



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3Q5I / pdb_00003q5i
Title : Crystal Structure of PBANKA_031420
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sortium (SGC)
Deposited on : 2010-12-28
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

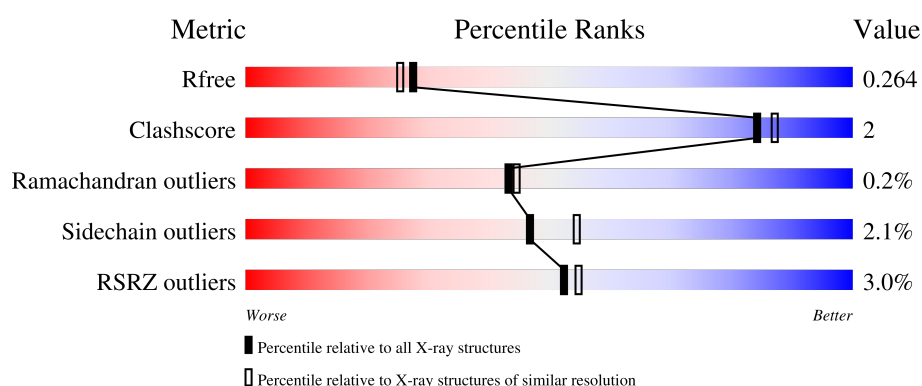
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	504	3% 88% 5% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4011 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 Protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	12	0
			3751	2405	621	706	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP Q4YRR5
A	21	HIS	-	expression tag	UNP Q4YRR5
A	22	HIS	-	expression tag	UNP Q4YRR5
A	23	HIS	-	expression tag	UNP Q4YRR5
A	24	HIS	-	expression tag	UNP Q4YRR5
A	25	HIS	-	expression tag	UNP Q4YRR5
A	26	HIS	-	expression tag	UNP Q4YRR5
A	27	SER	-	expression tag	UNP Q4YRR5
A	28	SER	-	expression tag	UNP Q4YRR5
A	29	GLY	-	expression tag	UNP Q4YRR5
A	30	ARG	-	expression tag	UNP Q4YRR5
A	31	GLU	-	expression tag	UNP Q4YRR5
A	32	ASN	-	expression tag	UNP Q4YRR5
A	33	LEU	-	expression tag	UNP Q4YRR5
A	34	TYR	-	expression tag	UNP Q4YRR5
A	35	PHE	-	expression tag	UNP Q4YRR5
A	36	GLN	-	expression tag	UNP Q4YRR5
A	37	GLY	-	expression tag	UNP Q4YRR5

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Ca	0	0
			6	6		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

