Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2022 – 04:07 pm BST

PDB ID	:	7QPN
Title	:	Crystal Structure of Phosphatidylinositol 5-Phosphate 4-Kinase (PI5P4K2C) bound to an allosteric inhibitor and AMP-PNP
Authors	:	Howard, T.D.; Ogg, D.T.
Deposited on	:	2022-01-05
Resolution	:	1.95 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

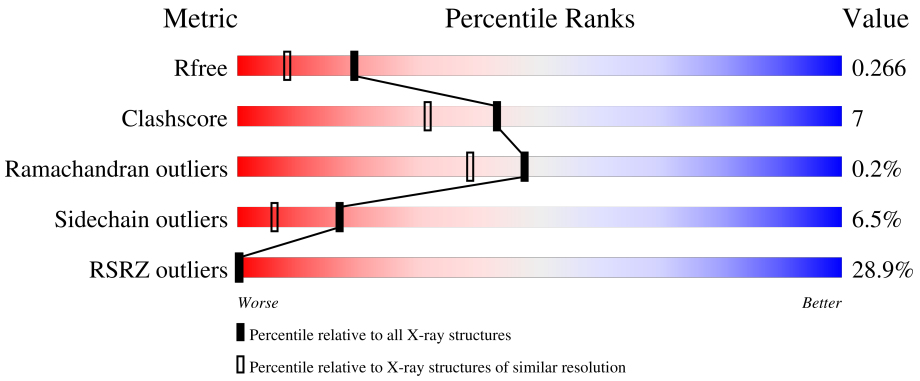
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	348	36% 71% 18% • 9%
1	B	348	16% 75% 14% • 10%

2 Entry composition

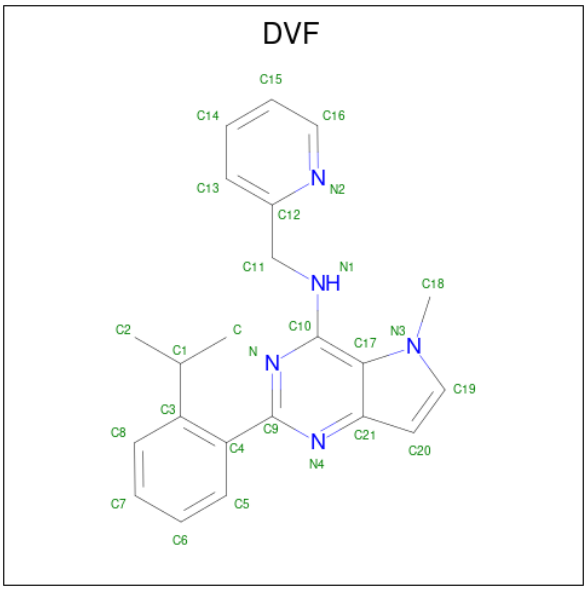
There are 4 unique types of molecules in this entry. The entry contains 5486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphatidylinositol 5-Phosphate 4-Kinase (PI5P4K2C).

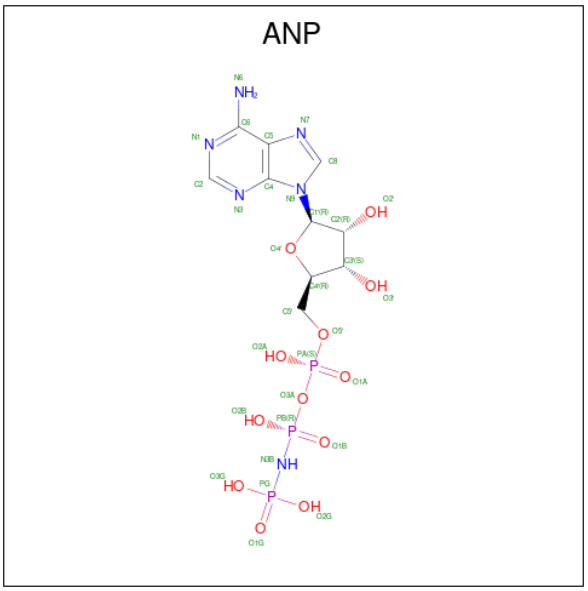
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2578	1661	439	467	11			
1	B	313	Total	C	N	O	S	0	5	0
			2555	1640	433	471	11			

- Molecule 2 is 5-methyl-2-(2-propan-2-ylphenyl)- {N}-(pyridin-2-ylmethyl)pyrrolo[3,2-d]pyrimidin-4-amine (three-letter code: DVF) (formula: $C_{22}H_{23}N_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			27	22	5		
2	B	1	Total	C	N	0	1
			54	44	10		

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

- Molecule 4 is water.

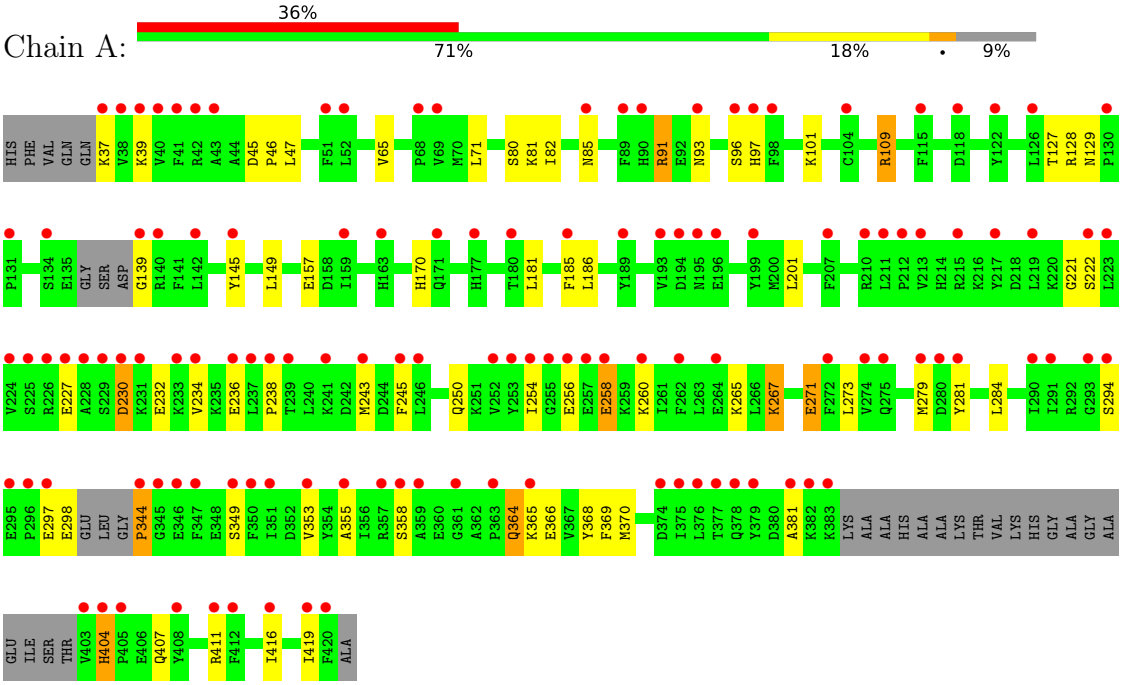
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	155	Total	O	0	0
			155	155		

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.

