



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2026 – 11:35 PM JST

PDB ID : 9WS6 / pdb_00009ws6
Title : Crystal structure of AMP-PNP-bound PAK2 kinase domain containing D368N mutant
Authors : Chen, F.Y.; Hu, H.-F.; Wang, J.; Luo, Z.P.; Wu, J.-W.; Wang, Z.-X.
Deposited on : 2025-09-12
Resolution : 2.00 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	:	1.8.5 (274361), 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

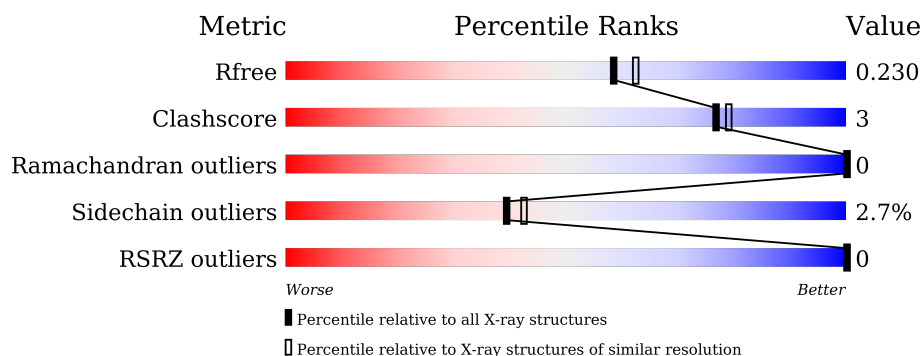
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	323	
1	B	323	
1	C	323	
1	D	323	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9673 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 PAK-2p34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2377	1516	391	452	18			
1	B	292	Total	C	N	O	S	0	0	0
			2281	1458	378	428	17			
1	C	309	Total	C	N	O	S	0	0	0
			2385	1525	392	450	18			
1	D	292	Total	C	N	O	S	0	0	0
			2274	1453	378	426	17			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MET	-	initiating methionine	UNP Q13177
A	203	GLY	-	expression tag	UNP Q13177
A	204	SER	-	expression tag	UNP Q13177
A	205	SER	-	expression tag	UNP Q13177
A	206	HIS	-	expression tag	UNP Q13177
A	207	HIS	-	expression tag	UNP Q13177
A	208	HIS	-	expression tag	UNP Q13177
A	209	HIS	-	expression tag	UNP Q13177
A	210	HIS	-	expression tag	UNP Q13177
A	211	HIS	-	expression tag	UNP Q13177
A	212	SER	-	expression tag	UNP Q13177
A	213	GLN	-	expression tag	UNP Q13177
A	214	ASP	-	expression tag	UNP Q13177
A	215	LEU	-	expression tag	UNP Q13177
A	216	GLU	-	expression tag	UNP Q13177
A	217	VAL	-	expression tag	UNP Q13177
A	218	LEU	-	expression tag	UNP Q13177
A	219	PHE	-	expression tag	UNP Q13177
A	220	GLN	-	expression tag	UNP Q13177
A	221	GLY	-	expression tag	UNP Q13177
A	222	PRO	-	expression tag	UNP Q13177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP Q13177
A	224	MET	-	expression tag	UNP Q13177
A	225	ALA	-	expression tag	UNP Q13177
A	226	SER	-	expression tag	UNP Q13177
A	368	ASN	ASP	engineered mutation	UNP Q13177
B	202	MET	-	initiating methionine	UNP Q13177
B	203	GLY	-	expression tag	UNP Q13177
B	204	SER	-	expression tag	UNP Q13177
B	205	SER	-	expression tag	UNP Q13177
B	206	HIS	-	expression tag	UNP Q13177
B	207	HIS	-	expression tag	UNP Q13177
B	208	HIS	-	expression tag	UNP Q13177
B	209	HIS	-	expression tag	UNP Q13177
B	210	HIS	-	expression tag	UNP Q13177
B	211	HIS	-	expression tag	UNP Q13177
B	212	SER	-	expression tag	UNP Q13177
B	213	GLN	-	expression tag	UNP Q13177
B	214	ASP	-	expression tag	UNP Q13177
B	215	LEU	-	expression tag	UNP Q13177
B	216	GLU	-	expression tag	UNP Q13177
B	217	VAL	-	expression tag	UNP Q13177
B	218	LEU	-	expression tag	UNP Q13177
B	219	PHE	-	expression tag	UNP Q13177
B	220	GLN	-	expression tag	UNP Q13177
B	221	GLY	-	expression tag	UNP Q13177
B	222	PRO	-	expression tag	UNP Q13177
B	223	HIS	-	expression tag	UNP Q13177
B	224	MET	-	expression tag	UNP Q13177
B	225	ALA	-	expression tag	UNP Q13177
B	226	SER	-	expression tag	UNP Q13177
B	368	ASN	ASP	engineered mutation	UNP Q13177
C	202	MET	-	initiating methionine	UNP Q13177
C	203	GLY	-	expression tag	UNP Q13177
C	204	SER	-	expression tag	UNP Q13177
C	205	SER	-	expression tag	UNP Q13177
C	206	HIS	-	expression tag	UNP Q13177
C	207	HIS	-	expression tag	UNP Q13177
C	208	HIS	-	expression tag	UNP Q13177
C	209	HIS	-	expression tag	UNP Q13177
C	210	HIS	-	expression tag	UNP Q13177
C	211	HIS	-	expression tag	UNP Q13177
C	212	SER	-	expression tag	UNP Q13177

