Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 08:42 PM EDT

PDB ID	:	4LGD
Title	:	Structural Basis for Autoactivation of Human Mst2 Kinase and Its Regulation by RASSF5
Authors	:	Luo, X.; Ni, L.; Tomchick, D.R.
Deposited on	:	2013-06-27
Resolution	:	3.05 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

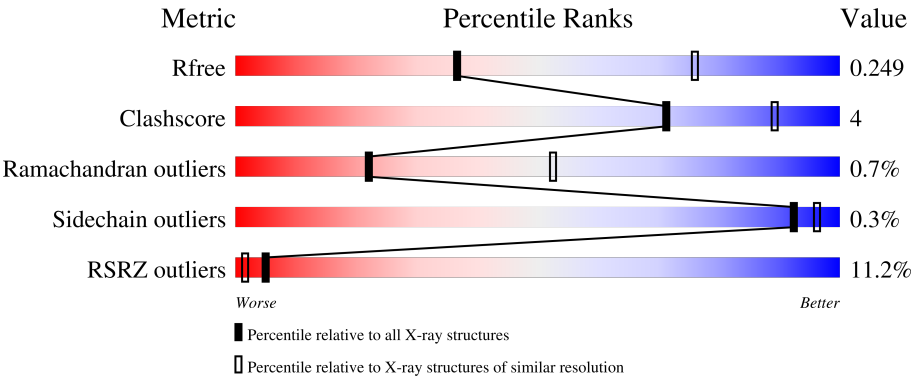
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	378	15% 82% 11% 7%
1	B	378	13% 84% 9% 7%
1	C	378	6% 84% 8% 8%
1	D	378	2% 82% 7% 11%
2	E	49	10% 84% 12%

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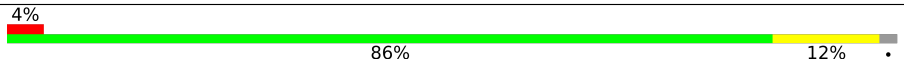
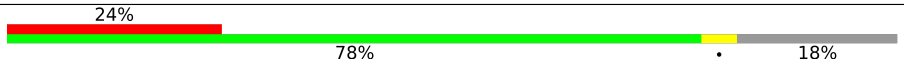
Mol	Chain	Length	Quality of chain
2	F	49	
2	G	49	
2	H	49	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	C	502	-	-	-	X
5	SO4	A	503	-	-	X	-
5	SO4	B	503	-	-	X	-
5	SO4	D	503	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25637 atoms, of which 12852 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 Serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	H	N	O	S	0	0	0
			5690	1799	2865	479	530	17			
1	B	350	Total	C	H	N	O	S	0	0	0
			5698	1794	2879	480	528	17			
1	C	349	Total	C	H	N	O	S	0	0	0
			5706	1800	2879	482	528	17			
1	D	338	Total	C	H	N	O	S	0	0	0
			5486	1731	2765	463	511	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q13188
A	1	HIS	-	expression tag	UNP Q13188
A	2	HIS	-	expression tag	UNP Q13188
A	3	HIS	-	expression tag	UNP Q13188
A	4	HIS	-	expression tag	UNP Q13188
A	5	HIS	-	expression tag	UNP Q13188
A	6	HIS	-	expression tag	UNP Q13188
A	7	GLY	-	expression tag	UNP Q13188
A	8	SER	-	expression tag	UNP Q13188
A	146	ASN	ASP	engineered mutation	UNP Q13188
B	0	MET	-	expression tag	UNP Q13188
B	1	HIS	-	expression tag	UNP Q13188
B	2	HIS	-	expression tag	UNP Q13188
B	3	HIS	-	expression tag	UNP Q13188
B	4	HIS	-	expression tag	UNP Q13188
B	5	HIS	-	expression tag	UNP Q13188
B	6	HIS	-	expression tag	UNP Q13188
B	7	GLY	-	expression tag	UNP Q13188
B	8	SER	-	expression tag	UNP Q13188
B	146	ASN	ASP	engineered mutation	UNP Q13188
C	0	MET	-	expression tag	UNP Q13188

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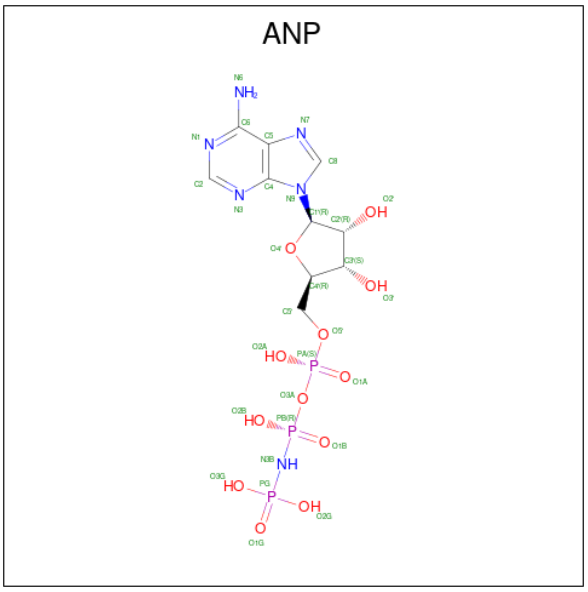
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	HIS	-	expression tag	UNP Q13188
C	2	HIS	-	expression tag	UNP Q13188
C	3	HIS	-	expression tag	UNP Q13188
C	4	HIS	-	expression tag	UNP Q13188
C	5	HIS	-	expression tag	UNP Q13188
C	6	HIS	-	expression tag	UNP Q13188
C	7	GLY	-	expression tag	UNP Q13188
C	8	SER	-	expression tag	UNP Q13188
C	146	ASN	ASP	engineered mutation	UNP Q13188
D	0	MET	-	expression tag	UNP Q13188
D	1	HIS	-	expression tag	UNP Q13188
D	2	HIS	-	expression tag	UNP Q13188
D	3	HIS	-	expression tag	UNP Q13188
D	4	HIS	-	expression tag	UNP Q13188
D	5	HIS	-	expression tag	UNP Q13188
D	6	HIS	-	expression tag	UNP Q13188
D	7	GLY	-	expression tag	UNP Q13188
D	8	SER	-	expression tag	UNP Q13188
D	146	ASN	ASP	engineered mutation	UNP Q13188

- Molecule 2 is a protein called Ras association domain family member 5, RASSF5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total	C	H	N	O	0	0	0
			810	260	403	67	80			
2	F	29	Total	C	H	N	O	0	0	0
			489	155	246	39	49			
2	G	48	Total	C	H	N	O	0	0	0
			825	265	409	68	83			
2	H	40	Total	C	H	N	O	0	0	0
			697	226	346	57	68			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

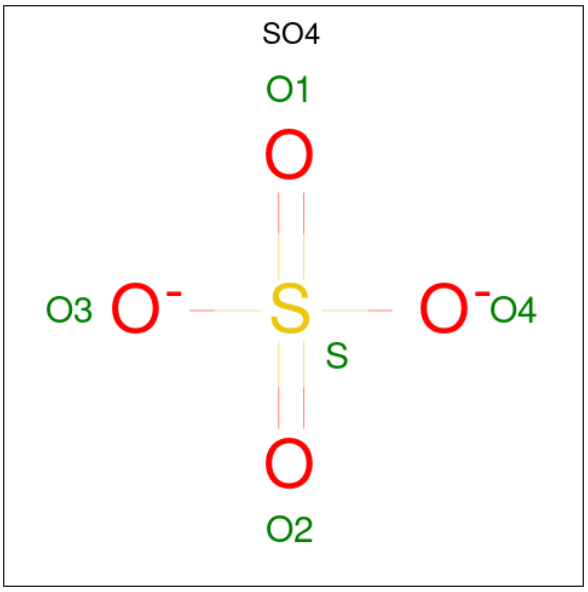


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	D	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