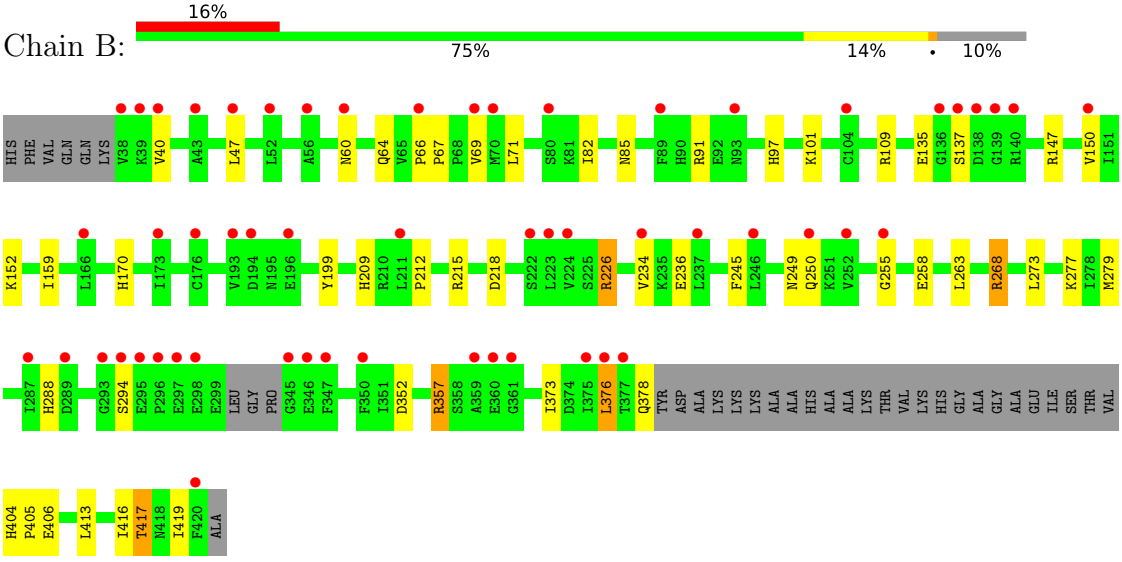
• Molecule 1: Phosphatidylinositol 5-Phosphate 4-Kinase (PI5P4K2C)

Chain A:



• Molecule 1: Phosphatidylinositol 5-Phosphate 4-Kinase (PI5P4K2C)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.92Å 65.62Å 117.12Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	116.94 – 1.95 116.94 – 1.95	Depositor EDS
% Data completeness (in resolution range)	74.0 (116.94-1.95) 74.0 (116.94-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.262 0.200 , 0.266	Depositor DCC
R_{free} test set	1877 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5486	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: DVF, 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	0.73	0/2637	0.84	0/3555
1	B	0.77	0/2613	0.92	3/3523 (0.1%)
All	All	0.75	0/5250	0.88	3/7078 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	226	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	109	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	147	ARG	NE-CZ-NH1	5.37	122.99	120.30

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	2578	0	2542	38	0
1	B	2555	0	2516	36	0
2	A	27	0	0	0	0
2	B	54	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	55	0	0	3	0
4	B	155	0	0	9	0
All	All	5486	0	5084	70	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 7.

All (70) 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:82:ILE:HD11	1:B:82:ILE:HD11	1.02	1.01
1:A:82:ILE:CD1	1:B:82:ILE:HD11	1.96	0.95
1:A:96:SER:OG	1:A:97:HIS:CD2	2.39	0.76
1:A:227:GLU:HG3	1:A:243:MET:HB2	1.73	0.70
1:B:215:ARG:NH1	4:B:602:HOH:O	2.27	0.68
1:A:404:HIS:HB2	1:A:407:GLN:NE2	2.11	0.66
1:A:82:ILE:HD11	1:B:82:ILE:CD1	1.99	0.66
1:A:358:SER:OG	1:A:366:GLU:N	2.31	0.63
1:A:404:HIS:HB2	1:A:407:GLN:HE22	1.63	0.63
1:A:101:LYS:NZ	3:A:502:ANP:O1B	2.34	0.60
1:A:129:ASN:HB2	1:A:145:TYR:CG	2.37	0.59
1:A:91:ARG:NH2	4:A:603:HOH:O	2.36	0.57
1:A:221:GLY:O	1:A:411:ARG:HD3	2.04	0.57
1:B:250:GLN:HA	4:B:656:HOH:O	2.05	0.57
1:B:263:LEU:HD13	1:B:417:THR:HG23	1.88	0.56
1:B:288:HIS:HE1	4:B:735:HOH:O	1.90	0.53
1:B:85:ASN:OD1	1:B:97:HIS:CD2	2.62	0.53
1:B:357:ARG:NH1	4:B:608:HOH:O	2.41	0.53
1:B:376[A]:LEU:HD12	1:B:376[A]:LEU:C	2.29	0.53
1:A:139:GLY:HA3	1:A:381:ALA:HB1	1.91	0.52
1:A:230:ASP:N	1:A:230:ASP:OD1	2.42	0.52
1:B:416:ILE:O	1:B:419:ILE:HG12	2.10	0.51
1:A:47:LEU:C	1:A:47:LEU:HD23	2.32	0.51
1:A:127:THR:O	1:A:128:ARG:C	2.48	0.51
1:B:406:GLU:H	1:B:406:GLU:CD	2.15	0.50
1:A:344:PRO:N	4:A:604:HOH:O	2.44	0.50
1:B:268:ARG:HD3	4:B:646:HOH:O	2.10	0.50
1:B:71:LEU:HD12	1:B:170:HIS:CE1	2.47	0.50
1:B:413:LEU:O	1:B:417:THR:OG1	2.30	0.50
1:B:255:GLY:HA3	1:B:258:GLU:OE1	2.13	0.49
1:B:60:ASN:HB2	4:B:614:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD12	1:A:170:HIS:CE1	2.49	0.48
1:B:236:GLU:H	1:B:236:GLU:CD	2.18	0.47
1:A:279:MET:O	1:A:281:TYR:CD2	2.67	0.47
1:A:96:SER:OG	1:A:97:HIS:HD2	1.91	0.47
1:A:81:LYS:HE3	1:B:85:ASN:ND2	2.30	0.47
1:A:267:LYS:HZ3	1:A:271:GLU:CD	2.17	0.46
1:A:355:ALA:HB2	1:A:369:PHE:CE1	2.50	0.46
1:A:232:GLU:O	1:A:238:PRO:HB3	2.16	0.46
1:B:47:LEU:C	1:B:47:LEU:HD23	2.36	0.45
1:B:245:PHE:CE1	1:B:250:GLN:CG	3.00	0.45
1:A:254:ILE:O	1:A:258:GLU:HG2	2.17	0.44
1:B:212:PRO:O	1:B:288:HIS:HD2	2.00	0.44
1:B:404:HIS:HB3	1:B:405:PRO:HD3	2.00	0.44
1:B:245:PHE:CE1	1:B:250:GLN:HG3	2.52	0.44
1:A:245:PHE:CE2	1:A:250:GLN:HG2	2.52	0.44
1:B:357:ARG:CZ	4:B:608:HOH:O	2.66	0.44
1:A:85:ASN:OD1	1:A:97:HIS:CE1	2.71	0.43
1:A:355:ALA:HA	1:A:368:TYR:O	2.18	0.43
1:B:249:ASN:ND2	4:B:621:HOH:O	2.52	0.43
1:A:149:LEU:HD22	1:A:186:LEU:HD12	2.01	0.42
1:B:209:HIS:HD2	1:B:352:ASP:OD1	2.02	0.42
1:A:65:VAL:O	1:A:109:ARG:NH2	2.45	0.42
1:A:416:ILE:O	1:A:419:ILE:HG12	2.20	0.42
1:B:137:SER:OG	1:B:152:LYS:HE3	2.19	0.42
1:A:284:LEU:O	1:A:370:MET:HA	2.19	0.42
1:A:297:GLU:O	1:A:298:GLU:C	2.57	0.42
1:B:97:HIS:HE1	4:B:738:HOH:O	2.02	0.41
1:B:159:ILE:HG13	1:B:199:TYR:CD2	2.55	0.41
1:B:376[A]:LEU:HD12	1:B:376[A]:LEU:O	2.20	0.41
1:A:185:PHE:CE1	1:A:201:LEU:HD21	2.55	0.41
1:A:364:GLN:HE21	1:A:364:GLN:HB2	1.77	0.41
1:A:129:ASN:HB2	1:A:145:TYR:CD2	2.56	0.41
4:A:611:HOH:O	1:B:64:GLN:HG3	2.20	0.40
1:B:66:PRO:HA	1:B:67:PRO:HD3	1.97	0.40
1:B:218:ASP:O	1:B:226:ARG:NH2	2.54	0.40
1:B:101:LYS:NZ	3:B:501:ANP:O2A	2.48	0.40
1:B:373:ILE:HD12	1:B:378[A]:GLN:HA	2.02	0.40
1:A:45:ASP:OD1	1:A:46:PRO:HD2	2.22	0.40
1:A:181:LEU:HG	1:A:265:LYS:HD2	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	309/348 (89%)	286 (93%)	23 (7%)	0	100 100
1	B	307/348 (88%)	295 (96%)	11 (4%)	1 (0%)	41 30
All	All	616/696 (88%)	581 (94%)	34 (6%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	VAL

