wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2023 – 03:27 am GMT

PDB ID	:	2VWB
Title	:	Structure of the archaeal Kae1-Bud32 fusion protein MJ1130: a model for the eukaryotic EKC-KEOPS subcomplex involved in transcription and telomere homeostasis.
Authors	:	Hecker, A.; Lopreiato, R.; Graille, M.; Collinet, B.; Forterre, P.; Domenico, L.; van Tilbeurgh, H.
Deposited on	:	2008-06-20
Resolution	:	3.05 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 (i) 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 (i)) were used in the production of this report:

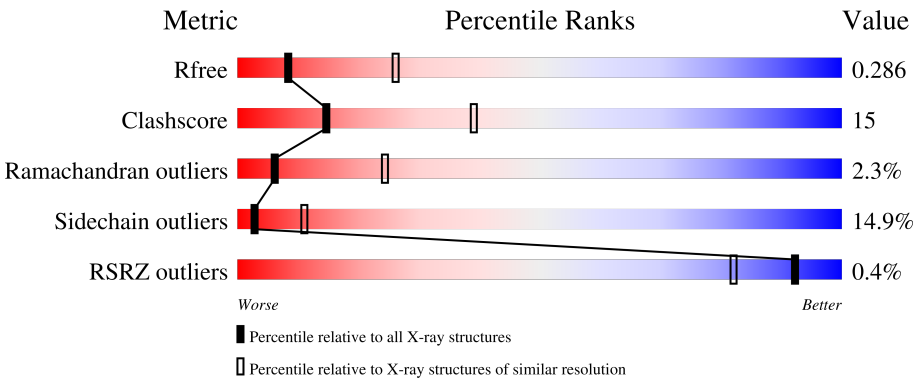
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

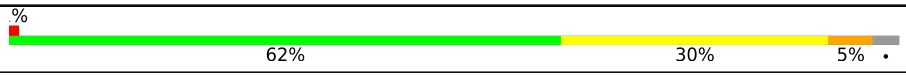
The reported resolution of this entry is 3.05 Å.

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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	535	
1	B	535	

2 Entry composition (i)

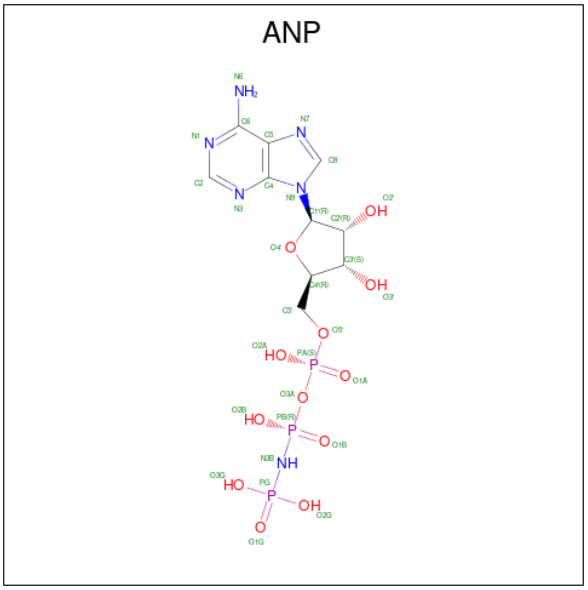
There are 2 unique types of molecules in this entry. The entry contains 8210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4125	2636	698	770	21	0	0	0
1	B	507	4023	2568	680	754	21	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