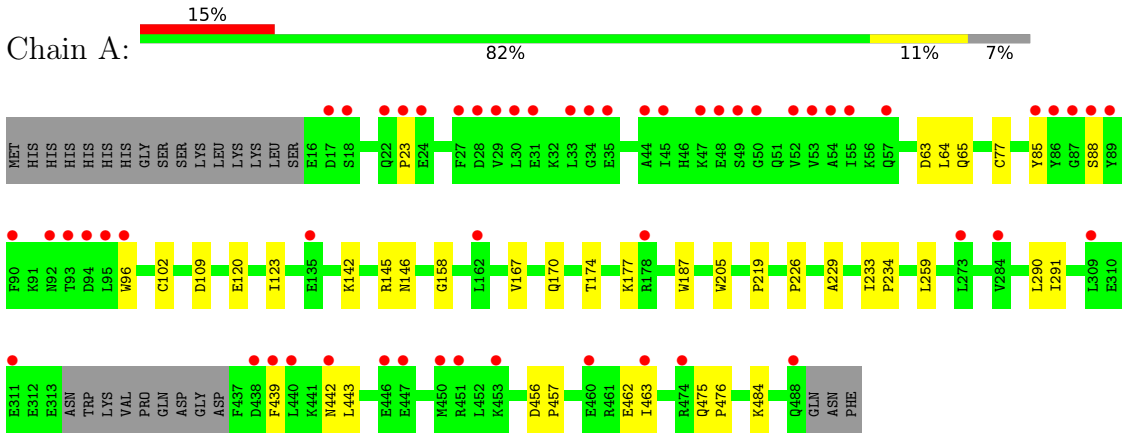
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total Na 2 2	0	0
6	D	1	Total Na 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

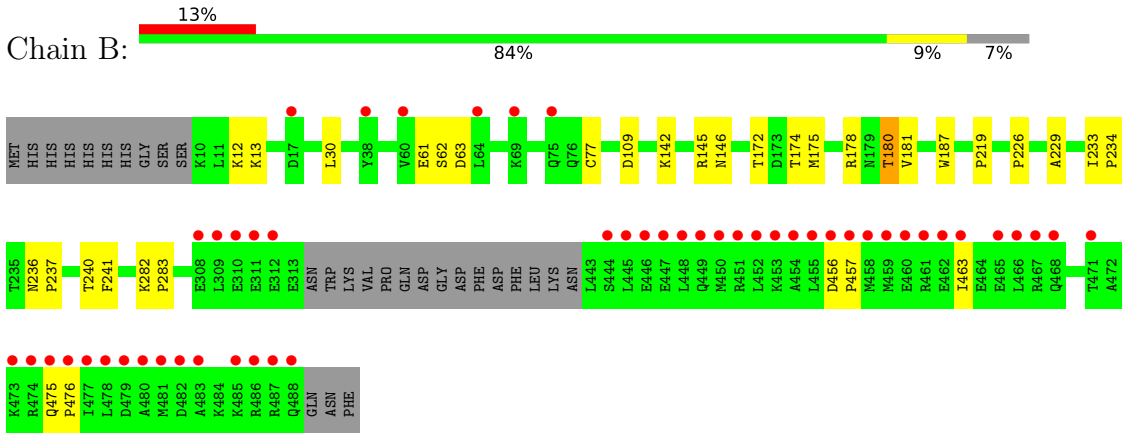
• Molecule 1: Serine/threonine-protein kinase 3

Chain A:



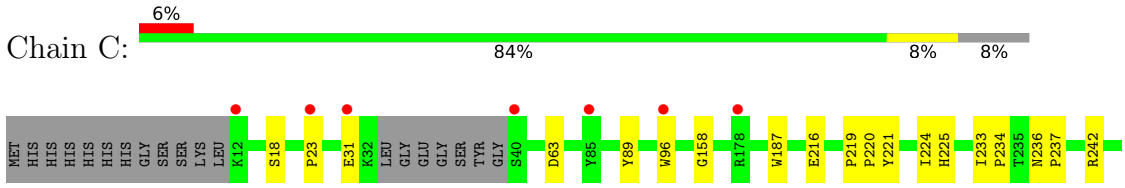
• Molecule 1: Serine/threonine-protein kinase 3

Chain B:

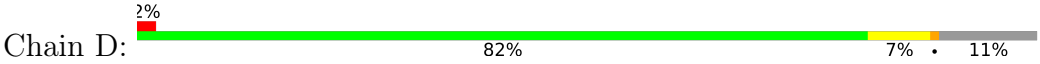


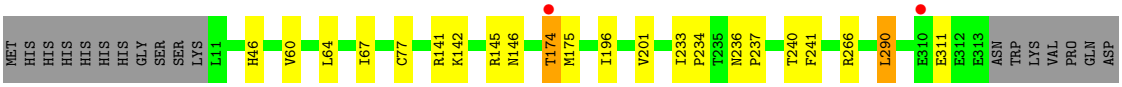
• Molecule 1: Serine/threonine-protein kinase 3

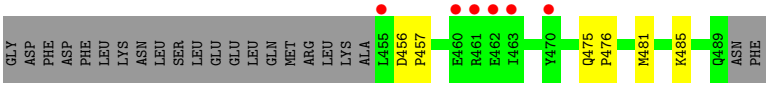
Chain C:



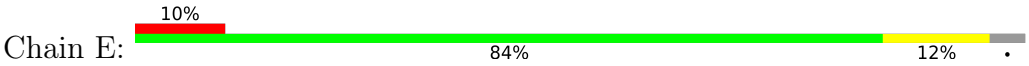
• Molecule 1: Serine/threonine-protein kinase 3

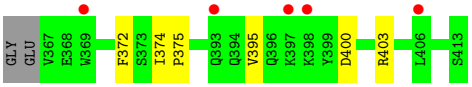




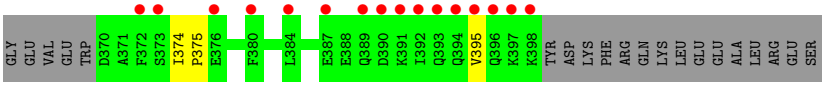


• Molecule 2: Ras association domain family member 5, RASSF5

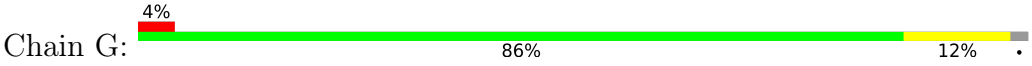


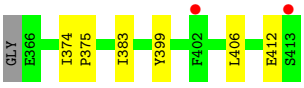


• Molecule 2: Ras association domain family member 5, RASSF5

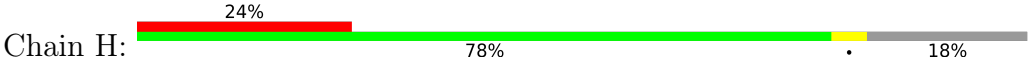


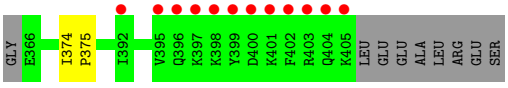
• Molecule 2: Ras association domain family member 5, RASSF5





• Molecule 2: Ras association domain family member 5, RASSF5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.40Å 237.14Å 95.86Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 46.05 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-3.05) 98.6 (46.05-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.199 , 0.244 0.210 , 0.249	Depositor DCC
R_{free} test set	2530 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 94.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25637	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: SO4, NA, 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	0.21	0/2879	0.38	0/3882
1	B	0.22	0/2871	0.41	0/3869
1	C	0.21	0/2879	0.38	0/3879
1	D	0.22	0/2773	0.40	0/3740
2	E	0.22	0/413	0.34	0/552
2	F	0.21	0/245	0.32	0/327
2	G	0.22	0/422	0.34	0/564
2	H	0.22	0/357	0.30	0/477
All	All	0.22	0/12839	0.39	0/17290

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	2825	2865	2858	25	0
1	B	2819	2879	2872	24	0
1	C	2827	2879	2872	17	0
1	D	2721	2765	2758	19	0
2	E	407	403	403	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	243	246	246	2	0
2	G	416	409	409	7	0
2	H	351	346	346	1	0
3	A	31	15	13	2	0
3	B	31	15	13	1	0
3	C	31	15	13	0	0
3	D	31	15	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	2	0
5	B	20	0	0	3	0
5	C	5	0	0	0	0
5	D	15	0	0	3	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
All	All	12785	12852	12816	90	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 4.