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	282/313 (90%)	258 (92%)	24 (8%)	10 3
1	B	284/313 (91%)	271 (95%)	13 (5%)	27 14
All	All	566/626 (90%)	529 (94%)	37 (6%)	17 6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	39	LYS
1	A	80	SER
1	A	91	ARG
1	A	93	ASN

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	157	GLU
1	A	222	SER
1	A	230	ASP
1	A	234	VAL
1	A	236	GLU
1	A	256	GLU
1	A	258	GLU
1	A	260	LYS
1	A	267	LYS
1	A	271	GLU
1	A	273	LEU
1	A	294	SER
1	A	344	PRO
1	A	349	SER
1	A	353	VAL
1	A	364	GLN
1	A	365	LYS
1	A	404	HIS
1	B	69	VAL
1	B	91	ARG
1	B	135	GLU
1	B	150	VAL
1	B	234	VAL
1	B	268	ARG
1	B	273	LEU
1	B	277	LYS
1	B	279	MET
1	B	294	SER
1	B	357	ARG
1	B	376[A]	LEU
1	B	417	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	247	ASN
1	A	364	GLN
1	B	209	HIS
1	B	247	ASN
1	B	288	HIS

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Mol	Chain	Res	Type
1	B	364	GLN

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

5 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	$\#\|Z\| > 2$
3	ANP	A	502	-	29,33,33	1.28	4 (13%)	31,52,52	1.22	4 (12%)
2	DVF	B	502[B]	-	27,30,30	0.61	0	28,42,42	1.15	3 (10%)
2	DVF	A	501	-	27,30,30	0.67	1 (3%)	28,42,42	0.66	1 (3%)
2	DVF	B	502[A]	-	27,30,30	0.58	0	28,42,42	0.74	1 (3%)
3	ANP	B	501	-	29,33,33	1.30	5 (17%)	31,52,52	1.31	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	502	-	-	2/14/38/38	0/3/3/3
2	DVF	B	502[B]	-	-	9/13/13/13	0/4/4/4
2	DVF	A	501	-	-	0/13/13/13	0/4/4/4
2	DVF	B	502[A]	-	-	1/13/13/13	0/4/4/4
3	ANP	B	501	-	-	4/14/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ANP	PG-O1G	3.42	1.51	1.46
3	A	502	ANP	PG-O1G	3.24	1.51	1.46
3	A	502	ANP	PB-O3A	3.18	1.63	1.59
3	B	501	ANP	PB-O1B	3.09	1.51	1.46
3	A	502	ANP	PB-O1B	2.97	1.50	1.46
2	A	501	DVF	C10-N	2.32	1.36	1.32
3	B	501	ANP	PB-O3A	2.26	1.61	1.59
3	A	502	ANP	PB-O2B	-2.22	1.50	1.56
3	B	501	ANP	PG-O3G	-2.03	1.51	1.56
3	B	501	ANP	PB-O2B	-2.01	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502[B]	DVF	C12-C11-N1	-3.92	104.40	113.07
3	A	502	ANP	O2B-PB-O1B	3.74	117.75	109.92
3	B	501	ANP	O2B-PB-O1B	3.56	117.38	109.92
2	B	502[B]	DVF	C17-C10-N	3.04	121.50	117.72
3	B	501	ANP	O2G-PG-O1G	-3.02	105.85	113.45
2	B	502[A]	DVF	C17-C10-N	2.48	120.81	117.72
3	B	501	ANP	O3G-PG-O1G	-2.46	107.27	113.45
3	B	501	ANP	C5-C6-N6	2.26	123.78	120.35
2	B	502[B]	DVF	C2-C1-C3	-2.23	107.88	111.76
3	A	502	ANP	C5-C6-N6	2.21	123.72	120.35
3	A	502	ANP	O1G-PG-N3B	-2.09	108.69	111.77
3	A	502	ANP	O3G-PG-O1G	-2.08	108.21	113.45
2	A	501	DVF	C17-C10-N	2.05	120.27	117.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502[B]	DVF	C17-C10-N1-C11

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Mol	Chain	Res	Type	Atoms
3	A	502	ANP	PB-N3B-PG-O1G
3	B	501	ANP	PB-N3B-PG-O1G
3	B	501	ANP	O4'-C4'-C5'-O5'
3	B	501	ANP	C3'-C4'-C5'-O5'
2	B	502[B]	DVF	C5-C4-C9-N4
2	B	502[B]	DVF	C5-C4-C9-N
2	B	502[B]	DVF	C12-C11-N1-C10
2	B	502[B]	DVF	C3-C4-C9-N4
2	B	502[B]	DVF	C3-C4-C9-N
2	B	502[B]	DVF	N-C10-N1-C11
3	A	502	ANP	PB-O3A-PA-O2A
3	B	501	ANP	PB-O3A-PA-O2A
2	B	502[B]	DVF	N1-C11-C12-C13
2	B	502[A]	DVF	C5-C4-C9-N
2	B	502[B]	DVF	N1-C11-C12-N2

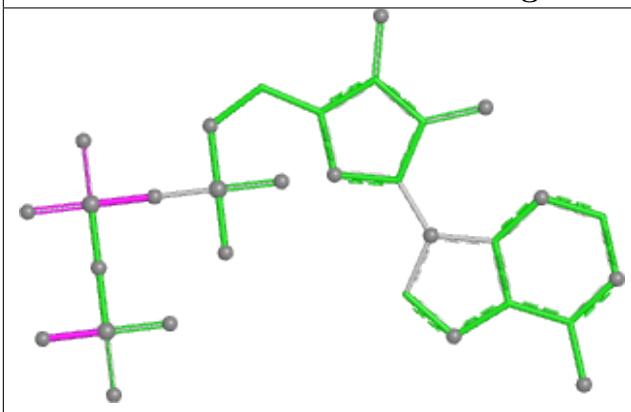
There are no ring outliers.

