Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 06:19 PM EDT

PDB ID	:	7JXQ
Title	:	EGFR kinase (T790M/V948R) in complex with allosteric inhibitor JBJ-09-063
Authors	:	Beyett, T.S.; Eck, M.J.
Deposited on	:	2020-08-27
Resolution	:	1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

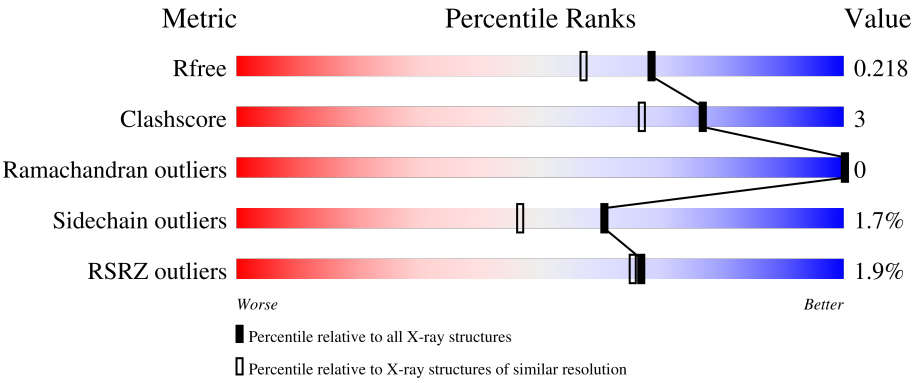
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	331	81% 7% • 11%
1	B	331	81% 8% 10%
1	C	331	83% 7% 10%
1	D	331	83% 7% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10431 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	298	Total	C	N	O	S	0	2	0
			2411	1549	409	432	21			
1	A	296	Total	C	N	O	S	0	2	0
			2399	1544	407	427	21			
1	B	297	Total	C	N	O	S	0	1	0
			2395	1541	407	427	20			
1	C	298	Total	C	N	O	S	0	1	0
			2397	1541	405	431	20			

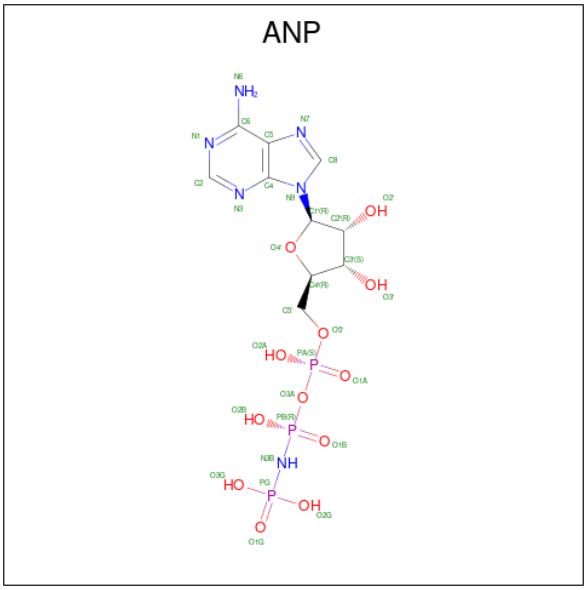
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

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

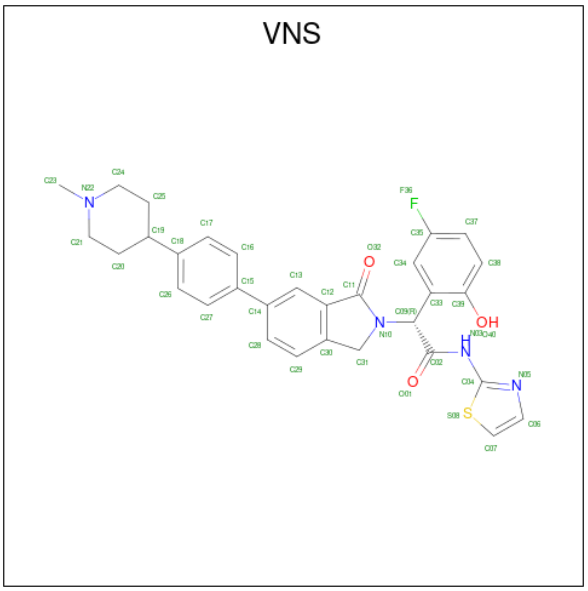
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 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
3	D	1	Total C N O P 31 10 6 12 3	0	0
3	A	1	Total C N O P 31 10 6 12 3	0	0
3	B	1	Total C N O P 31 10 6 12 3	0	0
3	C	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 4 is (2R)-2-(5-fluoro-2-hydroxyphenyl)-2-{6-[4-(1-methylpiperidin-4-yl)phenyl]-1-oxo-1,3-dihydro-2H-isoindol-2-yl}-N-(1,3-thiazol-2-yl)acetamide (three-letter code: VNS) (formula: $C_{31}H_{29}FN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	S	0	0
			40	31	1	4	3	1		
4	A	1	Total	C	F	N	O	S	0	0
			40	31	1	4	3	1		
4	B	1	Total	C	F	N	O	S	0	0
			40	31	1	4	3	1		
4	C	1	Total	C	F	N	O	S	0	0
			40	31	1	4	3	1		

- Molecule 5 is water.

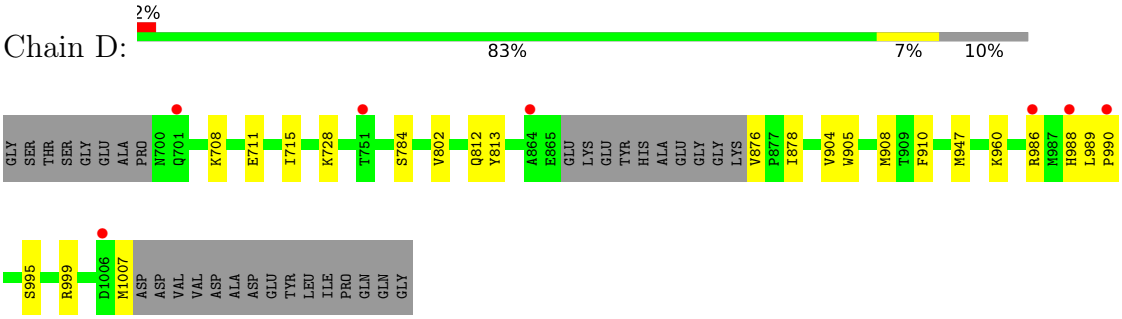
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	138	Total	O	0	0
			138	138		
5	A	120	Total	O	0	0
			120	120		
5	B	127	Total	O	0	0
			127	127		
5	C	156	Total	O	0	0
			156	156		

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.

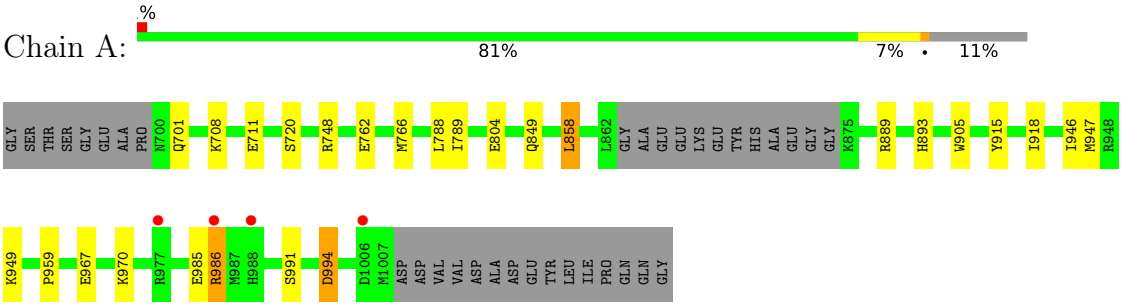
• Molecule 1: Epidermal growth factor receptor

Chain D:



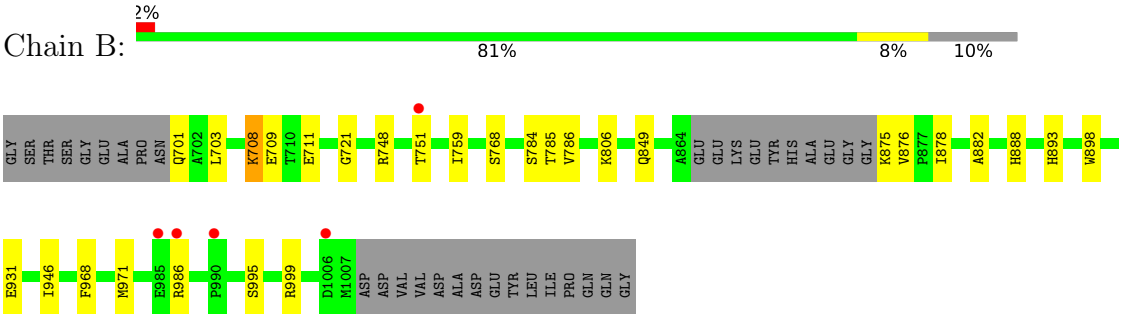
• Molecule 1: Epidermal growth factor receptor

Chain A:



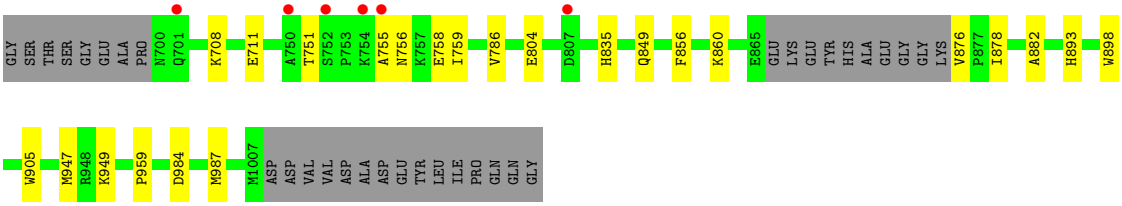
• Molecule 1: Epidermal growth factor receptor

Chain B:



• Molecule 1: Epidermal growth factor receptor

Chain C:


GLY SER THR SER GLY GLU ALA PRO N700 Q701 K708 E711 A750 T751 S752 P753 K754 A755 N756 K757 E758 I759 V786 E804 D807 H835 Q849 F856 K860 E865 GLU LYS GLU TYR HIS ALA GLU GLY LYS V876 P877 I878 A882 H893 W898
W905 M947 R948 K949 P959 D984 M987 M1007 ASP ASP VAL VAL ASP ALA ASP GLU TYR LEU ILE PRO GLN GLN GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.32Å 74.60Å 150.57Å 90.00° 98.69° 90.00°	Depositor
Resolution (Å)	66.69 – 1.83 66.69 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.9 (66.69-1.83) 90.2 (66.69-1.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.54 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.184 , 0.218 0.184 , 0.218	Depositor DCC
R_{free} test set	2002 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10431	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% 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: ANP, VNS, 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	0.40	0/2457	0.57	0/3319
1	B	0.41	0/2450	0.57	0/3310
1	C	0.45	0/2452	0.59	0/3315
1	D	0.43	0/2466	0.58	0/3332
All	All	0.42	0/9825	0.58	0/13276

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	2399	0	2463	16	0
1	B	2395	0	2456	15	0
1	C	2397	0	2444	13	0
1	D	2411	0	2463	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	0	0
3	C	31	0	13	0	0
3	D	31	0	13	0	0
4	A	40	0	0	2	0
4	B	40	0	0	1	0
4	C	40	0	0	0	0
4	D	40	0	0	1	0
5	A	120	0	0	3	0
5	B	127	0	0	2	0
5	C	156	0	0	2	0
5	D	138	0	0	0	0
All	All	10431	0	9878	60	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 3.