The chemical structure of ANP (Angiotensinogen Nucleotide Phosphate) is shown. It consists of a nucleotide moiety (adenine, ribose, and phosphate) and a phosphate group. The nucleotide moiety is composed of an adenine base (N1, N3, N7, N9, C2, C4, C6, C8) linked to a ribose sugar (C1', C2', C3', C4', C5') via an N-glycosidic bond. The ribose sugar is linked to a phosphate group (P1, O1, O2, O3, O4) via an O-phosphate bond. The phosphate group is linked to a second phosphate group (P2, O5, O6, O7, O8) via an O-phosphate bond. The second phosphate group is linked to a third phosphate group (P3, O9, O10, O11, O12) via an O-phosphate bond. The third phosphate group is linked to a fourth phosphate group (P4, O13, O14, O15, O16) via an O-phosphate bond. The fourth phosphate group is linked to a fifth phosphate group (P5, O17, O18, O19, O20) via an O-phosphate bond. The fifth phosphate group is linked to a sixth phosphate group (P6, O21, O22, O23, O24) via an O-phosphate bond. The sixth phosphate group is linked to a seventh phosphate group (P7, O25, O26, O27, O28) via an O-phosphate bond. The seventh phosphate group is linked to an eighth phosphate group (P8, O29, O30, O31, O32) via an O-phosphate bond. The eighth phosphate group is linked to a ninth phosphate group (P9, O33, O34, O35, O36) via an O-phosphate bond. The ninth phosphate group is linked to a tenth phosphate group (P10, O37, O38, O39, O40) via an O-phosphate bond. The tenth phosphate group is linked to an eleventh phosphate group (P11, O41, O42, O43, O44) via an O-phosphate bond. The eleventh phosphate group is linked to a twelfth phosphate group (P12, O45, O46, O47, O48) via an O-phosphate bond. The twelfth phosphate group is linked to a thirteenth phosphate group (P13, O49, O50, O51, O52) via an O-phosphate bond. The thirteenth phosphate group is linked to a fourteenth phosphate group (P14, O53, O54, O55, O56) via an O-phosphate bond. The fourteenth phosphate group is linked to a fifteenth phosphate group (P15, O57, O58, O59, O60) via an O-phosphate bond. The fifteenth phosphate group is linked to a sixteenth phosphate group (P16, O61, O62, O63, O64) via an O-phosphate bond. The sixteenth phosphate group is linked to a seventeenth phosphate group (P17, O65, O66, O67, O68) via an O-phosphate bond. The seventeenth phosphate group is linked to an eighteenth phosphate group (P18, O69, O70, O71, O72) via an O-phosphate bond. The eighteenth phosphate group is linked to a nineteenth phosphate group (P19, O73, O74, O75, O76) via an O-phosphate bond. The nineteenth phosphate group is linked to a twentieth phosphate group (P20, O77, O78, O79, O80) via an O-phosphate bond. The twentieth phosphate group is linked to a twenty-first phosphate group (P21, O81, O82, O83, O84) via an O-phosphate bond. The twenty-first phosphate group is linked to a twenty-second phosphate group (P22, O85, O86, O87, O88) via an O-phosphate bond. The twenty-second phosphate group is linked to a twenty-third phosphate group (P23, O89, O90, O91, O92) via an O-phosphate bond. The twenty-third phosphate group is linked to a twenty-fourth phosphate group (P24, O93, O94, O95, O96) via an O-phosphate bond. The twenty-fourth phosphate group is linked to a twenty-fifth phosphate group (P25, O97, O98, O99, O100) via an O-phosphate bond. The twenty-fifth phosphate group is linked to a twenty-sixth phosphate group (P26, O101, O102, O103, O104) via an O-phosphate bond. The twenty-sixth phosphate group is linked to a twenty-seventh phosphate group (P27, O105, O106, O107, O108) via an O-phosphate bond. The twenty-seventh phosphate group is linked to a twenty-eighth phosphate group (P28, O109, O110, O111, O112) via an O-phosphate bond. The twenty-eighth phosphate group is linked to a twenty-ninth phosphate group (P29, O113, O114, O115, O116) via an O-phosphate bond. The twenty-ninth phosphate group is linked to a thirtieth phosphate group (P30, O117, O118, O119, O120) via an O-phosphate bond. The thirtieth phosphate group is linked to a thirty-first phosphate group (P31, O121, O122, O123, O124) via an O-phosphate bond. The thirty-first phosphate group is linked to a thirty-second phosphate group (P32, O125, O126, O127, O128) via an O-phosphate bond. The thirty-second phosphate group is linked to a thirty-third phosphate group (P33, O129, O130, O131, O132) via an O-phosphate bond. The thirty-third phosphate group is linked to a thirty-fourth phosphate group (P34, O133, O134, O135, O136) via an O-phosphate bond. The thirty-fourth phosphate group is linked to a thirty-fifth phosphate group (P35, O137, O138, O139, O140) via an O-phosphate bond. The thirty-fifth phosphate group is linked to a thirty-sixth phosphate group (P36, O141, O142, O143, O144) via an O-phosphate bond. The thirty-sixth phosphate group is linked to a thirty-seventh phosphate group (P37, O145, O146, O147, O148) via an O-phosphate bond. The thirty-seventh phosphate group is linked to a thirty-eighth phosphate group (P38, O149, O150, O151, O152) via an O-phosphate bond. The thirty-eighth phosphate group is linked to a thirty-ninth phosphate group (P39, O153, O154, O155, O156) via an O-phosphate bond. The thirty-ninth phosphate group is linked to a fortieth phosphate group (P40, O157, O158, O159, O160) via an O-phosphate bond. The fortieth phosphate group is linked to a forty-first phosphate group (P41, O161, O162, O163, O164) via an O-phosphate bond. The forty-first phosphate group is linked to a forty-second phosphate group (P42, O165, O166, O167, O168) via an O-phosphate bond. The forty-second phosphate group is linked to a forty-third phosphate group (P43, O169, O170, O171, O172) via an O-phosphate bond. The forty-third phosphate group is linked to a forty-fourth phosphate group (P44, O173, O174, O175, O176) via an O-phosphate bond. The forty-fourth phosphate group is linked to a