WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 02:16 PM JST

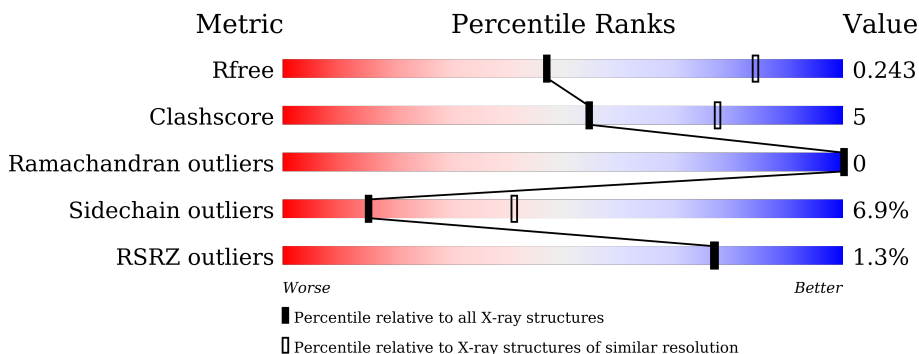|		
PDB ID	:	7CTX
Title	:	Crystal structure of Arabidopsis thaliana SOBIR1 kinase domain(residues 388-401 deleted) in complex with AMP-PNP and magnesium
Authors	:	Wei, X.; Wang, Y.L.; Gu, T.Y.; Xin, F.J.
Deposited on	:	2020-08-20
Resolution	:	2.91 Å(reported)

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 2.91 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		6.9%
RSRZ outliers		1.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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	323	.% 76% 13% · 9%
1	B	323	2% 77% 14% · 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	702	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4598 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 Leucine-rich repeat receptor-like serine/threonine/tyrosine-pr otein kinase SOBIR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total 2252	C 1445	N 379	O 413	S 15	0	0	0
1	B	299	Total 2282	C 1458	N 390	O 419	S 15	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	MET	-	initiating methionine	UNP Q9SKB2
A	306	GLY	-	expression tag	UNP Q9SKB2
A	307	SER	-	expression tag	UNP Q9SKB2
A	308	SER	-	expression tag	UNP Q9SKB2
A	309	HIS	-	expression tag	UNP Q9SKB2
A	310	HIS	-	expression tag	UNP Q9SKB2
A	311	HIS	-	expression tag	UNP Q9SKB2
A	312	HIS	-	expression tag	UNP Q9SKB2
A	313	HIS	-	expression tag	UNP Q9SKB2
A	314	HIS	-	expression tag	UNP Q9SKB2
A	315	SER	-	expression tag	UNP Q9SKB2
A	316	SER	-	expression tag	UNP Q9SKB2
A	317	GLY	-	expression tag	UNP Q9SKB2
A	318	LEU	-	expression tag	UNP Q9SKB2
A	319	VAL	-	expression tag	UNP Q9SKB2
A	320	PRO	-	expression tag	UNP Q9SKB2
A	321	ARG	-	expression tag	UNP Q9SKB2
A	322	GLY	-	expression tag	UNP Q9SKB2
A	323	SER	-	expression tag	UNP Q9SKB2
A	324	HIS	-	expression tag	UNP Q9SKB2
A	325	MET	-	expression tag	UNP Q9SKB2
A	?	-	LEU	deletion	UNP Q9SKB2
A	?	-	THR	deletion	UNP Q9SKB2
A	?	-	ASP	deletion	UNP Q9SKB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q9SKB2
A	?	-	ASP	deletion	UNP Q9SKB2
A	?	-	SER	deletion	UNP Q9SKB2
A	?	-	LYS	deletion	UNP Q9SKB2
A	?	-	PHE	deletion	UNP Q9SKB2
A	?	-	LEU	deletion	UNP Q9SKB2
A	?	-	ASN	deletion	UNP Q9SKB2
A	?	-	LYS	deletion	UNP Q9SKB2
A	?	-	LYS	deletion	UNP Q9SKB2
A	?	-	MET	deletion	UNP Q9SKB2
B	305	MET	-	initiating methionine	UNP Q9SKB2
B	306	GLY	-	expression tag	UNP Q9SKB2
B	307	SER	-	expression tag	UNP Q9SKB2
B	308	SER	-	expression tag	UNP Q9SKB2
B	309	HIS	-	expression tag	UNP Q9SKB2
B	310	HIS	-	expression tag	UNP Q9SKB2
B	311	HIS	-	expression tag	UNP Q9SKB2
B	312	HIS	-	expression tag	UNP Q9SKB2
B	313	HIS	-	expression tag	UNP Q9SKB2
B	314	HIS	-	expression tag	UNP Q9SKB2
B	315	SER	-	expression tag	UNP Q9SKB2
B	316	SER	-	expression tag	UNP Q9SKB2
B	317	GLY	-	expression tag	UNP Q9SKB2
B	318	LEU	-	expression tag	UNP Q9SKB2
B	319	VAL	-	expression tag	UNP Q9SKB2
B	320	PRO	-	expression tag	UNP Q9SKB2
B	321	ARG	-	expression tag	UNP Q9SKB2
B	322	GLY	-	expression tag	UNP Q9SKB2
B	323	SER	-	expression tag	UNP Q9SKB2
B	324	HIS	-	expression tag	UNP Q9SKB2
B	325	MET	-	expression tag	UNP Q9SKB2
B	?	-	LEU	deletion	UNP Q9SKB2
B	?	-	THR	deletion	UNP Q9SKB2
B	?	-	ASP	deletion	UNP Q9SKB2
B	?	-	GLU	deletion	UNP Q9SKB2
B	?	-	ASP	deletion	UNP Q9SKB2
B	?	-	SER	deletion	UNP Q9SKB2
B	?	-	LYS	deletion	UNP Q9SKB2
B	?	-	PHE	deletion	UNP Q9SKB2
B	?	-	LEU	deletion	UNP Q9SKB2
B	?	-	ASN	deletion	UNP Q9SKB2
B	?	-	LYS	deletion	UNP Q9SKB2

