



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 01:08 pm BST

PDB ID : 9RUK / pdb_00009ruk
Title : Streptococcus pneumoniae StkP catalytic domain T167A/T169A double mutant in complex with AMP-PNP and Mn²⁺
Authors : Hamidi, M.; Ravaud, S.; Grangeasse, C.
Deposited on : 2025-07-04
Resolution : 1.88 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

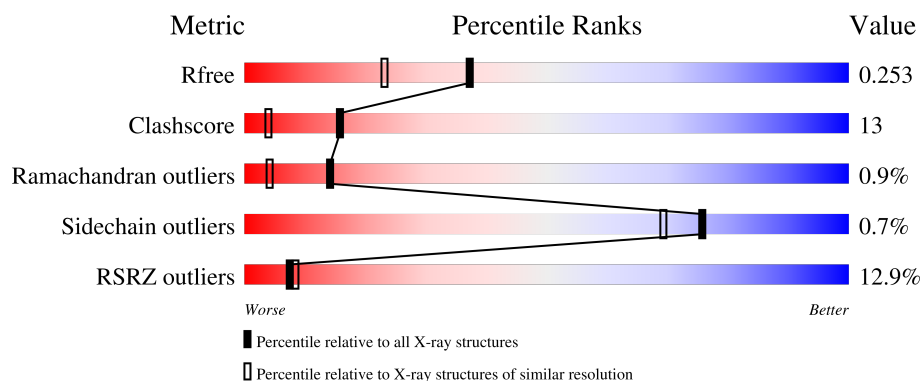
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	309	<div> <div>17%</div> <div>59%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>
1	B	309	<div> <div>6%</div> <div>79%</div> <div>13%</div> <div>•</div> <div>7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4528 atoms, of which 26 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 StkP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2026	1283	357	378	8			
1	B	286	Total	C	N	O	S	0	0	0
			2241	1416	393	423	9			

There are 48 discrepancies between the modelled and reference sequences:

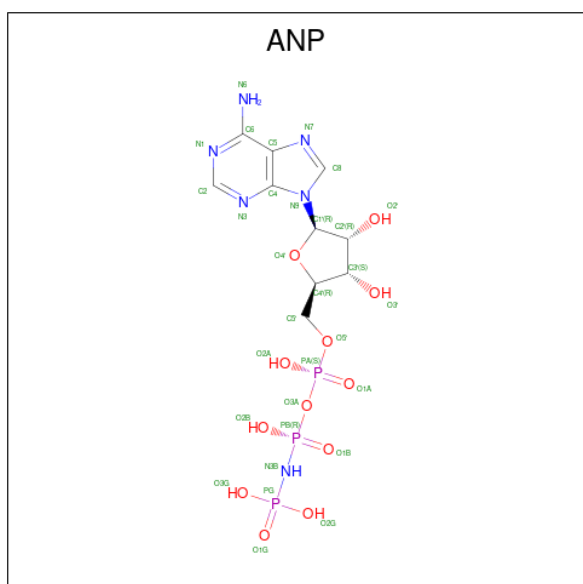
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q8DNS0
A	-20	GLY	-	expression tag	UNP Q8DNS0
A	-19	GLY	-	expression tag	UNP Q8DNS0
A	-18	HIS	-	expression tag	UNP Q8DNS0
A	-17	HIS	-	expression tag	UNP Q8DNS0
A	-16	HIS	-	expression tag	UNP Q8DNS0
A	-15	HIS	-	expression tag	UNP Q8DNS0
A	-14	HIS	-	expression tag	UNP Q8DNS0
A	-13	HIS	-	expression tag	UNP Q8DNS0
A	-12	HIS	-	expression tag	UNP Q8DNS0
A	-11	GLY	-	expression tag	UNP Q8DNS0
A	-10	GLY	-	expression tag	UNP Q8DNS0
A	-9	GLY	-	expression tag	UNP Q8DNS0
A	-8	ARG	-	expression tag	UNP Q8DNS0
A	-7	GLU	-	expression tag	UNP Q8DNS0
A	-6	ASN	-	expression tag	UNP Q8DNS0
A	-5	LEU	-	expression tag	UNP Q8DNS0
A	-4	TYR	-	expression tag	UNP Q8DNS0
A	-3	PHE	-	expression tag	UNP Q8DNS0
A	-2	GLN	-	expression tag	UNP Q8DNS0
A	-1	GLY	-	expression tag	UNP Q8DNS0
A	0	HIS	-	expression tag	UNP Q8DNS0
A	167	ALA	THR	engineered mutation	UNP Q8DNS0
A	169	ALA	THR	engineered mutation	UNP Q8DNS0
B	-21	MET	-	initiating methionine	UNP Q8DNS0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	GLY	-	expression tag	UNP Q8DNS0
B	-19	GLY	-	expression tag	UNP Q8DNS0
B	-18	HIS	-	expression tag	UNP Q8DNS0
B	-17	HIS	-	expression tag	UNP Q8DNS0
B	-16	HIS	-	expression tag	UNP Q8DNS0
B	-15	HIS	-	expression tag	UNP Q8DNS0
B	-14	HIS	-	expression tag	UNP Q8DNS0
B	-13	HIS	-	expression tag	UNP Q8DNS0
B	-12	HIS	-	expression tag	UNP Q8DNS0
B	-11	GLY	-	expression tag	UNP Q8DNS0
B	-10	GLY	-	expression tag	UNP Q8DNS0
B	-9	GLY	-	expression tag	UNP Q8DNS0
B	-8	ARG	-	expression tag	UNP Q8DNS0
B	-7	GLU	-	expression tag	UNP Q8DNS0
B	-6	ASN	-	expression tag	UNP Q8DNS0
B	-5	LEU	-	expression tag	UNP Q8DNS0
B	-4	TYR	-	expression tag	UNP Q8DNS0
B	-3	PHE	-	expression tag	UNP Q8DNS0
B	-2	GLN	-	expression tag	UNP Q8DNS0
B	-1	GLY	-	expression tag	UNP Q8DNS0
B	0	HIS	-	expression tag	UNP Q8DNS0
B	167	ALA	THR	engineered mutation	UNP Q8DNS0
B	169	ALA	THR	engineered mutation	UNP Q8DNS0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