All (60) 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:D:812:GLN:HG2	1:D:989:LEU:HG	1.64	0.77
1:A:720:SER:OG	1:A:748:ARG:NH1	2.26	0.69
1:A:849:GLN:NE2	5:A:1203:HOH:O	2.30	0.63
1:B:759:ILE:HD13	1:B:786:VAL:HG21	1.81	0.63
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.63	0.63
1:A:985:GLU:HG2	1:A:986:ARG:HD3	1.81	0.62
1:B:708:LYS:HE3	1:B:709:GLU:H	1.65	0.61
1:A:991:SER:HB3	1:A:994:ASP:HB2	1.84	0.59
1:B:876:VAL:HG23	1:B:878:ILE:HG12	1.86	0.57
1:B:893:HIS:HD2	5:B:1267:HOH:O	1.88	0.57
1:C:758:GLU:OE2	1:C:860:LYS:HD2	2.03	0.56
1:B:849:GLN:NE2	5:B:1202:HOH:O	2.30	0.56
1:C:949:LYS:HB3	1:C:959:PRO:HD3	1.89	0.55
1:C:876:VAL:HG23	1:C:878:ILE:HG12	1.89	0.55
1:B:751:THR:HG22	1:B:786:VAL:HG23	1.88	0.54
1:D:989:LEU:HB3	1:D:990:PRO:HD2	1.90	0.53
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.43	0.53
1:A:893:HIS:HD2	5:A:1286:HOH:O	1.90	0.53
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.73	0.53
1:D:876:VAL:HG23	1:D:878:ILE:HG12	1.91	0.52
1:B:968:PHE:HA	1:B:971:MET:HE3	1.93	0.51
1:A:905:TRP:CD1	1:A:947:MET:HE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ILE:HD13	1:C:786:VAL:HG21	1.93	0.50
1:D:812:GLN:HG2	1:D:989:LEU:CG	2.39	0.50
1:A:762:GLU:O	1:A:766[B]:MET:HG2	2.11	0.50
4:A:1102:VNS:O01	4:A:1102:VNS:S08	2.70	0.49
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.13	0.48
1:D:802:VAL:CG1	1:D:910:PHE:HA	2.43	0.48
1:A:915:TYR:HB3	1:A:918:ILE:HD12	1.94	0.48
4:B:1103:VNS:O01	4:B:1103:VNS:S08	2.72	0.48
1:A:946:ILE:HD11	1:A:967:GLU:HG2	1.97	0.47
1:B:703:LEU:HD13	1:B:768:SER:HA	1.97	0.47
1:B:708:LYS:O	1:B:711:GLU:HG2	2.13	0.47
4:D:1103:VNS:O01	4:D:1103:VNS:S08	2.74	0.45
1:B:995:SER:O	1:B:999:ARG:HG3	2.16	0.45
1:B:721:GLY:O	1:B:748:ARG:NH1	2.51	0.44
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.82	0.44
1:D:802:VAL:HG12	1:D:910:PHE:HA	2.00	0.44
1:D:988:HIS:CG	1:D:989:LEU:N	2.86	0.44
1:A:804:GLU:OE1	5:A:1201:HOH:O	2.21	0.44
1:C:849:GLN:NE2	5:C:1206:HOH:O	2.46	0.44
1:D:904:VAL:O	1:D:908[B]:MET:HG3	2.18	0.43
1:A:708:LYS:O	1:A:711:GLU:HG2	2.19	0.43
1:C:893:HIS:HD2	5:C:1256:HOH:O	2.01	0.43
1:C:835:HIS:CD2	1:C:856:PHE:HB3	2.54	0.43
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.54	0.43
1:B:888:HIS:NE2	1:C:755:ALA:HB2	2.34	0.42
1:D:708:LYS:O	1:D:711:GLU:HG2	2.19	0.42
1:B:751:THR:CG2	1:B:786:VAL:HG23	2.51	0.41
1:B:946:ILE:CD1	1:B:971:MET:HE1	2.50	0.41
1:C:751:THR:HB	1:C:756:ASN:OD1	2.21	0.41
1:D:715:ILE:HG12	1:D:728:LYS:O	2.21	0.41
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.55	0.41
1:C:984:ASP:HA	1:C:987:MET:HG3	2.02	0.41
1:A:858:LEU:HD11	4:A:1102:VNS:C12	2.50	0.41
1:A:970:LYS:HE2	1:A:970:LYS:HB3	1.91	0.41
1:D:995:SER:O	1:D:999:ARG:HG3	2.21	0.40
1:C:708:LYS:O	1:C:711:GLU:HG2	2.21	0.40
1:A:788:LEU:C	1:A:789:ILE:HD12	2.42	0.40
1:A:949:LYS:HB3	1:A:959:PRO:HD3	2.03	0.40

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	294/331 (89%)	289 (98%)	5 (2%)	0	100	100
1	B	294/331 (89%)	288 (98%)	6 (2%)	0	100	100
1	C	295/331 (89%)	290 (98%)	5 (2%)	0	100	100
1	D	296/331 (89%)	290 (98%)	6 (2%)	0	100	100
All	All	1179/1324 (89%)	1157 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	267/290 (92%)	262 (98%)	5 (2%)	57	42
1	B	265/290 (91%)	257 (97%)	8 (3%)	41	23
1	C	265/290 (91%)	264 (100%)	1 (0%)	91	88
1	D	267/290 (92%)	263 (98%)	4 (2%)	65	52
All	All	1064/1160 (92%)	1046 (98%)	18 (2%)	60	47

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	784	SER
1	D	960	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	986	ARG
1	D	1007	MET
1	A	701	GLN
1	A	858	LEU
1	A	889	ARG
1	A	986	ARG
1	A	994	ASP
1	B	701	GLN
1	B	708	LYS
1	B	784	SER
1	B	785	THR
1	B	806	LYS
1	B	875	LYS
1	B	931	GLU
1	B	986	ARG
1	C	804	GLU

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	VNS	D	1103	-	43,45,45	2.20	18 (41%)	54,65,65	3.85	21 (38%)
3	ANP	C	1103	2	29,33,33	0.95	1 (3%)	31,52,52	1.08	3 (9%)
4	VNS	C	1102	-	43,45,45	2.20	13 (30%)	54,65,65	3.64	21 (38%)
3	ANP	A	1103	2	29,33,33	0.97	2 (6%)	31,52,52	1.08	2 (6%)
3	ANP	B	1102	2	29,33,33	1.11	2 (6%)	31,52,52	1.00	2 (6%)
4	VNS	B	1103	-	43,45,45	2.13	14 (32%)	54,65,65	3.83	22 (40%)
3	ANP	D	1102	2	29,33,33	0.94	1 (3%)	31,52,52	1.16	4 (12%)
4	VNS	A	1102	-	43,45,45	2.37	13 (30%)	54,65,65	3.96	24 (44%)

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
4	VNS	D	1103	-	-	3/22/46/46	0/6/6/6
3	ANP	C	1103	2	-	5/14/38/38	0/3/3/3
4	VNS	C	1102	-	-	4/22/46/46	0/6/6/6
3	ANP	A	1103	2	-	5/14/38/38	0/3/3/3
3	ANP	B	1102	2	-	4/14/38/38	0/3/3/3
4	VNS	B	1103	-	-	1/22/46/46	0/6/6/6
3	ANP	D	1102	2	-	5/14/38/38	0/3/3/3
4	VNS	A	1102	-	-	2/22/46/46	0/6/6/6