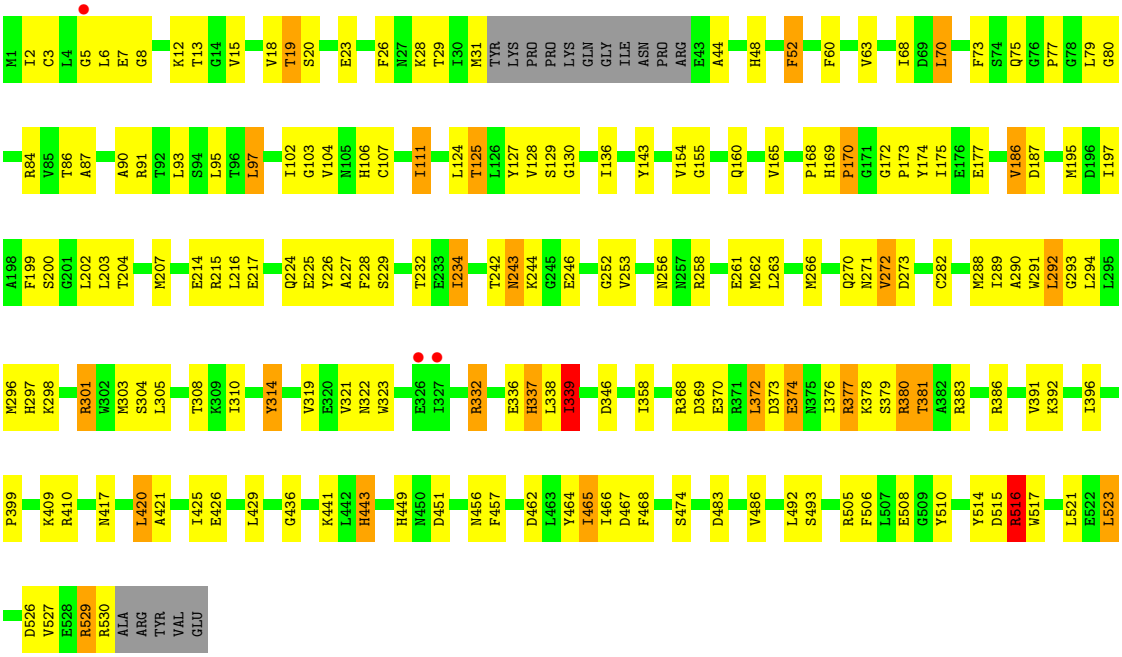
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0
2	B	1	31	10	6	12	3	0	0

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.

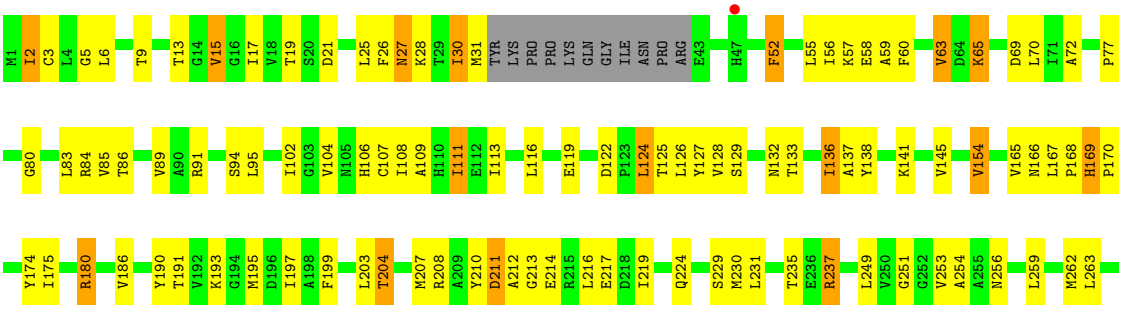
• Molecule 1: PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE

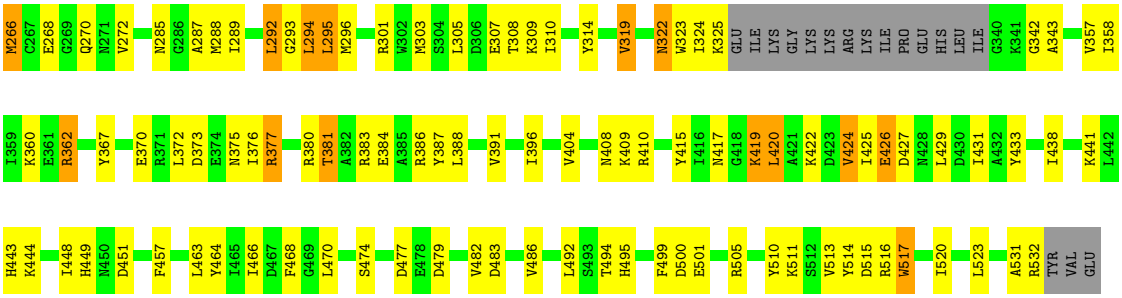
Chain A:



• Molecule 1: PUTATIVE O-SIALOGLYCOPROTEIN ENDOPEPTIDASE

Chain B:




M266 C267 E268 G269 Q270 N271 V272 N285 G286 A287 M288 I289 L292 G293 L294 L295 M296 R301 W302 M303 S304 L305 D306 E307 T308 K309 I310 Y314 V319 N322 W323 I324 K325 GLU ILE LYS GLY LYS LYS ARG LYS ILE PRO GLU HIS LEU ILE G340 K341 G342 A343 V357 I358
I359 K360 E361 R362 Y367 E370 R371 L372 D373 E374 N375 I376 R377 R380 T381 A382 R383 E384 A385 R386 Y387 L388 V391 I396 V404 N408 K409 R410 Y415 I416 N417 G418 K419 L420 A421 K422 D423 V424 I425 E426 D427 N428 L429 D430 I431 A432 Y433 I438 K441 L442
H443 K444 I448 H449 N450 D451 F457 L463 Y464 I465 I466 D467 F468 G469 L470 S474 D477 E478 D479 V482 D483 V486 L492 S493 T494 H495 F499 D500 E501 R505 Y510 K511 S512 V513 Y514 D515 R516 W517 I520 L523 A531 R532 TYR VAL GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	147.42Å 148.95Å 65.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.05 19.95 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.95-3.05) 94.4 (19.95-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.301 0.210 , 0.286	Depositor DCC
R_{free} test set	1319 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	0/4199	0.70	1/5660 (0.0%)
1	B	0.54	0/4094	0.72	1/5520 (0.0%)
All	All	0.54	0/8293	0.71	2/11180 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	LEU	CA-CB-CG	5.87	128.80	115.30
1	B	124	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	HIS	Peptide

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	4125	0	4181	122	0
1	B	4023	0	4060	131	0
2	A	31	0	13	2	0
2	B	31	0	13	1	0
All	All	8210	0	8267	252	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 15.

The worst 5 of 252 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:516:ARG:HH11	1:A:516:ARG:HG2	1.13	1.13
1:B:104:VAL:HG13	1:B:292:LEU:HD12	1.34	1.08
1:A:242:THR:HG21	1:A:244:LYS:HG2	1.37	1.06
1:A:242:THR:CG2	1:A:244:LYS:HG2	1.90	1.01
1:A:107:CYS:HG	1:A:127:TYR:HE2	1.09	0.99

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	515/535 (96%)	454 (88%)	51 (10%)	10 (2%)	8 29
1	B	501/535 (94%)	425 (85%)	63 (13%)	13 (3%)	5 22
All	All	1016/1070 (95%)	879 (86%)	114 (11%)	23 (2%)	6 24

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	337	HIS
1	A	339	ILE
1	B	166	ASN
1	A	80	GLY

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	443/457 (97%)	372 (84%)	71 (16%)	2 9
1	B	431/457 (94%)	372 (86%)	59 (14%)	3 14
All	All	874/914 (96%)	744 (85%)	130 (15%)	3 11

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	377	ARG
1	B	404	VAL
1	A	386	ARG
1	A	381	THR
1	B	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	GLN
1	B	285	ASN
1	B	443	HIS
1	B	271	ASN
1	B	297	HIS

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)

2 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	ANP	B	1533	-	29,33,33	2.00	7 (24%)	31,52,52	1.64	6 (19%)
2	ANP	A	1531	-	29,33,33	1.90	5 (17%)	31,52,52	1.75	8 (25%)

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	1533	-	-	4/14/38/38	0/3/3/3
2	ANP	A	1531	-	-	1/14/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1533	ANP	PG-N3B	5.30	1.77	1.63
2	A	1531	ANP	PG-N3B	5.19	1.76	1.63
2	B	1533	ANP	PB-N3B	5.11	1.76	1.63
2	A	1531	ANP	PB-N3B	5.04	1.76	1.63
2	B	1533	ANP	PB-O1B	3.76	1.52	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1531	ANP	O2B-PB-O1B	4.15	118.63	109.92
2	B	1533	ANP	O2G-PG-O3G	3.76	117.65	107.64
2	A	1531	ANP	O2G-PG-O3G	3.68	117.44	107.64
2	B	1533	ANP	O2B-PB-O1B	3.34	116.93	109.92
2	A	1531	ANP	N3-C2-N1	-3.34	123.46	128.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1531	ANP	PG-N3B-PB-O3A
2	B	1533	ANP	C5'-O5'-PA-O1A
2	B	1533	ANP	C3'-C4'-C5'-O5'
2	B	1533	ANP	O4'-C4'-C5'-O5'
2	B	1533	ANP	C5'-O5'-PA-O3A