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Chain	Residue	Modelled	Actual	Comment	Reference
C	213	GLN	-	expression tag	UNP Q13177
C	214	ASP	-	expression tag	UNP Q13177
C	215	LEU	-	expression tag	UNP Q13177
C	216	GLU	-	expression tag	UNP Q13177
C	217	VAL	-	expression tag	UNP Q13177
C	218	LEU	-	expression tag	UNP Q13177
C	219	PHE	-	expression tag	UNP Q13177
C	220	GLN	-	expression tag	UNP Q13177
C	221	GLY	-	expression tag	UNP Q13177
C	222	PRO	-	expression tag	UNP Q13177
C	223	HIS	-	expression tag	UNP Q13177
C	224	MET	-	expression tag	UNP Q13177
C	225	ALA	-	expression tag	UNP Q13177
C	226	SER	-	expression tag	UNP Q13177
C	368	ASN	ASP	engineered mutation	UNP Q13177
D	202	MET	-	initiating methionine	UNP Q13177
D	203	GLY	-	expression tag	UNP Q13177
D	204	SER	-	expression tag	UNP Q13177
D	205	SER	-	expression tag	UNP Q13177
D	206	HIS	-	expression tag	UNP Q13177
D	207	HIS	-	expression tag	UNP Q13177
D	208	HIS	-	expression tag	UNP Q13177
D	209	HIS	-	expression tag	UNP Q13177
D	210	HIS	-	expression tag	UNP Q13177
D	211	HIS	-	expression tag	UNP Q13177
D	212	SER	-	expression tag	UNP Q13177
D	213	GLN	-	expression tag	UNP Q13177
D	214	ASP	-	expression tag	UNP Q13177
D	215	LEU	-	expression tag	UNP Q13177
D	216	GLU	-	expression tag	UNP Q13177
D	217	VAL	-	expression tag	UNP Q13177
D	218	LEU	-	expression tag	UNP Q13177
D	219	PHE	-	expression tag	UNP Q13177
D	220	GLN	-	expression tag	UNP Q13177
D	221	GLY	-	expression tag	UNP Q13177
D	222	PRO	-	expression tag	UNP Q13177
D	223	HIS	-	expression tag	UNP Q13177
D	224	MET	-	expression tag	UNP Q13177
D	225	ALA	-	expression tag	UNP Q13177
D	226	SER	-	expression tag	UNP Q13177
D	368	ASN	ASP	engineered mutation	UNP Q13177

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | B | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | C | 1 | Total Mg
1 1 | 0 | 0 |
| 3 | D | 1 | Total Mg
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | A | 1 | Total Cl
1 1 | 0 | 0 |
| 4 | B | 1 | Total Cl
1 1 | 0 | 0 |



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

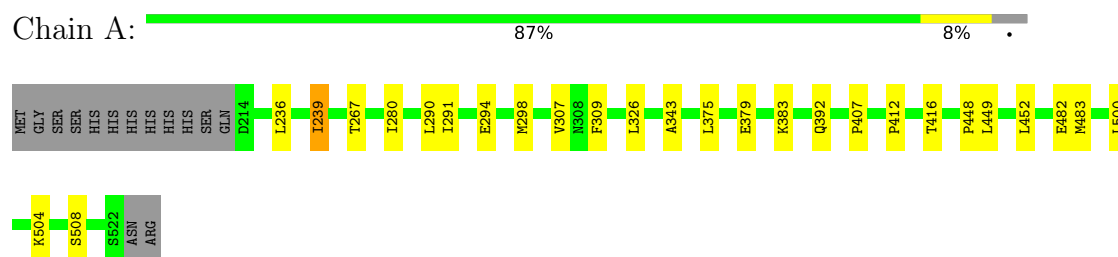
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total 78	O 78	0	0
5	B	63	Total 63	O 63	0	0
5	C	85	Total 85	O 85	0	0
5	D	60	Total 60	O 60	0	0