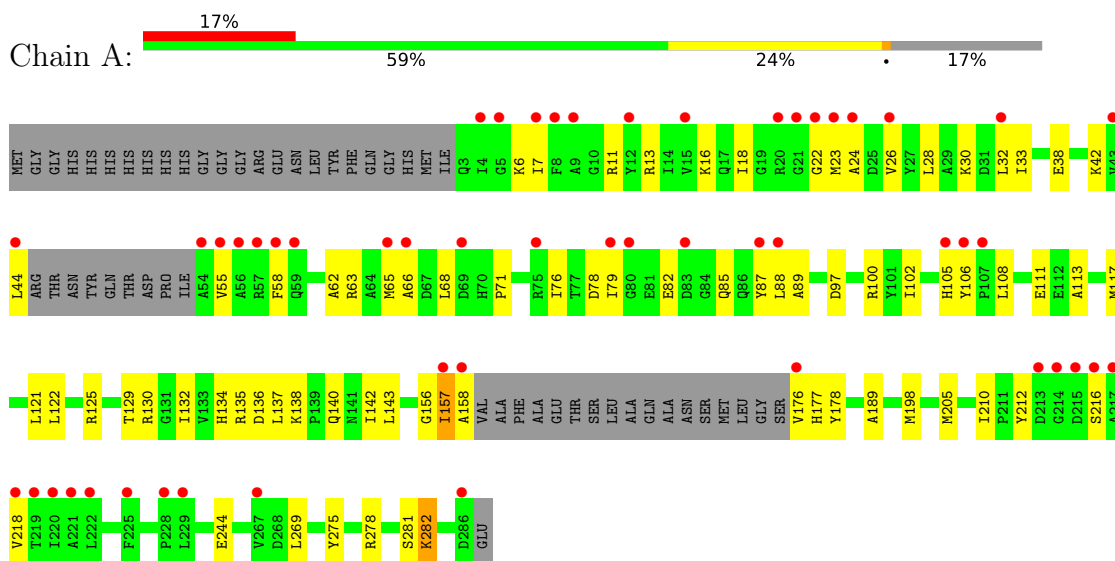
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	144	Total	O	0	0
			144	144		

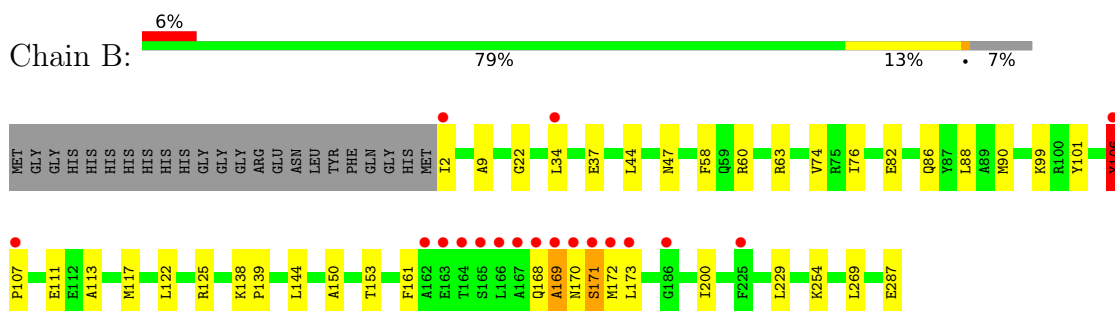
3 Residue-property plots [i](#)

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 StkP



- Molecule 1: Serine/threonine-protein kinase StkP



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.53Å 51.79Å 82.54Å 90.00° 104.21° 90.00°	Depositor
Resolution (Å)	59.21 – 1.88 59.21 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.7 (59.21-1.88) 96.7 (59.21-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.211 , 0.252 0.212 , 0.253	Depositor DCC
R_{free} test set	2280 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4528	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MN

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	0.23	0/2059	0.43	0/2781
1	B	0.36	0/2279	0.56	0/3083
All	All	0.30	0/4338	0.50	0/5864

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2026	0	2045	73	0
1	B	2241	0	2261	45	0
2	A	31	13	13	4	0
2	B	31	13	13	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	0	0	0
4	B	144	0	0	1	0
All	All	4502	26	4332	115	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 13.