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	VNS	C11-N10	6.55	1.42	1.36
4	C	1102	VNS	C11-N10	6.53	1.42	1.36
4	D	1103	VNS	C11-N10	6.18	1.42	1.36
4	C	1102	VNS	C31-N10	5.58	1.51	1.46
4	B	1103	VNS	C11-N10	5.55	1.41	1.36
4	A	1102	VNS	C09-C02	5.43	1.60	1.54
4	A	1102	VNS	C31-N10	5.38	1.51	1.46
4	A	1102	VNS	C33-C09	5.17	1.58	1.52
4	D	1103	VNS	C31-N10	4.67	1.50	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	VNS	C02-N03	4.56	1.45	1.35
4	B	1103	VNS	C33-C09	4.48	1.58	1.52
4	A	1102	VNS	C02-N03	4.27	1.45	1.35
4	C	1102	VNS	C02-N03	3.93	1.44	1.35
4	C	1102	VNS	C09-N10	-3.55	1.43	1.46
4	B	1103	VNS	C09-N10	-3.54	1.43	1.46
4	B	1103	VNS	C31-N10	3.52	1.49	1.46
4	D	1103	VNS	C33-C09	3.48	1.56	1.52
4	C	1102	VNS	C33-C09	3.27	1.56	1.52
4	D	1103	VNS	C02-N03	3.24	1.42	1.35
4	C	1102	VNS	C34-C35	3.23	1.43	1.37
4	D	1103	VNS	C39-C33	3.19	1.43	1.40
4	D	1103	VNS	C17-C16	3.12	1.44	1.38
4	B	1103	VNS	C34-C35	3.03	1.42	1.37
4	A	1102	VNS	C17-C16	2.99	1.44	1.38
3	B	1102	ANP	PB-O3A	-2.91	1.55	1.59
4	D	1103	VNS	C31-C30	2.89	1.54	1.50
4	A	1102	VNS	C39-C33	2.82	1.43	1.40
4	D	1103	VNS	C18-C19	2.81	1.57	1.52
4	A	1102	VNS	C18-C19	2.78	1.57	1.52
4	B	1103	VNS	C17-C16	2.76	1.43	1.38
4	C	1102	VNS	C17-C16	2.72	1.43	1.38
4	D	1103	VNS	C37-C35	2.72	1.42	1.37
4	D	1103	VNS	C34-C35	2.71	1.42	1.37
4	A	1102	VNS	C34-C35	2.69	1.42	1.37
4	B	1103	VNS	C37-C35	2.68	1.42	1.37
4	C	1102	VNS	C37-C35	2.66	1.42	1.37
3	D	1102	ANP	PG-N3B	2.64	1.70	1.63
4	D	1103	VNS	C28-C14	2.60	1.44	1.39
4	D	1103	VNS	C15-C14	2.58	1.55	1.49
3	B	1102	ANP	PG-N3B	2.55	1.70	1.63
4	B	1103	VNS	C04-N03	2.53	1.41	1.36
4	B	1103	VNS	C39-C33	2.49	1.43	1.40
4	C	1102	VNS	C39-C33	2.48	1.43	1.40
4	A	1102	VNS	C37-C35	2.48	1.41	1.37
4	D	1103	VNS	C29-C30	2.47	1.43	1.39
4	C	1102	VNS	C29-C28	2.47	1.43	1.38
3	A	1103	ANP	PB-O3A	-2.43	1.56	1.59
4	D	1103	VNS	C29-C28	2.37	1.43	1.38
4	B	1103	VNS	C29-C28	2.36	1.43	1.38
4	B	1103	VNS	O01-C02	-2.34	1.18	1.23
4	A	1102	VNS	C15-C14	2.31	1.54	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1103	ANP	PB-O1B	2.28	1.49	1.46
4	D	1103	VNS	C27-C26	2.18	1.42	1.38
4	D	1103	VNS	C17-C18	2.18	1.42	1.39
4	A	1102	VNS	C29-C28	2.18	1.42	1.38
4	C	1102	VNS	C28-C14	2.17	1.43	1.39
4	B	1103	VNS	C17-C18	2.13	1.42	1.39
4	C	1102	VNS	C04-N03	2.12	1.40	1.36
4	A	1102	VNS	C17-C18	2.07	1.42	1.39
4	D	1103	VNS	C09-C02	2.06	1.56	1.54
3	A	1103	ANP	PG-O1G	2.06	1.49	1.46
4	C	1102	VNS	C15-C14	2.05	1.54	1.49
4	D	1103	VNS	C09-N10	-2.04	1.44	1.46
4	B	1103	VNS	C27-C26	2.01	1.42	1.38

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	VNS	C31-N10-C11	-16.91	106.16	113.12
4	C	1102	VNS	C31-N10-C11	-15.93	106.56	113.12
4	D	1103	VNS	C31-N10-C11	-15.88	106.59	113.12
4	B	1103	VNS	C31-N10-C11	-15.44	106.77	113.12
4	B	1103	VNS	C30-C31-N10	11.11	105.88	102.18
4	A	1102	VNS	C30-C31-N10	11.11	105.88	102.18
4	C	1102	VNS	C30-C31-N10	10.71	105.75	102.18
4	D	1103	VNS	C30-C31-N10	10.51	105.68	102.18
4	A	1102	VNS	C12-C11-N10	9.42	112.00	106.44
4	D	1103	VNS	C12-C11-N10	9.13	111.83	106.44
4	B	1103	VNS	C12-C11-N10	8.83	111.65	106.44
4	C	1102	VNS	C12-C11-N10	8.49	111.45	106.44
4	B	1103	VNS	O32-C11-N10	-8.46	118.89	125.24
4	A	1102	VNS	O32-C11-N10	-8.09	119.18	125.24
4	D	1103	VNS	O32-C11-N10	-7.96	119.27	125.24
4	C	1102	VNS	O32-C11-N10	-7.83	119.37	125.24
4	D	1103	VNS	C24-C25-C19	6.87	119.17	111.04
4	B	1103	VNS	C24-N22-C21	6.43	118.51	109.52
4	D	1103	VNS	C21-C20-C19	5.59	117.66	111.04
4	A	1102	VNS	C30-C12-C11	-5.42	106.04	108.94
4	B	1103	VNS	C30-C12-C11	-5.34	106.08	108.94
4	B	1103	VNS	C20-C19-C18	-5.17	100.67	112.79
4	D	1103	VNS	C20-C19-C18	-5.03	101.00	112.79
4	A	1102	VNS	C24-C25-C19	5.03	116.99	111.04
4	A	1102	VNS	C24-N22-C21	4.98	116.48	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	VNS	C21-C20-C19	4.59	116.47	111.04
4	A	1102	VNS	C20-C21-N22	4.43	117.16	111.22
4	D	1103	VNS	C30-C12-C11	-4.40	106.58	108.94
4	A	1102	VNS	C16-C15-C14	4.40	128.97	121.36
4	B	1103	VNS	C20-C21-N22	4.35	117.06	111.22
4	A	1102	VNS	C20-C19-C18	-4.18	102.99	112.79
4	C	1102	VNS	C24-N22-C21	4.17	115.35	109.52
4	C	1102	VNS	C30-C12-C11	-4.13	106.73	108.94
4	C	1102	VNS	C23-N22-C24	-4.00	104.68	110.66
4	C	1102	VNS	C20-C19-C18	-3.97	103.48	112.79
4	D	1103	VNS	C16-C15-C14	3.87	128.06	121.36
4	B	1103	VNS	C21-C20-C19	3.85	115.60	111.04
4	A	1102	VNS	C23-N22-C24	-3.85	104.90	110.66
4	A	1102	VNS	C23-N22-C21	-3.71	105.11	110.66
4	D	1103	VNS	C24-N22-C21	3.69	114.68	109.52
4	B	1103	VNS	C04-N03-C02	-3.60	121.02	129.02
4	C	1102	VNS	C24-C25-C19	3.60	115.29	111.04
4	D	1103	VNS	C26-C18-C17	-3.56	113.85	118.29
4	B	1103	VNS	C23-N22-C21	-3.54	105.37	110.66
4	C	1102	VNS	C23-N22-C21	-3.41	105.56	110.66
4	C	1102	VNS	C16-C15-C14	3.40	127.25	121.36
4	B	1103	VNS	C23-N22-C24	-3.40	105.57	110.66
4	B	1103	VNS	C16-C15-C14	3.28	127.04	121.36
4	C	1102	VNS	C31-N10-C09	3.14	126.79	123.86
3	A	1103	ANP	O3G-PG-O1G	-3.12	105.60	113.45
4	A	1102	VNS	C26-C18-C17	-3.02	114.52	118.29
4	D	1103	VNS	C23-N22-C21	-3.01	106.16	110.66
4	D	1103	VNS	C04-N03-C02	-2.96	122.44	129.02
4	A	1102	VNS	C31-N10-C09	2.92	126.59	123.86
4	D	1103	VNS	C31-N10-C09	2.84	126.52	123.86
4	B	1103	VNS	C26-C18-C17	-2.83	114.76	118.29
4	D	1103	VNS	C25-C24-N22	2.82	115.01	111.22
4	D	1103	VNS	C20-C21-N22	2.81	115.00	111.22
4	D	1103	VNS	C37-C35-C34	-2.81	119.64	123.29
4	A	1102	VNS	C04-N03-C02	-2.80	122.79	129.02
4	C	1102	VNS	C26-C18-C17	-2.78	114.83	118.29
4	C	1102	VNS	C37-C35-C34	-2.77	119.69	123.29
3	D	1102	ANP	O1G-PG-N3B	-2.75	107.72	111.77
4	B	1103	VNS	C31-N10-C09	2.74	126.42	123.86
3	D	1102	ANP	O1B-PB-N3B	2.62	115.62	111.77
4	A	1102	VNS	C33-C34-C35	2.60	121.97	118.59
4	C	1102	VNS	C21-C20-C19	2.58	114.09	111.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1103	ANP	O3G-PG-O1G	-2.54	107.06	113.45
4	B	1103	VNS	C33-C34-C35	2.53	121.88	118.59
4	D	1103	VNS	C23-N22-C24	-2.53	106.87	110.66
4	C	1102	VNS	C04-N03-C02	-2.52	123.41	129.02
4	B	1103	VNS	C37-C35-C34	-2.51	120.03	123.29
4	C	1102	VNS	C28-C14-C15	2.42	125.56	121.36
4	D	1103	VNS	C33-C34-C35	2.42	121.74	118.59
4	B	1103	VNS	C25-C19-C18	2.41	118.43	112.79
4	D	1103	VNS	C27-C15-C16	-2.40	112.80	117.59
4	C	1102	VNS	C20-C21-N22	2.39	114.43	111.22
4	A	1102	VNS	C37-C35-C34	-2.32	120.27	123.29
4	C	1102	VNS	C33-C34-C35	2.31	121.59	118.59
4	A	1102	VNS	C27-C15-C14	-2.30	117.37	121.36
4	B	1103	VNS	C24-C25-C19	2.24	113.69	111.04
3	D	1102	ANP	O2B-PB-O1B	-2.23	105.25	109.92
4	B	1103	VNS	C28-C29-C30	-2.22	118.47	121.39
3	B	1102	ANP	C5-C6-N6	2.20	123.69	120.35
4	B	1103	VNS	C38-C39-C33	2.18	122.40	120.41
3	C	1103	ANP	C5-C6-N6	2.17	123.65	120.35
4	C	1102	VNS	C27-C15-C16	-2.14	113.33	117.59
4	D	1103	VNS	C26-C27-C15	2.13	124.20	121.13
4	A	1102	VNS	C38-C39-C33	2.12	122.35	120.41
3	B	1102	ANP	O2G-PG-O3G	2.12	113.27	107.64
4	A	1102	VNS	C27-C15-C16	-2.11	113.39	117.59
3	A	1103	ANP	C5-C6-N6	2.09	123.52	120.35
4	A	1102	VNS	C26-C27-C15	2.08	124.13	121.13
3	C	1103	ANP	O2G-PG-O1G	-2.07	108.25	113.45
4	B	1103	VNS	C27-C15-C16	-2.06	113.47	117.59
4	C	1102	VNS	C26-C27-C15	2.05	124.09	121.13
4	A	1102	VNS	C17-C18-C19	2.05	126.44	121.11
3	D	1102	ANP	C5-C6-N6	2.04	123.45	120.35
4	A	1102	VNS	C29-C30-C12	-2.01	118.49	120.31

