



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:47 am BST

PDB ID : 4K2R
Title : Structural basis for activation of ZAP-70 by phosphorylation of the SH2-kinase linker
Authors : Yan, Q.; Barros, T.; Visperas, P.R.; Deindl, S.; Kadlecsek, T.A.; Weiss, A.; Kuriyan, J.
Deposited on : 2013-04-09
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

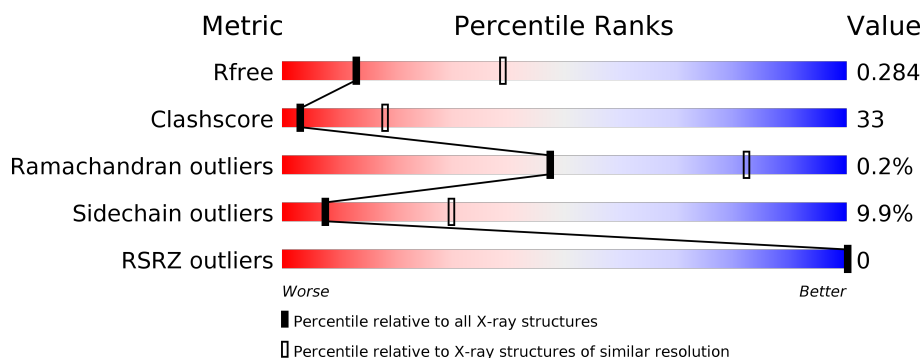
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	614	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4435 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 Tyrosine-protein kinase ZAP-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4398	2815	758	789	36			

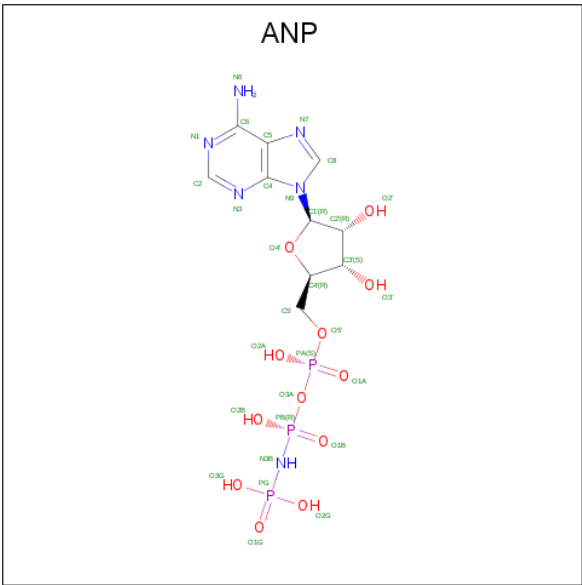
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	ASN	ASP	ENGINEERED MUTATION	UNP P43403
A	607	GLY	-	EXPRESSION TAG	UNP P43403
A	608	SER	-	EXPRESSION TAG	UNP P43403
A	609	GLY	-	EXPRESSION TAG	UNP P43403
A	610	LEU	-	EXPRESSION TAG	UNP P43403
A	611	GLU	-	EXPRESSION TAG	UNP P43403
A	612	VAL	-	EXPRESSION TAG	UNP P43403
A	613	LEU	-	EXPRESSION TAG	UNP P43403
A	614	PHE	-	EXPRESSION TAG	UNP P43403

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

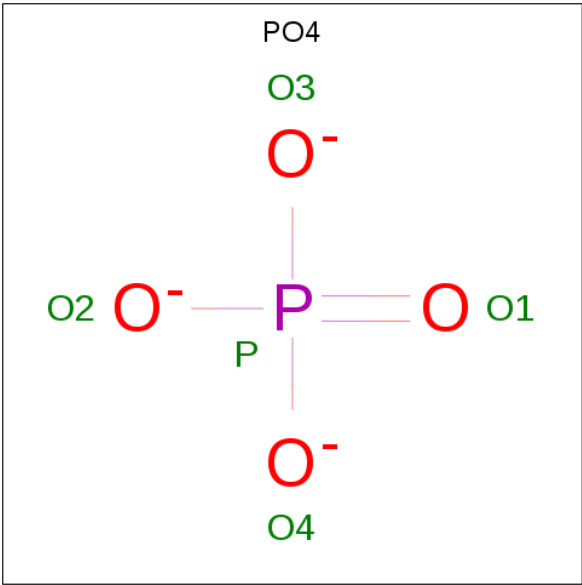
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

These plots are drawn for all protein, RNA and DNA 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.