All (115) 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:24:ALA:HB2	1:A:44:LEU:HD23	1.48	0.92
1:A:16:LYS:HZ1	1:A:18:ILE:HG22	1.33	0.92
1:A:68:LEU:HD21	1:A:130:ARG:HD2	1.52	0.89
1:B:172:MET:H	1:B:172:MET:HE2	1.39	0.86
1:A:176:VAL:HG13	1:A:178:TYR:H	1.43	0.81
1:A:62:ALA:HB1	1:A:88:LEU:HD21	1.63	0.80
1:A:24:ALA:HB2	1:A:44:LEU:CD2	2.12	0.80
1:A:16:LYS:NZ	1:A:18:ILE:HG22	1.97	0.79
1:B:22:GLY:H	1:B:172:MET:HE3	1.48	0.79
1:A:68:LEU:CD2	1:A:130:ARG:HD2	2.14	0.77
1:B:22:GLY:H	1:B:172:MET:CE	1.99	0.74
1:B:22:GLY:N	1:B:172:MET:HE3	2.03	0.74
1:B:171:SER:HB2	2:B:301:ANP:O2B	1.88	0.73
1:B:22:GLY:CA	1:B:172:MET:HE3	2.18	0.72
1:B:76:ILE:HD13	1:B:90:MET:HG2	1.72	0.71
1:A:22:GLY:O	1:A:23:MET:HB3	1.90	0.70
1:A:23:MET:HE3	1:A:24:ALA:HB3	1.74	0.70
1:B:22:GLY:HA3	1:B:172:MET:HE3	1.73	0.70
1:A:58:PHE:HZ	1:A:88:LEU:HG	1.59	0.68
1:A:55:VAL:O	1:A:55:VAL:HG12	1.93	0.68
1:A:63:ARG:HG2	1:A:79:ILE:HD12	1.77	0.67
1:B:168:GLN:HB2	1:B:172:MET:CB	2.26	0.66
1:B:34:LEU:HD12	1:B:37:GLU:HB3	1.77	0.66
1:A:58:PHE:HD2	1:A:157:ILE:HG22	1.66	0.61
1:A:275:TYR:O	1:A:278:ARG:HG2	2.00	0.61
1:B:60:ARG:HD3	4:B:500:HOH:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:CZ	1:A:88:LEU:HG	2.35	0.60
1:A:62:ALA:CB	1:A:88:LEU:HD21	2.31	0.59
1:B:168:GLN:HB2	1:B:172:MET:HB3	1.83	0.59
1:A:122:LEU:HD13	1:B:122:LEU:HD13	1.85	0.57
2:A:301:ANP:H8	2:A:301:ANP:H5'1	1.87	0.57
1:B:138:LYS:NZ	1:B:171:SER:HB3	2.20	0.57
1:A:157:ILE:O	1:A:158:ALA:HB3	2.03	0.56
1:A:210:ILE:HD13	1:A:212:TYR:O	2.04	0.56
1:B:254:LYS:HG3	1:B:287:GLU:OE1	2.05	0.56
1:B:200:ILE:HD13	1:B:229:LEU:HD11	1.86	0.56
1:A:176:VAL:HG22	1:A:177:HIS:H	1.70	0.56
1:B:168:GLN:HG2	1:B:169:ALA:N	2.21	0.56
1:B:172:MET:HE2	1:B:172:MET:N	2.17	0.55
1:A:106:TYR:O	1:A:108:LEU:N	2.39	0.54
1:A:134:HIS:O	1:A:135:ARG:HB2	2.08	0.54
1:A:65:MET:HG2	1:A:76:ILE:HD12	1.90	0.54
1:A:11:ARG:O	1:A:32:LEU:HD23	2.08	0.54
1:A:65:MET:HE2	1:A:76:ILE:HG13	1.90	0.54
1:B:76:ILE:HD12	1:B:88:LEU:CD1	2.38	0.54
1:A:136:ASP:OD2	2:A:301:ANP:O3G	2.27	0.53
1:A:65:MET:SD	1:A:76:ILE:HD11	2.49	0.53
1:A:11:ARG:HD2	1:A:33:ILE:HD12	1.91	0.52
1:A:102:ILE:HD11	1:A:205:MET:HG2	1.91	0.52
1:B:34:LEU:HD12	1:B:34:LEU:O	2.08	0.52
1:A:157:ILE:O	1:A:158:ALA:CB	2.57	0.52
1:A:23:MET:HE1	2:A:301:ANP:O1G	2.10	0.52
1:A:58:PHE:CD2	1:A:157:ILE:HG22	2.44	0.52
1:A:244:GLU:OE2	1:A:282:LYS:HE3	2.09	0.52
1:A:24:ALA:CB	1:A:44:LEU:HD23	2.31	0.52
1:A:156:GLY:O	1:A:157:ILE:C	2.53	0.52
1:B:101:TYR:CG	1:B:144:LEU:HD12	2.45	0.52
1:B:113:ALA:O	1:B:117:MET:HG3	2.09	0.52
1:B:168:GLN:O	1:B:169:ALA:HB2	2.10	0.50
1:B:172:MET:HE1	2:B:301:ANP:HNB1	1.77	0.50
1:B:138:LYS:HZ1	1:B:171:SER:HB3	1.77	0.50
