



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UIE
Title : Crystal structure of adenosine 5'-phosphosulfate kinase from Arabidopsis Thaliana in Complex with AMPPNP and APS
Authors : Ravilious, G.E.; Jez, J.M.
Deposited on : 2011-11-04
Resolution : 1.79 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

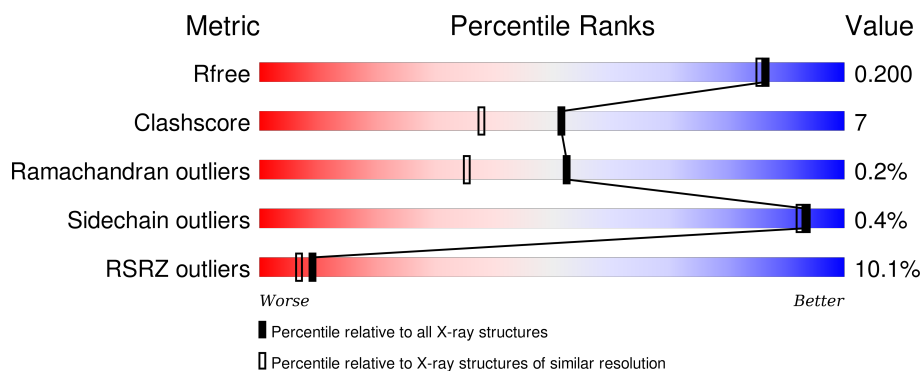
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	<div> <div>10%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	B	200	<div> <div>9%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	C	200	<div> <div>11%</div> <div>84%</div> <div>10%</div> <div>7%</div> </div>

2 Entry composition [i](#)

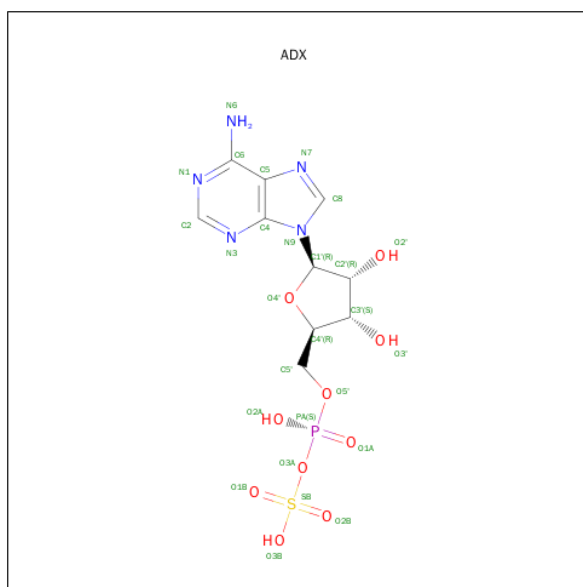
There are 5 unique types of molecules in this entry. The entry contains 5178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenylyl-sulfate kinase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	7	0
			1495	937	259	285	14			
1	B	197	Total	C	N	O	S	0	6	0
			1550	972	270	294	14			
1	C	187	Total	C	N	O	S	0	8	0
			1477	931	255	279	12			

- Molecule 2 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: C₁₀H₁₄N₅O₁₀PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			27	10	5	10	1 1		
2	B	1	Total	C	N	O	P S	0	0
			27	10	5	10	1 1		
2	C	1	Total	C	N	O	P S	0	0
			27	10	5	10	1 1		

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- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

- Molecule 5 is water.

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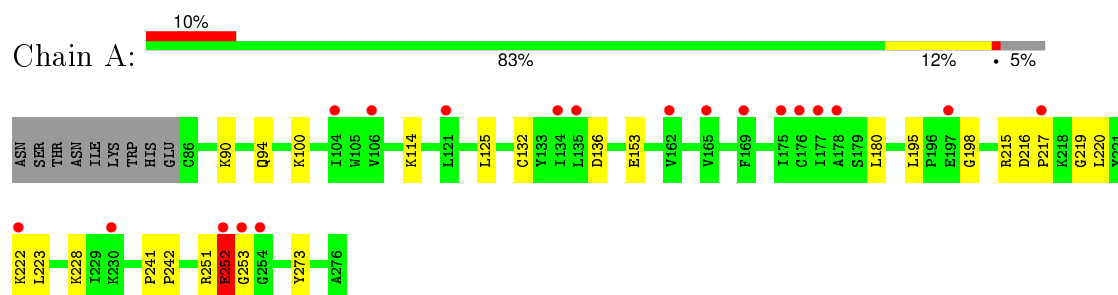
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	115	Total	O	0	0
			115	115		