All (90) 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:85:TYR:OH	1:A:88:SER:OG	2.08	0.71
1:D:145:ARG:NH1	5:D:503:SO4:S	2.72	0.63
1:B:145:ARG:NH1	5:B:503:SO4:S	2.73	0.61
1:B:145:ARG:NH1	5:B:503:SO4:O2	2.34	0.61
1:B:77:CYS:SG	1:B:142:LYS:NZ	2.73	0.61
1:A:484:LYS:NZ	2:E:372:PHE:O	2.36	0.58
2:E:374:ILE:HB	2:E:375:PRO:HD3	1.86	0.58
1:D:64:LEU:HD11	2:G:383:ILE:HG21	1.86	0.56
1:D:77:CYS:SG	1:D:142:LYS:NZ	2.76	0.55
1:A:77:CYS:SG	1:A:142:LYS:NZ	2.79	0.55
2:F:374:ILE:HB	2:F:375:PRO:HD3	1.90	0.54
1:B:475:GLN:HB3	1:B:476:PRO:HD3	1.91	0.52
1:D:475:GLN:N	1:D:476:PRO:CD	2.73	0.52
2:G:374:ILE:HB	2:G:375:PRO:HD3	1.92	0.51
1:B:236:ASN:HB3	1:B:237:PRO:CD	2.41	0.51
1:A:145:ARG:NH1	5:A:503:SO4:O1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:NH1	5:B:503:SO4:O1	2.44	0.50
1:B:240:THR:OG1	1:B:241:PHE:N	2.44	0.50
1:B:233:ILE:HB	1:B:234:PRO:HD3	1.94	0.50
2:E:400:ASP:OD2	2:E:403:ARG:NH1	2.44	0.50
1:D:233:ILE:HB	1:D:234:PRO:HD3	1.93	0.49
1:B:109:ASP:OD1	3:B:501:ANP:O2'	2.26	0.49
1:D:201:VAL:CG1	1:D:266:ARG:HD2	2.42	0.49
1:D:240:THR:OG1	1:D:241:PHE:N	2.46	0.48
1:C:187:TRP:CZ2	1:C:219:PRO:HG3	2.48	0.48
1:A:226:PRO:HG2	1:B:178:ARG:NH1	2.28	0.47
1:B:30:LEU:N	1:B:30:LEU:HD12	2.29	0.47
1:D:145:ARG:NH1	5:D:503:SO4:O4	2.47	0.47
1:A:23:PRO:HB2	1:A:96:TRP:CZ3	2.49	0.47
1:D:64:LEU:O	1:D:67:ILE:N	2.47	0.47
1:A:158:GLY:HA2	1:A:291:ILE:CD1	2.45	0.47
1:A:109:ASP:OD1	3:A:501:ANP:O2'	2.32	0.47
1:A:187:TRP:CZ2	1:A:219:PRO:HG3	2.50	0.47
1:A:145:ARG:NH1	5:A:503:SO4:S	2.84	0.47
1:D:60:VAL:O	1:D:64:LEU:HG	2.14	0.47
1:C:158:GLY:HA2	1:C:291:ILE:CD1	2.45	0.46
1:D:174:THR:HG22	1:D:175:MET:N	2.30	0.46
1:C:23:PRO:HB2	1:C:96:TRP:CE3	2.50	0.46
1:A:475:GLN:N	1:A:476:PRO:CD	2.78	0.46
1:C:456:ASP:HB2	1:C:457:PRO:HD3	1.98	0.46
1:A:233:ILE:HB	1:A:234:PRO:HD3	1.97	0.46
1:B:174:THR:HG22	1:B:175:MET:N	2.30	0.45
1:B:226:PRO:O	1:B:229:ALA:N	2.50	0.45
1:C:220:PRO:O	1:C:221:TYR:HB2	2.17	0.45
1:C:236:ASN:HB3	1:C:237:PRO:CD	2.47	0.45
1:C:224:ILE:HG22	1:C:225:HIS:N	2.31	0.45
1:B:463:ILE:HG22	2:F:395:VAL:HG11	1.98	0.45
1:C:233:ILE:HB	1:C:234:PRO:HD3	1.98	0.45
1:B:282:LYS:HB3	1:B:283:PRO:HD2	2.00	0.44
1:C:290:LEU:C	1:C:290:LEU:HD12	2.38	0.44
1:A:290:LEU:C	1:A:290:LEU:HD12	2.37	0.44
1:C:459:MET:HB2	2:G:399:TYR:CD1	2.53	0.44
2:H:374:ILE:HB	2:H:375:PRO:HD3	2.00	0.44
1:A:462:GLU:HG2	2:E:395:VAL:HG21	2.00	0.43
1:B:236:ASN:HB3	1:B:237:PRO:HD2	2.00	0.43
1:A:475:GLN:HB3	1:A:476:PRO:HD3	1.99	0.43
1:C:282:LYS:HB3	1:C:283:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:O	1:A:123:ILE:N	2.51	0.43
1:B:456:ASP:HB2	1:B:457:PRO:HD3	2.01	0.43
1:D:290:LEU:HD12	1:D:290:LEU:C	2.39	0.43
1:B:456:ASP:N	1:B:457:PRO:CD	2.82	0.43
1:C:475:GLN:HB3	1:C:476:PRO:HD3	2.00	0.43
1:D:64:LEU:CD1	2:G:383:ILE:HG21	2.49	0.43
1:C:481:MET:HE3	1:C:485:LYS:HE3	2.02	0.42
1:B:12:LYS:O	1:B:13:LYS:C	2.57	0.42
2:G:412:GLU:HA	2:G:412:GLU:OE1	2.20	0.42
1:C:440:LEU:HD22	2:G:406:LEU:CD2	2.50	0.42
1:D:46:HIS:NE2	5:D:504:SO4:O2	2.53	0.42
1:D:141:ARG:HG2	1:D:141:ARG:O	2.20	0.42
1:D:456:ASP:N	1:D:457:PRO:CD	2.82	0.42
1:A:463:ILE:HG22	2:E:395:VAL:HG11	2.02	0.42
1:B:180:THR:CG2	1:B:181:VAL:N	2.82	0.42
1:B:237:PRO:HG3	1:D:237:PRO:HG3	2.02	0.42
1:B:172:THR:HG22	1:B:172:THR:O	2.20	0.42
1:D:481:MET:O	1:D:485:LYS:HG2	2.19	0.42
1:A:64:LEU:HD12	1:A:65:GLN:N	2.34	0.41
1:A:226:PRO:O	1:A:229:ALA:N	2.53	0.41
2:G:374:ILE:N	2:G:375:PRO:CD	2.83	0.41
1:A:102:CYS:O	3:A:501:ANP:C2	2.68	0.41
1:A:439:PHE:O	1:A:443:LEU:HB2	2.20	0.41
1:A:456:ASP:HB2	1:A:457:PRO:HD3	2.02	0.41
1:C:224:ILE:CG2	1:C:225:HIS:N	2.84	0.41
1:A:456:ASP:N	1:A:457:PRO:CD	2.83	0.41
1:B:61:GLU:HG3	1:B:62:SER:N	2.35	0.41
1:C:18:SER:O	1:C:89:TYR:OH	2.28	0.41
1:C:216:GLU:OE1	1:C:242:ARG:NH2	2.53	0.41
1:A:170:GLN:HB2	1:A:177:LYS:HE2	2.02	0.40
1:A:205:TRP:CE3	1:A:259:LEU:HA	2.56	0.40
1:B:187:TRP:CZ2	1:B:219:PRO:HG3	2.56	0.40
1:D:236:ASN:HB3	1:D:237:PRO:CD	2.50	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	346/378 (92%)	319 (92%)	24 (7%)	3 (1%)	17	47
1	B	346/378 (92%)	328 (95%)	16 (5%)	2 (1%)	25	55
1	C	343/378 (91%)	325 (95%)	16 (5%)	2 (1%)	25	55
1	D	334/378 (88%)	314 (94%)	16 (5%)	4 (1%)	13	40
2	E	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
2	F	27/49 (55%)	26 (96%)	1 (4%)	0	100	100
2	G	46/49 (94%)	46 (100%)	0	0	100	100
2	H	38/49 (78%)	38 (100%)	0	0	100	100
All	All	1525/1708 (89%)	1440 (94%)	74 (5%)	11 (1%)	22	52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	GLU
1	A	174	THR
1	C	31	GLU
1	D	174	THR
1	A	63	ASP
1	B	146	ASN
1	A	146	ASN
1	B	63	ASP
1	C	63	ASP
1	D	146	ASN
1	D	196	ILE