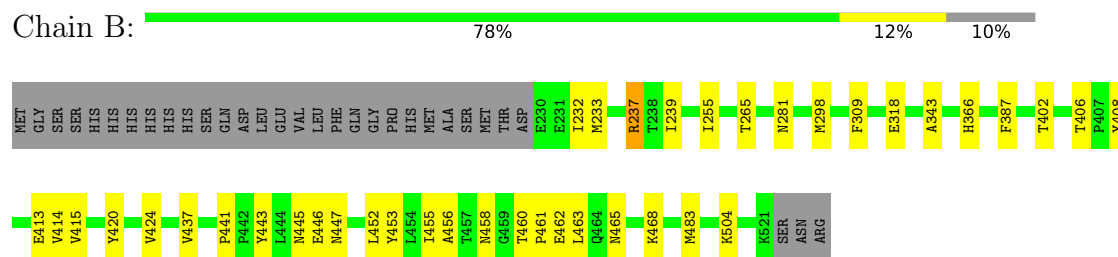
3 Residue-property plots [i](#)

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.

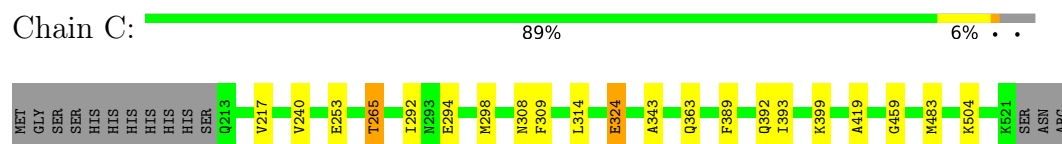
• Molecule 1: PAK-2p34



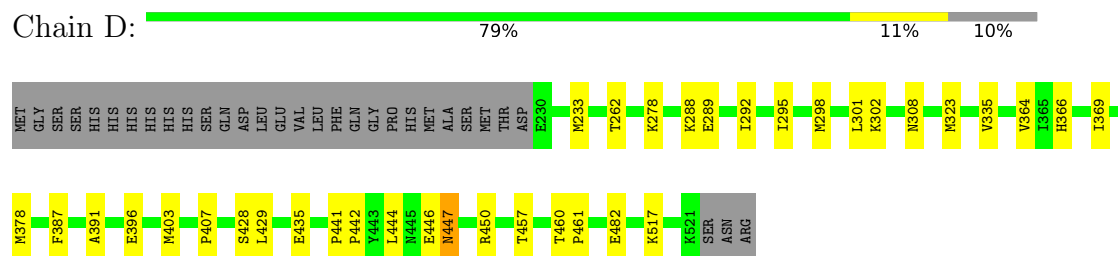
• Molecule 1: PAK-2p34



• Molecule 1: PAK-2p34



• Molecule 1: PAK-2p34



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.94Å 67.05Å 183.32Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	22.70 – 2.00 22.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (22.70-2.00) 90.5 (22.70-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.195 , 0.228 0.199 , 0.230	Depositor DCC
R_{free} test set	4306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.028 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.033 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.030 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.155 for -h,-k,l	Xtriage
Reported twinning fraction	0.884 for H, K, L 0.116 for -h,-k,l	Depositor
Outliers	0 of 86803 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9673	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 6.40% 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: CL, 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	0.61	0/2417	0.96	0/3272
1	B	0.62	0/2320	1.00	0/3137
1	C	0.63	0/2426	1.01	0/3285
1	D	0.62	0/2313	1.02	0/3128
All	All	0.62	0/9476	1.00	0/12822