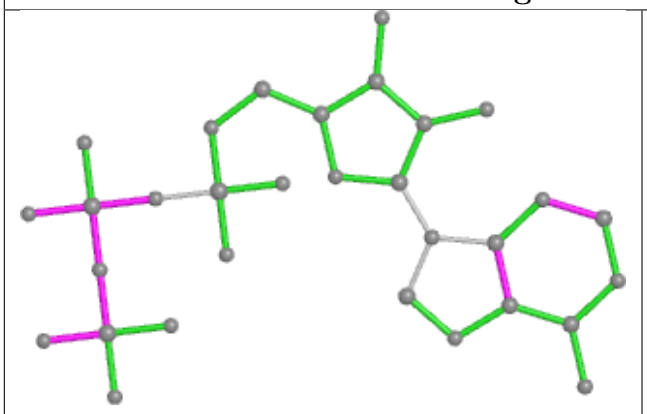
There are no ring outliers.

2 monomers are involved in 3 short contacts:

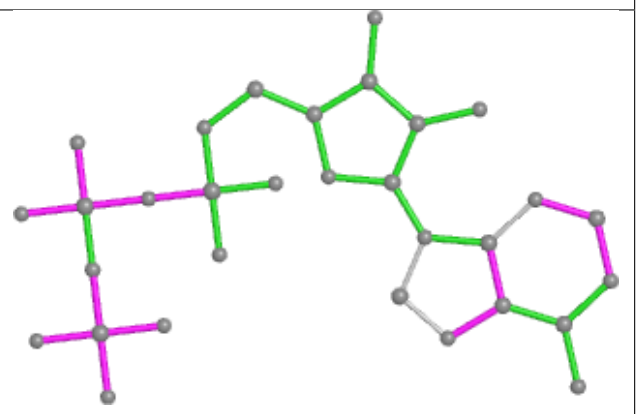
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1533	ANP	1	0
2	A	1531	ANP	2	0

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.