2 monomers are involved in 2 short contacts:

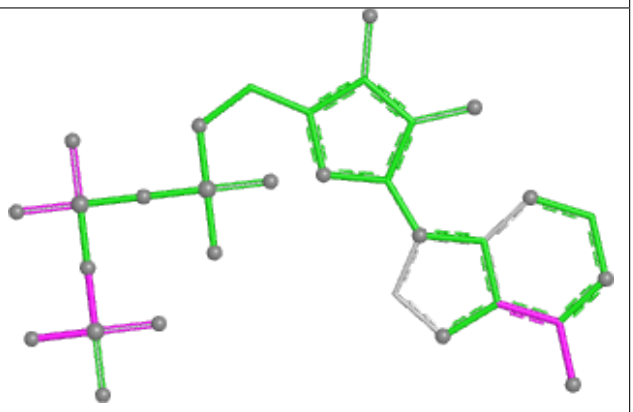
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ANP	1	0
3	B	501	ANP	1	0

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.

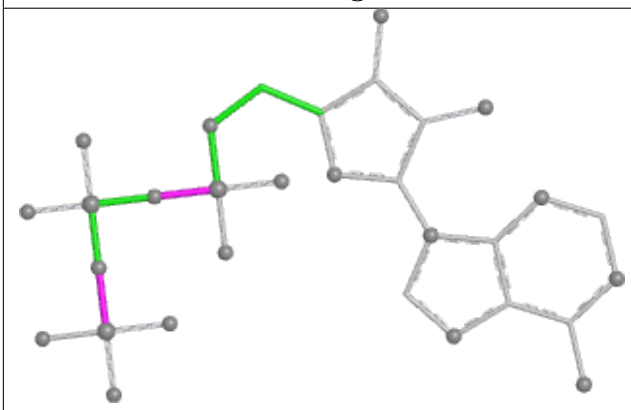
Ligand ANP A 502



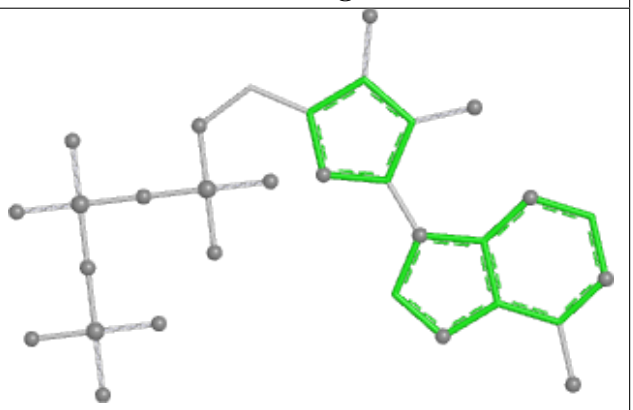
Bond lengths



Bond angles

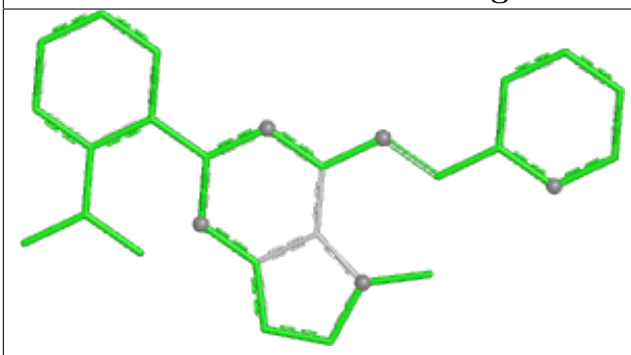


Torsions

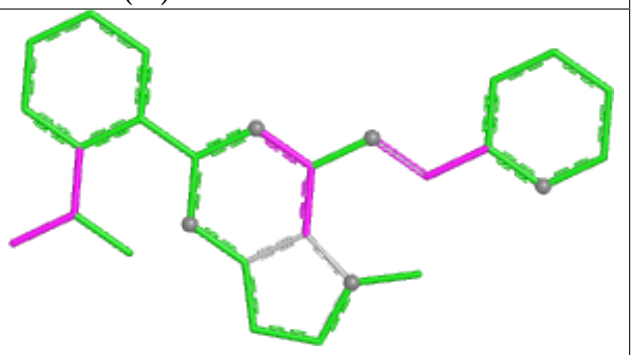


Rings

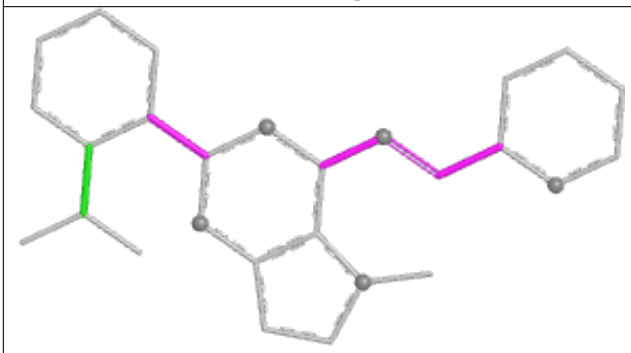
Ligand DVF B 502 (B)