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 [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	2377	0	2395	12	0
1	B	2281	0	2347	18	0
1	C	2385	0	2414	10	0
1	D	2274	0	2334	19	0
2	A	31	0	13	0	0
2	C	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	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	78	0	0	0	0
5	B	63	0	0	0	0
5	C	85	0	0	0	0
5	D	60	0	0	0	0
All	All	9673	0	9516	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (55) 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:B:406:THR:HG21	1:B:445:ASN:HB2	1.65	0.78
1:A:416:THR:HA	1:D:447:ASN:HB3	1.70	0.72
1:C:298:MET:HB3	1:C:309:PHE:HB2	1.74	0.68
1:D:366:HIS:CD2	1:D:387:PHE:HB3	2.29	0.67
1:C:363:GLN:HA	1:C:393:ILE:HD12	1.75	0.67
1:D:446:GLU:HB3	1:D:450:ARG:HB3	1.79	0.64
1:B:458:ASN:HB2	1:B:461:PRO:HD3	1.80	0.63
1:D:278:LYS:HD2	1:D:391:ALA:HA	1.83	0.61
1:B:255:ILE:HD13	1:B:265:THR:HG23	1.83	0.60
1:A:407:PRO:HG2	1:A:448:PRO:HB3	1.84	0.59
1:A:298:MET:HB3	1:A:309:PHE:HB2	1.85	0.58
1:A:236:LEU:HD23	1:A:239:ILE:HD11	1.88	0.56
1:A:449:LEU:HB2	1:D:407:PRO:HG2	1.91	0.52
1:B:456:ALA:HB1	1:B:483:MET:HB2	1.91	0.51
1:A:326:LEU:HD11	1:A:383:LYS:HD2	1.93	0.51
1:A:307:VAL:HG21	1:A:375:LEU:HD12	1.91	0.51
1:B:366:HIS:CD2	1:B:387:PHE:HB3	2.47	0.49
1:B:455:ILE:HG12	1:B:462:GLU:HB2	1.94	0.48
1:A:379:GLU:CD	1:A:379:GLU:H	2.22	0.48
1:C:459:GLY:HA2	1:C:483:MET:SD	2.55	0.47
1:D:289:GLU:HA	1:D:292:ILE:HD12	1.97	0.46
1:D:447:ASN:OD1	1:D:450:ARG:HB2	2.16	0.46
1:A:280:ILE:HD13	1:A:291:ILE:HD12	1.98	0.46
1:D:295:ILE:HA	1:D:298:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:MET:HB3	1:B:309:PHE:HB2	1.98	0.46
1:C:217:VAL:HG13	1:C:292:ILE:HD12	1.97	0.46
1:B:415:VAL:HG21	1:B:452:LEU:HD11	1.98	0.45
1:D:378:MET:HE1	1:D:517:LYS:HE2	1.98	0.45
1:B:281:ASN:HA	1:B:318:GLU:HG2	1.98	0.45
1:B:406:THR:HG21	1:B:445:ASN:CB	2.43	0.44
1:C:399:LYS:HA	1:C:419:ALA:HA	2.00	0.44
1:D:369:ILE:HB	1:D:428:SER:HB2	1.99	0.44
1:C:253:GLU:HB2	1:C:265:THR:HG22	1.99	0.44
1:D:444:LEU:HD11	1:D:461:PRO:HB3	1.99	0.44
1:B:402:THR:HG21	1:C:389:PHE:CZ	2.53	0.44
1:A:452:LEU:HD11	1:D:403:MET:HE1	1.99	0.43
1:B:413:GLU:OE2	1:B:424:VAL:HG12	2.18	0.42
1:B:465:ASN:O	1:B:468:LYS:HG2	2.19	0.42
1:D:335:VAL:HG11	1:D:435:GLU:HG2	2.02	0.42
1:D:302:LYS:HA	1:D:308:ASN:OD1	2.19	0.42
1:B:233:MET:O	1:B:237:ARG:HD3	2.19	0.42
1:D:323:MET:HE3	1:D:323:MET:HB2	1.87	0.42
1:A:412:PRO:HG2	1:A:483:MET:SD	2.60	0.42
1:D:301:LEU:HD11	1:D:364:VAL:HG21	2.03	0.41
1:C:294:GLU:HG2	1:C:298:MET:HE2	2.02	0.41
1:A:343:ALA:HB3	1:A:504:LYS:HE2	2.02	0.41
1:C:343:ALA:HB3	1:C:504:LYS:HE2	2.02	0.41
1:B:343:ALA:HB3	1:B:504:LYS:HE2	2.02	0.41
1:B:414:VAL:HG22	1:B:420:TYR:CD2	2.56	0.41
1:D:233:MET:HE3	1:D:288:LYS:HD3	2.02	0.40
1:C:308:ASN:HB3	1:C:324:GLU:HB3	2.04	0.40
1:D:447:ASN:CG	1:D:450:ARG:HB2	2.47	0.40
1:D:441:PRO:HA	1:D:442:PRO:HD3	1.92	0.40
1:B:408:TYR:CD1	1:B:441:PRO:HB3	2.56	0.40
1:B:460:THR:HA	1:B:463:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	307/323 (95%)	297 (97%)	10 (3%)	0	100	100
1	B	290/323 (90%)	279 (96%)	11 (4%)	0	100	100
1	C	307/323 (95%)	295 (96%)	12 (4%)	0	100	100
1	D	290/323 (90%)	281 (97%)	9 (3%)	0	100	100
All	All	1194/1292 (92%)	1152 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	258/282 (92%)	250 (97%)	8 (3%)	35	37
1	B	253/282 (90%)	245 (97%)	8 (3%)	34	35
1	C	259/282 (92%)	254 (98%)	5 (2%)	50	56
1	D	251/282 (89%)	244 (97%)	7 (3%)	38	41
All	All	1021/1128 (90%)	993 (97%)	28 (3%)	39	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ILE
1	A	267	THR
1	A	290	LEU
1	A	294	GLU
1	A	392	GLN
1	A	482	GLU
1	A	500	LEU
1	A	508	SER
1	B	232	ILE
1	B	237	ARG