- Chain A: 47% 37% 6% 10%

Residue	Protein Structure	Sequence
L571	TYR	E408
M572	THR	A409
S573	ALA	L330
D574	ARG	L412
C575	SER	E415
M576	ALA	E415
I577	GLY	G419
L578	LYS	F425
R583	W501	F425
F586	L503	R430
L587	K504	E431
E590	A507	E432
Q591	C510	I433
R594	R514	N437
Y597	K515	E440
S599	L441	L441
L600	S518	L442
V604	R519	H443
B605	S520	Q444
S608	D521	V445
G609	S446	S446
L610	M523	N447
F614	G448	G448
	M449	M449
	K450	K362
	S534	K369
	Y535	V370
	Y540	E454
	K541	Y451
	K542	L452
	M543	E453
	K544	E454
	G545	R460
	F546	N461
	E547	N466
	V548	E381
	M549	E382
	A550	R383
	F551	M384
	K556	R385
	R557	D311
	M558	A387
	E559	Q388
	C560	I389
	P561	Q392
	F563	L393
	C564	A394
	P565	I395
	E567	G396
	L568	A397
	V569	I398
	A570	ASP
	L571	ASP
	L572	ASP
	L573	ASP
	L574	ASP
	L575	ASP
	L576	ASP
	L577	ASP
	L578	ASP
	L579	ASP
	L580	ASP
	L581	ASP
	L582	ASP
	L583	ASP
	L584	ASP
	L585	ASP
	L586	ASP
	L587	ASP
	L588	ASP
	L589	ASP
	L590	ASP
	L591	ASP
	L592	ASP
	L593	ASP
	L594	ASP
	L595	ASP
	L596	ASP
	L597	ASP
	L598	ASP
	L599	ASP
	L600	ASP
	L601	ASP
	L602	ASP
	L603	ASP
	L604	ASP
	L605	ASP
	L606	ASP
	L607	ASP
	L608	ASP
	L609	ASP
	L610	ASP
	L611	ASP
	L612	ASP
	L613	ASP
	L614	ASP
	L615	ASP
	L616	ASP
	L617	ASP
	L618	ASP
	L619	ASP
	L620	ASP
	L621	ASP
	L622	ASP
	L623	ASP
	L624	ASP
	L625	ASP
	L626	ASP
	L627	ASP
	L628	ASP
	L629	ASP
	L630	ASP
	L631	ASP
	L632	ASP
	L633	ASP
	L634	ASP
	L635	ASP
	L636	ASP
	L637	ASP
	L638	ASP
	L639	ASP
	L640	ASP
	L641	ASP
	L642	ASP
	L643	ASP
	L644	ASP
	L645	ASP
	L646	ASP
	L647	ASP
	L648	ASP
	L649	ASP
	L650	ASP
	L651	ASP
	L652	ASP
	L653	ASP
	L654	ASP
	L655	ASP
	L656	ASP
	L657	ASP
	L658	ASP
	L659	ASP
	L660	ASP
	L661	ASP
	L662	ASP
	L663	ASP
	L664	ASP
	L665	ASP
	L666	ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.53Å 53.15Å 68.96Å 106.10° 93.26° 104.40°	Depositor
Resolution (Å)	49.09 – 3.00 49.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (49.09-3.00) 93.9 (49.09-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.287 0.209 , 0.284	Depositor DCC
R_{free} test set	579 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4435	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ANP, MG

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	0.64	2/4507 (0.0%)	0.71	0/6081

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	TRP	CD2-CE2	5.55	1.48	1.41
1	A	233	TRP	CD2-CE2	5.14	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4398	0	4374	294	0
2	A	1	0	0	0	0
3	A	31	0	13	0	0
4	A	5	0	0	0	0
All	All	4435	0	4387	294	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 33.

The worst 5 of 294 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:2:PRO:HD2	1:A:150:GLU:OE1	1.39	1.19
1:A:108:LEU:HD23	1:A:109:GLU:N	1.58	1.19
1:A:133:LEU:O	1:A:134:GLU:HG2	1.47	1.12
1:A:375:THR:HG22	1:A:377:LYS:O	1.48	1.12
1:A:519:ARG:CG	1:A:519:ARG:HH11	1.70	1.03

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	545/614 (89%)	493 (90%)	51 (9%)	1 (0%)	47 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

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	466/521 (89%)	420 (90%)	46 (10%)	8 30