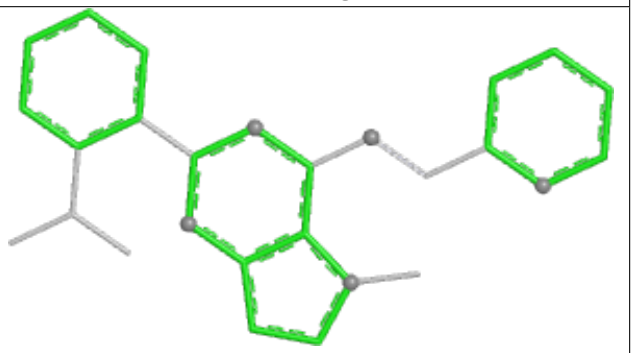
Bond lengths



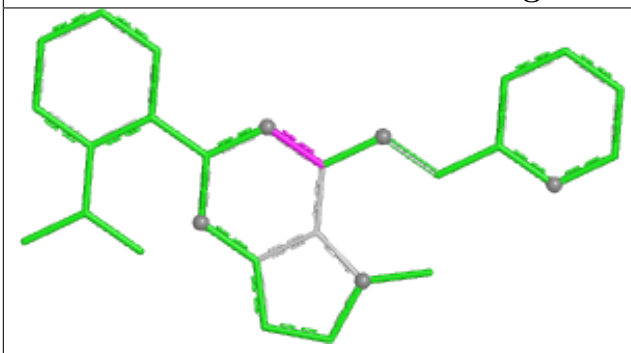
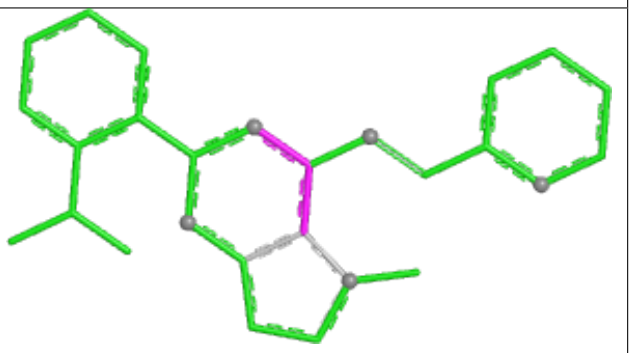
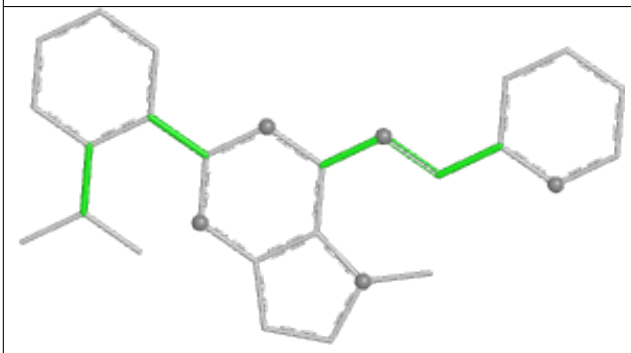
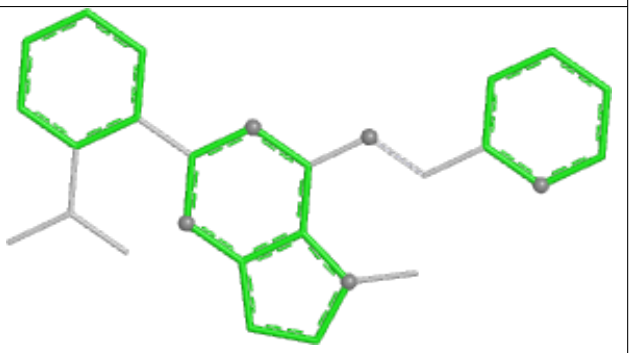
Bond angles

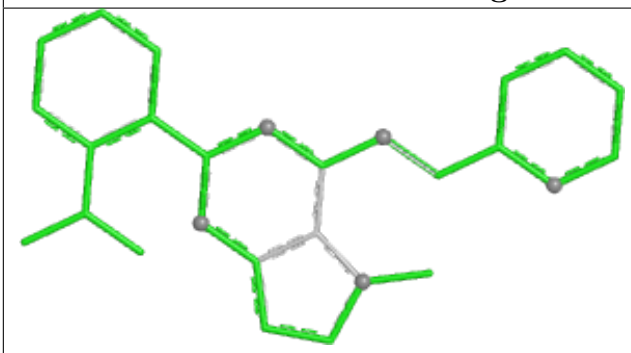
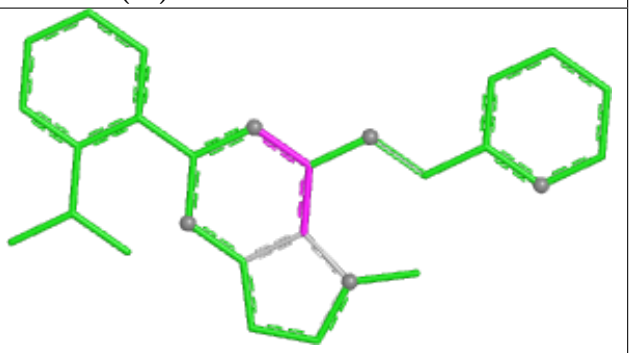
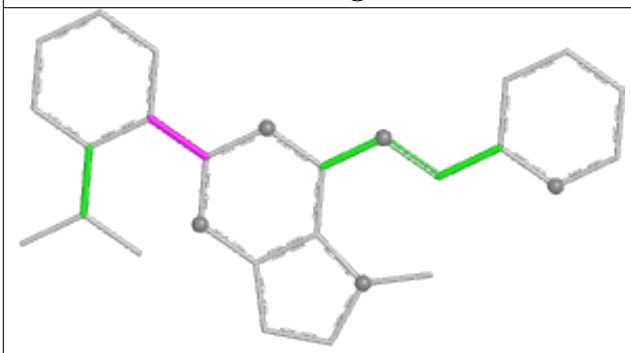
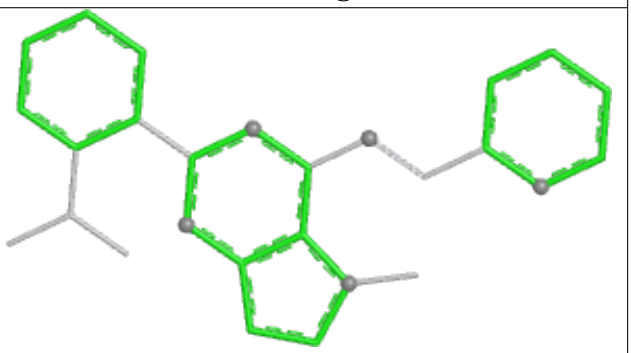