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1102	ANP	PB-N3B-PG-O1G
3	D	1102	ANP	PG-N3B-PB-O1B
3	D	1102	ANP	PG-N3B-PB-O3A
3	D	1102	ANP	PA-O3A-PB-O1B
3	D	1102	ANP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1103	ANP	PB-N3B-PG-O1G
3	A	1103	ANP	PG-N3B-PB-O1B
3	A	1103	ANP	PG-N3B-PB-O3A
3	A	1103	ANP	PA-O3A-PB-O1B
3	A	1103	ANP	PA-O3A-PB-O2B
3	B	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PG-N3B-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O2B
3	C	1103	ANP	PB-N3B-PG-O1G
3	C	1103	ANP	PG-N3B-PB-O1B
3	C	1103	ANP	PA-O3A-PB-O1B
3	C	1103	ANP	PA-O3A-PB-O2B
4	A	1102	VNS	C02-C09-C33-C39
3	C	1103	ANP	PG-N3B-PB-O3A
4	C	1102	VNS	C02-C09-C33-C39
4	D	1103	VNS	C33-C09-N10-C31
4	B	1103	VNS	C33-C09-N10-C31
4	C	1102	VNS	C33-C09-N10-C31
4	C	1102	VNS	C13-C14-C15-C27
4	D	1103	VNS	C02-C09-C33-C34
4	A	1102	VNS	C02-C09-C33-C34
4	C	1102	VNS	C02-C09-C33-C34
4	D	1103	VNS	C02-C09-C33-C39

There are no ring outliers.

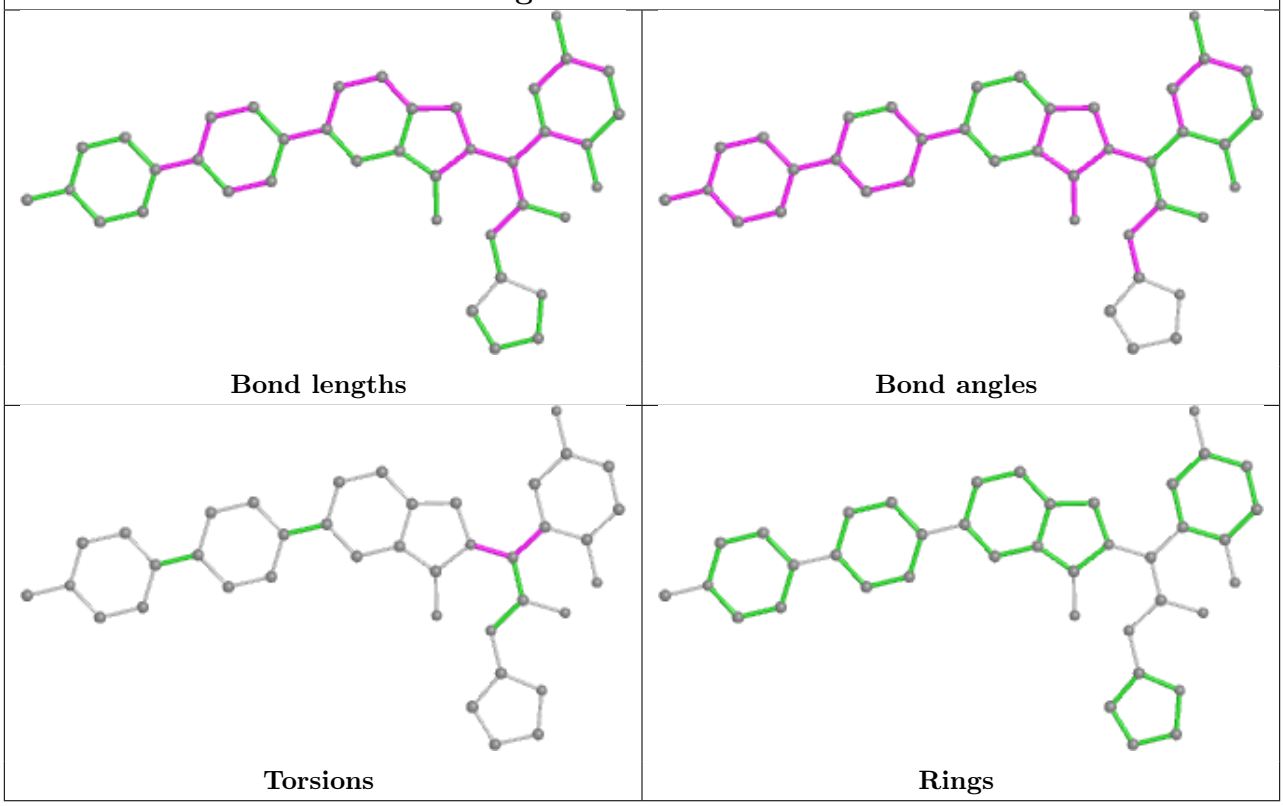
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1103	VNS	1	0
4	B	1103	VNS	1	0
4	A	1102	VNS	2	0

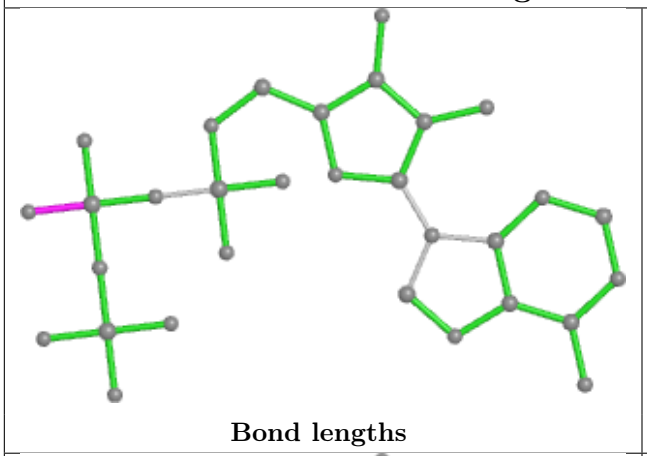
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