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	311/337 (92%)	309 (99%)	2 (1%)	86 93
1	B	311/337 (92%)	310 (100%)	1 (0%)	92 96
1	C	313/337 (93%)	313 (100%)	0	100 100
1	D	300/337 (89%)	299 (100%)	1 (0%)	92 96
2	E	45/46 (98%)	45 (100%)	0	100 100
2	F	28/46 (61%)	28 (100%)	0	100 100
2	G	46/46 (100%)	46 (100%)	0	100 100
2	H	39/46 (85%)	39 (100%)	0	100 100
All	All	1393/1532 (91%)	1389 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	VAL
1	A	442	ASN
1	B	180	THR
1	D	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.05	0
3	ANP	C	501	4	29,33,33	1.54	9 (31%)	31,52,52	1.62	4 (12%)
5	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.07	0
5	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.04	0
3	ANP	B	501	4	29,33,33	1.56	9 (31%)	31,52,52	1.60	5 (16%)
5	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.06	0
3	ANP	D	501	4	29,33,33	1.56	9 (31%)	31,52,52	1.71	6 (19%)
5	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.08	0
3	ANP	A	501	4	29,33,33	1.59	9 (31%)	31,52,52	1.55	4 (12%)
5	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.05	0

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	D	501	4	-	3/14/38/38	0/3/3/3
3	ANP	C	501	4	-	4/14/38/38	0/3/3/3
3	ANP	A	501	4	-	7/14/38/38	0/3/3/3
3	ANP	B	501	4	-	6/14/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	ANP	C2'-C1'	-3.76	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ANP	C2'-C1'	-3.60	1.48	1.53
3	C	501	ANP	C2'-C1'	-3.56	1.48	1.53
3	A	501	ANP	C2'-C1'	-3.48	1.48	1.53
3	D	501	ANP	C6-N6	3.09	1.45	1.34
3	B	501	ANP	C6-N6	3.08	1.45	1.34
3	A	501	ANP	C6-N6	3.00	1.45	1.34
3	C	501	ANP	C6-N6	2.99	1.44	1.34
3	A	501	ANP	PB-O1B	2.40	1.50	1.46
3	B	501	ANP	C2-N3	2.37	1.35	1.32
3	A	501	ANP	PG-O1G	2.36	1.49	1.46
3	B	501	ANP	PB-O1B	2.35	1.49	1.46
3	C	501	ANP	C2-N3	2.35	1.35	1.32
3	D	501	ANP	C2-N3	2.34	1.35	1.32
3	A	501	ANP	C2-N3	2.32	1.35	1.32
3	A	501	ANP	O4'-C4'	-2.31	1.39	1.45
3	A	501	ANP	C2'-C3'	-2.25	1.47	1.53
3	C	501	ANP	O4'-C4'	-2.24	1.40	1.45
3	C	501	ANP	PB-O1B	2.23	1.49	1.46
3	D	501	ANP	O4'-C4'	-2.23	1.40	1.45
3	A	501	ANP	O2'-C2'	-2.23	1.37	1.43
3	B	501	ANP	O2'-C2'	-2.18	1.37	1.43
3	C	501	ANP	PG-O1G	2.16	1.49	1.46
3	D	501	ANP	O2'-C2'	-2.15	1.37	1.43
3	B	501	ANP	PG-O1G	2.12	1.49	1.46
3	C	501	ANP	O2'-C2'	-2.12	1.38	1.43
3	B	501	ANP	O4'-C4'	-2.11	1.40	1.45
3	D	501	ANP	PB-O1B	2.11	1.49	1.46
3	B	501	ANP	C2'-C3'	-2.11	1.47	1.53
3	D	501	ANP	C2'-C3'	-2.09	1.47	1.53
3	C	501	ANP	C2'-C3'	-2.09	1.47	1.53
3	A	501	ANP	O3'-C3'	-2.07	1.38	1.43
3	D	501	ANP	PG-O1G	2.07	1.49	1.46
3	B	501	ANP	O3'-C3'	-2.02	1.38	1.43
3	C	501	ANP	O3'-C3'	-2.01	1.38	1.43
3	D	501	ANP	O3'-C3'	-2.00	1.38	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ANP	N3-C2-N1	-5.54	120.02	128.68
3	C	501	ANP	N3-C2-N1	-5.43	120.19	128.68
3	B	501	ANP	N3-C2-N1	-5.31	120.38	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	ANP	N3-C2-N1	-5.28	120.43	128.68
3	B	501	ANP	PB-O3A-PA	-4.42	117.04	132.62
3	D	501	ANP	PB-O3A-PA	-3.94	118.75	132.62
3	C	501	ANP	PB-O3A-PA	-3.60	119.95	132.62
3	A	501	ANP	PB-O3A-PA	-3.54	120.14	132.62
3	D	501	ANP	O1G-PG-N3B	-3.21	107.05	111.77
3	B	501	ANP	O3A-PB-N3B	2.38	113.18	106.59
3	D	501	ANP	O3A-PB-N3B	2.37	113.18	106.59
3	C	501	ANP	O1G-PG-N3B	-2.24	108.47	111.77
3	A	501	ANP	O1B-PB-N3B	-2.23	108.48	111.77
3	C	501	ANP	O1B-PB-N3B	-2.18	108.56	111.77
3	B	501	ANP	C4-C5-N7	-2.17	107.14	109.40
3	D	501	ANP	O2B-PB-O3A	2.10	111.66	104.64
3	A	501	ANP	O2G-PG-O1G	-2.10	108.17	113.45
3	B	501	ANP	O1G-PG-N3B	-2.08	108.70	111.77
3	D	501	ANP	C4-C5-N7	-2.02	107.29	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ANP	PB-N3B-PG-O1G
3	A	501	ANP	PG-N3B-PB-O1B
3	A	501	ANP	PA-O3A-PB-O1B
3	A	501	ANP	PA-O3A-PB-O2B
3	A	501	ANP	C5'-O5'-PA-O3A
3	B	501	ANP	PB-N3B-PG-O1G
3	B	501	ANP	PG-N3B-PB-O1B
3	B	501	ANP	PG-N3B-PB-O3A
3	B	501	ANP	PB-O3A-PA-O5'
3	C	501	ANP	PG-N3B-PB-O1B
3	C	501	ANP	PG-N3B-PB-O3A
3	C	501	ANP	PA-O3A-PB-O1B
3	C	501	ANP	PA-O3A-PB-O2B
3	D	501	ANP	PG-N3B-PB-O1B
3	D	501	ANP	PA-O3A-PB-O1B
3	D	501	ANP	PA-O3A-PB-O2B
3	B	501	ANP	O4'-C4'-C5'-O5'
3	A	501	ANP	C5'-O5'-PA-O2A
3	B	501	ANP	C3'-C4'-C5'-O5'
3	A	501	ANP	C5'-O5'-PA-O1A