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q9SKB2
B	?	-	MET	deletion	UNP Q9SKB2

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
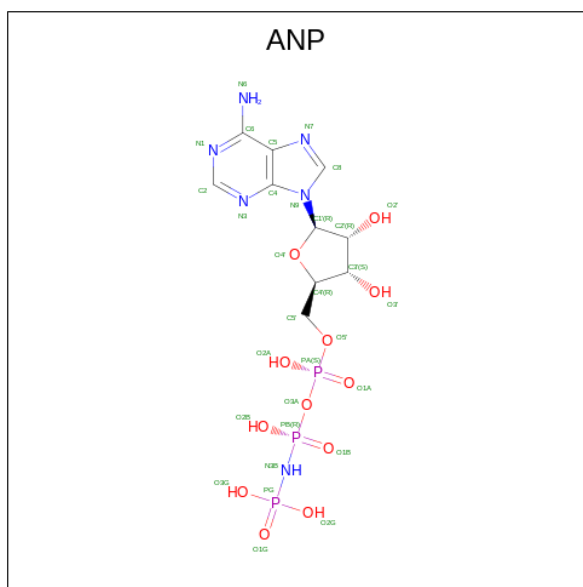
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	31	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	31	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

3 Residue-property plots ⓘ

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: Leucine-rich repeat receptor-like serine/threonine/tyrosine-protein kinase SO-BIR1

Chain A:

• Molecule 1: Leucine-rich repeat receptor-like serine/threonine/tyrosine-protein kinase SO-BIR1