forty-fifth phosphate group (P45, O177, O178, O179, O180) via an O-phosphate bond. The forty-fifth phosphate group is linked to a forty-sixth phosphate group (P46, O181, O182, O183, O184) via an O-phosphate bond. The forty-sixth phosphate group is linked to a forty-seventh phosphate group (P47, O185, O186, O187, O188) via an O-phosphate bond. The forty-seventh phosphate group is linked to a forty-eighth phosphate group (P48, O189, O190, O191, O192) via an O-phosphate bond. The forty-eighth phosphate group is linked to a forty-ninth phosphate group (P49, O193, O194, O195, O196) via an O-phosphate bond. The forty-ninth phosphate group is linked to a fiftieth phosphate group (P50, O197, O198, O199, O200) via an O-phosphate bond. The fiftieth phosphate group is linked to a fifty-first phosphate group (P51, O201, O202, O203, O204) via an O-phosphate bond. The fifty-first phosphate group is linked to a fifty-second phosphate group (P52, O205, O206, O207, O208) via an O-phosphate bond. The fifty-second phosphate group is linked to a fifty-third phosphate group (P53, O209, O210, O211, O212) via an O-phosphate bond. The fifty-third phosphate group is linked to a fifty-fourth phosphate group (P54, O213, O214, O215, O216) via an O-phosphate bond. The fifty-fourth phosphate group is linked to a fifty-fifth phosphate group (P55, O217, O218, O219, O220) via an O-phosphate bond. The fifty-fifth phosphate group is linked to a fifty-sixth phosphate group (P56, O221, O222, O223, O224) via an O-phosphate bond. The fifty-sixth phosphate group is linked to a fifty-seventh phosphate group (P57, O225, O226, O227, O228) via an O-phosphate bond. The fifty-seventh phosphate group is linked to a fifty-eighth phosphate group (P58, O229, O230, O231, O232) via an O-phosphate bond. The fifty-eighth phosphate group is linked to a fifty-ninth phosphate group (P59, O233, O234, O235, O236) via an O-phosphate bond. The fifty-ninth phosphate group is linked to a sixtieth phosphate group (P60, O237, O238, O239, O240) via an O-phosphate bond. The sixtieth phosphate group is linked to a sixty-first phosphate group (P61, O241, O242, O243, O244) via an O-phosphate bond. The sixty-first phosphate group is linked to a sixty-second phosphate group (P62, O245, O246, O247, O248) via an O-phosphate bond. The sixty-second phosphate group is linked to a sixty-third phosphate group (P63, O249, O250, O251, O252) via an O-phosphate bond. The sixty-third phosphate group is linked to a sixty-fourth phosphate group (P64, O253, O254, O255, O256) via an O-phosphate bond. The sixty-fourth phosphate group is linked to a sixty-fifth phosphate group (P65, O257, O258, O259, O260) via an O-phosphate bond. The sixty-fifth phosphate group is linked to a sixty-sixth phosphate group (P66, O261, O262, O263, O264) via an O-phosphate bond. The sixty-sixth phosphate group is linked to a sixty-seventh phosphate group (P67, O265, O266, O267, O268) via an O-phosphate bond. The sixty-seventh phosphate group is linked to a sixty-eighth phosphate group (P68, O269, O270, O271, O272) via an O-phosphate bond. The sixty-eighth phosphate group is linked to a sixty-ninth phosphate group (P69, O273, O274, O275, O276) via an O-phosphate bond. The sixty-ninth phosphate group is linked to a seventieth phosphate group (P70, O277, O278, O279, O280) via an O-phosphate bond. The seventieth phosphate group is linked to a seventy-first phosphate group (P71, O281, O282, O283, O284) via an O-phosphate bond. The seventy-first phosphate group is linked to a seventy-second phosphate group (P72, O285, O286, O287, O288) via an O-phosphate bond. The seventy-second phosphate group is linked to a seventy-third phosphate group (P73, O289, O290, O291, O292) via an O-phosphate bond. The seventy-third phosphate group is linked to a seventy-fourth phosphate group (P74, O293, O294, O295, O296) via an O-phosphate bond. The seventy-fourth phosphate group is linked to a seventy-fifth phosphate group (P75, O297, O298, O299, O300) via an O-phosphate bond. The seventy-fifth phosphate group is linked to a seventy-sixth phosphate group (P76, O301, O302, O303, O304) via an O-phosphate bond. The seventy-sixth phosphate group is linked to a seventy-seventh phosphate group (P77, O305, O306, O307, O308) via an O-phosphate bond. The seventy-seventh phosphate group is linked to a seventy-eighth phosphate group (P78, O309, O310, O311, O312) via an O-phosphate bond. The seventy-eighth phosphate group is linked to a seventy-ninth phosphate group (P79, O313, O314, O315, O316) via an O-phosphate bond. The seventy-ninth phosphate group is linked to an eightieth phosphate group (P80, O317, O318, O319, O320) via an O-phosphate bond. The eightieth phosphate group is linked to an eighty-first phosphate group (P81, O321, O322, O323, O324) via an O-phosphate bond. The eighty-first phosphate group is linked to an eighty-second phosphate group (P82, O325, O326, O327, O328) via an O-phosphate bond. The eighty-second phosphate group is linked to an eighty-third phosphate group (P83, O329, O330, O331, O332) via an O-phosphate bond. The eighty-third phosphate group is linked to an eighty-fourth phosphate group (P84, O333, O334, O335, O336) via an O-phosphate bond. The eighty-fourth phosphate group is linked to an eighty-fifth phosphate group (P85, O337, O338, O339, O340) via an O-phosphate bond. The eighty-fifth phosphate group is linked to an eighty-sixth phosphate group (P86, O341, O342, O343, O344) via an O-phosphate bond. The eighty-sixth phosphate group is linked to an eighty-seventh phosphate group (P87, O345, O346, O347, O348) via an O-phosphate bond. The eighty-seventh phosphate group is linked to an eighty-eighth phosphate group (P88, O349, O350, O351, O352) via an O-phosphate bond. The eighty-eighth phosphate group is linked to an eighty-ninth phosphate group (P89, O353, O354, O355, O356)