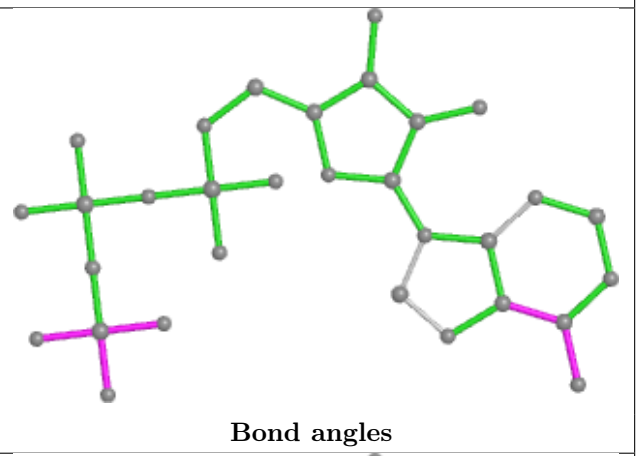
Ligand VNS D 1103



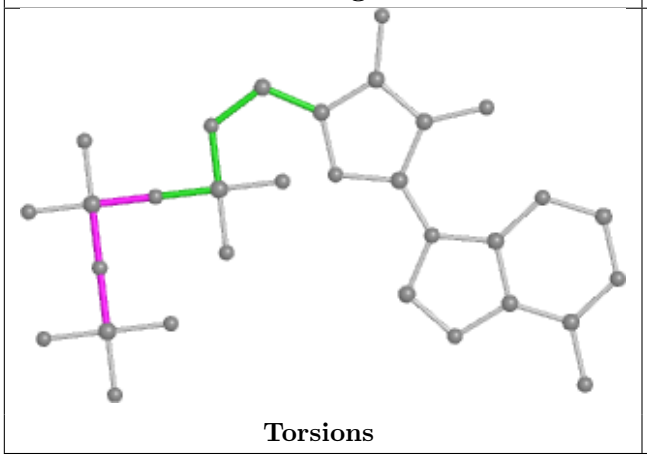
Ligand ANP C 1103



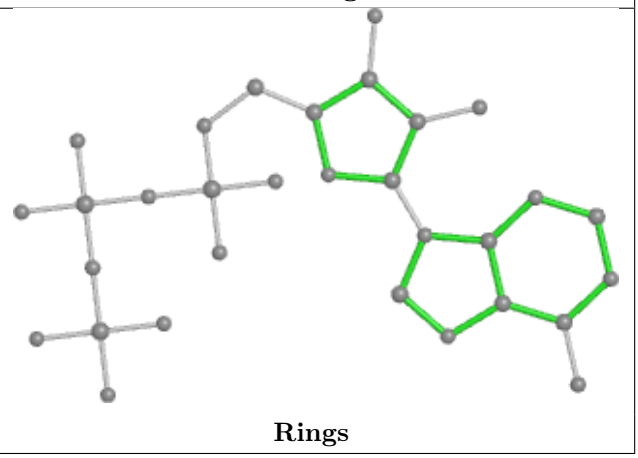
Bond lengths



Bond angles

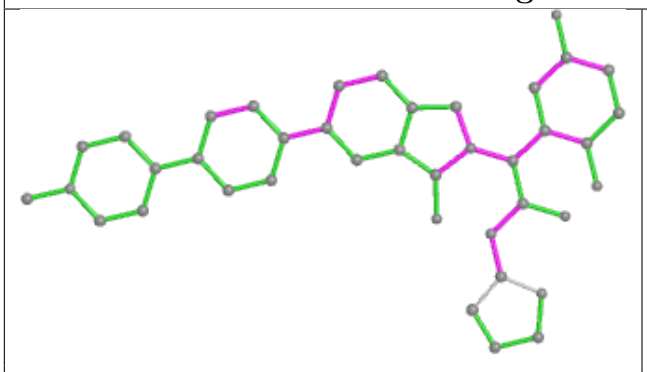


Torsions

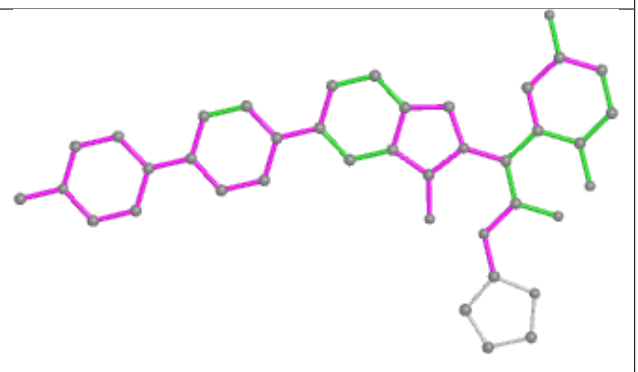


Rings

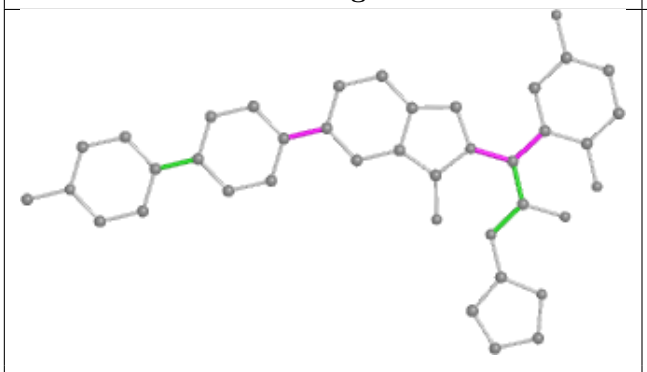
Ligand VNS C 1102



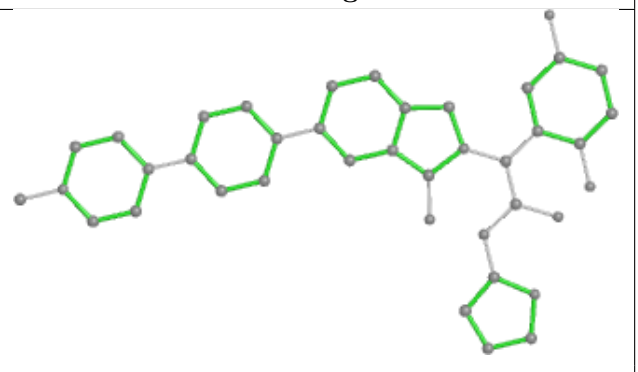
Bond lengths



Bond angles

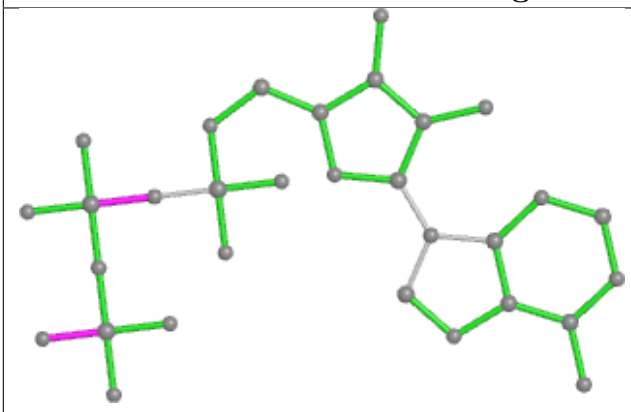


Torsions

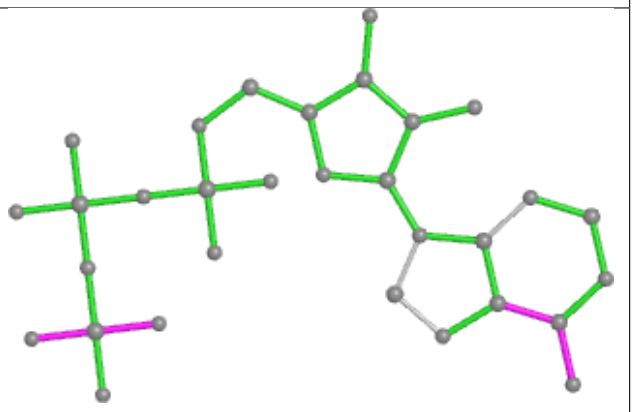


Rings

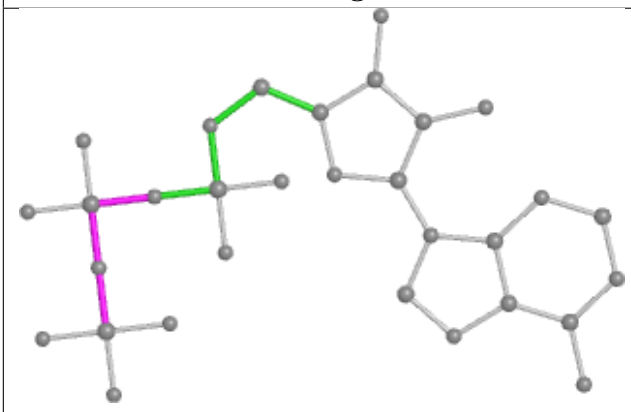
Ligand ANP A 1103



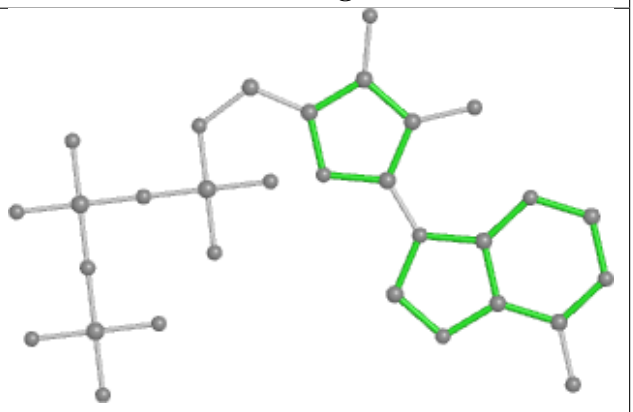
Bond lengths



Bond angles

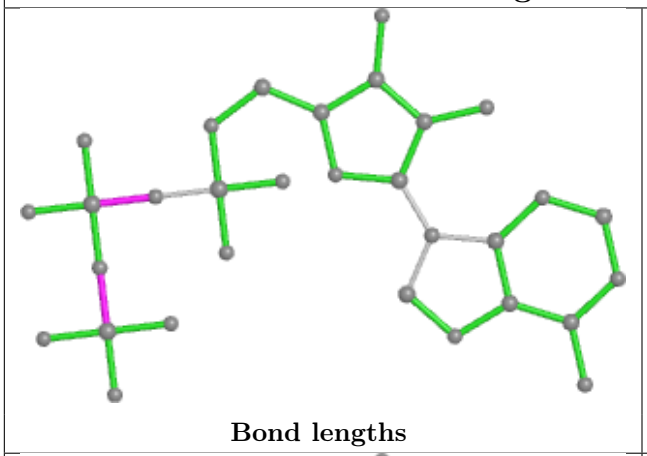


Torsions

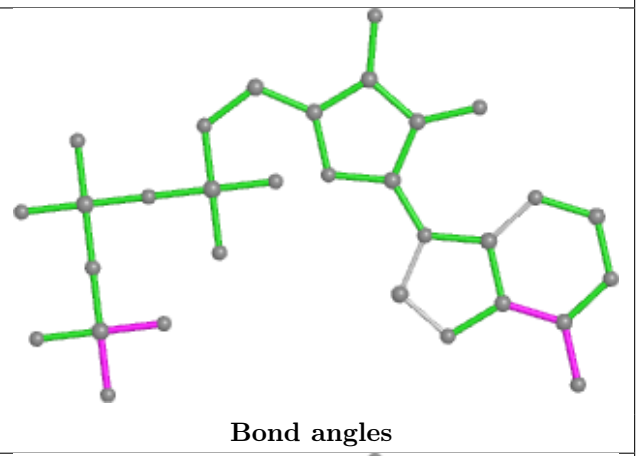


Rings

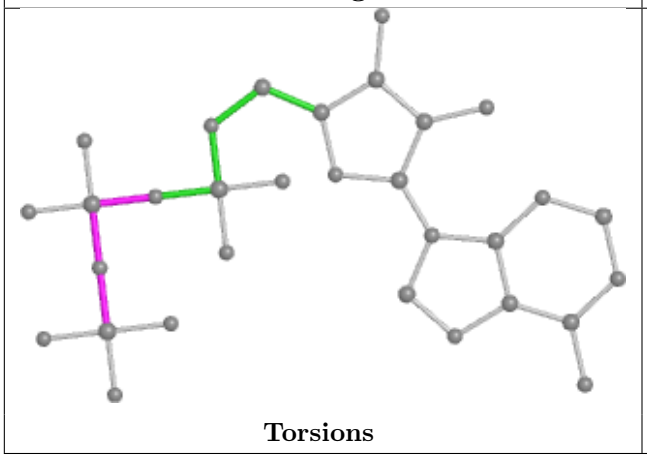
Ligand ANP B 1102



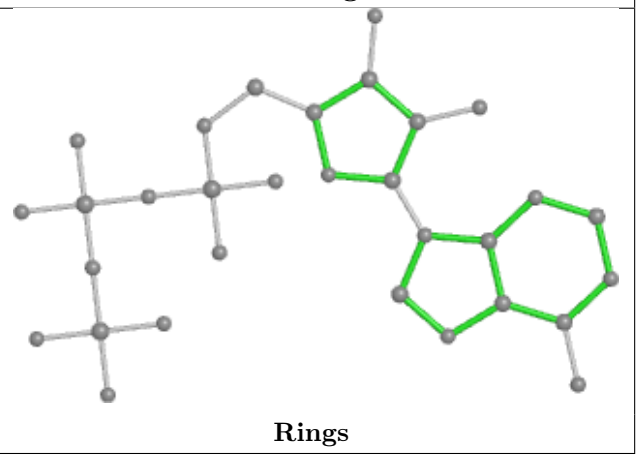
Bond lengths



Bond angles

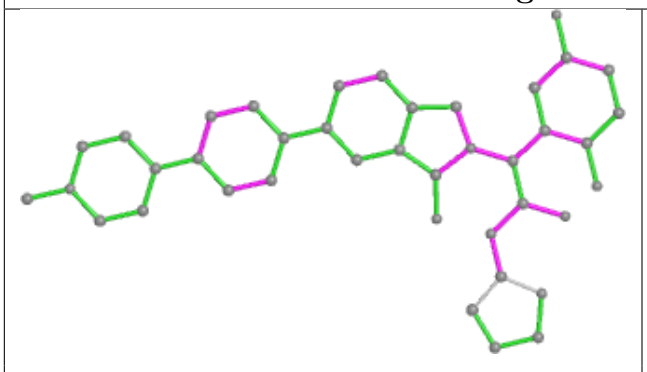


Torsions

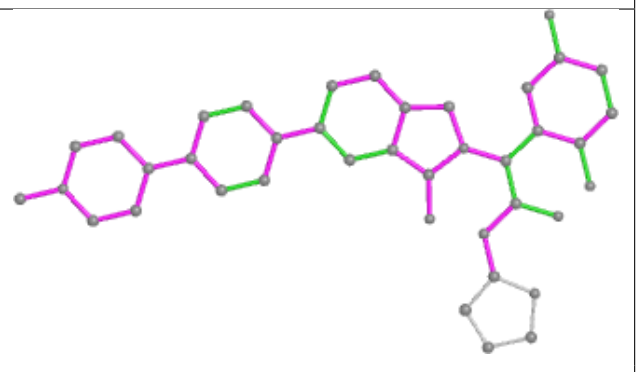


Rings