Chain B:
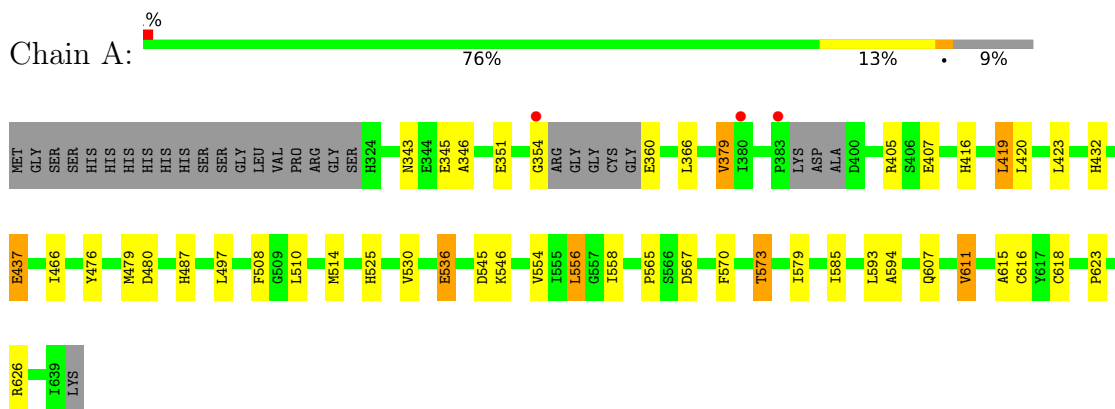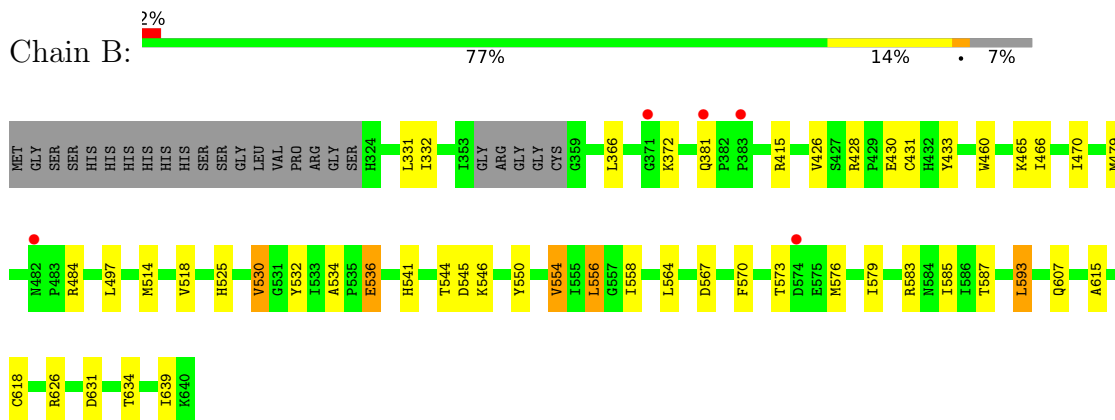
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.39Å 50.73Å 93.07Å 90.00° 106.65° 90.00°	Depositor
Resolution (Å)	28.63 – 2.91 29.35 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.63-2.91) 98.1 (29.35-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.225 , 0.243 0.224 , 0.243	Depositor DCC
R_{free} test set	725 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.0	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5494e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: MG, ANP

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	0.26	0/2300	0.42	0/3127
1	B	0.26	0/2330	0.42	0/3167
All	All	0.26	0/4630	0.42	0/6294

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	2252	0	2202	21	0
1	B	2282	0	2226	27	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	4598	0	4454	47	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.

The worst 5 of 47 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:426:VAL:HG22	1:B:433:TYR:HB2	1.81	0.61
1:B:460:TRP:HE1	1:B:607:GLN:HG2	1.68	0.58
1:A:554:VAL:HG22	1:A:579:ILE:HD11	1.85	0.57
1:A:416:HIS:HB3	1:A:419:LEU:HB2	1.86	0.57
1:B:556:LEU:HB3	1:B:615:ALA:HB2	1.89	0.55

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	289/323 (90%)	282 (98%)	7 (2%)	0	100	100
1	B	295/323 (91%)	290 (98%)	5 (2%)	0	100	100
All	All	584/646 (90%)	572 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2　Protein sidechains ⓘ

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	237/280 (85%)	217 (92%)	20 (8%)	11	31
1	B	238/280 (85%)	225 (94%)	13 (6%)	21	53

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	475/560 (85%)	442 (93%)	33 (7%)	15 41

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	554	VAL
1	B	556	LEU
1	B	593	LEU
1	A	536	GLU
1	A	530	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
2	ANP	B	701	3	29,33,33	4.86	15 (51%)	31,52,52	2.47	5 (16%)
2	ANP	A	701	3	29,33,33	4.90	15 (51%)	31,52,52	2.54	5 (16%)

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	ANP	B	701	3	-	9/14/38/38	0/3/3/3
2	ANP	A	701	3	-	9/14/38/38	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ANP	C2'-C1'	-16.49	1.28	1.53
2	B	701	ANP	C2'-C1'	-16.33	1.29	1.53
2	A	701	ANP	O4'-C1'	15.12	1.62	1.41
2	B	701	ANP	O4'-C1'	14.93	1.61	1.41
2	B	701	ANP	PB-O2B	-5.36	1.42	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	ANP	C5-C6-N6	9.24	134.40	120.35
2	B	701	ANP	C5-C6-N6	9.07	134.14	120.35
2	A	701	ANP	N6-C6-N1	-6.24	105.61	118.57
2	B	701	ANP	N6-C6-N1	-6.05	106.01	118.57
2	B	701	ANP	N3-C2-N1	-5.58	119.96	128.68