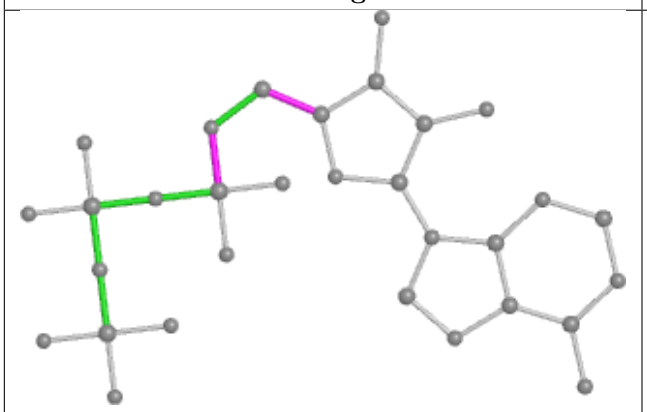
Ligand ANP B 1533



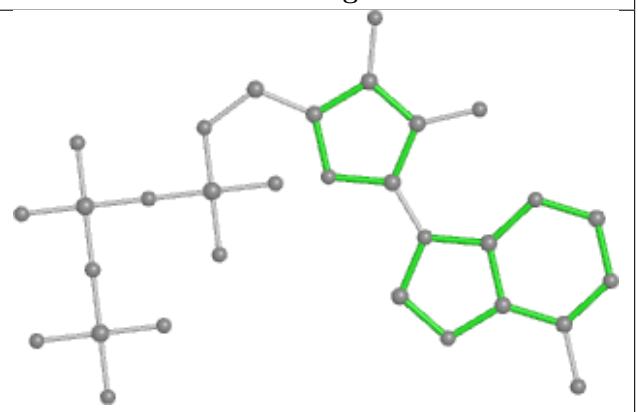
Bond lengths



Bond angles

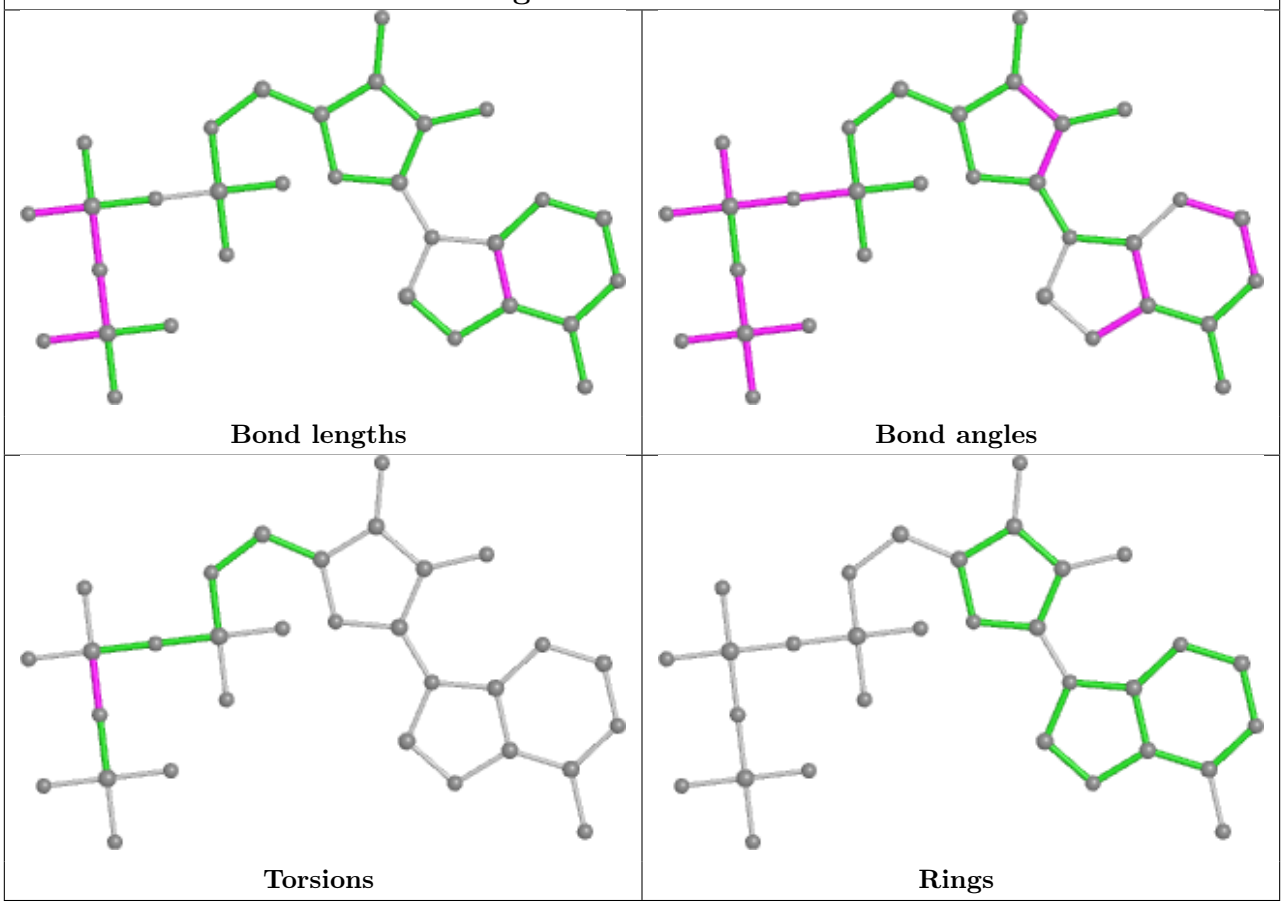


Torsions



Rings

Ligand ANP A 1531



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	519/535 (97%)	-0.33	3 (0%)	89	76	34, 56, 85, 107	0
1	B	507/535 (94%)	-0.34	1 (0%)	95	89	35, 60, 93, 112	0
All	All	1026/1070 (95%)	-0.33	4 (0%)	92	82	34, 58, 90, 112	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	2.8
1	A	326	GLU	2.4
1	B	47	HIS	2.2
1	A	327	ILE	2.2

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, 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
2	ANP	A	1531	31/31	0.96	0.13	43,45,74,74	0

Continued on next page...