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

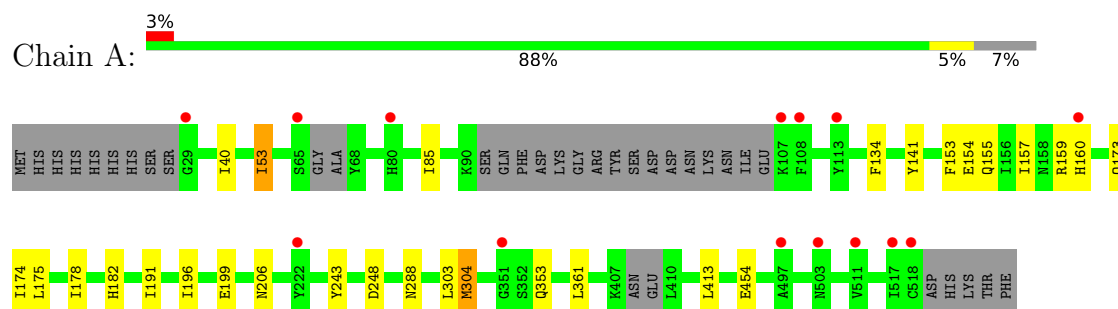
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | A | 1 | Total Mg
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5 | A | 222 | Total O
222 222 | 0 | 0 |