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Mol	Chain	Res	Type
1	B	239	ILE
1	B	437	VAL
1	B	443	TYR
1	B	446	GLU
1	B	447	ASN
1	B	453	TYR
1	C	240	VAL
1	C	265	THR
1	C	314	LEU
1	C	324	GLU
1	C	392	GLN
1	D	262	THR
1	D	396	GLU
1	D	429	LEU
1	D	447	ASN
1	D	457	THR
1	D	460	THR
1	D	482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	305	ASN
1	A	392	GLN
1	A	458	ASN
1	B	305	ASN
1	B	354	GLN
1	B	465	ASN
1	C	279	GLN
1	C	305	ASN
1	C	354	GLN
1	D	293	ASN
1	D	305	ASN
1	D	354	GLN
1	D	362	ASN
1	D	445	ASN
1	D	447	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 10 ligands modelled in this entry, 8 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	C	601	3	32,33,33	1.31	4 (12%)	44,52,52	1.03	3 (6%)
2	ANP	A	601	3	32,33,33	1.22	4 (12%)	44,52,52	1.18	3 (6%)

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	C	601	3	-	3/18/38/38	0/3/3/3
2	ANP	A	601	3	-	4/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ANP	PB-O1B	4.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ANP	PG-O1G	3.90	1.52	1.46
2	A	601	ANP	PB-O1B	3.74	1.52	1.46
2	A	601	ANP	PG-O1G	3.40	1.51	1.46
2	A	601	ANP	PG-O3G	-2.66	1.49	1.56
2	C	601	ANP	PB-O3A	2.36	1.62	1.59
2	A	601	ANP	PB-O2B	-2.14	1.51	1.56
2	C	601	ANP	PG-O3G	-2.08	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ANP	O2B-PB-O1B	4.95	120.31	109.92
2	C	601	ANP	O2B-PB-O1B	4.41	119.17	109.92
2	C	601	ANP	O3G-PG-O1G	-2.40	107.43	113.45
2	A	601	ANP	O1B-PB-N3B	-2.38	108.27	111.77
2	A	601	ANP	O3G-PG-O1G	-2.32	107.62	113.45
2	C	601	ANP	O1G-PG-N3B	2.03	114.76	111.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