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	ARG
1	A	384	MET
1	A	564	CYS
1	A	356	VAL
1	A	372	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	363	GLN
1	A	392	GLN
1	A	140	GLN
1	A	388	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	702	2	29,33,33	1.92	6 (20%)	31,52,52	1.79	8 (25%)
4	PO4	A	703	-	4,4,4	0.81	0	6,6,6	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	702	2	-	4/14/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ANP	PG-N3B	4.67	1.75	1.63
3	A	702	ANP	PB-N3B	4.39	1.74	1.63
3	A	702	ANP	PB-O3A	4.10	1.64	1.59
3	A	702	ANP	C5-C4	3.07	1.49	1.40
3	A	702	ANP	C2-N3	2.55	1.36	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ANP	C3'-C2'-C1'	4.21	107.32	100.98
3	A	702	ANP	O1B-PB-N3B	-3.47	106.66	111.77
3	A	702	ANP	N3-C2-N1	-3.33	123.47	128.68
3	A	702	ANP	O2B-PB-O3A	3.19	115.30	104.64
3	A	702	ANP	C4-C5-N7	-2.47	106.82	109.40

There are no chirality outliers.

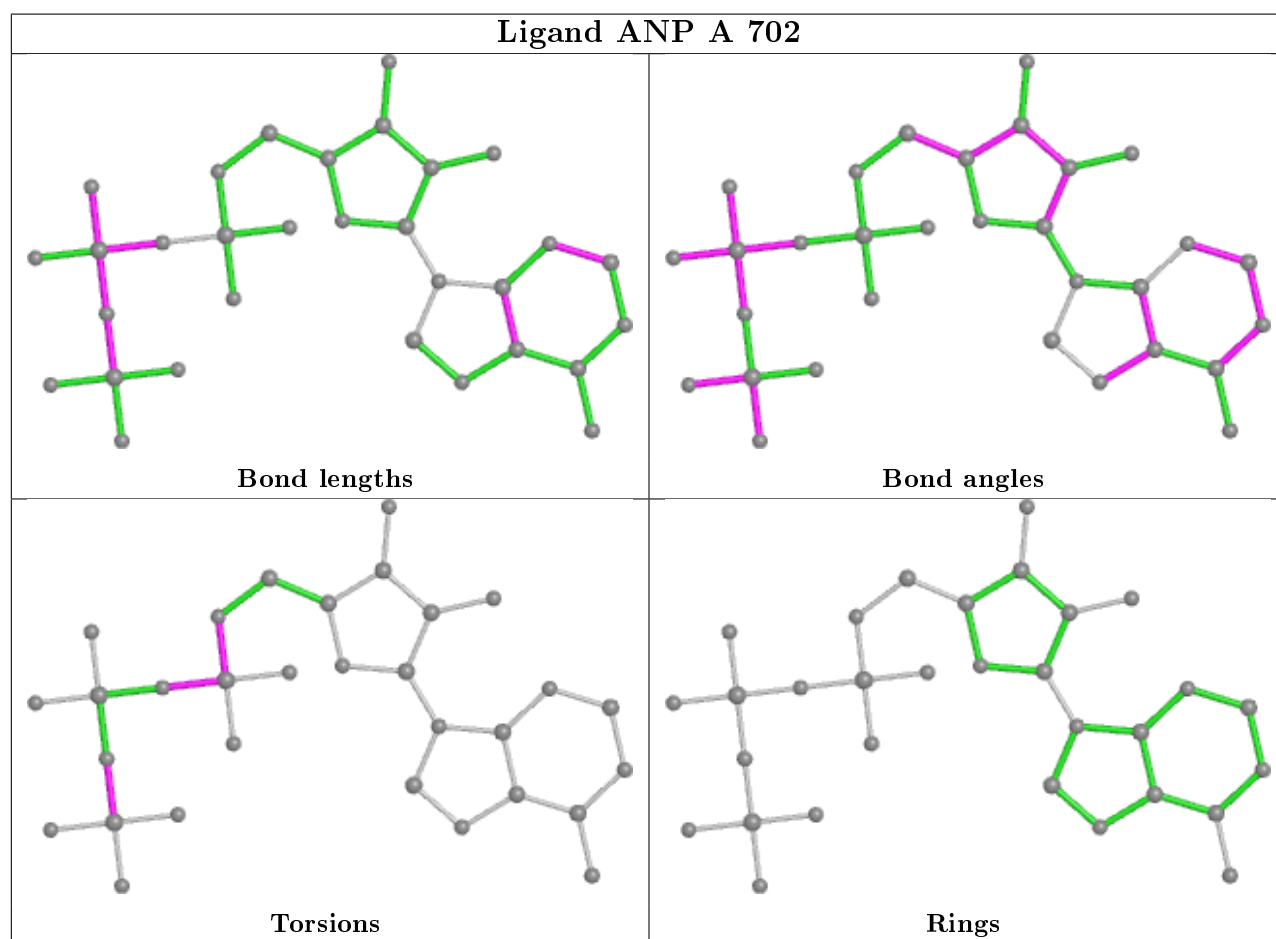
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ANP	PB-N3B-PG-O1G
3	A	702	ANP	PB-O3A-PA-O5'
3	A	702	ANP	C5'-O5'-PA-O3A
3	A	702	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/614 (89%)	-0.50	0 100 100	22, 46, 79, 111	0