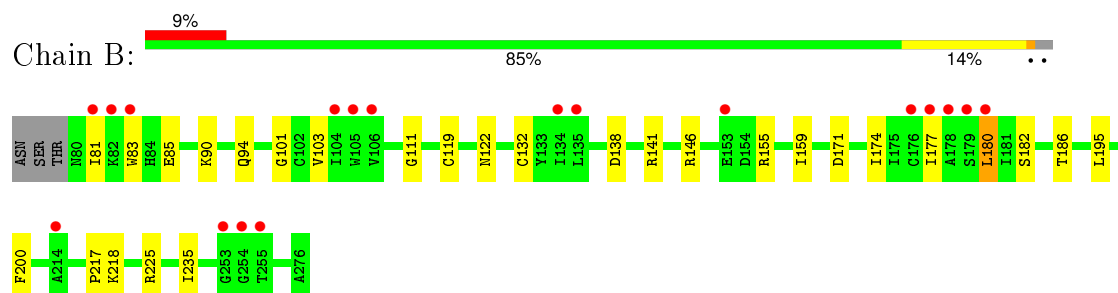
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

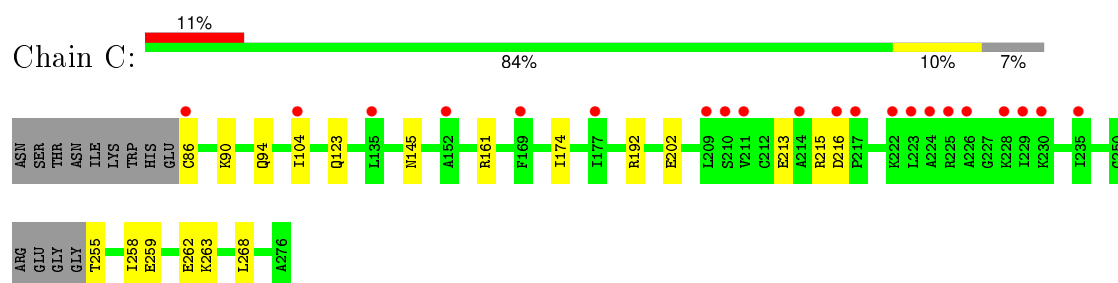
- Molecule 1: Adenylyl-sulfate kinase 1, chloroplastic



- Molecule 1: Adenylyl-sulfate kinase 1, chloroplastic



- Molecule 1: Adenylyl-sulfate kinase 1, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.14Å 95.31Å 73.33Å 90.00° 114.08° 90.00°	Depositor
Resolution (Å)	30.50 – 1.79 30.54 – 1.79	Depositor EDS
% Data completeness (in resolution range)	87.1 (30.50-1.79) 87.0 (30.54-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.173 , 0.201 0.172 , 0.200	Depositor DCC
R_{free} test set	3510 reflections (5.98%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 69365 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5178	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP, ADX

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	0.37	0/1532	0.70	3/2062 (0.1%)
1	B	0.35	0/1584	0.50	1/2133 (0.0%)
1	C	0.30	0/1519	0.46	0/2044
All	All	0.34	0/4635	0.56	4/6239 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLU	OE1-CD-OE2	-18.38	101.25	123.30
1	A	252	GLU	CG-CD-OE1	10.51	139.32	118.30
1	A	180	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	180	LEU	CA-CB-CG	5.50	127.95	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	1495	0	1514	22	2
1	B	1550	0	1552	27	0
1	C	1477	0	1509	16	0
2	A	27	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	13	1	0
2	C	27	0	13	0	0
3	A	31	0	13	3	0
3	B	31	0	13	1	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	177	0	0	3	0
5	B	187	0	0	7	0
5	C	115	0	0	2	0
All	All	5178	0	4653	64	2