1:B:34:LEU:CD1	1:B:37:GLU:HB3	2.43	0.49
1:B:144:LEU:HD23	1:B:150:ALA:HA	1.93	0.49
1:A:111:GLU:HG2	1:B:111:GLU:HG2	1.95	0.48
1:A:97:ASP:OD1	1:A:100:ARG:HG3	2.13	0.48
1:A:125:ARG:O	1:A:129:THR:HG23	2.14	0.48
1:B:169:ALA:O	1:B:173:LEU:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:CD1	1:A:106:TYR:C	2.89	0.47
1:A:68:LEU:HD11	1:A:132:ILE:HD12	1.96	0.47
1:A:135:ARG:HH11	1:A:189:ALA:HB3	1.79	0.47
1:A:138:LYS:HD2	1:A:140:GLN:OE1	2.15	0.47
1:B:269:LEU:C	1:B:269:LEU:HD13	2.40	0.47
1:A:210:ILE:HD12	1:A:210:ILE:C	2.40	0.46
1:A:82:GLU:O	1:A:85:GLN:HB2	2.15	0.46
1:A:7:ILE:CD1	1:A:13:ARG:HB2	2.46	0.46
1:A:26:VAL:HG21	2:A:301:ANP:H5'2	1.99	0.45
1:B:63:ARG:HH11	1:B:63:ARG:HG2	1.82	0.45
1:A:121:LEU:HD12	1:A:269:LEU:HD22	1.98	0.44
1:B:106:TYR:CD2	1:B:106:TYR:O	2.70	0.44
1:B:76:ILE:HD12	1:B:88:LEU:HD12	1.98	0.44
1:B:101:TYR:CD1	1:B:144:LEU:HD12	2.52	0.44
1:A:122:LEU:CD1	1:B:122:LEU:HD13	2.48	0.44
1:A:6:LYS:HD2	1:A:6:LYS:HA	1.76	0.44
1:A:7:ILE:HD13	1:A:13:ARG:HA	2.00	0.43
1:A:130:ARG:HE	1:A:130:ARG:HB3	1.58	0.43
1:A:30:LYS:O	1:A:32:LEU:HD22	2.19	0.43
1:A:42:LYS:O	1:A:87:TYR:HA	2.19	0.43
1:A:71:PRO:HD3	1:B:125:ARG:CZ	2.48	0.43
1:A:244:GLU:OE2	1:A:282:LYS:CE	2.66	0.43
1:A:157:ILE:O	1:A:157:ILE:HD12	2.18	0.43
1:A:216:SER:OG	1:A:218:VAL:HG12	2.18	0.43
1:A:134:HIS:O	1:A:135:ARG:CB	2.66	0.42
1:A:66:ALA:HA	1:A:76:ILE:HB	2.01	0.42
1:A:102:ILE:O	1:A:106:TYR:HA	2.19	0.42
1:B:2:ILE:O	1:B:2:ILE:HG22	2.18	0.42
1:A:32:LEU:HD22	1:A:32:LEU:N	2.35	0.42
1:A:7:ILE:HD13	1:A:7:ILE:HA	1.84	0.42
1:A:142:ILE:C	1:A:143:LEU:HD23	2.45	0.42
1:A:113:ALA:O	1:A:117:MET:HG3	2.20	0.42
1:A:269:LEU:O	1:A:269:LEU:HG	2.13	0.41
1:A:78:ASP:HB3	1:A:89:ALA:HB3	2.02	0.41
1:B:47:ASN:OD1	1:B:47:ASN:C	2.63	0.41
1:B:171:SER:CB	2:B:301:ANP:O2B	2.63	0.41
1:A:55:VAL:O	1:A:55:VAL:CG1	2.63	0.41
1:A:105:HIS:O	1:A:106:TYR:C	2.62	0.41
1:B:76:ILE:CD1	1:B:88:LEU:HD12	2.50	0.41
1:A:137:LEU:HD13	1:A:198:MET:HG3	2.02	0.41
1:B:74:VAL:HG21	1:B:153:THR:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH1	1:A:189:ALA:HB3	2.36	0.41
1:B:99:LYS:HB2	1:B:139:PRO:HB2	2.02	0.41
1:B:44:LEU:HD22	1:B:161:PHE:CE2	2.56	0.40
1:A:28:LEU:HD11	1:A:38:GLU:HB3	2.03	0.40
1:B:9:ALA:HA	1:B:82:GLU:CD	2.46	0.40
1:A:135:ARG:HH11	1:A:135:ARG:HG2	1.86	0.40
1:B:58:PHE:CE2	1:B:86:GLN:HB3	2.56	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	252/309 (82%)	235 (93%)	16 (6%)	1 (0%)	30	18
1	B	284/309 (92%)	271 (95%)	9 (3%)	4 (1%)	9	1
All	All	536/618 (87%)	506 (94%)	25 (5%)	5 (1%)	14	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
1	B	106	TYR
1	B	107	PRO
1	B	169	ALA
1	B	170	ASN