There are no RSRZ outliers to report.

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](#)

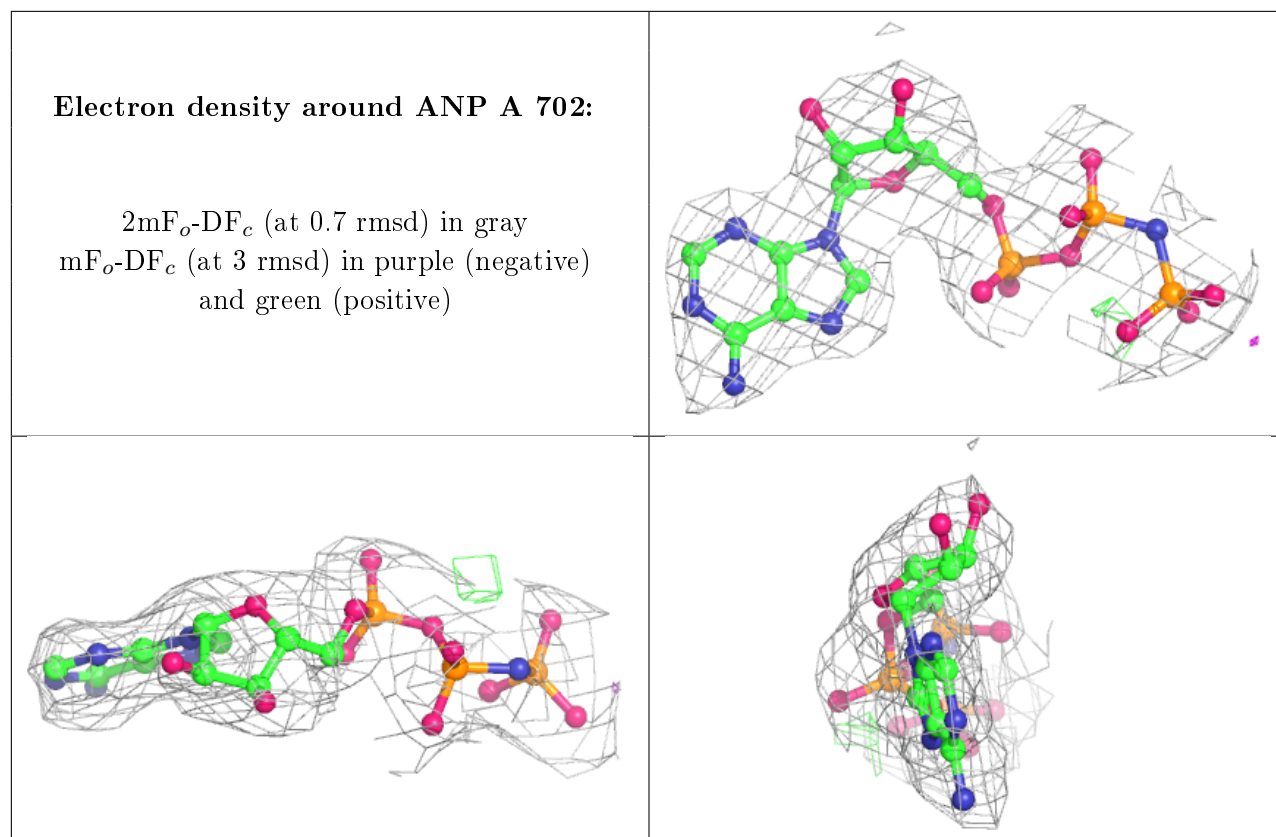
There are no carbohydrates in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	A	703	5/5	0.94	0.22	72,81,81,87	0
3	ANP	A	702	31/31	0.95	0.16	31,39,50,51	0
2	MG	A	701	1/1	0.97	0.07	32,32,32,32	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.