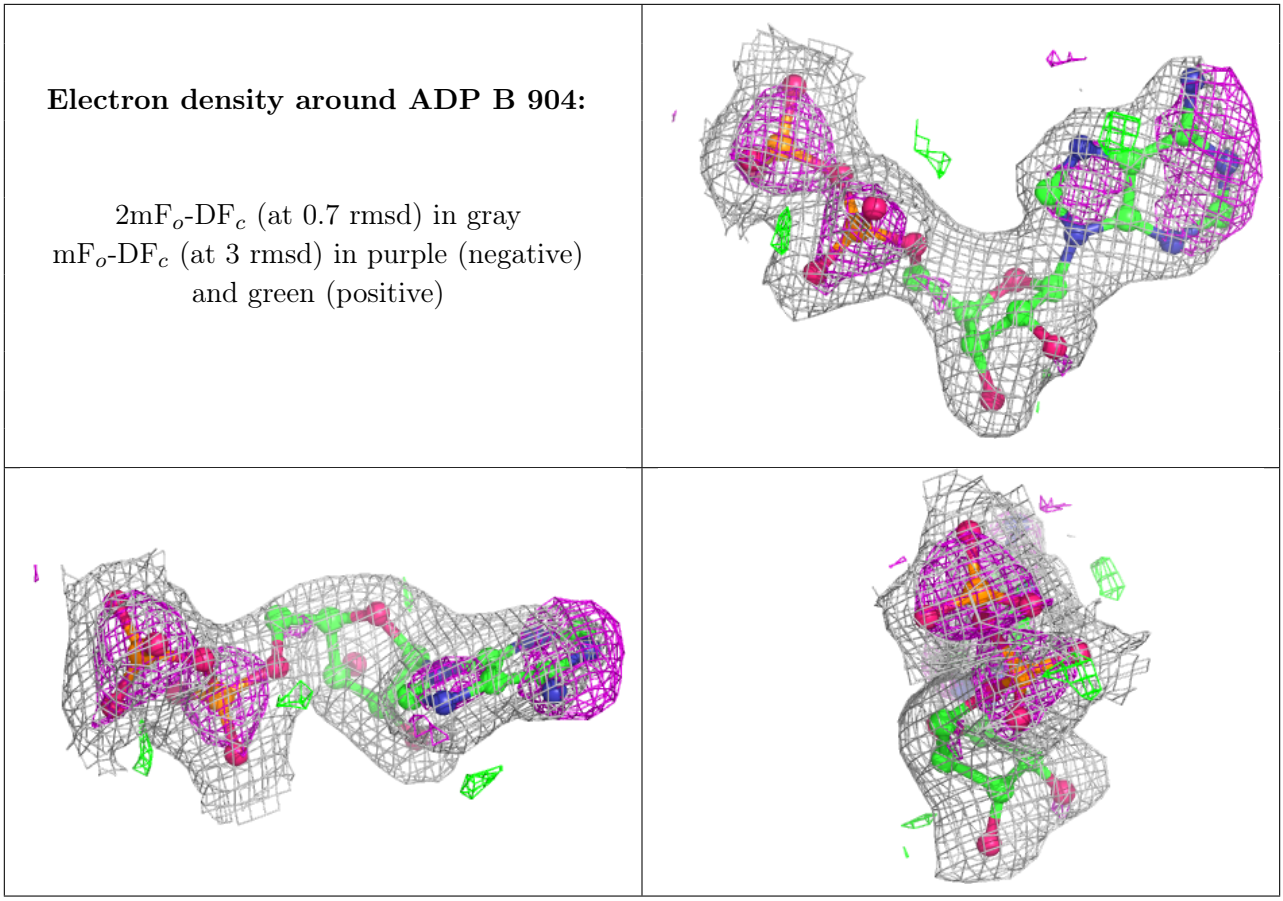
Electron density around ADP A 900:

$2mF_o$-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 904:

$2mF_o$-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.