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: Protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.47Å 107.14Å 54.30Å 90.00° 108.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.10) 99.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109, TNT	Depositor
R, R_{free}	0.194 , 0.250 0.213 , 0.264	Depositor DCC
R_{free} test set	1545 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4011	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: CA, 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	0.89	1/3826 (0.0%)	0.97	1/5150 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	MET	SD-CE	-5.44	1.66	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	TYR	N-CA-C	5.27	115.50	108.38

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	3751	0	3567	14	0
2	A	6	0	0	0	0
3	A	31	0	13	3	0
4	A	1	0	0	0	0
5	A	222	0	0	1	0
All	All	4011	0	3580	17	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 2.

The worst 5 of 17 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)
3:A:1634:ANP:H5'2	3:A:1634:ANP:O3G	1.78	0.84
1:A:178:ILE:HD11	1:A:191:ILE:HD11	1.83	0.60
1:A:178:ILE:HD11	1:A:191:ILE:CD1	2.34	0.57
1:A:153:PHE:CE2	1:A:157:ILE:HD11	2.43	0.54
1:A:175:LEU:HD21	1:A:304:MET:HE1	1.92	0.52

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	468/504 (93%)	456 (97%)	11 (2%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	HIS

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	387/455 (85%)	379 (98%)	8 (2%)	47 54

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	GLU
1	A	413	LEU
1	A	303	LEU
1	A	288[A]	ASN
1	A	353	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	109	HIS
1	A	155	GLN
1	A	272	GLN
1	A	515	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	1634	4,2	33,33,33	2.15	11 (33%)	45,52,52	2.45	18 (40%)

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	1634	4,2	-	6/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1634	ANP	PB-O3A	5.21	1.65	1.59
3	A	1634	ANP	PG-O1G	4.12	1.52	1.46
3	A	1634	ANP	C5-C4	4.10	1.46	1.39
3	A	1634	ANP	PB-O1B	3.90	1.52	1.46
3	A	1634	ANP	C5-N7	-3.41	1.32	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1634	ANP	C5-C4-N3	-6.27	118.08	126.72
3	A	1634	ANP	N3-C4-N9	5.61	136.72	127.17
3	A	1634	ANP	O5'-C5'-C4'	5.37	127.28	108.99
3	A	1634	ANP	O4'-C1'-N9	4.81	117.33	108.09
3	A	1634	ANP	O2G-PG-O3G	3.84	117.91	107.59