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

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:B:174:ILE:HD11	1:C:174[A]:ILE:HD11	1.49	0.94
1:A:136:ASP:OD1	5:A:552:HOH:O	1.93	0.85
1:C:192[B]:ARG:NH2	1:C:202:GLU:OE1	2.13	0.80
1:B:111:GLY:H	3:B:302:ANP:HNB1	1.35	0.72
1:A:217:PRO:HG3	3:A:402:ANP:H4'	1.71	0.71
1:B:138:ASP:HB2	5:B:433:HOH:O	1.91	0.71
1:B:119[A]:CYS:SG	5:C:447:HOH:O	2.52	0.67
5:B:586:HOH:O	1:C:123:GLN:NE2	2.32	0.61
1:A:251:ARG:O	1:A:252:GLU:HB2	2.00	0.60
1:C:192[B]:ARG:HH22	1:C:202:GLU:CD	2.04	0.59
1:A:100:LYS:HB2	1:A:273:TYR:HD1	1.68	0.59
1:B:174:ILE:CD1	1:C:174[A]:ILE:HD11	2.28	0.58
1:C:255:THR:HA	5:C:485:HOH:O	2.02	0.57
1:B:90:LYS:HE3	5:B:496:HOH:O	2.06	0.56
1:A:251:ARG:O	1:A:252:GLU:CB	2.55	0.54
1:B:83:TRP:HD1	1:B:85:GLU:HG3	1.72	0.54
1:B:103:VAL:HG21	1:B:195:LEU:HD11	1.88	0.54
1:C:192[B]:ARG:HH21	1:C:202:GLU:HB2	1.74	0.53
1:A:153:GLU:CD	1:A:153:GLU:H	2.12	0.52
1:A:90:LYS:HE2	1:A:94:GLN:OE1	2.10	0.52
1:B:83:TRP:CD1	1:B:85:GLU:HG3	2.46	0.51
1:B:132[B]:CYS:SG	1:B:177:ILE:CD1	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:OD1	1:B:132[B]:CYS:HB3	2.12	0.49
1:B:122:ASN:OD1	1:B:132[A]:CYS:HB2	2.12	0.49
1:B:94:GLN:NE2	1:B:101:GLY:H	2.10	0.49
1:A:125:LEU:HD13	1:A:132[A]:CYS:SG	2.53	0.48
1:A:216:ASP:OD2	1:A:222:LYS:HE3	2.14	0.48
1:B:90:LYS:HD2	1:B:171:ASP:HA	1.95	0.48
1:C:192[B]:ARG:NH2	1:C:202:GLU:HB2	2.27	0.48
1:B:81:ILE:O	5:B:581:HOH:O	2.20	0.47
1:A:220:LEU:HD11	2:A:401:ADX:O2'	2.14	0.46
2:B:301:ADX:H3'	2:B:301:ADX:N3	2.31	0.46
1:B:225:ARG:CZ	1:B:235:ILE:HD12	2.46	0.46
1:B:159:ILE:HD13	1:B:180:LEU:HD23	1.98	0.46
1:C:90:LYS:O	1:C:94:GLN:HG3	2.16	0.46
1:C:145:ASN:OD1	1:C:161:ARG:HD2	2.16	0.45
1:A:219:GLY:O	1:A:222:LYS:HG2	2.17	0.45
1:A:198:GLY:O	1:A:273:TYR:OH	2.31	0.45
1:B:217:PRO:HG2	5:B:444:HOH:O	2.16	0.45
1:A:251:ARG:HB3	5:A:603:HOH:O	2.18	0.44
1:A:198:GLY:HA2	5:A:644:HOH:O	2.17	0.44
1:C:104[B]:ILE:HD11	1:C:268:LEU:HD11	2.00	0.44
1:C:215:ARG:O	1:C:216:ASP:C	2.56	0.43
1:B:141:ARG:O	1:B:146:ARG:HA	2.18	0.43
1:C:259:GLU:O	1:C:263:LYS:HG3	2.18	0.43
1:A:223:LEU:HD23	1:A:228:LYS:HD3	1.99	0.43
1:A:125:LEU:CD1	1:A:132[A]:CYS:SG	3.06	0.43
1:C:213:GLU:O	1:C:216:ASP:HB2	2.19	0.43
1:B:186[B]:THR:HG23	5:B:413:HOH:O	2.18	0.42
1:A:252:GLU:HG3	1:A:253:GLY:N	2.34	0.42
1:B:218:LYS:HE3	5:B:536:HOH:O	2.18	0.42
1:C:258:ILE:O	1:C:262:GLU:HG3	2.20	0.42
1:B:155:ARG:O	1:B:159:ILE:HG12	2.18	0.42
1:B:103:VAL:CG2	1:B:195:LEU:HD11	2.48	0.42
1:A:241:PRO:HA	1:A:242:PRO:HD3	1.97	0.42
1:B:159:ILE:HD12	1:B:182:SER:HB3	2.02	0.42
1:A:217:PRO:HG2	3:A:402:ANP:H5'2	2.02	0.41
1:B:132[B]:CYS:SG	1:B:177:ILE:HD11	2.60	0.41
1:A:217:PRO:CG	3:A:402:ANP:H4'	2.46	0.41
1:B:195:LEU:HD12	1:B:200:PHE:HD1	1.85	0.41
1:A:114:LYS:HE2	1:A:114:LYS:HB2	1.90	0.41
1:C:90:LYS:HE2	1:C:94:GLN:OE1	2.21	0.40
1:A:215:ARG:O	1:A:216:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HD11	1:B:182:SER:HA	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:CD	1:A:252:GLU:OE1[2_554]	1.26	0.94
1:A:252:GLU:OE1	1:A:252:GLU:OE2[2_554]	1.94	0.26