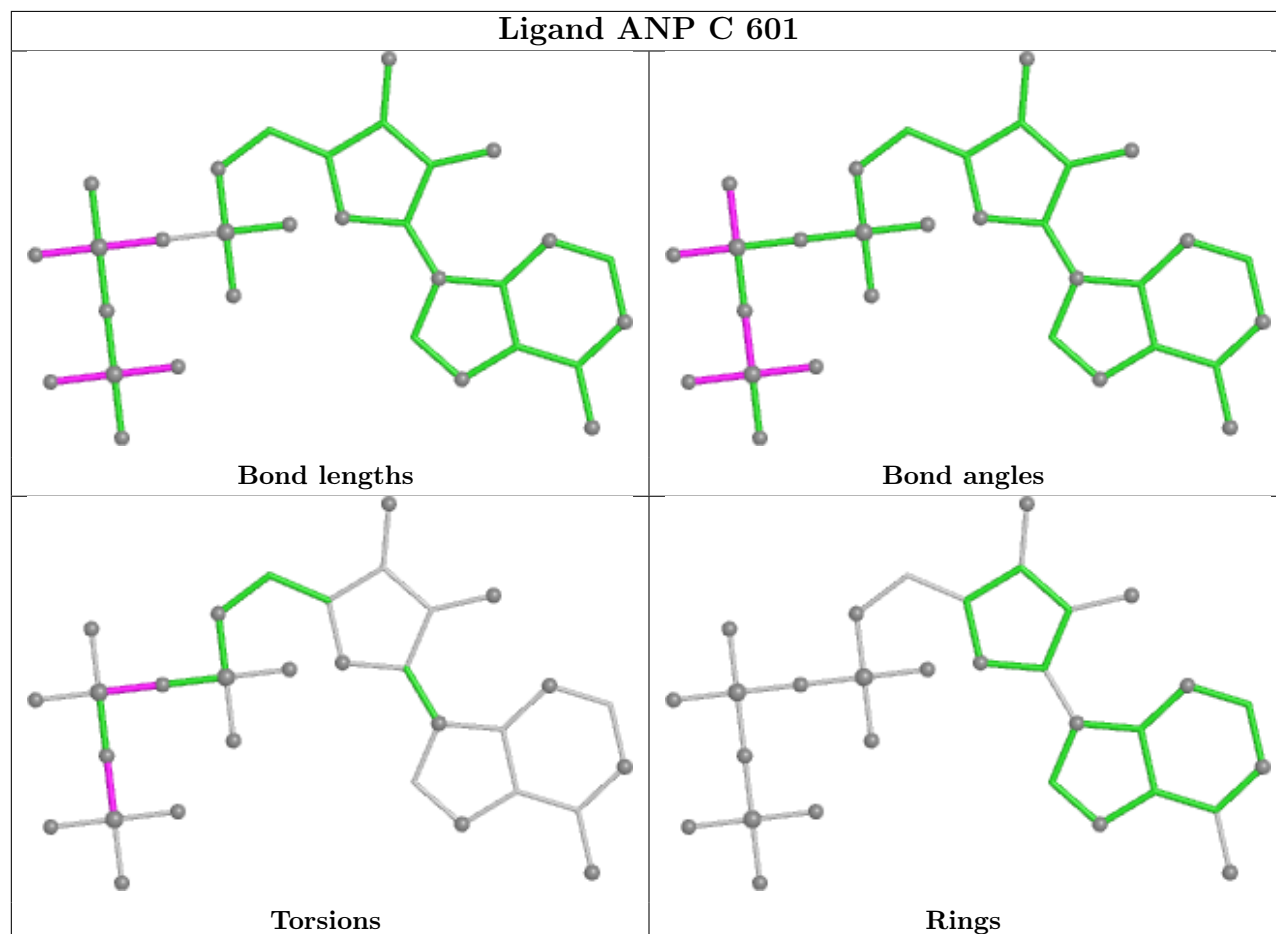
Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
2	C	601	ANP	PB-N3B-PG-O1G
2	C	601	ANP	PA-O3A-PB-O1B
2	C	601	ANP	PA-O3A-PB-O2B

