wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 07:10 am BST

PDB ID	:	2XB2
Title	:	Crystal structure of the core Mago-Y14-eIF4AIII-Barentsz-UPF3b assembly shows how the EJC is bridged to the NMD machinery
Authors	:	Buchwald, G.; Ebert, J.; Basquin, C.; Sauliere, J.; Jayachandran, U.; Bono, F.; Le Hir, H.; Conti, E.
Deposited on	:	2010-04-03
Resolution	:	3.40 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 following versions of software and data (see references (1)) were used in the production of this report:

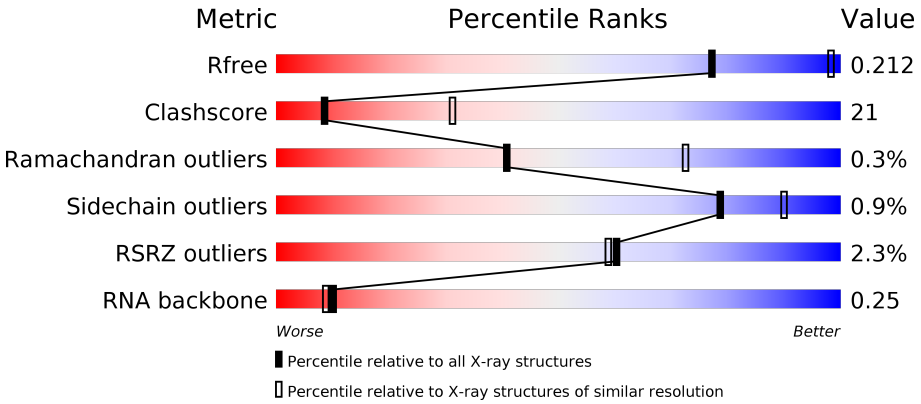
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 <=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	411	% 58% 36% • 5%
1	X	411	% 62% 31% • 5%
2	C	146	% 62% 35% ••
2	Y	146	4% 62% 36% •

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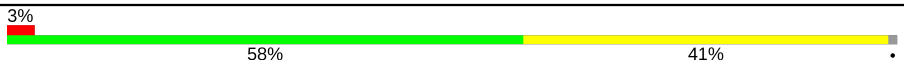
Mol	Chain	Length	Quality of chain
3	D	90	
3	Z	90	
4	E	15	
4	R	15	
5	F	3	
6	G	60	
6	U	60	
7	S	150	
7	T	150	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11710 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 EUKARYOTIC INITIATION FACTOR 4A-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3131	1976	546	590	19			
1	X	390	Total	C	N	O	S	0	0	0
			3131	1976	546	590	19			

- Molecule 2 is a protein called PROTEIN MAGO NASHI HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	143	Total	C	N	O	S	0	0	0
			1190	769	199	219	3			
2	Y	143	Total	C	N	O	S	0	0	0
			1190	769	199	219	3			

- Molecule 3 is a protein called RNA-BINDING PROTEIN 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			719	456	120	140	3			
3	Z	89	Total	C	N	O	S	0	0	0
			719	456	120	140	3			

- Molecule 4 is a RNA chain called RNA POLY-U-RIBONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	8	Total	C	N	O	P	0	0	0
			157	72	16	62	7			
4	R	7	Total	C	N	O	P	0	0	0
			137	63	14	54	6			

- Molecule 5 is a protein called PUTATIVE REGULATOR OF NONSENSE TRANSCRIPTS 3B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			25	14	6	5			

- Molecule 6 is a protein called REGULATOR OF NONSENSE TRANSCRIPTS 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	S	0	0	0
			124	77	25	21	1			
6	U	17	Total	C	N	O	S	0	0	1
			120	74	23	22	1			

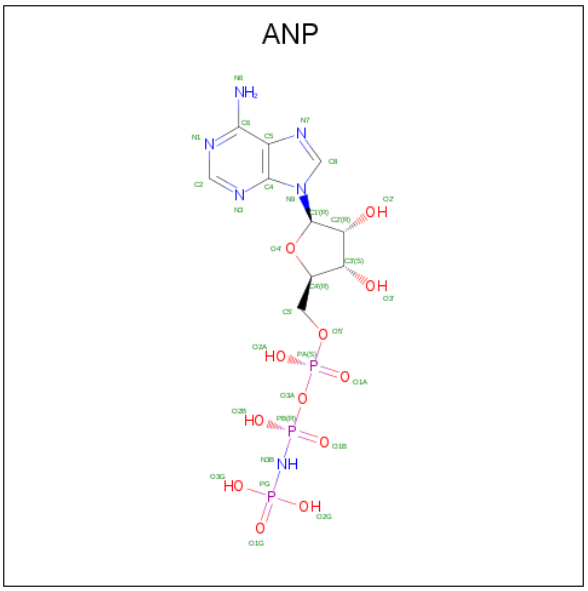
- Molecule 7 is a protein called PROTEIN CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	S	57	Total	C	N	O	0	0	0
			494	309	92	93			
7	T	59	Total	C	N	O	0	0	0
			509	318	96	95			