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	215/256 (84%)	213 (99%)	2 (1%)	70	63
1	B	239/256 (93%)	238 (100%)	1 (0%)	84	79
All	All	454/512 (89%)	451 (99%)	3 (1%)	76	69

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	SER
1	A	282	LYS
1	B	171	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
1	B	105	HIS
1	B	183	GLN
1	B	227	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ANP	A	301	3	32,33,33	2.30	4 (12%)	44,52,52	1.60	9 (20%)
2	ANP	B	301	3	32,33,33	2.16	5 (15%)	44,52,52	1.82	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	301	3	-	6/18/38/38	0/3/3/3
2	ANP	B	301	3	-	2/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ANP	PB-O3A	8.93	1.70	1.59
2	B	301	ANP	PB-O3A	7.94	1.69	1.59
2	B	301	ANP	PG-N3B	6.42	1.80	1.63
2	A	301	ANP	PG-N3B	6.38	1.80	1.63
2	A	301	ANP	PG-O1G	4.55	1.53	1.46
2	B	301	ANP	PG-O1G	4.26	1.52	1.46
2	B	301	ANP	PB-O1B	2.78	1.50	1.46
2	A	301	ANP	PB-O1B	2.62	1.50	1.46
2	B	301	ANP	PB-O2B	-2.05	1.51	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ANP	O2B-PB-O1B	5.11	120.63	109.92
2	B	301	ANP	O2B-PB-O1B	4.90	120.20	109.92
2	B	301	ANP	O1G-PG-N3B	-4.27	105.48	111.77
2	B	301	ANP	O2G-PG-O3G	3.87	117.95	107.64
2	B	301	ANP	O3'-C3'-C4'	3.62	121.50	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ANP	C2'-C3'-C4'	-3.35	96.13	102.64
2	A	301	ANP	O1G-PG-N3B	-3.33	106.87	111.77
2	B	301	ANP	C3'-C2'-C1'	3.15	107.41	101.43
2	A	301	ANP	O4'-C1'-N9	3.12	114.22	108.06
2	A	301	ANP	C2'-C1'-N9	-3.00	105.71	113.30
2	A	301	ANP	O3A-PB-N3B	-2.69	99.13	106.59
2	B	301	ANP	O3A-PB-N3B	-2.66	99.20	106.59
2	A	301	ANP	O2'-C2'-C3'	-2.51	103.70	111.82
2	A	301	ANP	O2G-PG-O3G	2.43	114.10	107.64
2	B	301	ANP	O4'-C1'-N9	2.34	112.68	108.06
2	B	301	ANP	C4-N9-C8	2.16	108.06	105.73
2	B	301	ANP	O1B-PB-N3B	2.14	114.93	111.77
2	A	301	ANP	O4'-C4'-C5'	-2.14	102.32	109.37
2	B	301	ANP	C2'-C1'-N9	-2.10	107.97	113.30
2	A	301	ANP	O2'-C2'-C1'	2.09	117.01	110.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ANP	PB-N3B-PG-O1G
2	A	301	ANP	PG-N3B-PB-O1B
2	A	301	ANP	PA-O3A-PB-O1B
2	A	301	ANP	PA-O3A-PB-O2B
2	B	301	ANP	PB-N3B-PG-O1G
2	B	301	ANP	PG-N3B-PB-O3A
2	A	301	ANP	O4'-C4'-C5'-O5'
2	A	301	ANP	C5'-O5'-PA-O1A

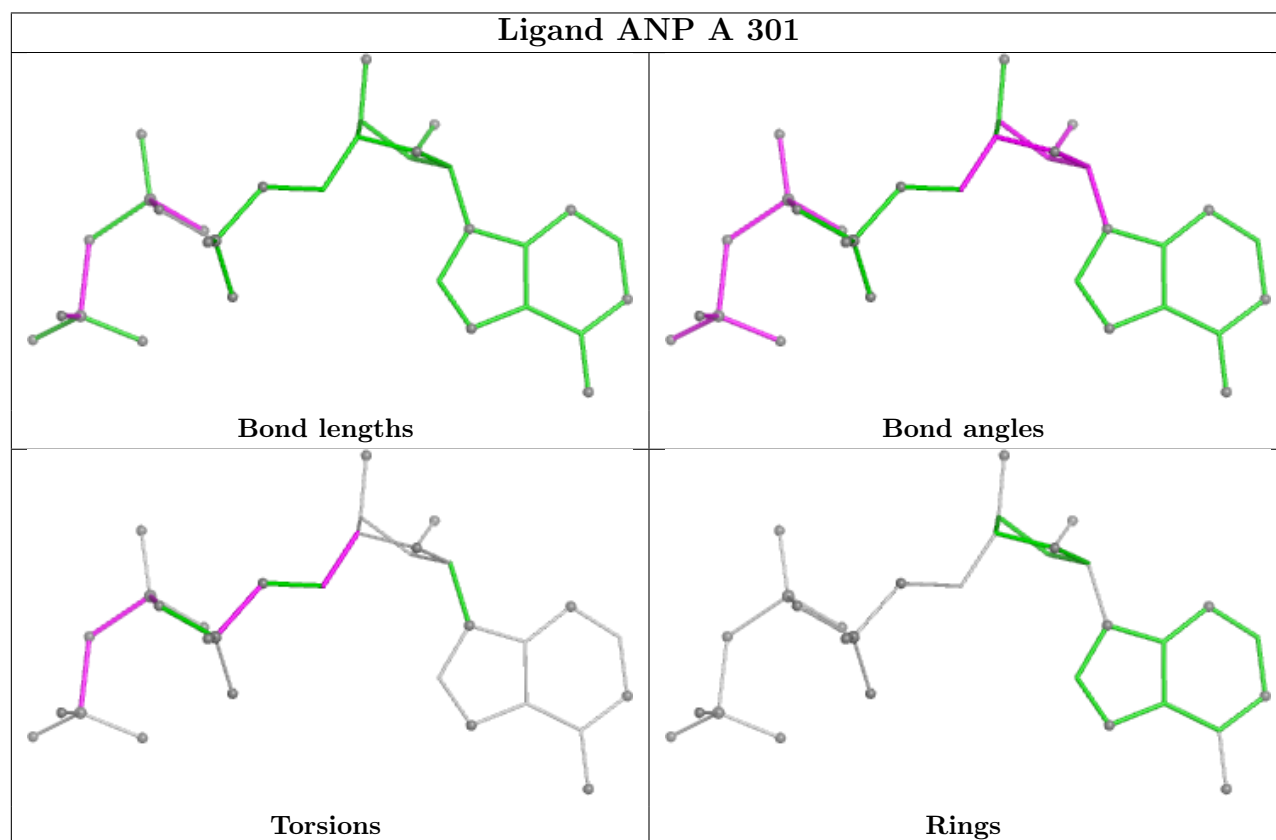
There are no ring outliers.