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	195/200 (98%)	190 (97%)	4 (2%)	1 (0%)	34	17
1	B	201/200 (100%)	196 (98%)	5 (2%)	0	100	100
1	C	191/200 (96%)	186 (97%)	5 (3%)	0	100	100
All	All	587/600 (98%)	572 (97%)	14 (2%)	1 (0%)	52	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLU

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	165/167 (99%)	164 (99%)	1 (1%)	90	88
1	B	169/167 (101%)	169 (100%)	0	100	100
1	C	164/167 (98%)	163 (99%)	1 (1%)	90	88
All	All	498/501 (99%)	496 (100%)	2 (0%)	93	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	C	86	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADX	A	401	-	22,29,29	1.51	4 (18%)	25,45,45	2.37	3 (12%)
3	ANP	A	402	4	27,33,33	3.58	10 (37%)	30,52,52	2.43	8 (26%)
2	ADX	B	301	-	22,29,29	1.54	3 (13%)	25,45,45	2.30	5 (20%)
3	ANP	B	302	4	27,33,33	3.76	10 (37%)	30,52,52	2.79	7 (23%)
2	ADX	C	301	-	22,29,29	1.46	4 (18%)	25,45,45	2.29	4 (16%)
3	ANP	C	302	4	27,33,33	3.83	9 (33%)	30,52,52	2.72	11 (36%)