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	X	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



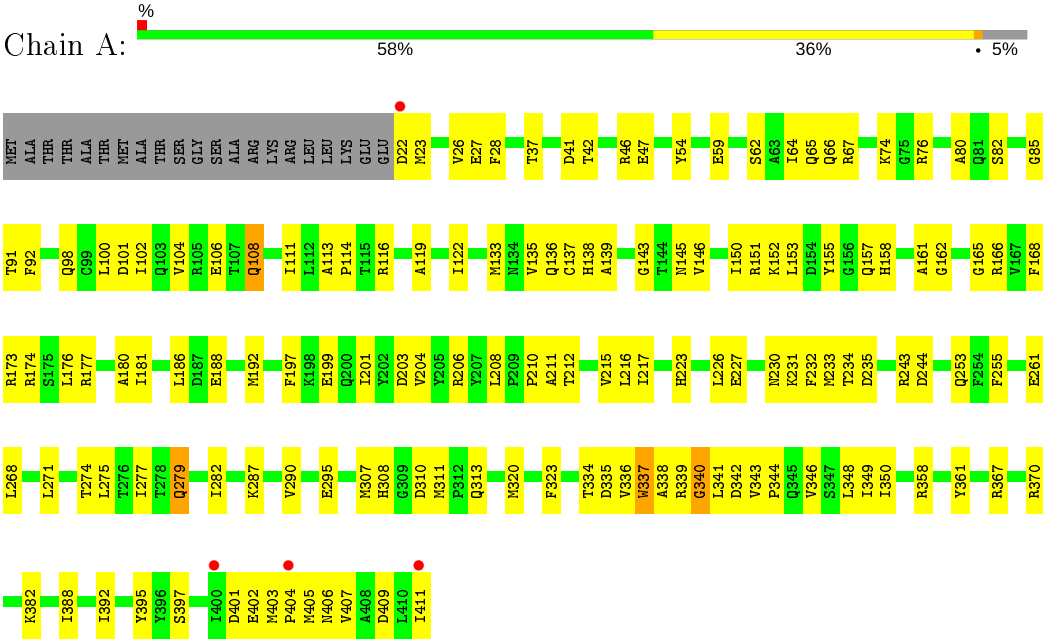
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
9	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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 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.

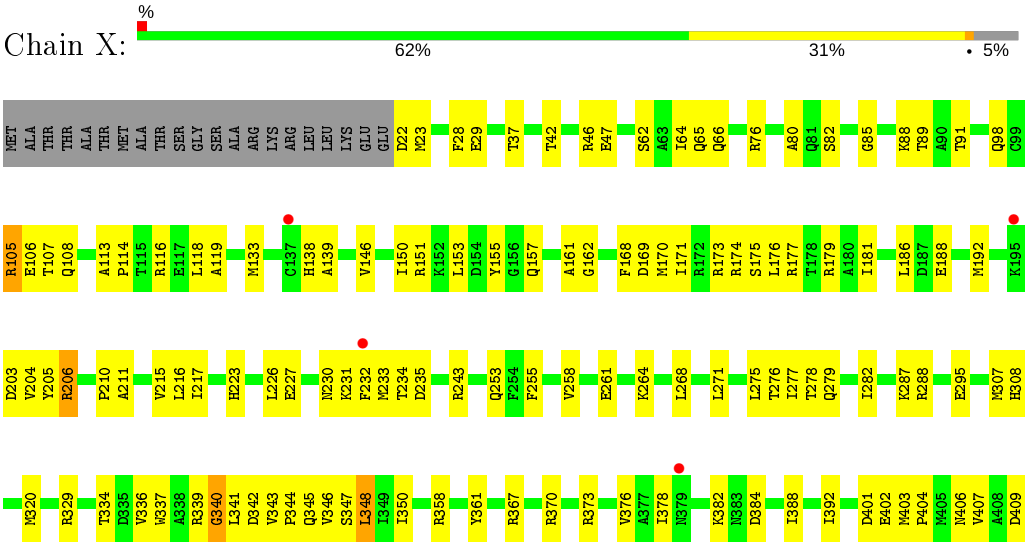
- Molecule 1: EUKARYOTIC INITIATION FACTOR 4A-III

Chain A:



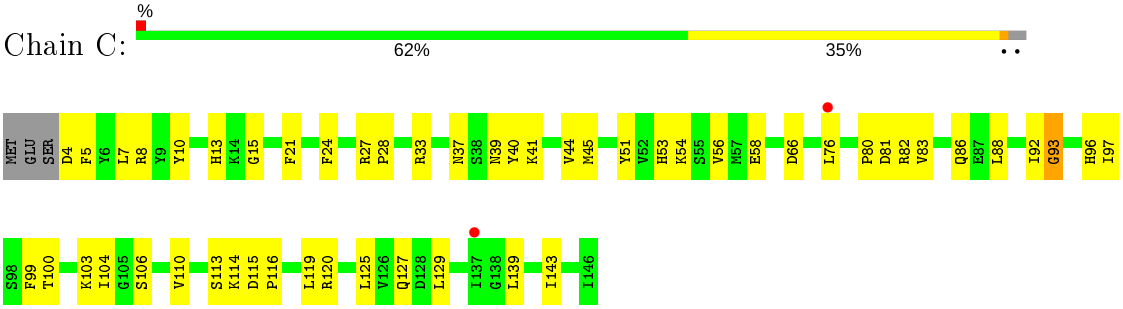
- Molecule 1: EUKARYOTIC INITIATION FACTOR 4A-III

Chain X:



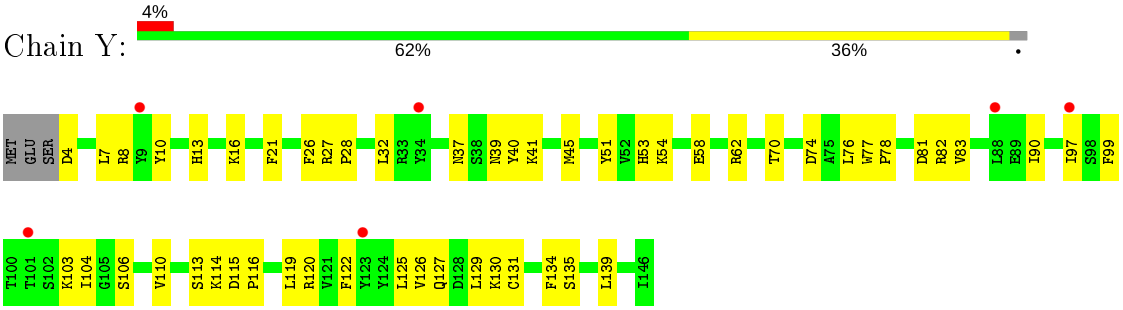
- Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain C:



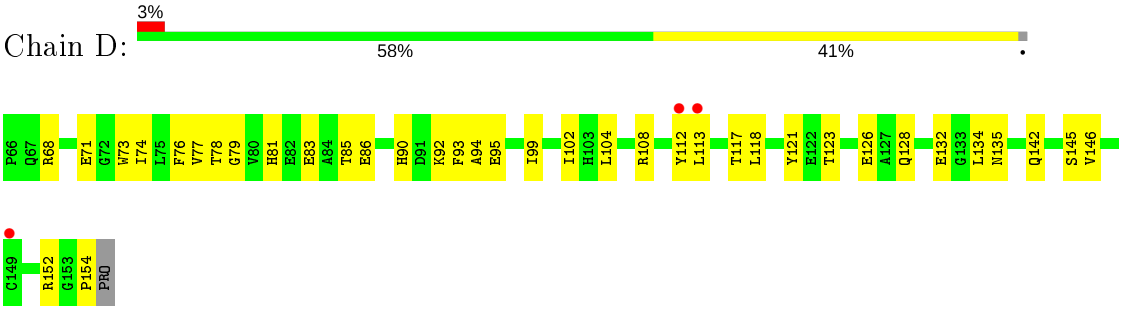
• Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain Y:



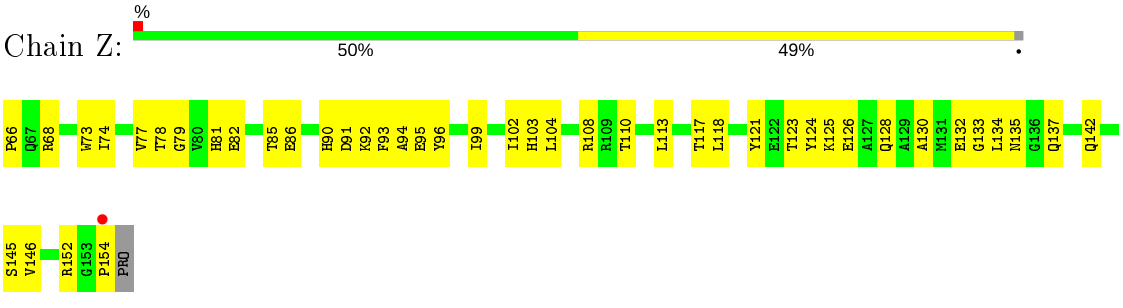
• Molecule 3: RNA-BINDING PROTEIN 8A

Chain D:



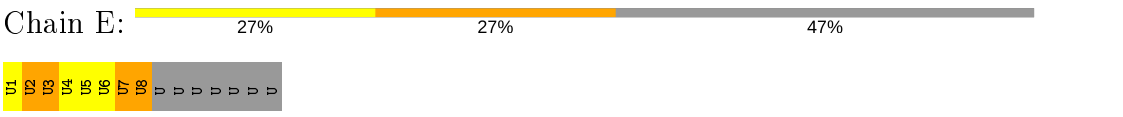
• Molecule 3: RNA-BINDING PROTEIN 8A

Chain Z:



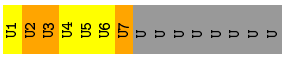
• Molecule 4: RNA POLY-U-RIBONUCLEOTIDE

Chain E:



• Molecule 4: RNA POLY-U-RIBONUCLEOTIDE

Chain R:

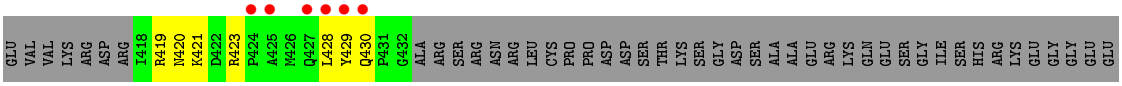


• Molecule 5: PUTATIVE REGULATOR OF NONSENSE TRANSCRIPTS 3B

Chain F:

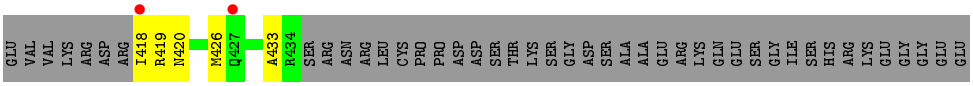
• Molecule 6: REGULATOR OF NONSENSE TRANSCRIPTS 3B

Chain G:



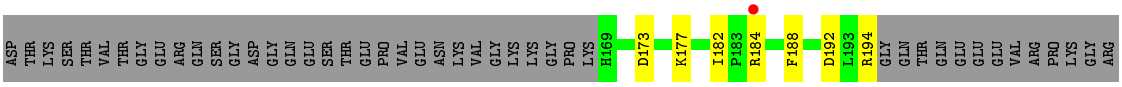
• Molecule 6: REGULATOR OF NONSENSE TRANSCRIPTS 3B

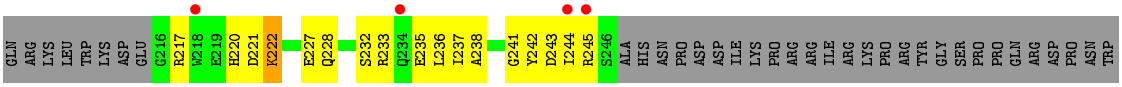
Chain U:



• Molecule 7: PROTEIN CASC3

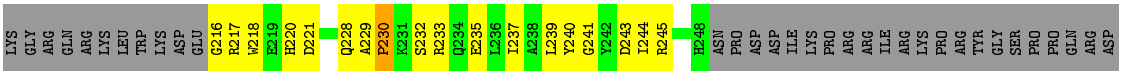
Chain S:





• Molecule 7: PROTEIN CASC3

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.80Å 134.80Å 227.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.40 67.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.00-3.40) 100.0 (67.40-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.260 0.215 , 0.212	Depositor DCC
R_{free} test set	1634 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11710	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	0.70	3/3180 (0.1%)	0.71	2/4291 (0.0%)
1	X	0.57	3/3180 (0.1%)	0.68	2/4291 (0.0%)
2	C	0.53	1/1219 (0.1%)	0.61	1/1640 (0.1%)
2	Y	0.56	2/1219 (0.2%)	0.59	0/1640
3	D	0.43	0/736	0.59	0/995
3	Z	0.52	1/736 (0.1%)	0.60	0/995
4	E	0.42	0/172	0.76	0/264
4	R	0.42	0/150	0.76	0/230
5	F	0.71	0/24	0.50	0/30
6	G	0.39	0/126	0.56	0/168
6	U	0.59	0/122	0.60	0/166
7	S	0.63	0/506	0.57	0/677
7	T	0.58	0/522	0.63	0/699
All	All	0.59	10/11892 (0.1%)	0.66	5/16086 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	VAL	CB-CG1	-15.69	1.19	1.52
1	A	26	VAL	CB-CG2	-14.93	1.21	1.52
1	X	29	GLU	CG-CD	-6.92	1.41	1.51
2	Y	39	ASN	CG-ND2	-5.56	1.19	1.32
1	X	206	ARG	CG-CD	-5.55	1.38	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	VAL	CG1-CB-CG2	-9.74	95.32	110.90
1	X	340	GLY	N-CA-C	7.15	130.97	113.10
1	A	340	GLY	N-CA-C	6.96	130.50	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	206	ARG	CG-CD-NE	5.58	123.51	111.80
2	C	93	GLY	N-CA-C	-5.02	100.55	113.10