There are no chirality outliers.
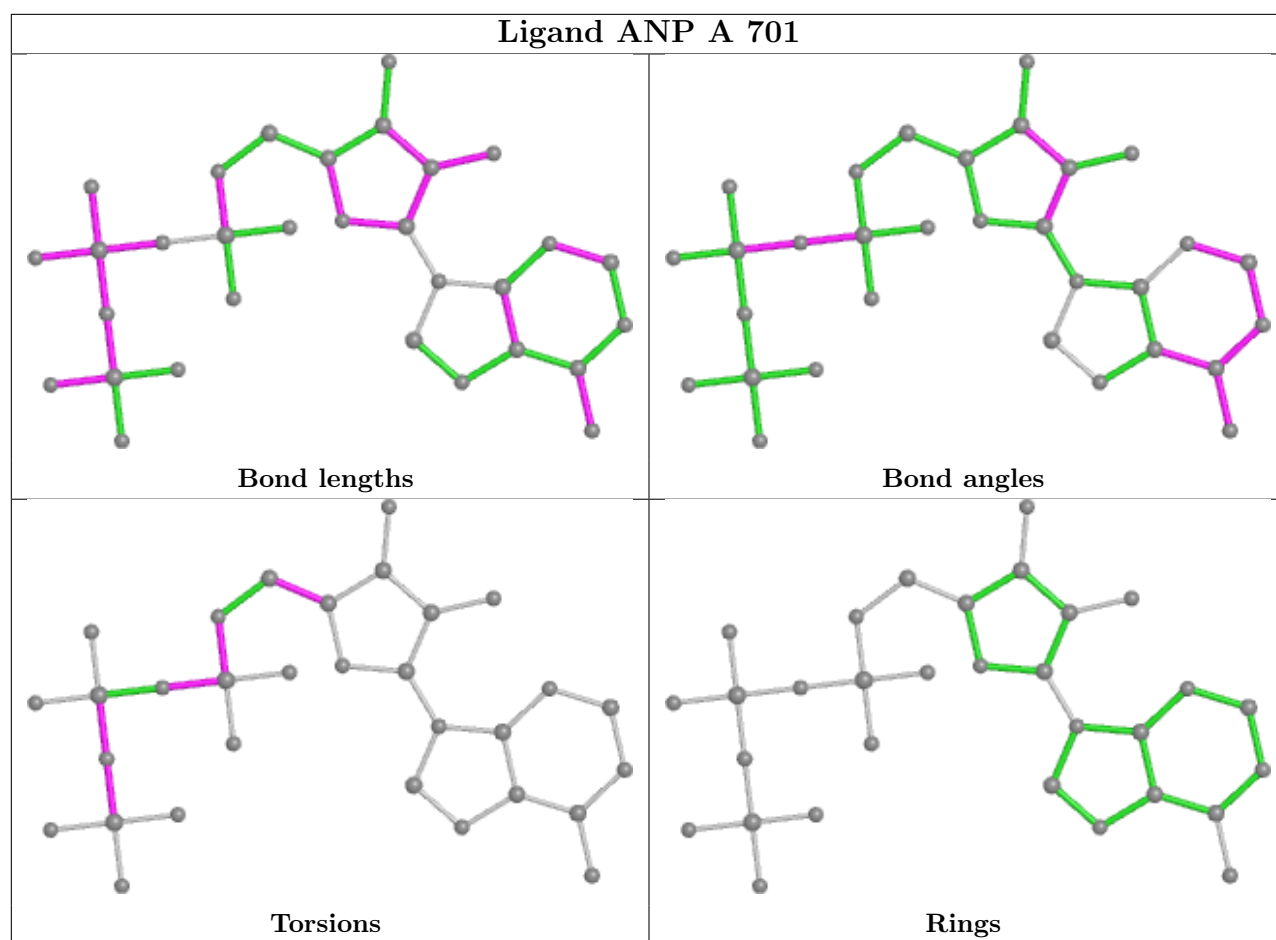
5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PB-N3B-PG-O1G
2	A	701	ANP	PG-N3B-PB-O1B
2	A	701	ANP	PG-N3B-PB-O3A
2	A	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	O4'-C4'-C5'-O5'

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 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 ANP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP A 701