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

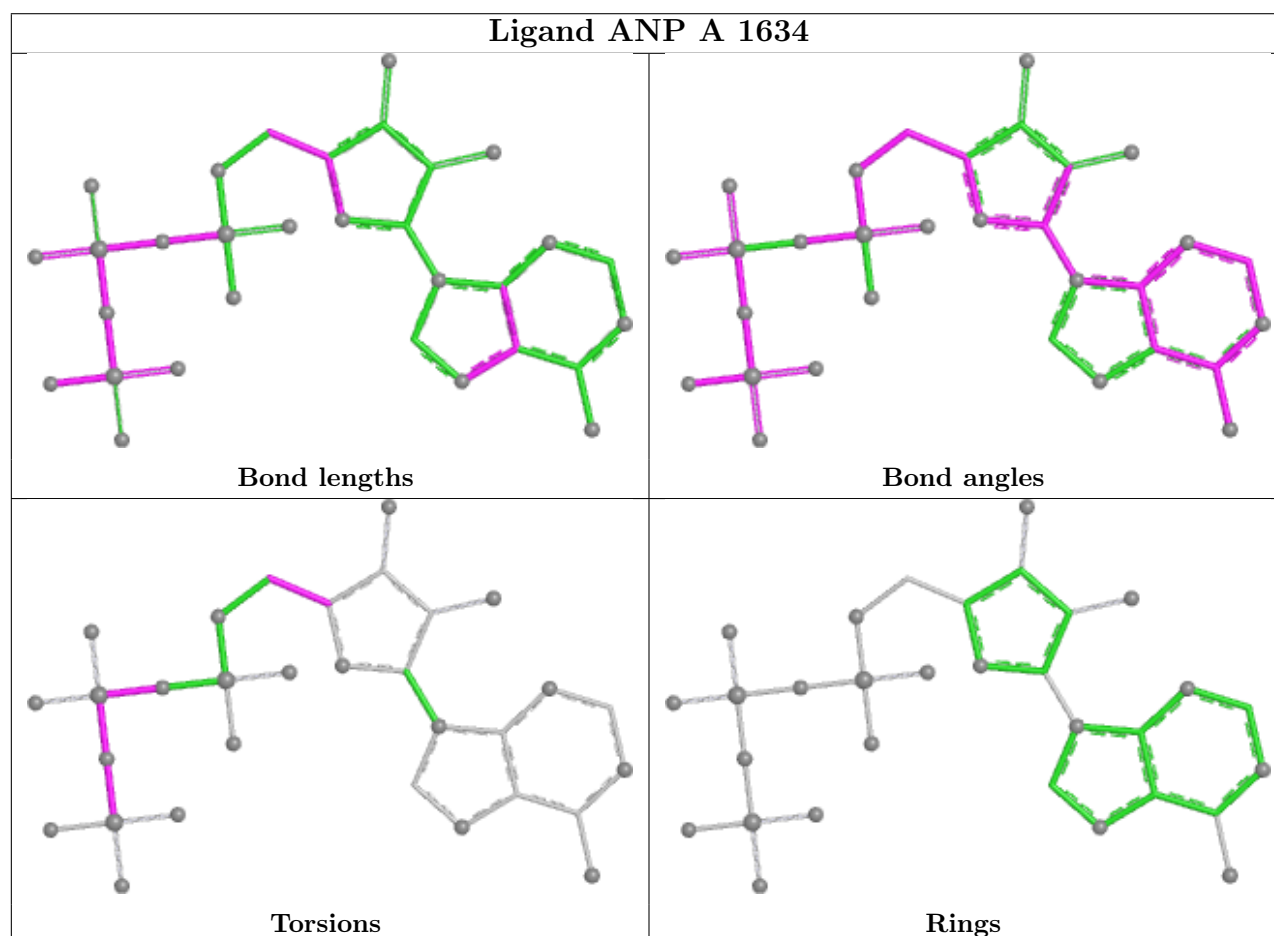
Mol	Chain	Res	Type	Atoms
3	A	1634	ANP	PB-N3B-PG-O1G
3	A	1634	ANP	PG-N3B-PB-O1B
3	A	1634	ANP	O4'-C4'-C5'-O5'
3	A	1634	ANP	C3'-C4'-C5'-O5'
3	A	1634	ANP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1634	ANP	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 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	470/504 (93%)	-0.14	14 (2%) 52 55	1, 9, 35, 67	12 (2%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PHE	4.5
1	A	511	VAL	3.0
1	A	160	HIS	2.8
1	A	518	CYS	2.7
1	A	503[A]	ASN	2.6

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 oligosaccharides 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.