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	3131	0	3173	153	0
1	X	3131	0	3172	135	0
2	C	1190	0	1177	47	0
2	Y	1190	0	1177	39	0
3	D	719	0	680	30	0
3	Z	719	0	680	35	0
4	E	157	0	82	14	0
4	R	137	0	72	15	0
5	F	25	0	26	1	0
6	G	124	0	126	14	0
6	U	120	0	109	3	0
7	S	494	0	459	35	0
7	T	509	0	471	32	0
8	A	1	0	0	0	0
8	X	1	0	0	0	0
9	A	31	0	13	6	0
9	X	31	0	13	6	0
All	All	11710	0	11430	478	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 21.

The worst 5 of 478 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:X:348:LEU:HD23	1:X:411:ILE:HD12	1.20	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:423:ARG:HH11	6:G:423:ARG:HG2	1.39	0.87
1:A:104:VAL:HG22	1:A:106:GLU:HG3	1.57	0.86
7:S:244:ILE:HD12	1:X:151:ARG:NH2	1.96	0.81
1:X:307:MET:HA	1:X:311:MET:SD	2.21	0.80

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	388/411 (94%)	365 (94%)	23 (6%)	0	100 100
1	X	388/411 (94%)	366 (94%)	21 (5%)	1 (0%)	41 72
2	C	141/146 (97%)	129 (92%)	12 (8%)	0	100 100
2	Y	141/146 (97%)	128 (91%)	13 (9%)	0	100 100
3	D	87/90 (97%)	81 (93%)	6 (7%)	0	100 100
3	Z	87/90 (97%)	81 (93%)	6 (7%)	0	100 100
5	F	1/3 (33%)	1 (100%)	0	0	100 100
6	G	13/60 (22%)	13 (100%)	0	0	100 100
6	U	15/60 (25%)	13 (87%)	1 (7%)	1 (7%)	1 8
7	S	53/150 (35%)	46 (87%)	6 (11%)	1 (2%)	8 31
7	T	55/150 (37%)	48 (87%)	6 (11%)	1 (2%)	8 32
All	All	1369/1717 (80%)	1271 (93%)	94 (7%)	4 (0%)	41 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	S	222	LYS
6	U	433	ALA

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Mol	Chain	Res	Type
1	X	384	ASP
7	T	230	PRO

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	345/361 (96%)	340 (99%)	5 (1%)	67 83
1	X	345/361 (96%)	340 (99%)	5 (1%)	67 83
2	C	131/134 (98%)	131 (100%)	0	100 100
2	Y	131/134 (98%)	131 (100%)	0	100 100
3	D	75/76 (99%)	75 (100%)	0	100 100
3	Z	75/76 (99%)	74 (99%)	1 (1%)	69 84
5	F	2/2 (100%)	2 (100%)	0	100 100
6	G	13/51 (26%)	13 (100%)	0	100 100
6	U	11/51 (22%)	11 (100%)	0	100 100
7	S	51/133 (38%)	51 (100%)	0	100 100
7	T	52/133 (39%)	52 (100%)	0	100 100
All	All	1231/1512 (81%)	1220 (99%)	11 (1%)	78 90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	TRP
1	X	105	ARG
1	X	337	TRP
1	A	279	GLN
1	X	201	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	430	GLN
1	X	194	ASN
3	Z	128	GLN
6	U	420	ASN
6	U	430	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	7/15 (46%)	4 (57%)	0
4	R	6/15 (40%)	3 (50%)	0
All	All	13/30 (43%)	7 (53%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	2	U
4	E	3	U
4	E	7	U
4	E	8	U
4	R	2	U

There are no RNA pucker outliers to report.