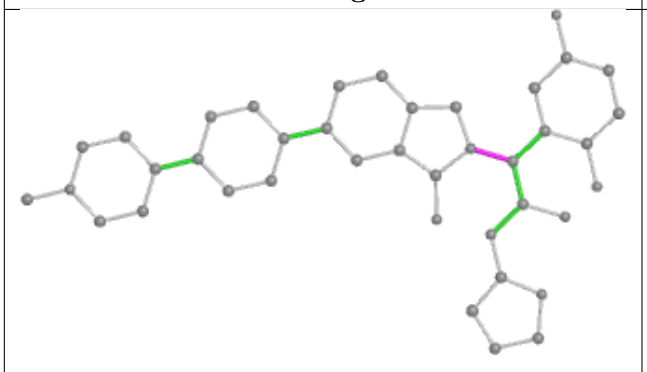
Ligand VNS B 1103



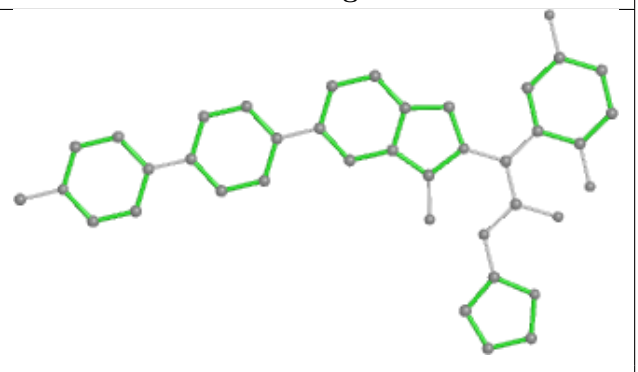
Bond lengths



Bond angles

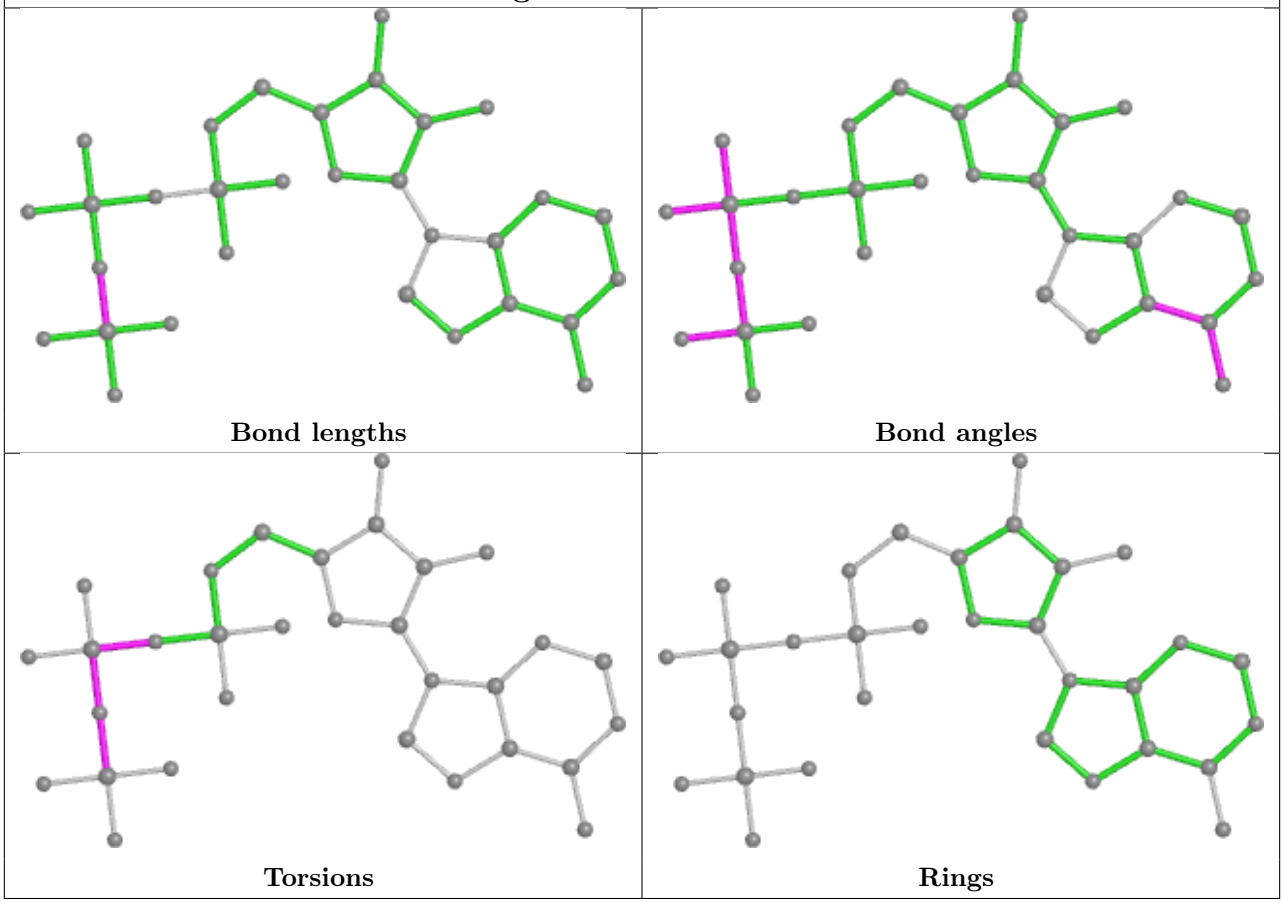


Torsions

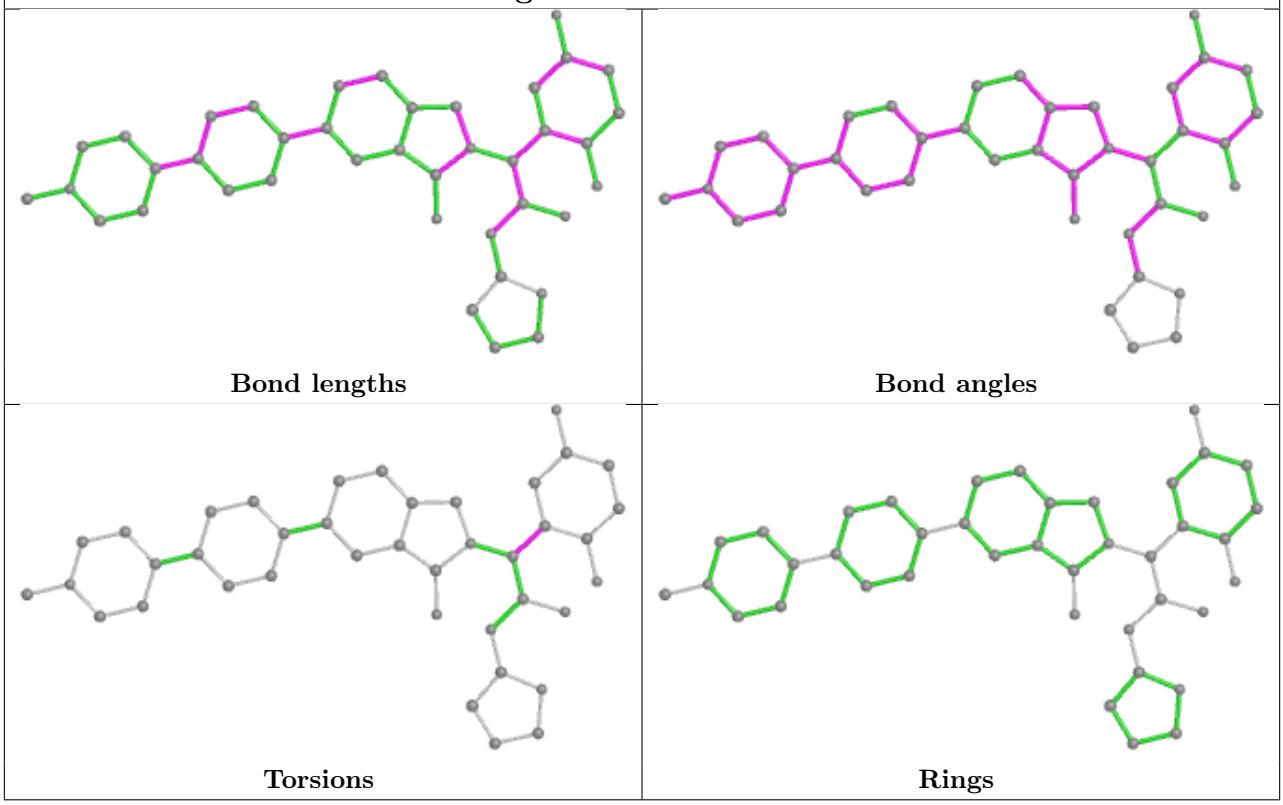


Rings

Ligand ANP D 1102



Ligand VNS A 1102



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	296/331 (89%)	-0.14	4 (1%)	75	75	26, 47, 72, 94	0
1	B	297/331 (89%)	-0.15	5 (1%)	70	69	25, 43, 72, 79	0
1	C	298/331 (90%)	-0.21	6 (2%)	65	64	26, 41, 66, 91	0
1	D	298/331 (90%)	-0.16	7 (2%)	60	58	25, 41, 67, 91	0
All	All	1189/1324 (89%)	-0.16	22 (1%)	66	65	25, 43, 71, 94	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	988	HIS	5.4
1	D	986	ARG	4.6
1	C	807	ASP	4.2
1	A	986	ARG	4.1
1	C	701	GLN	4.1
1	A	988	HIS	3.8
1	D	1006	ASP	3.6
1	D	864	ALA	3.1
1	B	1006	ASP	3.0
1	B	751	THR	3.0
1	B	985	GLU	2.8
1	B	986	ARG	2.7
1	C	750	ALA	2.7
1	D	990	PRO	2.7
1	C	752	SER	2.6
1	A	1006	ASP	2.5
1	A	977	ARG	2.5
1	D	701	GLN	2.4
1	D	751	THR	2.3
1	C	754	LYS	2.3
1	C	755	ALA	2.2
1	B	990	PRO	2.1