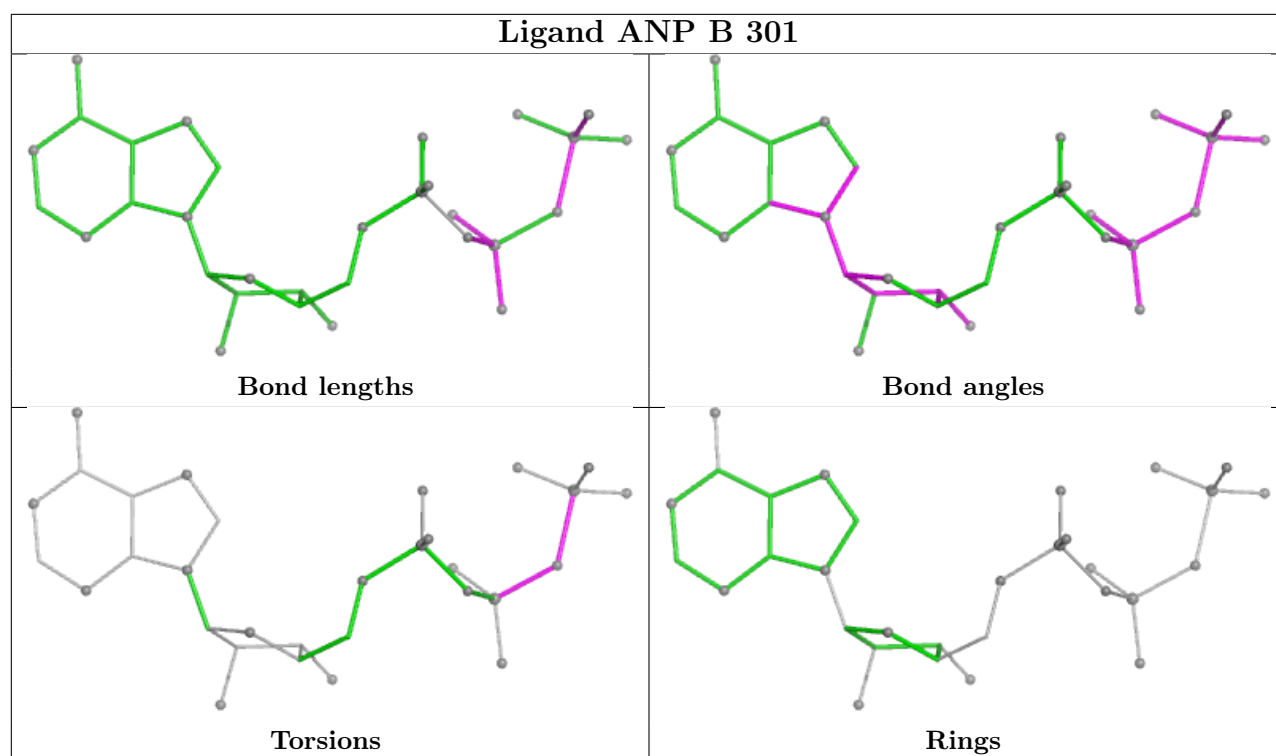
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ANP	4	0
2	B	301	ANP	3	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 than 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.





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/309 (83%)	1.23	52 (20%) 3 3	23, 42, 72, 92	0
1	B	286/309 (92%)	0.26	18 (6%) 26 28	15, 25, 47, 66	0
All	All	544/618 (88%)	0.72	70 (12%) 7 8	15, 32, 65, 92	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	9.8
1	B	172	MET	7.1
1	A	54	ALA	6.2
1	A	56	ALA	5.8
1	B	171	SER	5.7
1	A	214	GLY	5.6
1	A	23	MET	5.6
1	B	169	ALA	5.4
1	A	24	ALA	4.8
1	A	217	ALA	4.7
1	A	107	PRO	4.6
1	A	158	ALA	4.4
1	B	173	LEU	4.3
1	A	225	PHE	4.2
1	B	166	LEU	4.1
1	A	218	VAL	4.1
1	A	44	LEU	4.1
1	B	2	ILE	4.0
1	A	106	TYR	3.8
1	B	167	ALA	3.7
1	B	170	ASN	3.7
1	A	215	ASP	3.6
1	A	213	ASP	3.5
1	B	163	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	216	SER	3.4
1	B	164	THR	3.4
1	A	57	ARG	3.4
1	A	15	VAL	3.3
1	A	55	VAL	3.3
1	A	8	PHE	3.3
1	A	58	PHE	3.3
1	B	168	GLN	3.2
1	A	176	VAL	3.2
1	B	107	PRO	3.2
1	A	12	TYR	3.0
1	A	219	THR	3.0
1	A	4	ILE	3.0
1	A	157	ILE	2.9
1	A	220	ILE	2.9
1	A	9	ALA	2.8
1	A	7	ILE	2.8
1	A	32	LEU	2.7
1	A	22	GLY	2.6
1	A	286	ASP	2.5
1	A	79	ILE	2.5
1	A	87	TYR	2.5
1	A	75	ARG	2.5
1	A	267	VAL	2.5
1	A	222	LEU	2.4
1	B	225	PHE	2.4
1	A	83	ASP	2.4
1	B	186	GLY	2.4
1	B	165	SER	2.4
1	A	66	ALA	2.3
1	A	88	LEU	2.3
1	A	228	PRO	2.3
1	A	221	ALA	2.3
1	A	69	ASP	2.2
1	A	59	GLN	2.2
1	A	65	MET	2.1
1	A	21	GLY	2.1
1	A	105	HIS	2.1
1	A	5	GLY	2.1
1	A	43	VAL	2.1
1	B	34	LEU	2.1
1	A	20	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	GLY	2.1
1	A	229	LEU	2.1
1	B	106	TYR	2.0
1	A	26	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