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 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	$\#\|Z\| > 2$
9	ANP	X	1413	8	29,33,33	2.56	7 (24%)	31,52,52	2.93	13 (41%)
9	ANP	A	1413	8	29,33,33	2.56	7 (24%)	31,52,52	2.93	13 (41%)

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
9	ANP	X	1413	8	-	6/14/38/38	0/3/3/3
9	ANP	A	1413	8	-	6/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	X	1413	ANP	PG-O1G	8.18	1.59	1.46
9	A	1413	ANP	PG-O1G	8.14	1.59	1.46
9	A	1413	ANP	PB-O1B	7.31	1.57	1.46
9	X	1413	ANP	PB-O1B	7.29	1.57	1.46
9	A	1413	ANP	PB-O2B	-3.02	1.48	1.56

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1413	ANP	C1'-N9-C4	6.98	138.90	126.64
9	X	1413	ANP	C1'-N9-C4	6.97	138.89	126.64
9	X	1413	ANP	O2G-PG-O1G	-6.74	96.52	113.45
9	A	1413	ANP	O2G-PG-O1G	-6.72	96.55	113.45
9	X	1413	ANP	C3'-C2'-C1'	-6.67	90.93	100.98

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	X	1413	ANP	C5'-O5'-PA-O1A
9	X	1413	ANP	O4'-C4'-C5'-O5'
9	A	1413	ANP	PB-N3B-PG-O1G
9	A	1413	ANP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	A	1413	ANP	O4'-C4'-C5'-O5'

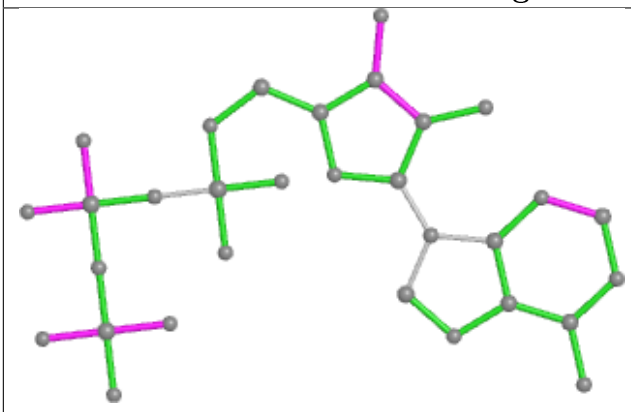
There are no ring outliers.

2 monomers are involved in 12 short contacts:

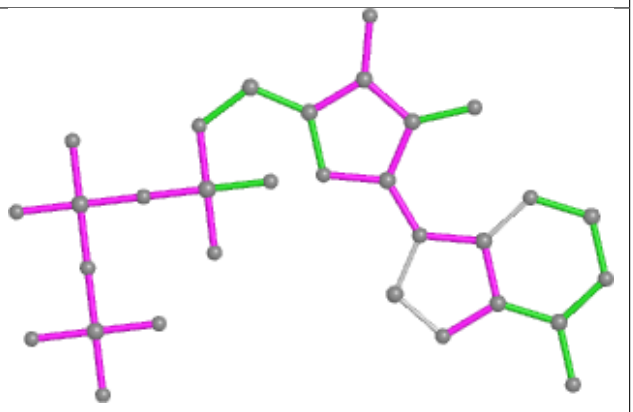
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	1413	ANP	6	0
9	A	1413	ANP	6	0

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.