Torsions

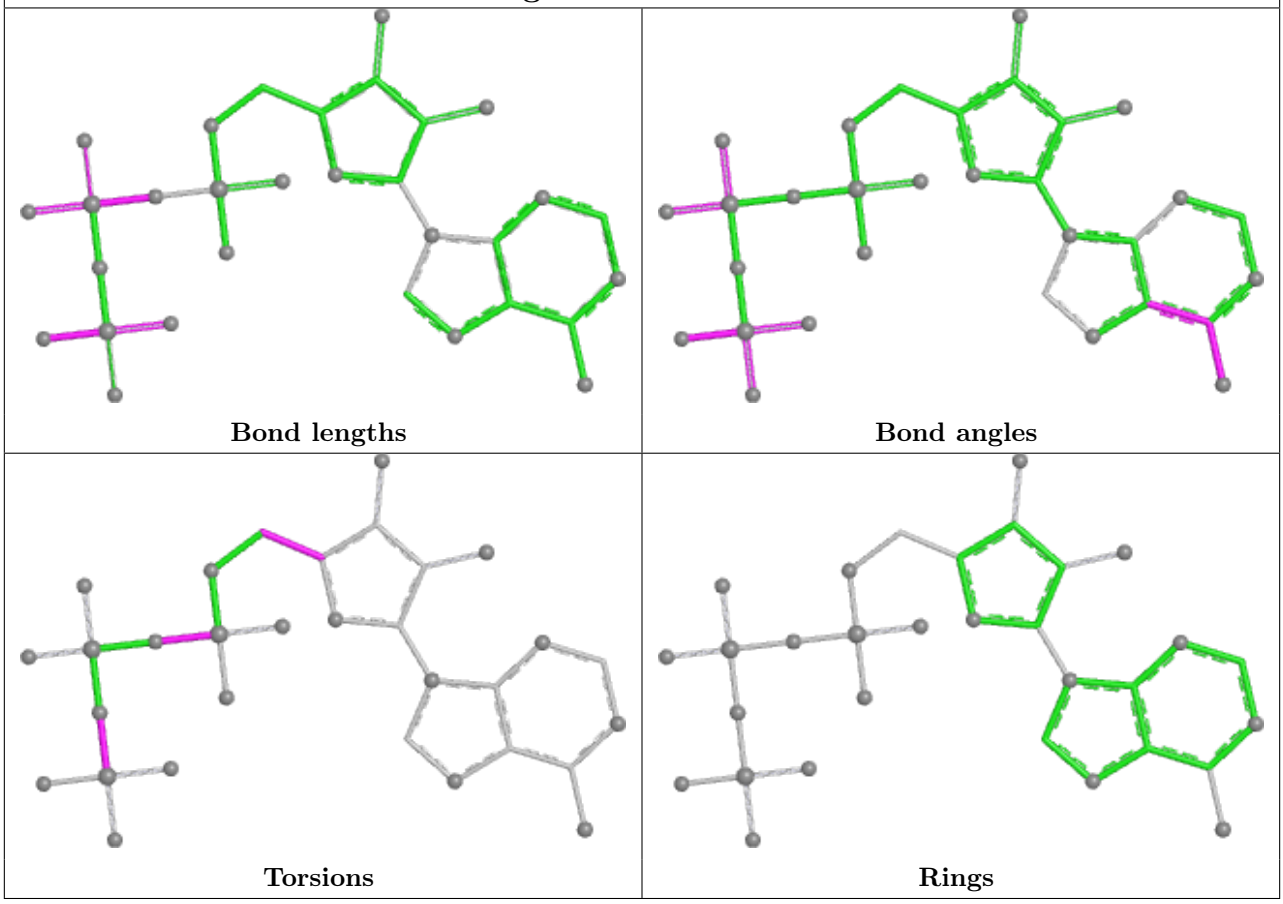


Rings

Ligand DVF A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DVF B 502 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP B 501



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	317/348 (91%)	2.08	126 (39%)	0	0	28, 56, 96, 113	0
1	B	313/348 (89%)	1.54	56 (17%)	1	1	22, 37, 72, 94	5 (1%)
All	All	630/696 (90%)	1.81	182 (28%)	0	0	22, 47, 90, 113	5 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	PHE	9.4
1	B	347	PHE	9.3
1	A	254	ILE	9.1
1	A	38	VAL	9.1
1	A	291	ILE	8.7
1	A	41	PHE	8.6
1	A	351	ILE	7.9
1	B	38	VAL	7.5
1	B	294	SER	7.4
1	A	229	SER	7.0
1	B	346	GLU	6.7
1	A	246	LEU	6.6
1	B	69	VAL	6.6
1	B	139	GLY	6.5
1	A	196	GLU	6.5
1	B	361	GLY	6.4
1	A	344	PRO	6.2
1	A	134	SER	6.2
1	A	403	VAL	6.1
1	B	295	GLU	6.0
1	A	359	ALA	5.8
1	A	139	GLY	5.7
1	A	234	VAL	5.7
1	A	363	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	5.6
1	A	383	LYS	5.4
1	A	39	LYS	5.3
1	A	361	GLY	5.2
1	A	69	VAL	5.0
1	A	213	VAL	4.9
1	A	145	TYR	4.7
1	A	375	ILE	4.7
1	A	131	PRO	4.5
1	A	224	VAL	4.5
1	A	237	LEU	4.4
1	B	345	GLY	4.4
1	A	194	ASP	4.3
1	A	345	GLY	4.3
1	A	40	VAL	4.3
1	B	194	ASP	4.2
1	A	295	GLU	4.2
1	A	411	ARG	4.2
1	A	223	LEU	4.2
1	A	381	ALA	4.1
1	A	353	VAL	4.0
1	B	350	PHE	3.9
1	A	42	ARG	3.9
1	A	274	VAL	3.9
1	A	97	HIS	3.9
1	B	250	GLN	3.8
1	A	231	LYS	3.8
1	A	253	TYR	3.8
1	B	377[A]	THR	3.8
1	B	193	VAL	3.8
1	A	222	SER	3.8
1	A	296	PRO	3.7
1	A	382	LYS	3.7
1	A	93	ASN	3.7
1	A	280	ASP	3.7
1	B	40	VAL	3.6
1	A	90	HIS	3.6
1	B	39	LYS	3.6
1	A	43	ALA	3.6
1	A	293	GLY	3.6
1	A	297	GLU	3.6
1	A	217	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	70	MET	3.6
1	B	234	VAL	3.6
1	A	225	SER	3.5
1	A	294	SER	3.5
1	B	138	ASP	3.5
1	A	346	GLU	3.4
1	A	230	ASP	3.4
1	A	219	LEU	3.4
1	A	365	LYS	3.4
1	B	375[A]	ILE	3.4
1	A	142	LEU	3.4
1	B	224	VAL	3.4
1	B	376[A]	LEU	3.4
1	A	96	SER	3.3
1	A	211	LEU	3.3
1	A	272	PHE	3.2
1	B	360	GLU	3.2
1	A	350	PHE	3.2
1	A	281	TYR	3.1
1	A	419	ILE	3.1
1	B	298	GLU	3.1
1	A	357	ARG	3.1
1	A	195	ASN	3.0
1	A	405	PRO	3.0
1	A	89	PHE	3.0
1	A	207	PHE	3.0
1	A	159	ILE	2.9
1	A	239	THR	2.9
1	B	255	GLY	2.9
1	A	275	GLN	2.8
1	A	243	MET	2.8
1	A	238	PRO	2.8
1	A	290	ILE	2.8
1	A	416	ILE	2.7
1	B	293	GLY	2.7
1	A	378	GLN	2.7
1	B	237	LEU	2.7
1	A	210	ARG	2.7
1	A	233	LYS	2.7
1	A	404	HIS	2.7
1	A	358	SER	2.7
1	A	245	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	2.6
1	B	196	GLU	2.6
1	A	140	ARG	2.6
1	B	211	LEU	2.6
1	A	257	GLU	2.6
1	B	296	PRO	2.6
1	A	262	PHE	2.6
1	A	264	GLU	2.6
1	A	199	TYR	2.5
1	B	223	LEU	2.5
1	A	37	LYS	2.5
1	B	66	PRO	2.5
1	B	93	ASN	2.5
1	A	185	PHE	2.5
1	A	126	LEU	2.5
1	B	52	LEU	2.5
1	B	89	PHE	2.4
1	A	227	GLU	2.4
1	B	56	ALA	2.4
1	B	252	VAL	2.4
1	A	255	GLY	2.4
1	A	374	ASP	2.4
1	B	287	ILE	2.4
1	A	177	HIS	2.4
1	B	246	LEU	2.4
1	A	226	ARG	2.4
1	B	150	VAL	2.4
1	B	176	CYS	2.4
1	B	104	CYS	2.3
1	B	43	ALA	2.3
1	A	408	TYR	2.3
1	A	193	VAL	2.3
1	B	173	ILE	2.3
1	B	136	GLY	2.3
1	A	212	PRO	2.3
1	A	163	HIS	2.3
1	A	241	LYS	2.3
1	A	355	ALA	2.3
1	A	122	TYR	2.2
1	B	289	ASP	2.3
1	A	51	PHE	2.2
1	A	412	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	CYS	2.2
1	A	258	GLU	2.2
1	B	60	ASN	2.2
1	B	359	ALA	2.2
1	B	80	SER	2.2
1	A	189	TYR	2.2
1	B	297	GLU	2.2
1	A	171	GLN	2.2
1	B	47	LEU	2.1
1	A	98	PHE	2.1
1	A	420	PHE	2.1
1	B	420	PHE	2.1
1	A	260	LYS	2.1
1	A	279	MET	2.1
1	A	180	THR	2.1
1	A	379	TYR	2.1
1	A	376	LEU	2.1
1	A	130	PRO	2.1
1	A	236	GLU	2.1
1	A	215	ARG	2.0
1	A	118	ASP	2.0
1	A	256	GLU	2.0
1	A	349	SER	2.0
1	B	137	SER	2.0
1	B	140	ARG	2.0
1	A	68	PRO	2.0
1	A	252	VAL	2.0
1	A	115	PHE	2.0
1	A	52	LEU	2.0
1	A	85	ASN	2.0
1	A	377	THR	2.0
1	B	222	SER	2.0