Bond lengths

Bond angles

Torsions

Rings
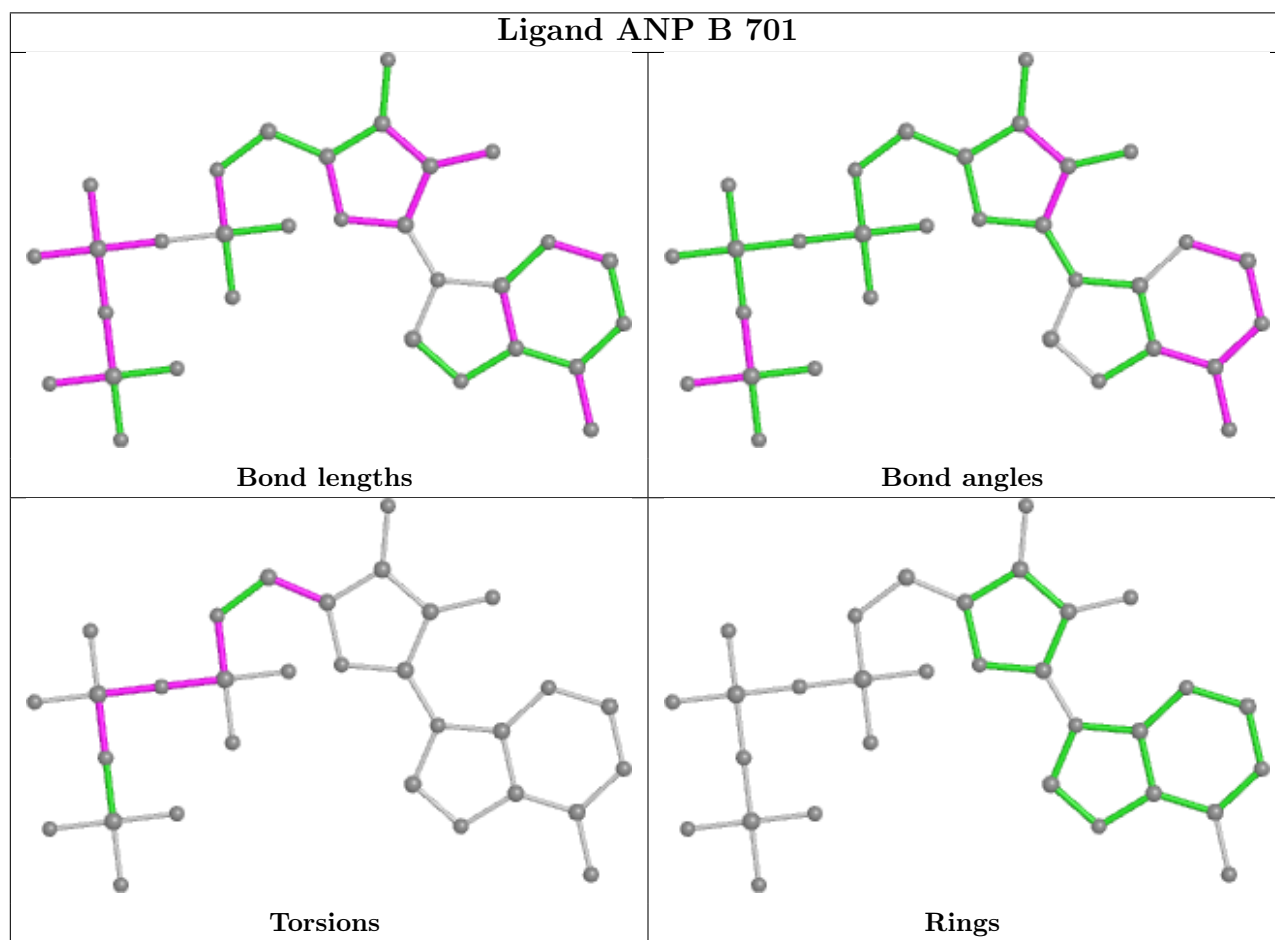
5.7 Other polymers ⓘ

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, 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	295/323 (91%)	-0.33	3 (1%)	82	82	35, 55, 88, 131	0
1	B	299/323 (92%)	-0.23	5 (1%)	70	69	33, 60, 98, 129	0
All	All	594/646 (91%)	-0.28	8 (1%)	77	77	33, 57, 95, 131	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	PRO	3.3
1	B	371	GLY	3.2
1	A	354	GLY	3.2
1	A	380	ILE	3.1
1	B	574	ASP	2.5

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 ⓘ

LIGAND-RSR INFOmissingINFO

6.5 Other polymers ⓘ

There are no such residues in this entry.