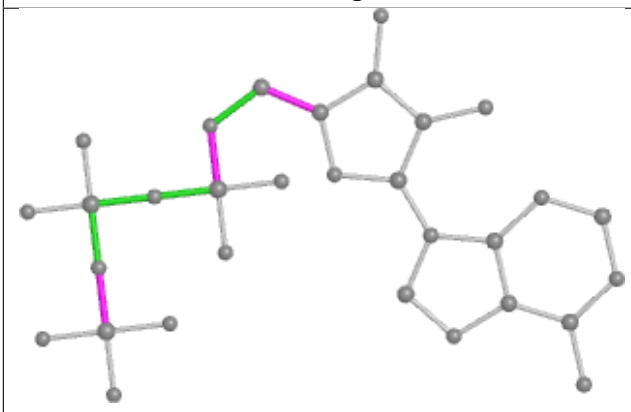
Ligand ANP X 1413



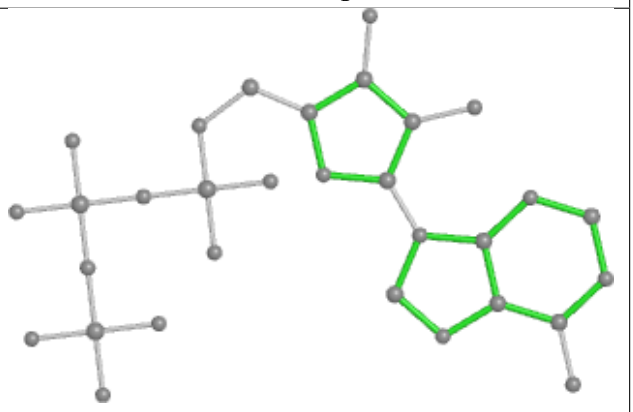
Bond lengths



Bond angles

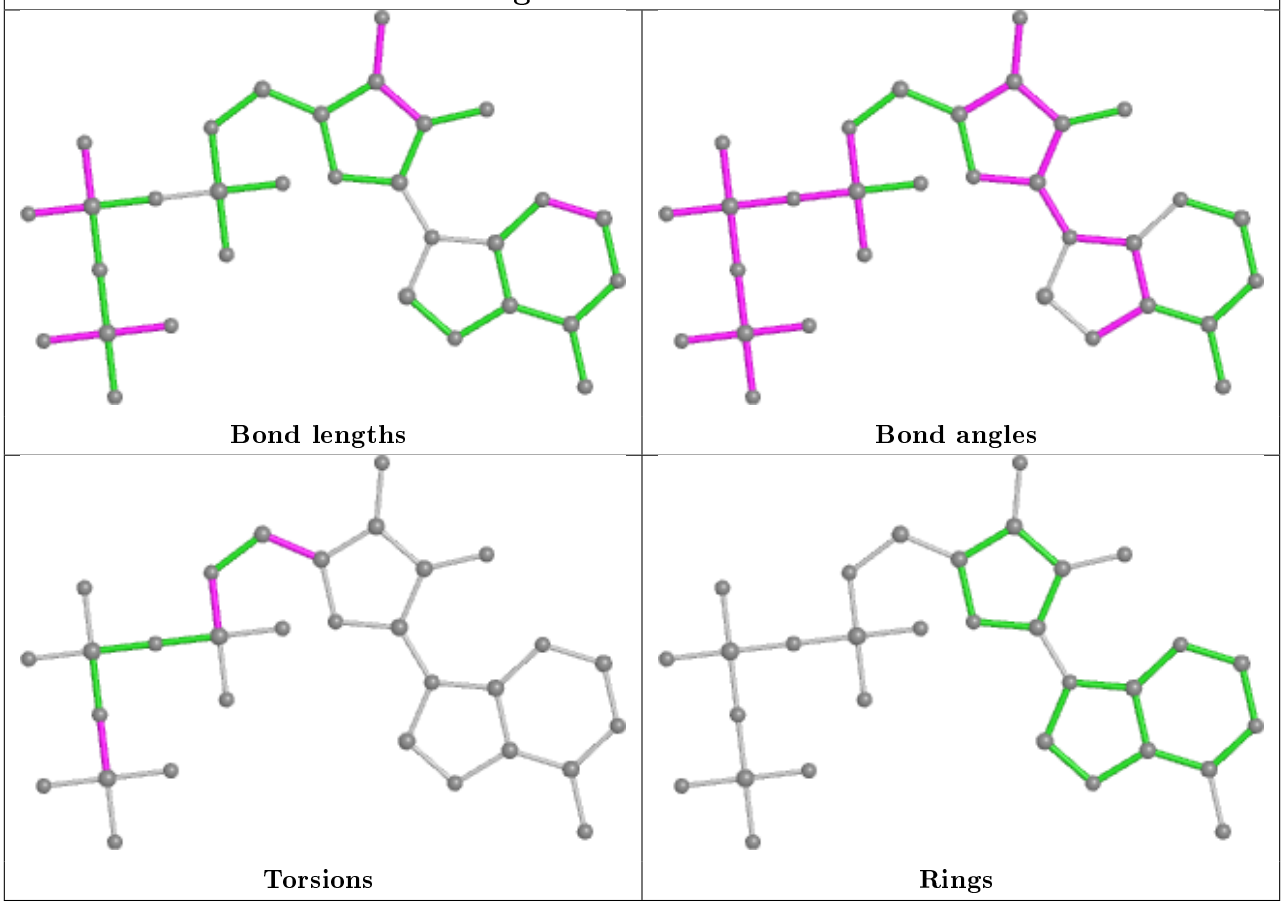


Torsions



Rings

Ligand ANP A 1413



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

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, 95^{th} 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	390/411 (94%)	0.32	4 (1%) 82 81	37, 69, 110, 155	0
1	X	390/411 (94%)	0.35	4 (1%) 82 81	49, 79, 100, 120	0
2	C	143/146 (97%)	0.50	2 (1%) 75 74	44, 80, 111, 152	0
2	Y	143/146 (97%)	0.76	6 (4%) 36 35	57, 77, 92, 111	0
3	D	89/90 (98%)	0.41	3 (3%) 45 44	56, 84, 137, 162	0
3	Z	89/90 (98%)	0.29	1 (1%) 80 79	57, 78, 106, 113	0
4	E	8/15 (53%)	0.57	0 100 100	75, 90, 135, 151	0
4	R	7/15 (46%)	0.53	0 100 100	75, 83, 113, 168	0
5	F	3/3 (100%)	0.69	0 100 100	91, 91, 99, 105	0
6	G	15/60 (25%)	1.37	6 (40%) 0 0	80, 110, 145, 147	0
6	U	17/60 (28%)	0.77	2 (11%) 4 5	66, 88, 133, 140	0
7	S	57/150 (38%)	0.67	5 (8%) 10 11	78, 92, 110, 117	0