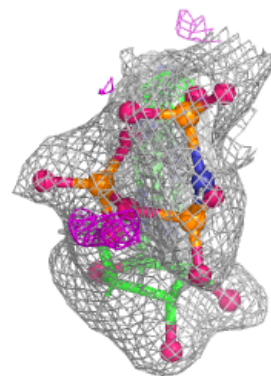
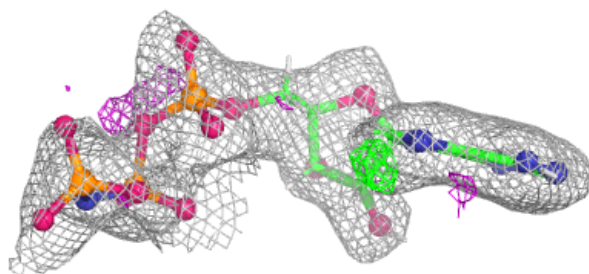
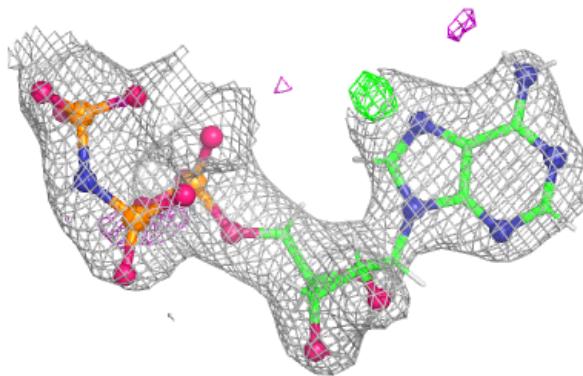
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ANP	A	301	31/31	0.86	0.10	39,55,68,74	0
2	ANP	B	301	31/31	0.97	0.06	17,24,30,32	0
3	MN	A	302	1/1	0.98	0.06	57,57,57,57	0
3	MN	B	302	1/1	0.99	0.03	19,19,19,19	0

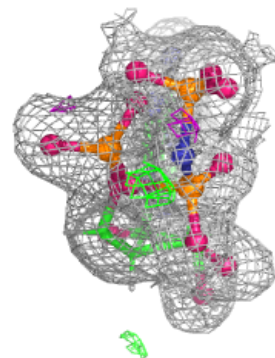
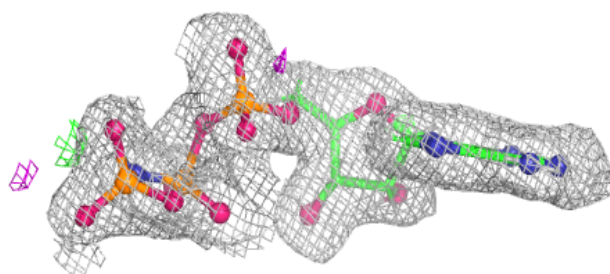
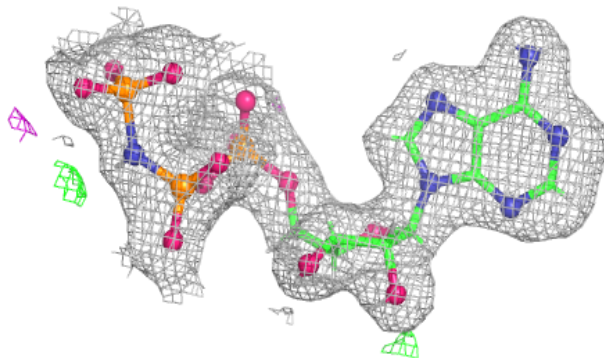
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 301:

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

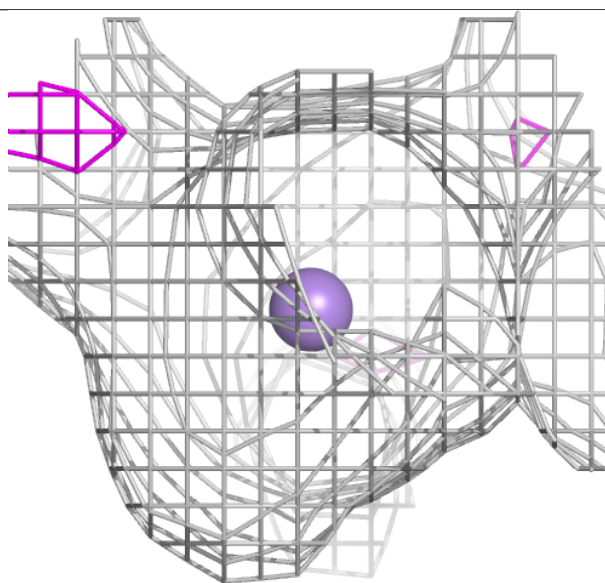
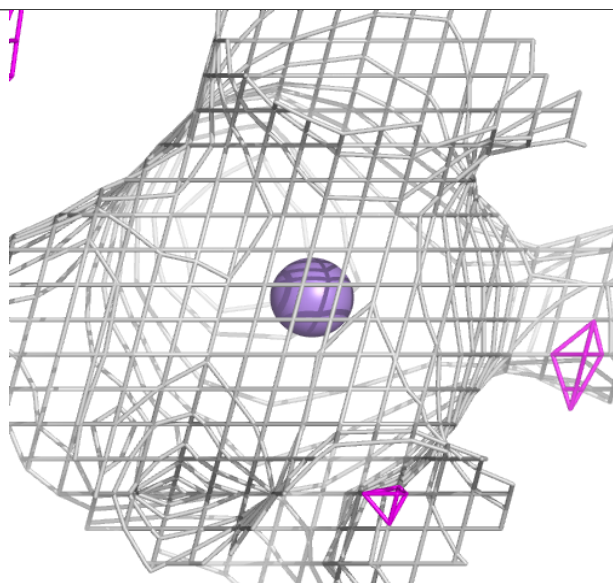
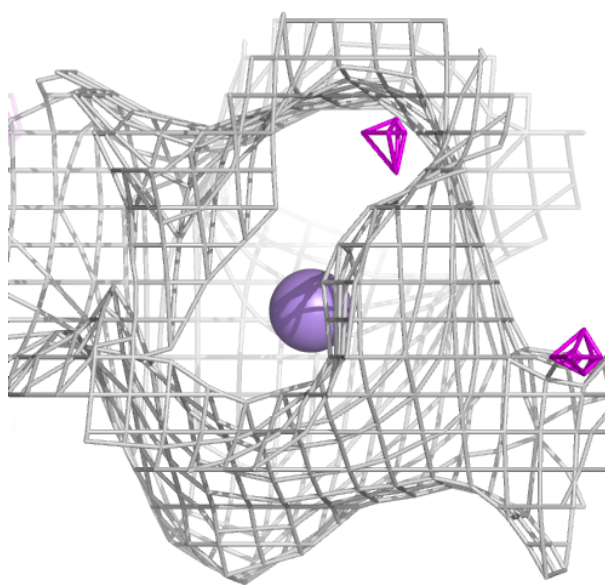
**Electron density around ANP B 301:**