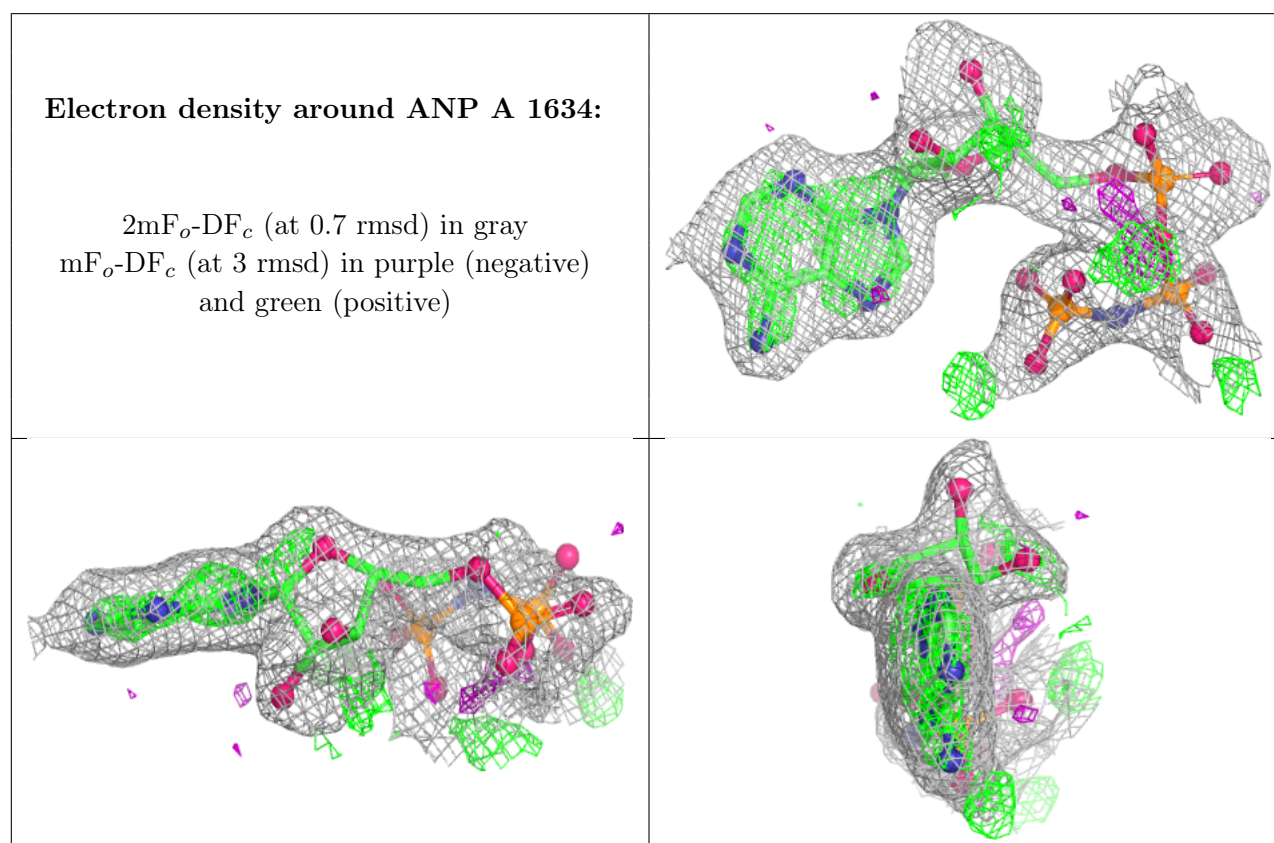
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	A	1634	31/31	0.82	0.17	19,32,46,48	31
2	CA	A	527	1/1	0.92	0.08	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	525	1/1	0.93	0.14	29,29,29,29	0
4	MG	A	529	1/1	0.93	0.16	28,28,28,28	0
2	CA	A	528	1/1	0.94	0.13	29,29,29,29	0
2	CA	A	1	1/1	0.97	0.04	2,2,2,2	0
2	CA	A	526	1/1	0.98	0.09	31,31,31,31	0
2	CA	A	524	1/1	0.99	0.14	23,23,23,23	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.