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	ADX	A	401	-	-	0/6/32/32	0/3/3/3
3	ANP	A	402	4	-	0/12/38/38	0/3/3/3
2	ADX	B	301	-	-	0/6/32/32	0/3/3/3
3	ANP	B	302	4	-	1/12/38/38	0/3/3/3
2	ADX	C	301	-	-	0/6/32/32	0/3/3/3
3	ANP	C	302	4	-	0/12/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ADX	C2'-C3'	-4.68	1.40	1.53
2	A	401	ADX	C2'-C3'	-4.56	1.41	1.53
2	C	301	ADX	C2'-C3'	-4.38	1.41	1.53
3	B	302	ANP	C5'-C4'	-2.82	1.42	1.51
3	C	302	ANP	C2'-C3'	-2.74	1.45	1.53
3	C	302	ANP	C5'-C4'	-2.74	1.42	1.51
3	A	402	ANP	C5'-C4'	-2.73	1.42	1.51
3	A	402	ANP	C2'-C3'	-2.69	1.46	1.53
3	B	302	ANP	C2'-C3'	-2.61	1.46	1.53
2	B	301	ADX	C5'-C4'	-2.52	1.43	1.51
3	B	302	ANP	C3'-C4'	-2.32	1.46	1.53
3	B	302	ANP	PG-O3G	-2.25	1.50	1.56
2	A	401	ADX	C5'-C4'	-2.25	1.44	1.51
2	C	301	ADX	C5'-C4'	-2.23	1.44	1.51
3	A	402	ANP	C3'-C4'	-2.18	1.47	1.53
3	C	302	ANP	C3'-C4'	-2.17	1.47	1.53
3	A	402	ANP	O4'-C1'	-2.03	1.38	1.41
2	A	401	ADX	C2-N3	2.00	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ADX	C2-N3	2.13	1.36	1.32
3	A	402	ANP	PG-N3B	2.23	1.69	1.63
3	A	402	ANP	PB-O3A	2.36	1.62	1.59
3	C	302	ANP	PG-N3B	2.38	1.69	1.63
3	B	302	ANP	PG-N3B	2.45	1.69	1.63
2	C	301	ADX	C6-N6	2.56	1.42	1.34
2	B	301	ADX	C6-N6	2.65	1.43	1.34
2	A	401	ADX	C6-N6	2.70	1.43	1.34
3	B	302	ANP	PB-N3B	2.92	1.71	1.63
3	A	402	ANP	PB-N3B	2.95	1.71	1.63
3	C	302	ANP	PB-N3B	3.06	1.71	1.63
3	B	302	ANP	PB-O3A	3.34	1.63	1.59
3	C	302	ANP	PB-O3A	3.52	1.63	1.59
3	A	402	ANP	C6-N6	3.60	1.46	1.34
3	C	302	ANP	C6-N6	3.61	1.46	1.34
3	B	302	ANP	C6-N6	3.69	1.46	1.34
3	A	402	ANP	PB-O1B	9.79	1.57	1.46
3	B	302	ANP	PB-O1B	11.17	1.59	1.46
3	C	302	ANP	PB-O1B	11.34	1.59	1.46
3	A	402	ANP	PG-O1G	13.45	1.61	1.46
3	B	302	ANP	PG-O1G	13.47	1.61	1.46
3	C	302	ANP	PG-O1G	13.92	1.62	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ADX	N3-C2-N1	-10.06	121.19	128.89
2	A	401	ADX	N3-C2-N1	-9.98	121.26	128.89
2	B	301	ADX	N3-C2-N1	-9.73	121.45	128.89
3	C	302	ANP	N3-C2-N1	-9.59	121.56	128.89
3	B	302	ANP	N3-C2-N1	-9.00	122.00	128.89
3	B	302	ANP	O1B-PB-N3B	-8.82	98.38	111.90
3	A	402	ANP	N3-C2-N1	-8.72	122.22	128.89
3	C	302	ANP	O1B-PB-N3B	-5.38	103.65	111.90
3	C	302	ANP	O3A-PB-N3B	-4.87	93.04	106.44
3	A	402	ANP	O3A-PB-N3B	-4.14	95.05	106.44
3	C	302	ANP	O2G-PG-O1G	-3.66	103.76	113.49
3	B	302	ANP	O2G-PG-O1G	-3.20	104.97	113.49
3	A	402	ANP	O2G-PG-O1G	-3.07	105.32	113.49
3	A	402	ANP	C2'-C1'-N9	-3.04	109.65	114.29
3	A	402	ANP	O1G-PG-N3B	-2.86	107.52	111.90
3	B	302	ANP	O3A-PB-N3B	-2.64	99.18	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ADX	O2'-C2'-C3'	-2.61	103.35	111.83
3	C	302	ANP	O1G-PG-N3B	-2.50	108.07	111.90
3	A	402	ANP	O1B-PB-N3B	-2.34	108.32	111.90
2	B	301	ADX	C4-C5-N7	-2.31	107.35	109.48
2	B	301	ADX	C5'-C4'-C3'	-2.31	106.06	115.21