7	T	59/150 (39%)	0.23	0 100 100	61, 92, 127, 144	0
All	All	1410/1747 (80%)	0.42	33 (2%) 60 59	37, 79, 113, 168	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	113	LEU	3.7
3	D	112	TYR	3.2
1	X	137	CYS	3.2
6	G	427	GLN	3.0
2	Y	88	LEU	2.8

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)

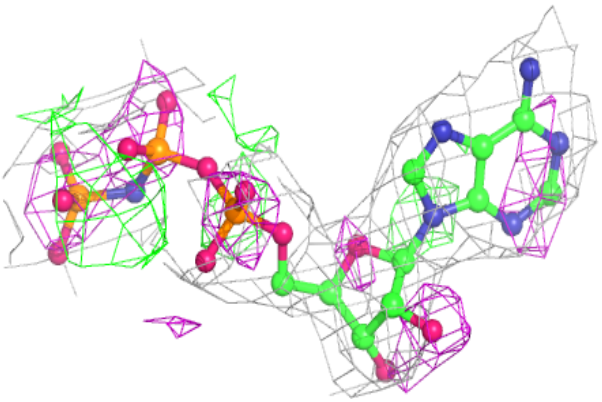
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

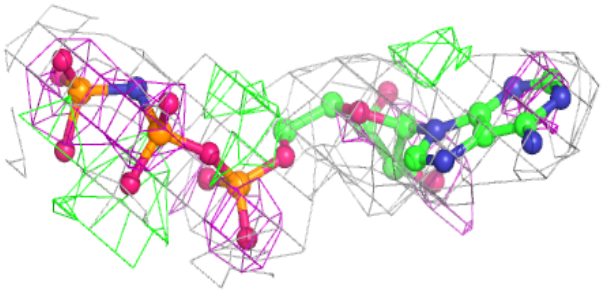
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	X	1412	1/1	0.76	0.32	81,81,81,81	0
8	MG	A	1412	1/1	0.88	0.34	81,81,81,81	0
9	ANP	A	1413	31/31	0.92	0.19	30,34,37,39	0
9	ANP	X	1413	31/31	0.93	0.19	30,34,37,39	0

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 1413:

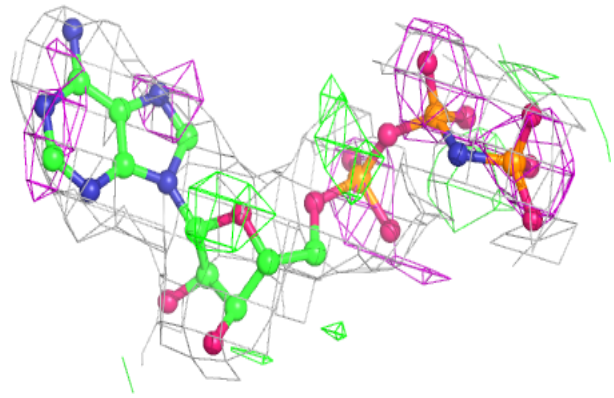
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

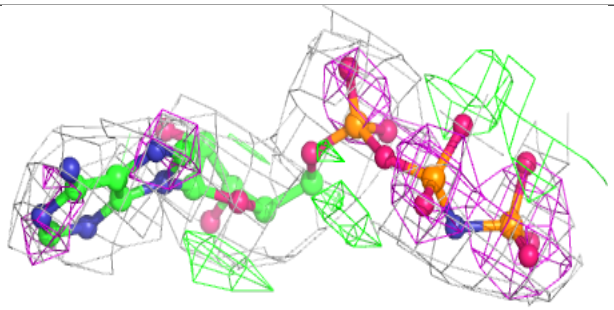


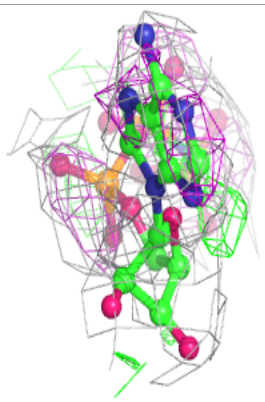


Electron density around ANP X 1413:

$2mF_o$-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

There are no such residues in this entry.