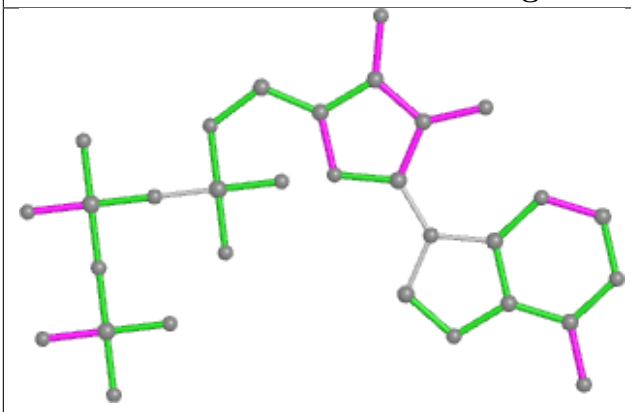
There are no ring outliers.

6 monomers are involved in 11 short contacts:

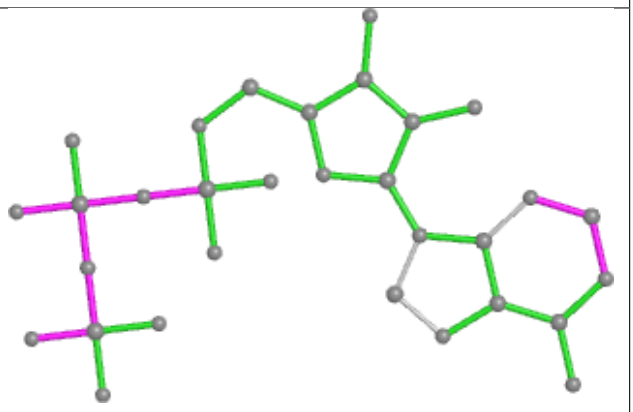
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	SO4	2	0
5	B	503	SO4	3	0
3	B	501	ANP	1	0
5	D	504	SO4	1	0
5	D	503	SO4	2	0
3	A	501	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