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)

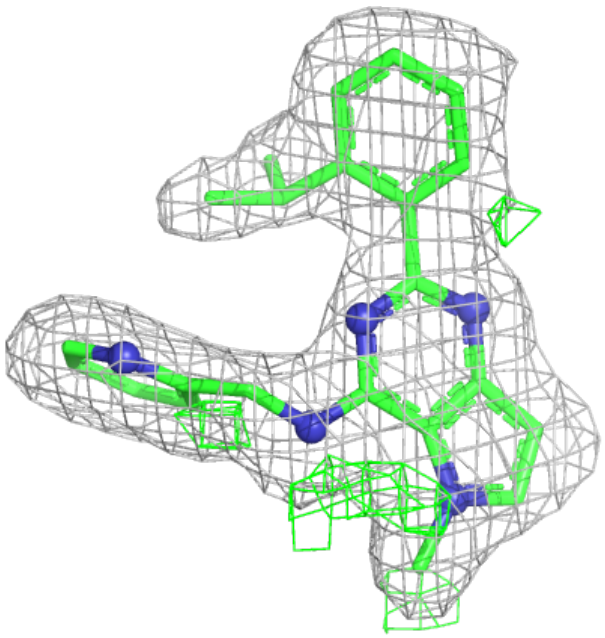
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

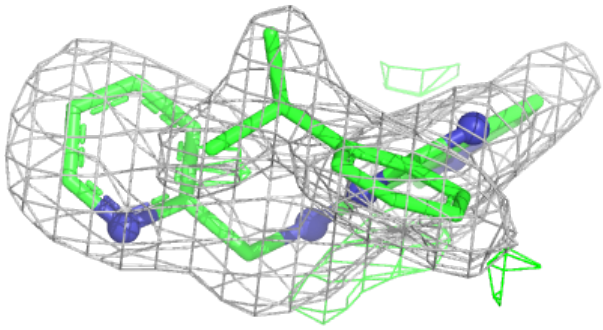
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DVF	B	502[A]	27/27	0.69	0.38	23,25,32,33	27
2	DVF	B	502[B]	27/27	0.69	0.38	10,14,16,17	27
3	ANP	A	502	31/31	0.71	0.36	66,92,121,132	0
3	ANP	B	501	31/31	0.81	0.23	51,74,90,104	0
2	DVF	A	501	27/27	0.85	0.21	42,47,55,56	0

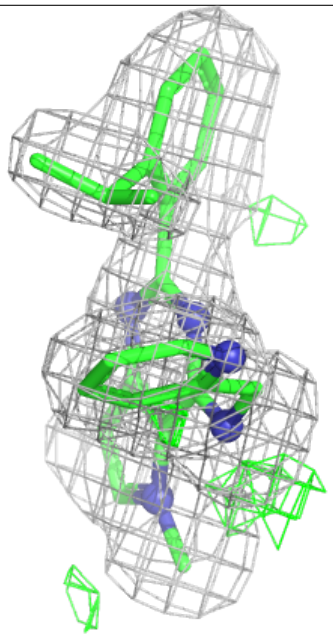
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DVF B 502 (A):

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

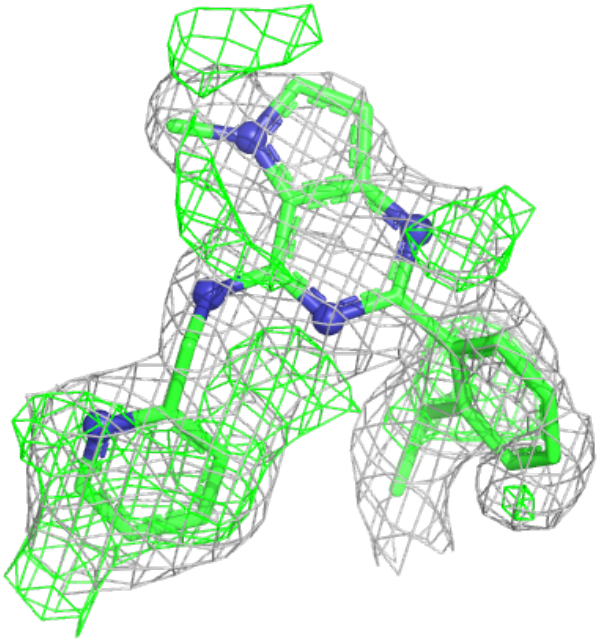


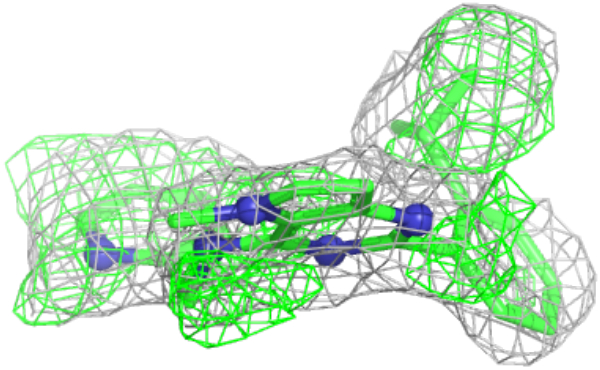


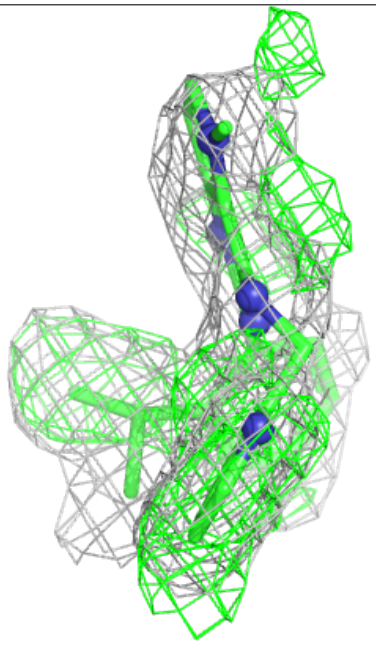


Electron density around DVF B 502 (B):