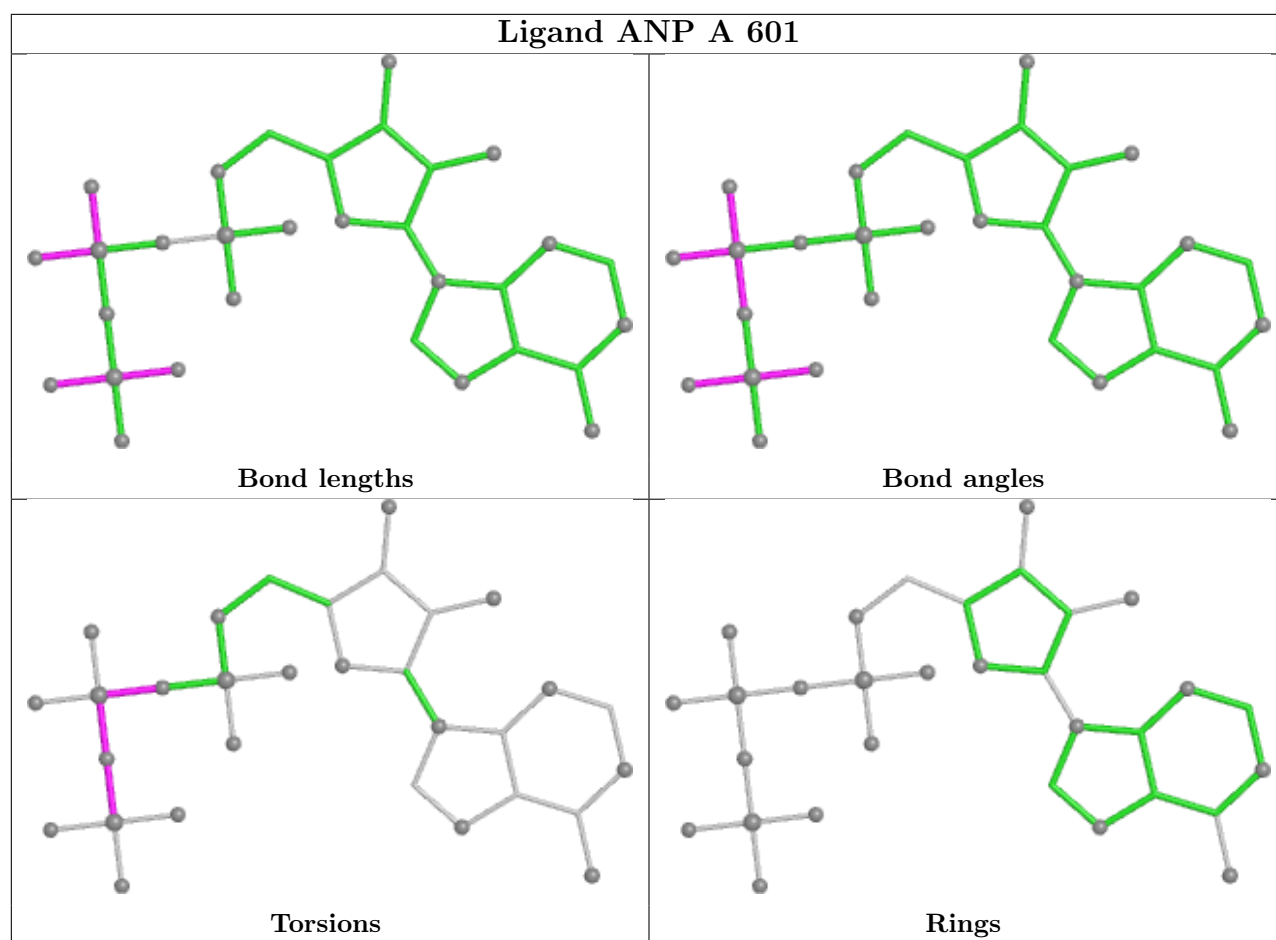
There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	309/323 (95%)	-1.19	0 100 100	27, 43, 89, 133	0
1	B	292/323 (90%)	-1.11	0 100 100	25, 45, 107, 123	0
1	C	309/323 (95%)	-1.27	0 100 100	25, 39, 86, 117	0
1	D	292/323 (90%)	-1.13	0 100 100	26, 46, 106, 143	0
All	All	1202/1292 (93%)	-1.18	0 100 100	25, 43, 99, 143	0

There are no RSRZ outliers to report.

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.