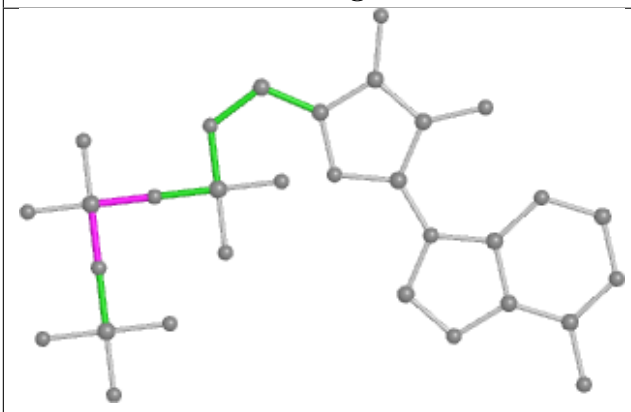
Ligand ANP C 501



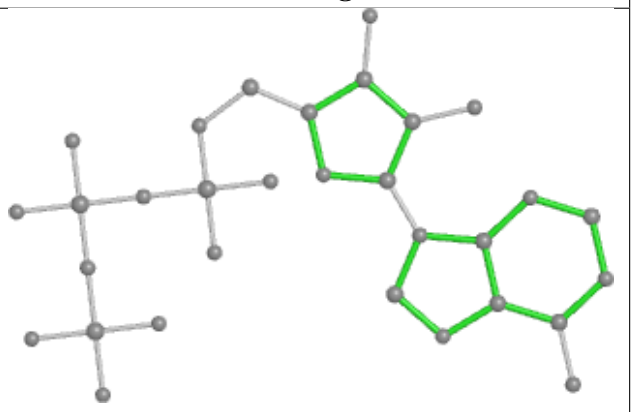
Bond lengths



Bond angles

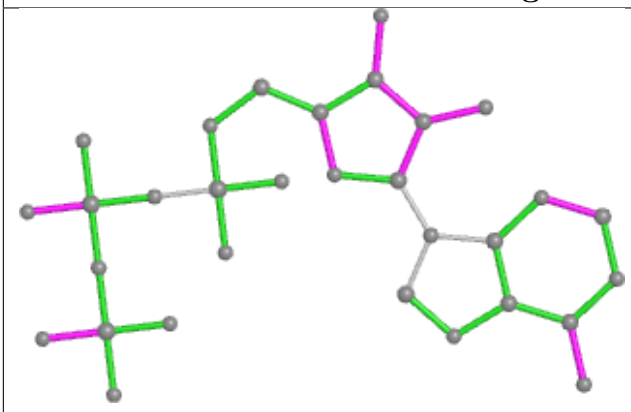


Torsions

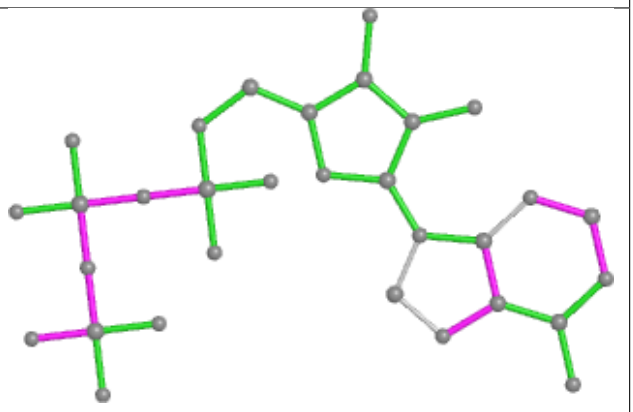


Rings

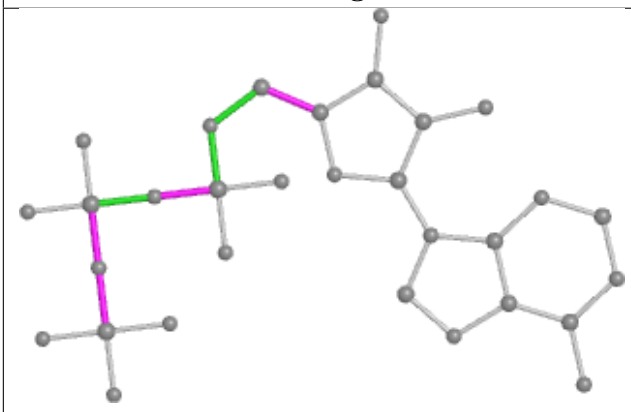
Ligand ANP B 501



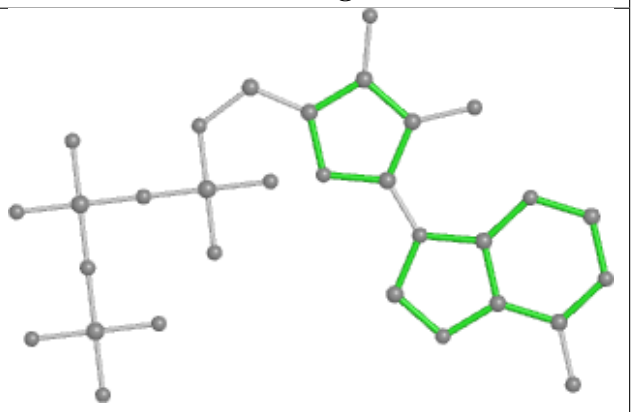
Bond lengths



Bond angles

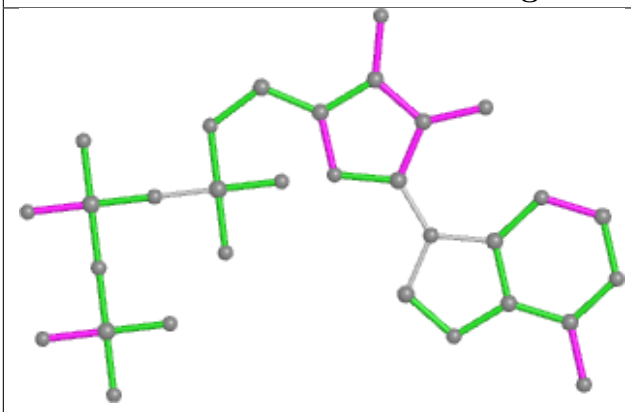


Torsions

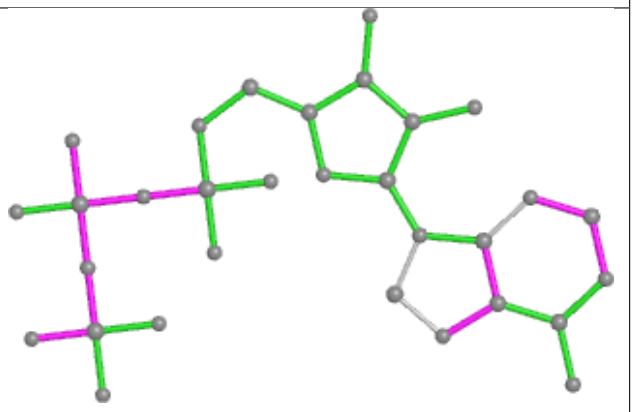


Rings

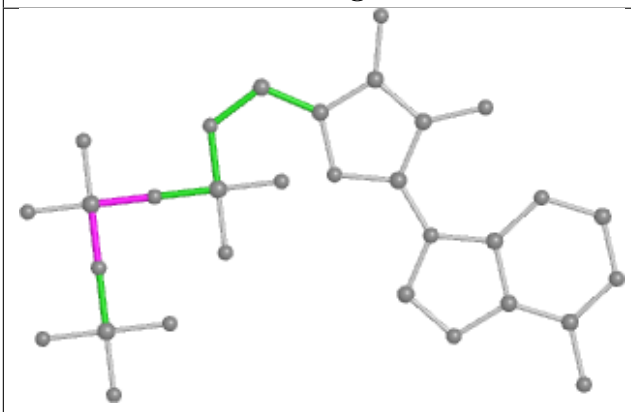
Ligand ANP D 501



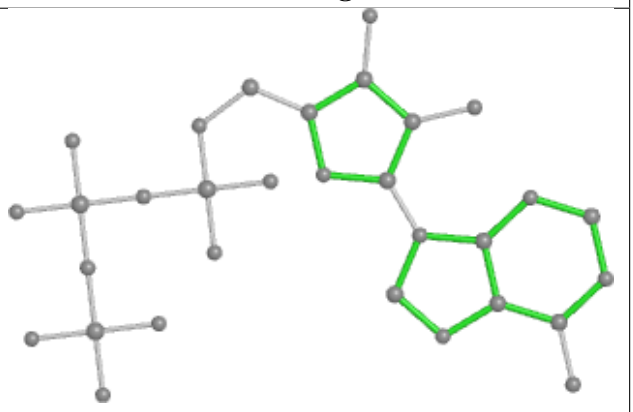
Bond lengths



Bond angles

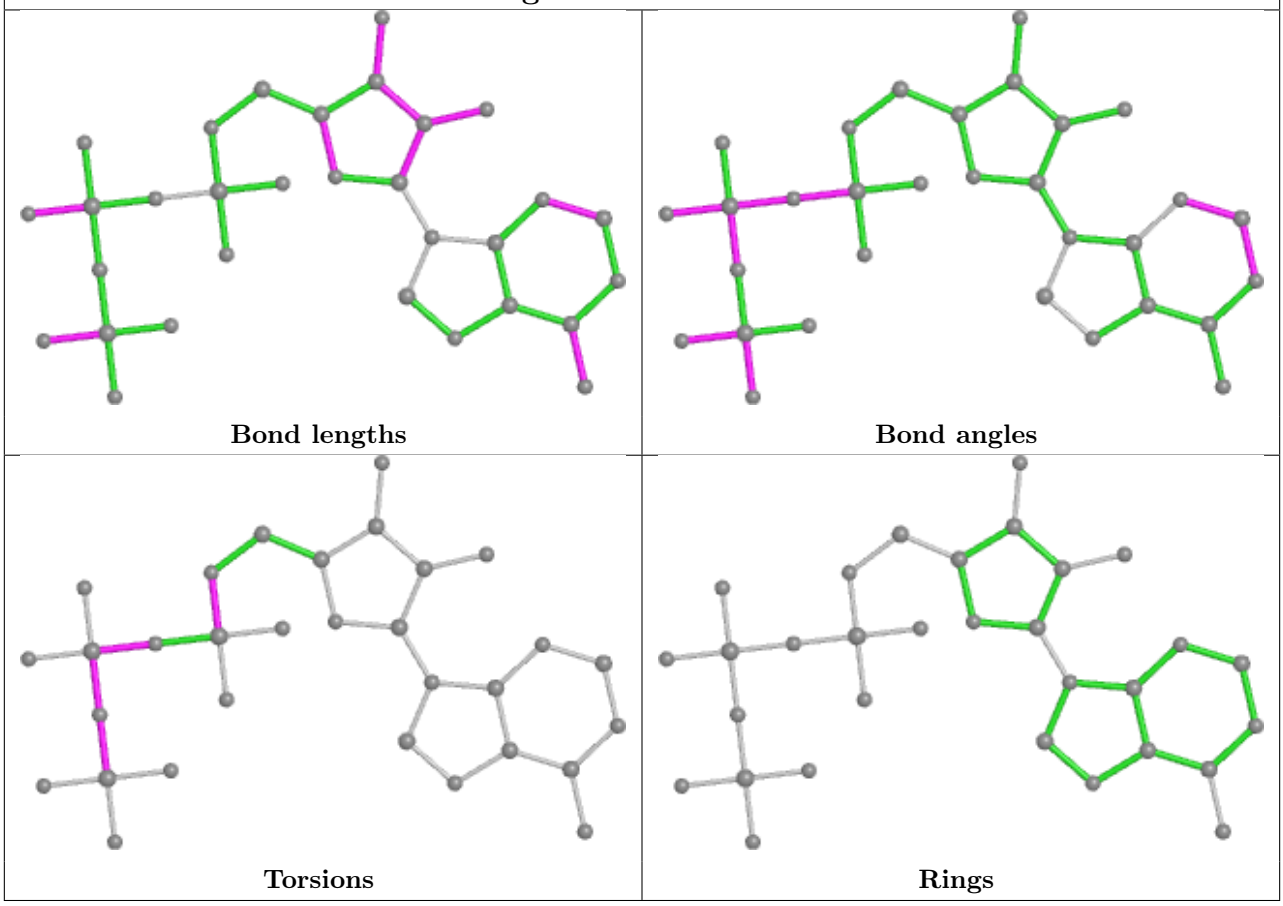


Torsions



Rings

Ligand ANP A 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	350/378 (92%)	1.00	55 (15%) 2 1	98, 160, 251, 332	0
1	B	350/378 (92%)	0.84	51 (14%) 2 1	57, 98, 245, 293	0
1	C	349/378 (92%)	0.66	24 (6%) 16 6	72, 122, 204, 242	0
1	D	338/378 (89%)	0.46	8 (2%) 59 34	57, 92, 175, 232	0
2	E	47/49 (95%)	0.85	5 (10%) 6 2	97, 128, 163, 181	0
2	F	29/49 (59%)	2.58	16 (55%) 0 0	179, 258, 279, 304	0
2	G	48/49 (97%)	0.59	2 (4%) 36 17	62, 119, 154, 180	0
2	H	40/49 (81%)	1.31	12 (30%) 0 0	119, 153, 213, 255	0
All	All	1551/1708 (90%)	0.79	173 (11%) 5 1	57, 122, 238, 332	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	450	MET	8.9
1	C	440	LEU	7.5
1	A	88	SER	7.4
1	B	451	ARG	7.0
2	F	391	LYS	6.8
1	B	452	LEU	6.7
1	B	457	PRO	6.6
1	A	96	TRP	6.5
1	B	463	ILE	6.1
1	A	23	PRO	6.1
1	A	94	ASP	5.9
1	B	456	ASP	5.8
1	A	89	TYR	5.8
1	A	85	TYR	5.8
1	C	437	PHE	5.6
2	F	392	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	477	ILE	5.4
1	A	31	GLU	5.3
1	B	454	ALA	5.3
2	F	384	LEU	5.3
1	B	447	GLU	5.2
1	D	460	GLU	5.2
2	F	380	PHE	5.2
1	B	460	GLU	5.1
1	B	453	LYS	5.1
1	A	45	ILE	5.1
2	F	389	GLN	4.9
1	B	455	LEU	4.8
1	A	47	LYS	4.8
1	A	27	PHE	4.7
2	F	372	PHE	4.7
1	A	50	GLY	4.5
1	B	479	ASP	4.5
1	B	478	LEU	4.5
1	A	33	LEU	4.4
1	B	449	GLN	4.4
1	A	44	ALA	4.3
1	A	17	ASP	4.3
1	A	87	GLY	4.2
1	C	441	LYS	4.1
2	H	404	GLN	4.1
2	F	396	GLN	4.1
1	A	442	ASN	4.0
1	A	93	THR	3.8
1	B	474	ARG	3.8
1	B	38	TYR	3.8
1	B	487	ARG	3.7
1	A	460	GLU	3.7
1	B	312	GLU	3.7
1	A	28	ASP	3.7
1	B	466	LEU	3.7
2	F	397	LYS	3.7
1	D	455	LEU	3.6
1	B	485	LYS	3.6