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



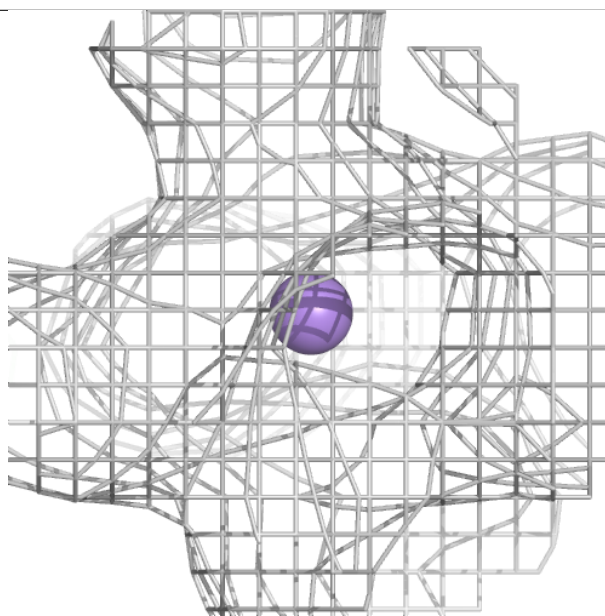
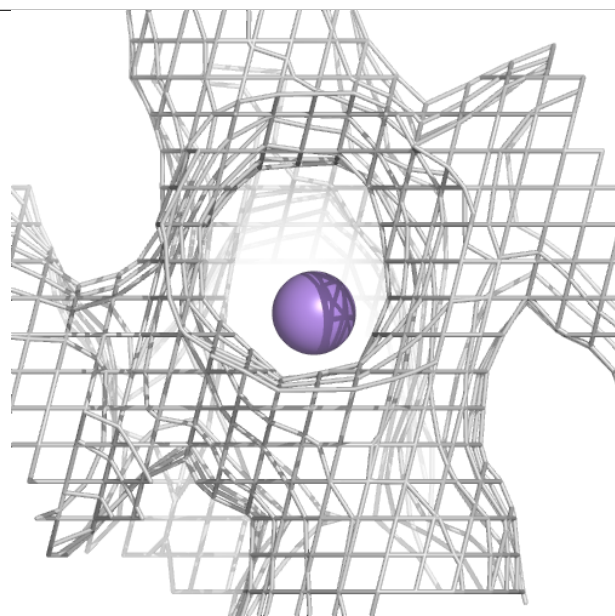
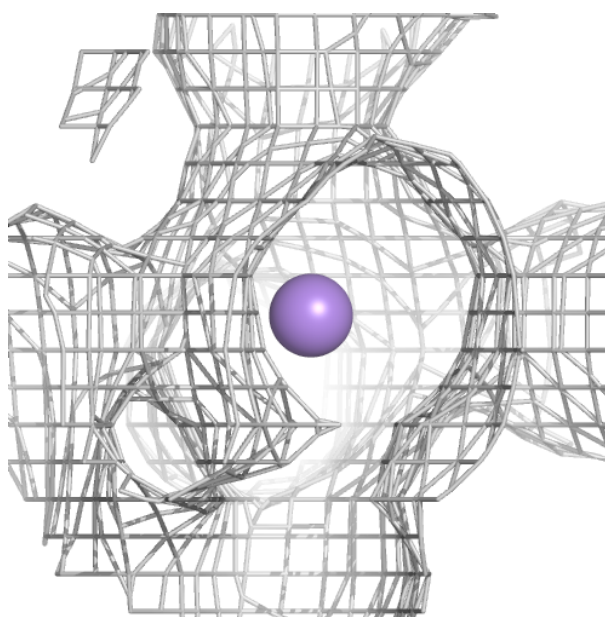
Electron density around MN A 302:

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



Electron density around MN B 302:

$2mF_o-DF_c$ (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.