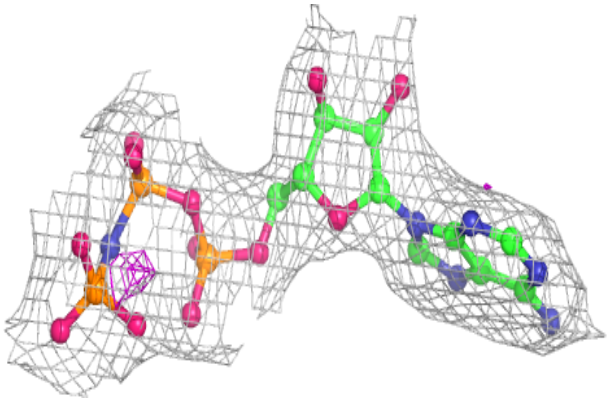
Continued from previous page...

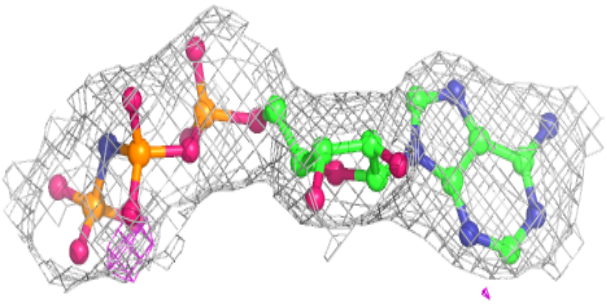
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ANP	B	1533	31/31	0.96	0.14	66,70,87,87	0

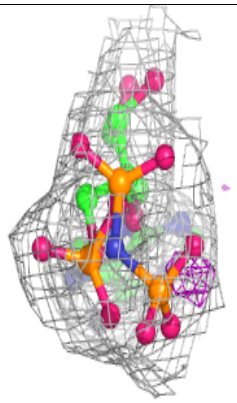
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP A 1531:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

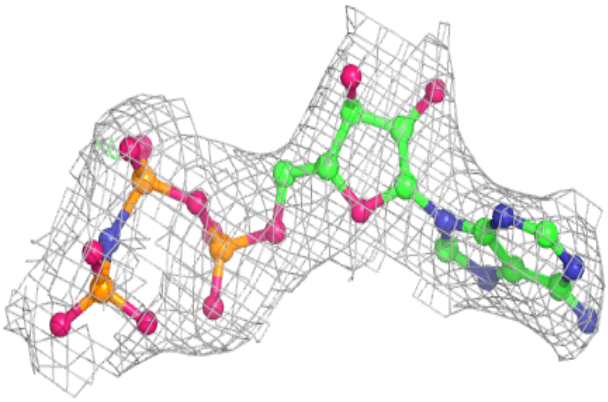


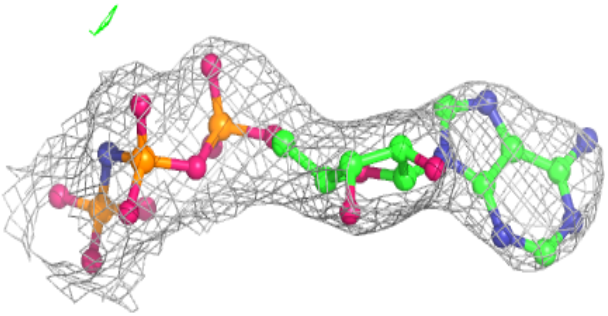


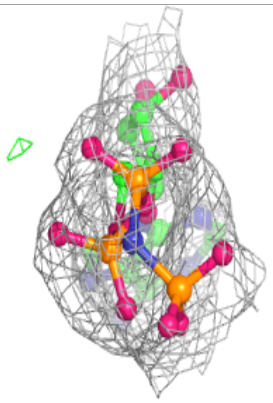


Electron density around ANP B 1533:

$2mF_o$-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 (i)

There are no such residues in this entry.