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

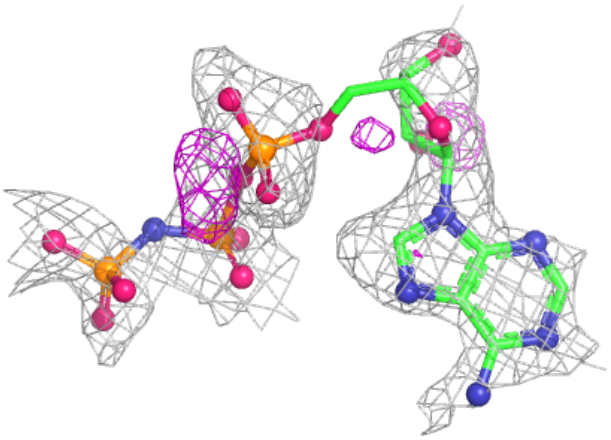


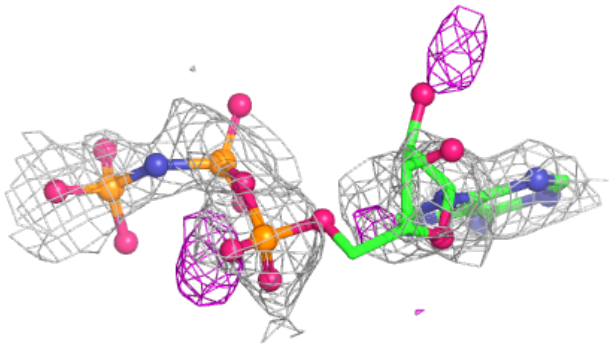


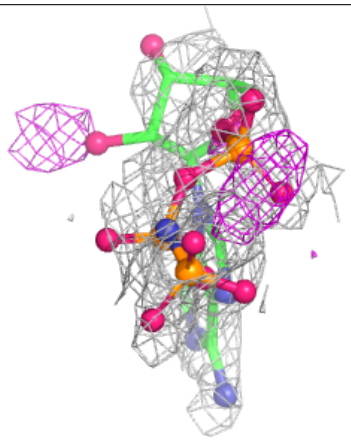


Electron density around ANP A 502:

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

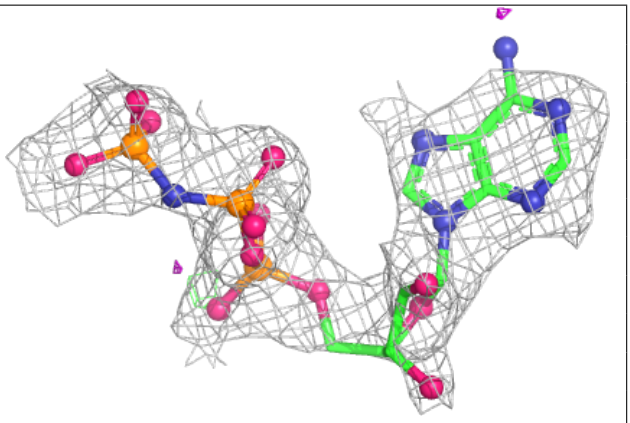


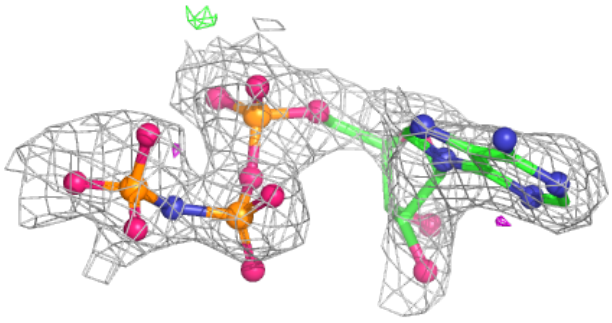


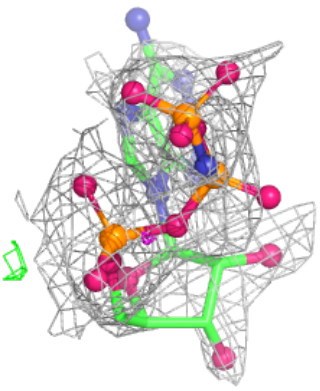


Electron density around ANP B 501:

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

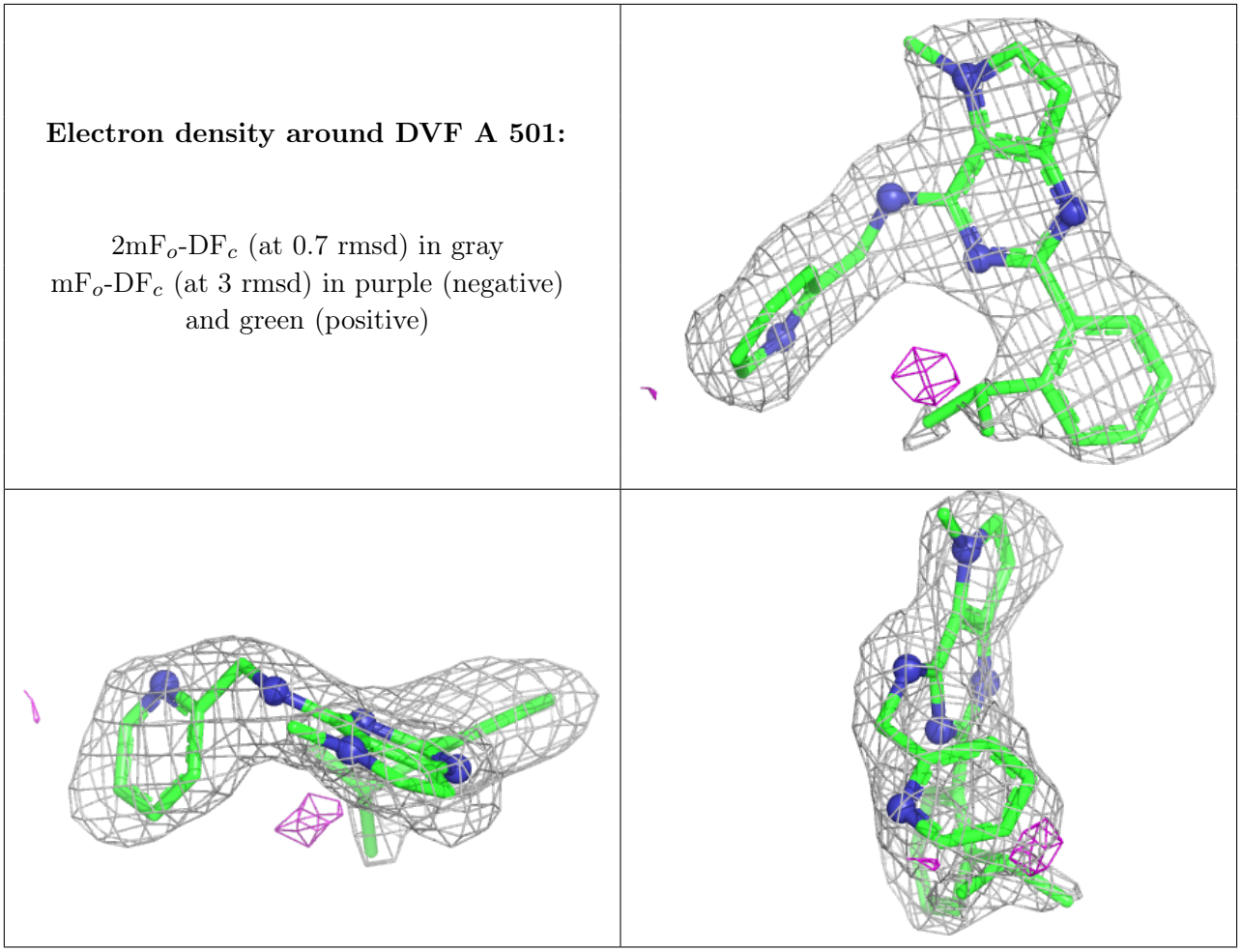






Electron density around DVF A 501:

$2mF_o$-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.