2	F	398	LYS	3.6
1	A	450	MET	3.6
1	A	178	ARG	3.5
2	H	402	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	397	LYS	3.5
1	B	311	GLU	3.5
1	B	467	ARG	3.5
2	H	403	ARG	3.4
2	F	395	VAL	3.4
2	H	400	ASP	3.4
1	B	459	MET	3.4
1	A	24	GLU	3.4
1	B	475	GLN	3.4
2	G	413	SER	3.4
1	B	476	PRO	3.4
2	H	395	VAL	3.4
1	A	22	GLN	3.3
1	A	447	GLU	3.3
1	C	455	LEU	3.3
1	B	482	ASP	3.3
1	C	23	PRO	3.2
2	G	402	PHE	3.2
1	B	310	GLU	3.2
1	A	52	VAL	3.2
1	B	308	GLU	3.2
1	B	486	ARG	3.1
1	C	85	TYR	3.1
1	A	438	ASP	3.1
1	C	445	LEU	3.1
2	H	392	ILE	3.1
1	C	96	TRP	3.1
2	H	396	GLN	3.1
1	A	86	TYR	3.0
1	B	445	LEU	3.0
2	E	369	TRP	3.0
1	C	442	ASN	3.0
2	F	376	GLU	3.0
1	D	174	THR	3.0
1	A	309	LEU	3.0
1	C	490	ASN	3.0
1	B	309	LEU	2.9
2	E	393	GLN	2.9
1	B	481	MET	2.9
1	A	53	VAL	2.9
1	D	310	GLU	2.9
1	A	48	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	401	LYS	2.8
1	C	178	ARG	2.8
1	A	54	ALA	2.8
1	B	473	LYS	2.8
1	A	453	LYS	2.8
1	A	18	SER	2.8
1	A	49	SER	2.8
2	F	393	GLN	2.8
1	C	313	GLU	2.8
2	F	373	SER	2.8
1	A	284	VAL	2.7
1	B	461	ARG	2.7
1	C	453	LYS	2.7
1	A	90	PHE	2.7
1	B	446	GLU	2.7
1	D	470	TYR	2.6
1	C	40	SER	2.6
1	A	29	VAL	2.6
2	H	399	TYR	2.6
1	A	440	LEU	2.6
1	C	307	ARG	2.6
1	B	444	SER	2.6
2	E	397	LYS	2.5
1	A	34	GLY	2.5
1	D	463	ILE	2.5
1	A	273	LEU	2.4
2	F	387	GLU	2.4
1	D	461	ARG	2.4
1	D	462	GLU	2.4
1	B	448	LEU	2.4
2	H	405	LYS	2.4
1	B	458	MET	2.4
1	B	483	ALA	2.4
1	A	57	GLN	2.3
1	C	462	GLU	2.3
2	F	390	ASP	2.3
2	E	406	LEU	2.3
1	B	60	VAL	2.3
1	B	64	LEU	2.3
1	C	452	LEU	2.3
1	B	17	ASP	2.3
1	C	448	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	480	ALA	2.2
1	C	12	LYS	2.2
2	H	398	LYS	2.2
1	A	474	ARG	2.2
1	B	468	GLN	2.2
1	A	162	LEU	2.2
1	A	451	ARG	2.2
2	F	394	GLN	2.2
1	A	92	ASN	2.2
1	C	31	GLU	2.2
1	A	439	PHE	2.2
1	C	303	GLU	2.2
1	B	75	GLN	2.2
1	A	463	ILE	2.2
1	B	471	THR	2.2
1	B	465	GLU	2.2
1	B	69	LYS	2.2
1	A	30	LEU	2.1
1	A	311	GLU	2.1
1	C	299	ALA	2.1
1	B	462	GLU	2.1
1	C	477	ILE	2.1
1	B	488	GLN	2.1
1	A	446	GLU	2.1
1	A	55	ILE	2.1
2	E	398	LYS	2.1
1	A	135	GLU	2.0
1	A	95	LEU	2.0
1	A	488	GLN	2.0
1	A	35	GLU	2.0
1	C	309	LEU	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)

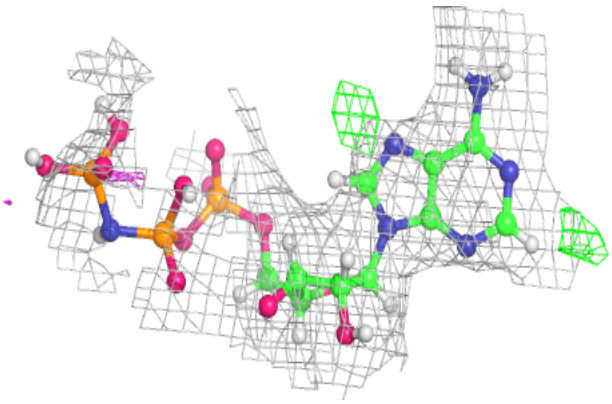
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