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)

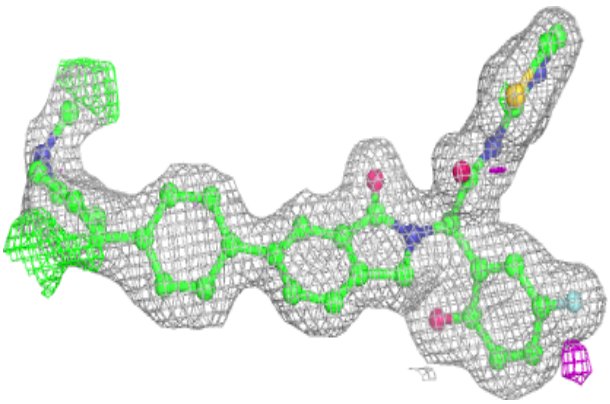
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

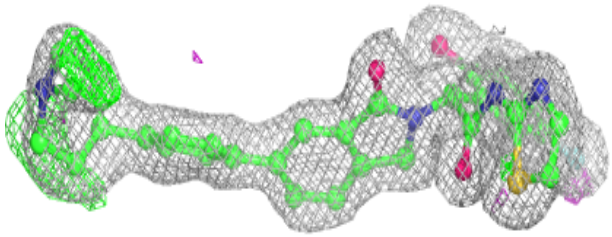
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	VNS	D	1103	40/40	0.95	0.11	25,31,56,67	0
4	VNS	A	1102	40/40	0.96	0.11	24,34,58,66	0
4	VNS	B	1103	40/40	0.96	0.11	26,37,58,72	0
4	VNS	C	1102	40/40	0.96	0.10	25,36,60,62	0
2	MG	A	1101	1/1	0.97	0.04	30,30,30,30	0
3	ANP	A	1103	31/31	0.97	0.09	23,32,40,42	0
3	ANP	D	1102	31/31	0.98	0.08	23,30,39,45	0
2	MG	C	1101	1/1	0.98	0.03	28,28,28,28	0
3	ANP	B	1102	31/31	0.98	0.09	24,31,38,39	0
3	ANP	C	1103	31/31	0.98	0.09	26,32,39,40	0
2	MG	B	1101	1/1	0.99	0.03	30,30,30,30	0
2	MG	D	1101	1/1	0.99	0.04	27,27,27,27	0

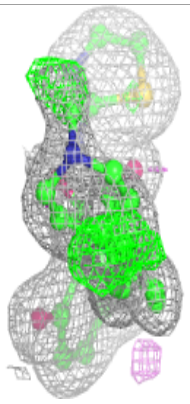
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VNS D 1103:

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

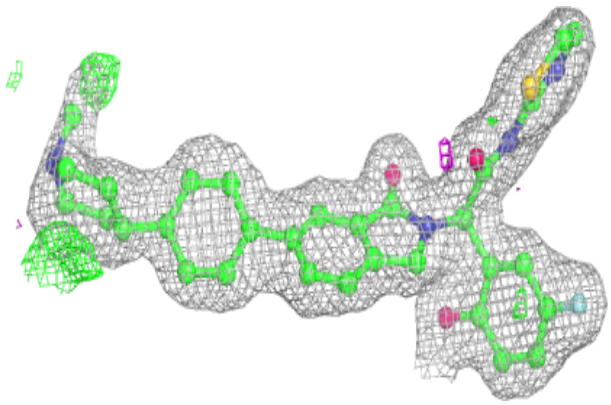


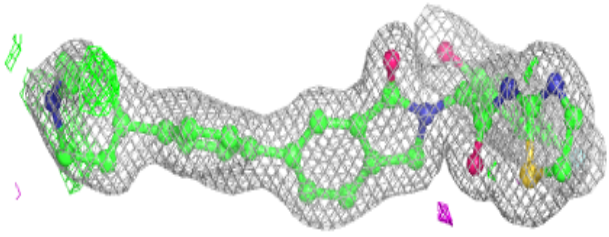


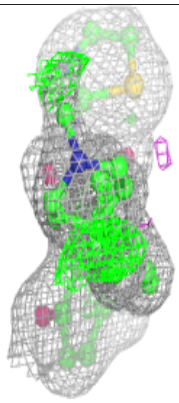


Electron density around VNS A 1102:

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

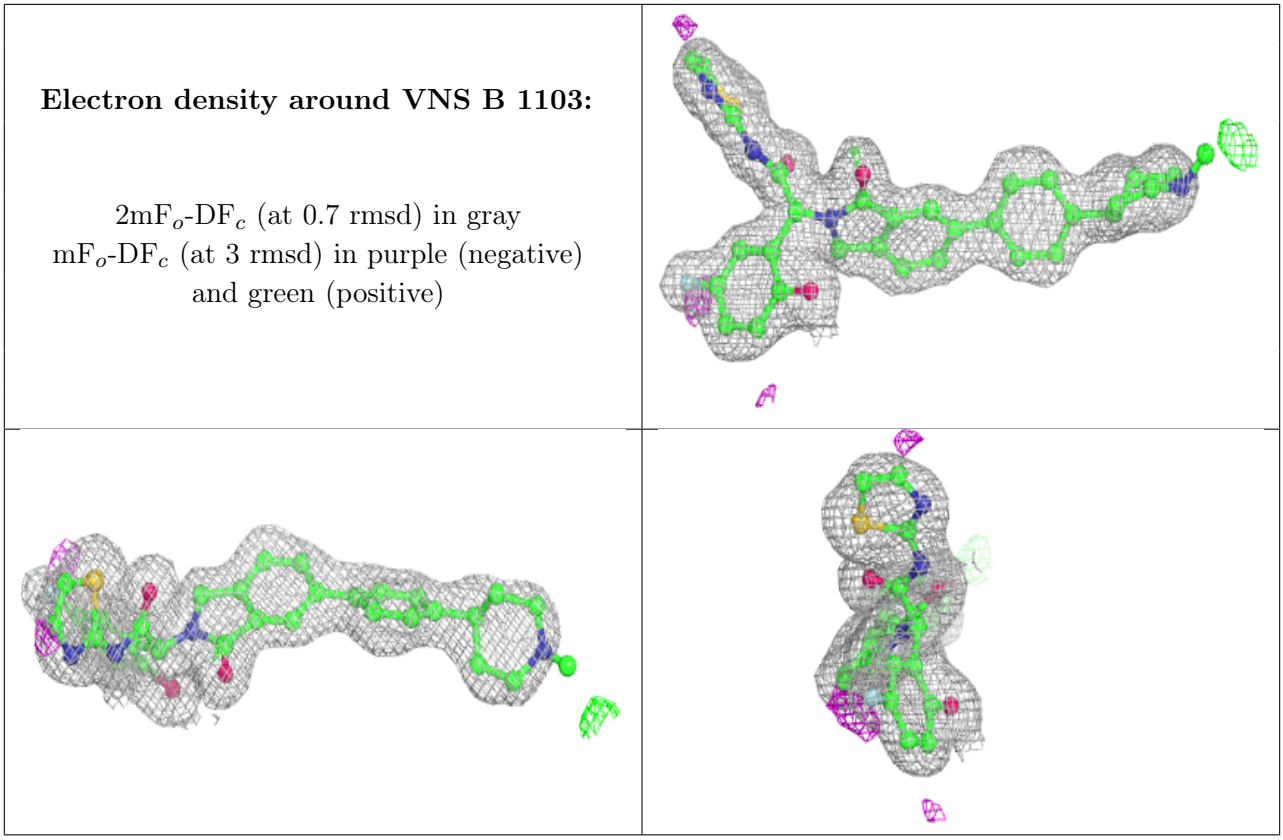






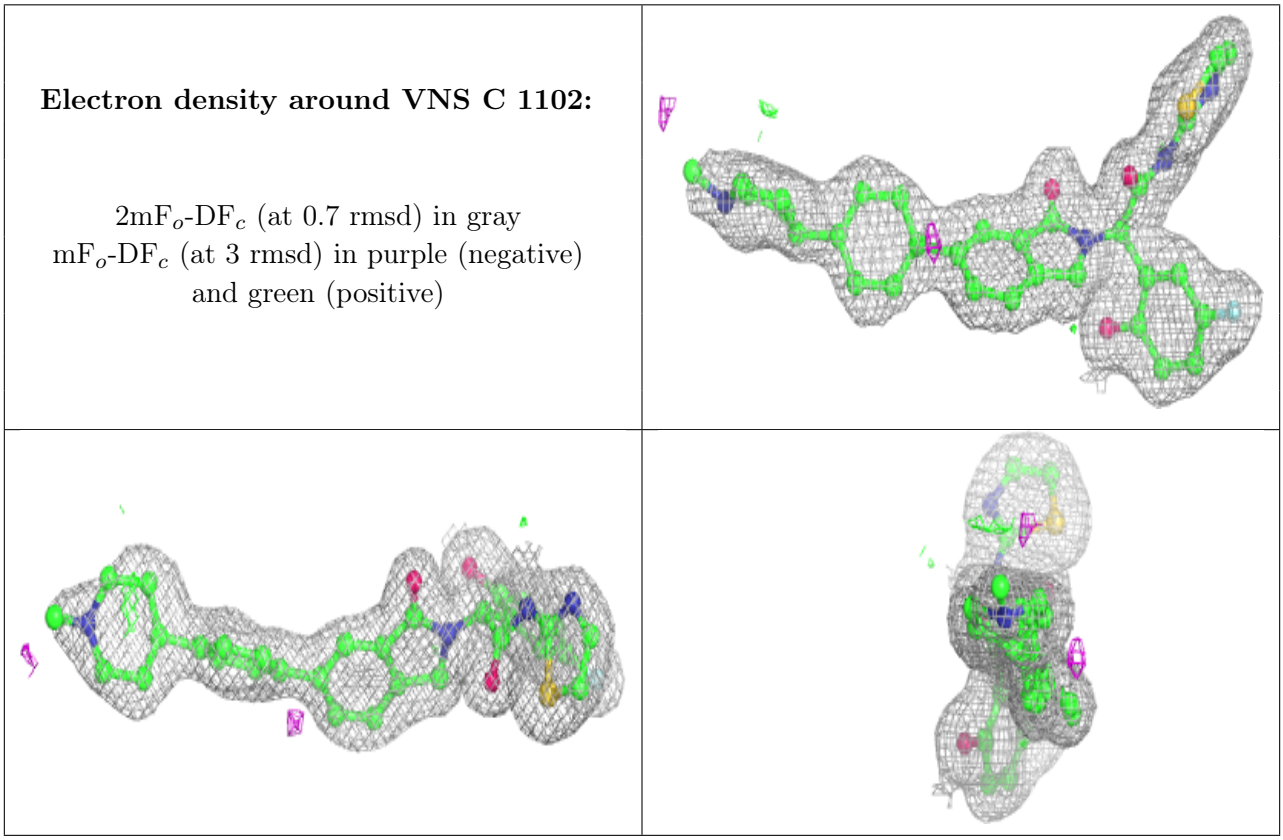
Electron density around VNS B 1103:

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



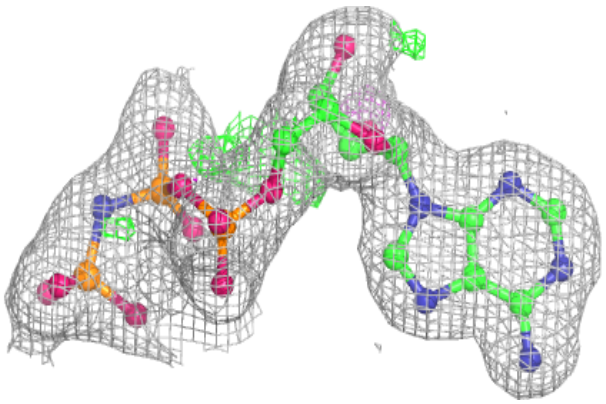
Electron density around VNS C 1102:

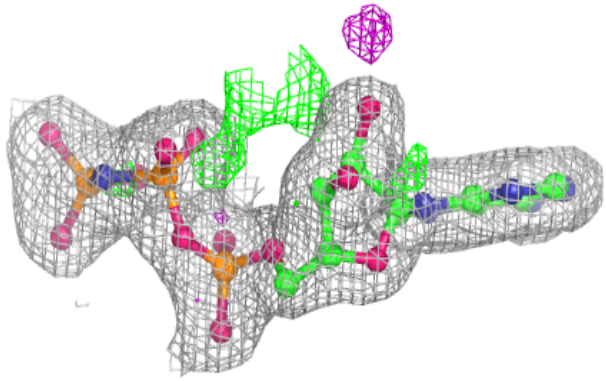
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

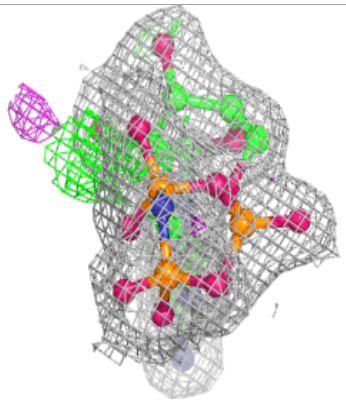


Electron density around ANP A 1103:

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

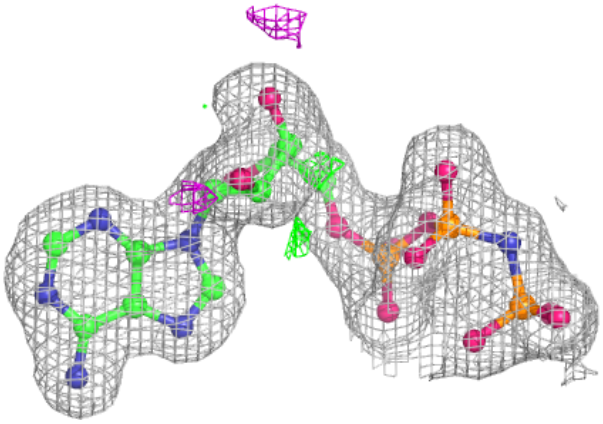


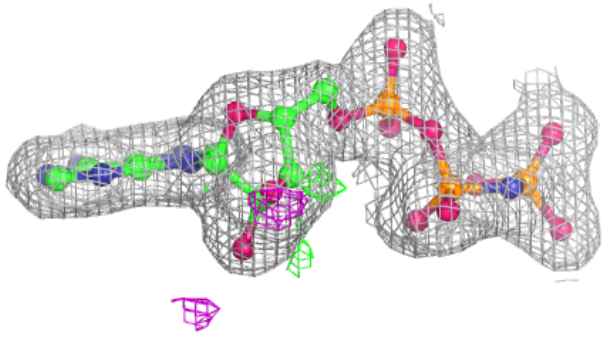


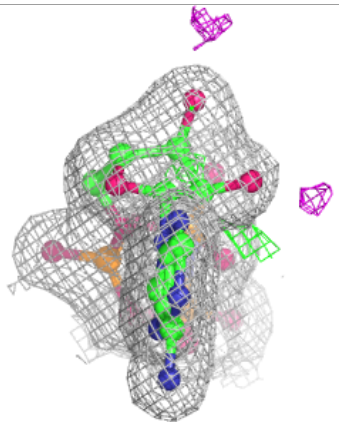


Electron density around ANP D 1102:

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

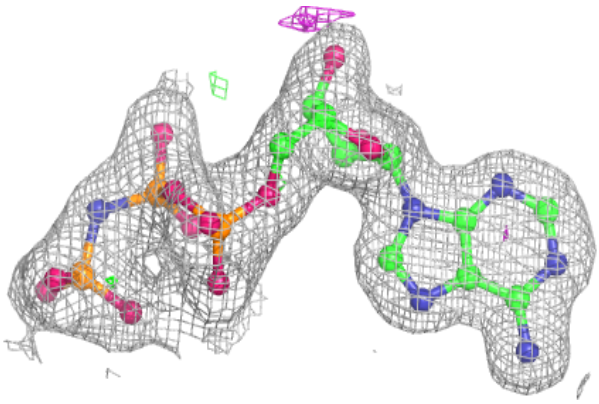


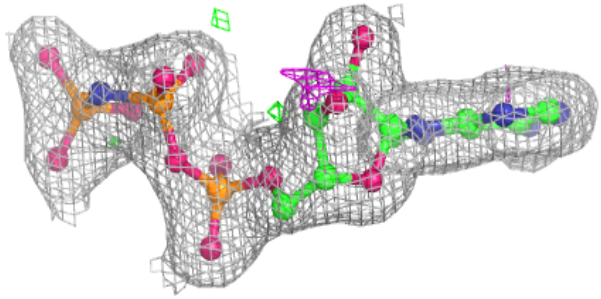


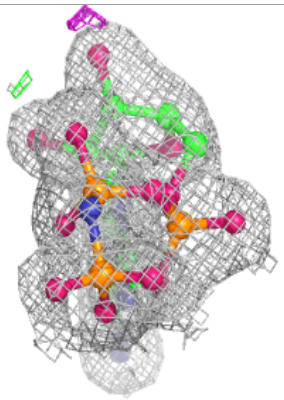


Electron density around ANP B 1102:

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

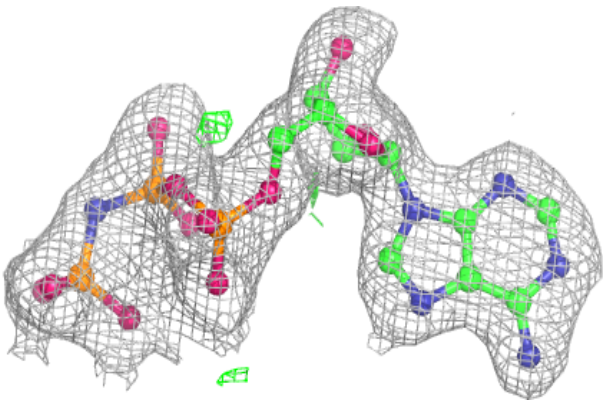


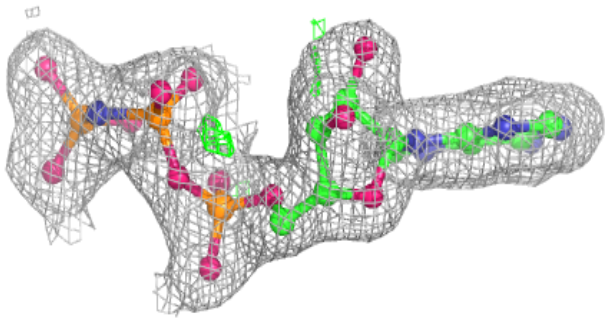


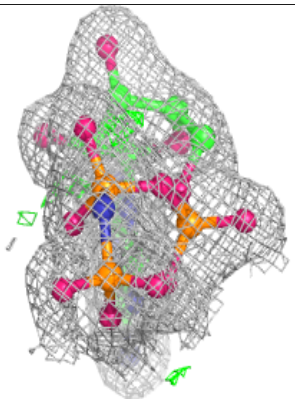


Electron density around ANP C 1103:

$2mF_o$-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.