3	B	302	ANP	PA-O3A-PB	-2.23	125.17	132.67
3	C	302	ANP	C4-C5-N7	-2.05	107.59	109.48
2	C	301	ADX	C4-C5-N7	-2.05	107.59	109.48
3	C	302	ANP	C1'-N9-C4	-2.03	123.88	126.94
3	C	302	ANP	O5'-C5'-C4'	2.03	116.59	109.12
3	A	402	ANP	O2A-PA-O3A	2.03	114.32	105.09
2	B	301	ADX	O5'-C5'-C4'	2.04	116.65	109.12
3	C	302	ANP	O4'-C1'-N9	2.15	112.60	108.10
2	C	301	ADX	O4'-C1'-N9	2.18	112.65	108.10
2	C	301	ADX	O5'-C5'-C4'	2.20	117.22	109.12
3	C	302	ANP	O2B-PB-O3A	2.23	115.21	105.09
2	A	401	ADX	O2A-PA-O3A	2.26	112.99	104.94
3	B	302	ANP	O2A-PA-O3A	2.62	116.98	105.09
2	A	401	ADX	O4'-C1'-N9	2.85	114.06	108.10
3	B	302	ANP	O2B-PB-O1B	3.79	117.91	110.00
3	C	302	ANP	O2B-PB-O1B	3.93	118.20	110.00
3	A	402	ANP	O2B-PB-O1B	4.05	118.45	110.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	ANP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADX	1	0
3	A	402	ANP	3	0
2	B	301	ADX	1	0
3	B	302	ANP	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/200 (95%)	0.29	19 (9%) 9 7	22, 30, 58, 105	0
1	B	197/200 (98%)	0.20	18 (9%) 11 9	25, 36, 56, 69	0
1	C	187/200 (93%)	0.42	21 (11%) 7 5	27, 41, 79, 107	0
All	All	575/600 (95%)	0.30	58 (10%) 9 7	22, 36, 67, 107	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLY	7.6
1	A	253	GLY	6.6
1	C	214	ALA	6.3
1	C	226	ALA	5.1
1	C	229	ILE	4.6
1	B	135	LEU	4.2
1	C	86	CYS	4.1
1	B	106	VAL	3.7
1	C	228	LYS	3.7
1	B	180	LEU	3.5
1	A	252	GLU	3.4
1	A	177	ILE	3.4
1	A	106	VAL	3.3
1	C	223	LEU	3.1
1	A	135	LEU	3.1
1	B	254	GLY	3.0
1	A	169	PHE	2.9
1	C	135	LEU	2.9
1	C	222	LYS	2.9
1	A	134	ILE	2.8
1	A	104	ILE	2.8
1	C	104[A]	ILE	2.8
1	A	162	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	2.7
1	B	179[A]	SER	2.7
1	C	230	LYS	2.6
1	C	210	SER	2.6
1	B	177	ILE	2.6
1	B	255	THR	2.5
1	B	178	ALA	2.5
1	A	230	LYS	2.5
1	C	216	ASP	2.5
1	A	197	GLU	2.4
1	A	178	ALA	2.4
1	B	104	ILE	2.4
1	A	217	PRO	2.4
1	A	121	LEU	2.3
1	B	153	GLU	2.3
1	B	82	LYS	2.3
1	B	81	ILE	2.3
1	B	214	ALA	2.3
1	B	176	CYS	2.3
1	C	217	PRO	2.3
1	B	134	ILE	2.2
1	A	222	LYS	2.2
1	C	225	ARG	2.2
1	C	211	VAL	2.2
1	B	105	TRP	2.2
1	C	152	ALA	2.2
1	C	169	PHE	2.1
1	B	253	GLY	2.1
1	A	176	CYS	2.1
1	C	177	ILE	2.1
1	C	224	ALA	2.1
1	A	165	VAL	2.1
1	C	209	LEU	2.1
1	C	235	ILE	2.1
1	B	83	TRP	2.0

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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADX	B	301	27/27	0.97	0.10	-0.12	29,44,62,81	0
3	ANP	B	302	31/31	0.97	0.10	-0.20	29,39,60,66	0
3	ANP	C	302	31/31	0.96	0.10	-0.21	31,44,60,64	0
2	ADX	A	401	27/27	0.97	0.09	-0.27	24,37,51,75	0
3	ANP	A	402	31/31	0.98	0.09	-0.48	26,34,54,63	0
4	MG	C	303	1/1	0.95	0.08	-0.92	44,44,44,44	0
2	ADX	C	301	27/27	0.97	0.07	-1.02	32,46,54,58	0
4	MG	A	403	1/1	0.98	0.04	-	32,32,32,32	0
4	MG	B	303	1/1	0.97	0.07	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.