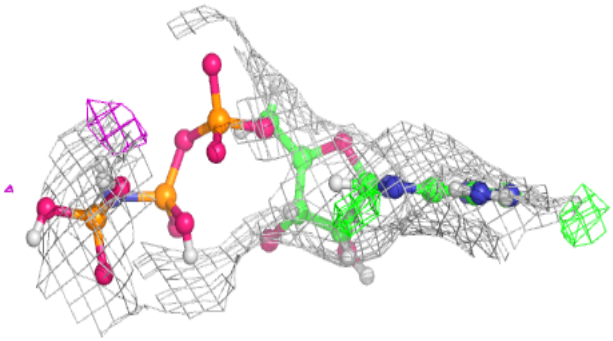
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	C	504	1/1	0.34	0.38	103,103,103,103	0
4	MG	C	502	1/1	0.66	0.57	221,221,221,221	0
3	ANP	A	501	31/31	0.74	0.26	144,191,249,314	0
3	ANP	C	501	31/31	0.75	0.34	140,192,243,292	0
5	SO4	D	504	5/5	0.76	0.28	125,138,149,156	0
6	NA	C	505	1/1	0.79	0.14	189,189,189,189	0
5	SO4	B	506	5/5	0.83	0.50	187,190,193,199	0
5	SO4	B	504	5/5	0.83	0.18	191,191,196,199	0
4	MG	B	502	1/1	0.84	0.43	104,104,104,104	0
5	SO4	D	505	5/5	0.87	0.34	128,150,162,168	0
4	MG	A	502	1/1	0.88	0.59	219,219,219,219	0
5	SO4	B	505	5/5	0.89	0.24	113,128,140,166	0
6	NA	D	506	1/1	0.89	0.22	65,65,65,65	0
4	MG	D	502	1/1	0.92	0.55	87,87,87,87	0
5	SO4	B	503	5/5	0.92	0.24	108,110,116,132	0
5	SO4	D	503	5/5	0.93	0.27	77,78,105,145	0
5	SO4	A	503	5/5	0.93	0.16	133,149,152,155	0
3	ANP	D	501	31/31	0.95	0.28	57,93,183,229	0
3	ANP	B	501	31/31	0.95	0.27	57,101,168,247	0
5	SO4	C	503	5/5	0.96	0.20	94,96,107,133	0

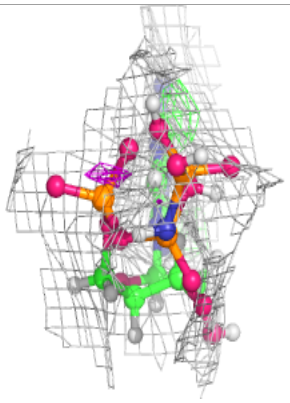
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 501:

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

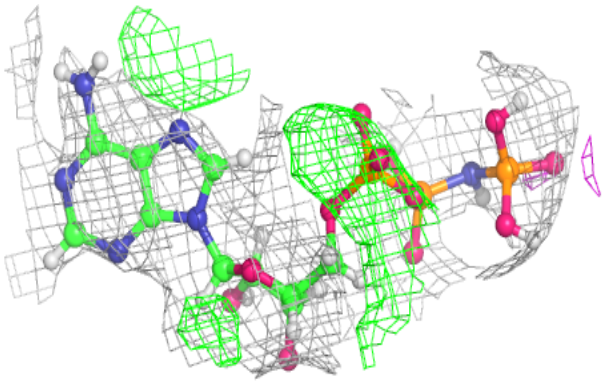


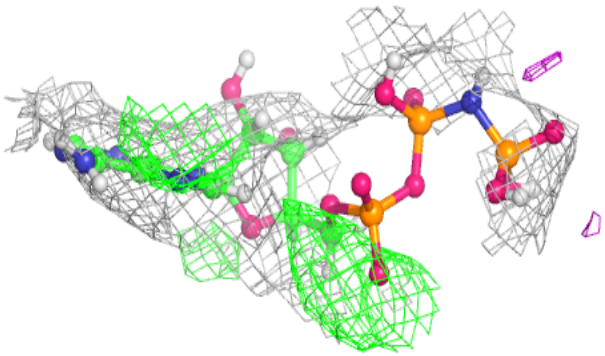


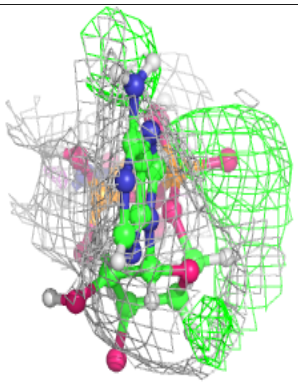


Electron density around ANP C 501:

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

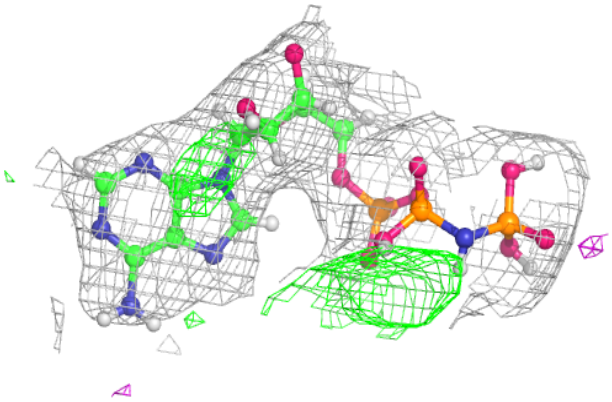


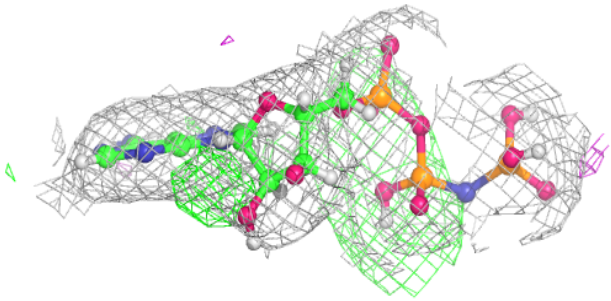


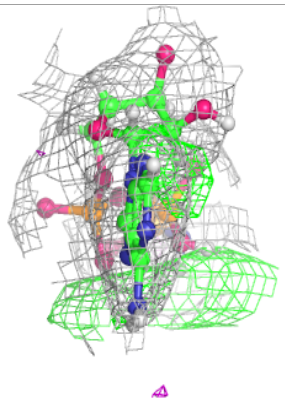


Electron density around ANP D 501:

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

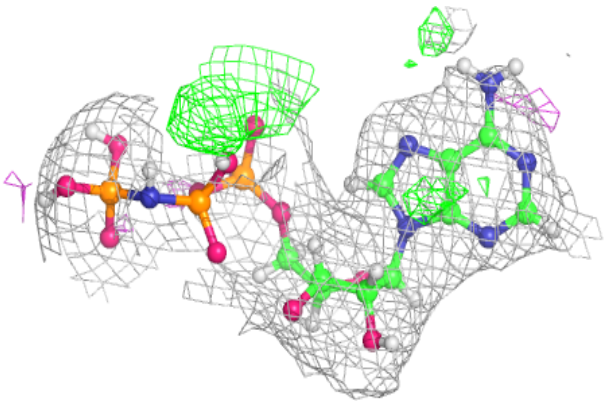


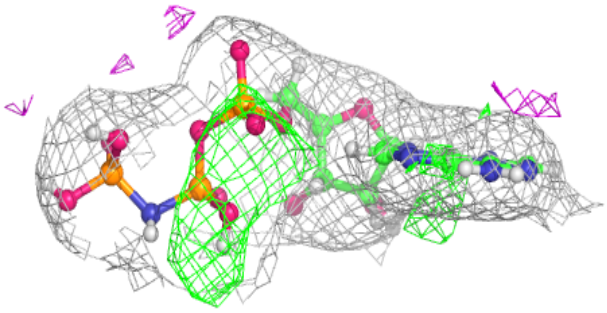


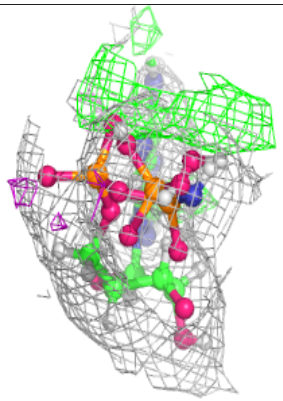


Electron density around ANP B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.