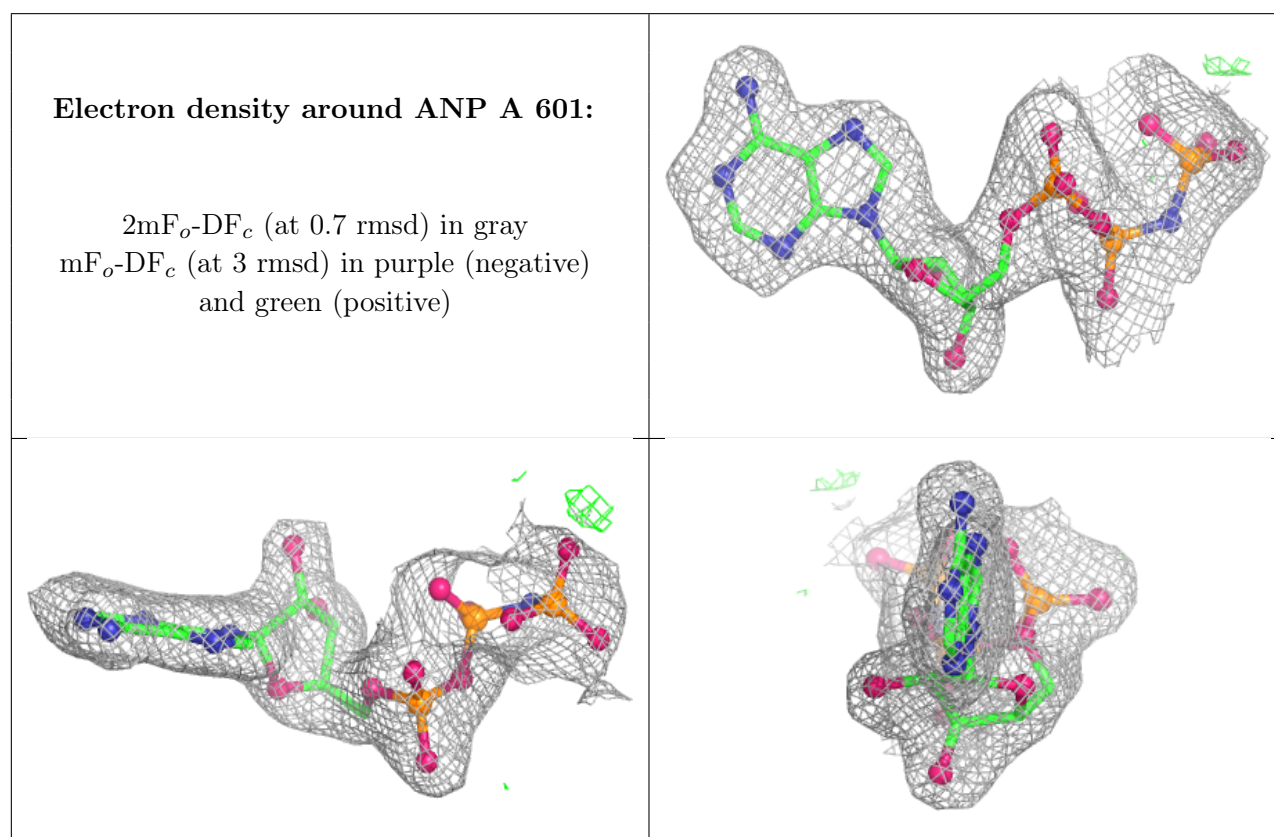
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ANP	A	601	31/31	0.99	0.03	33,47,56,64	0
2	ANP	C	601	31/31	0.99	0.03	31,41,54,62	0
3	MG	A	602	1/1	0.99	0.04	49,49,49,49	0
3	MG	C	602	1/1	0.99	0.05	46,46,46,46	0

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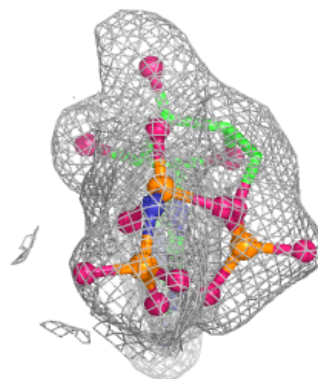
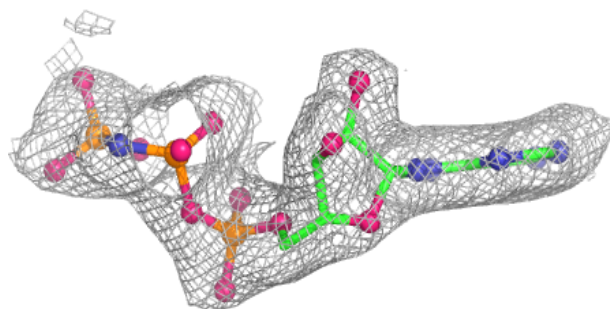
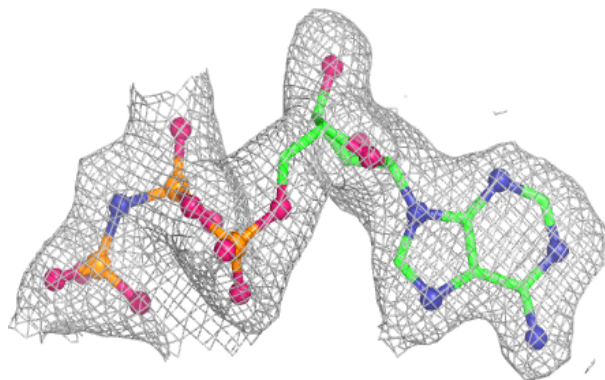
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	603	1/1	0.99	0.04	58,58,58,58	0
4	CL	B	602	1/1	0.99	0.04	53,53,53,53	0
4	CL	C	603	1/1	0.99	0.04	53,53,53,53	0
4	CL	D	602	1/1	0.99	0.04	51,51,51,51	0
3	MG	B	601	1/1	1.00	0.01	37,37,37,37	0
3	MG	D	601	1/1	1.00	0.01	32,32,32,32	0

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.



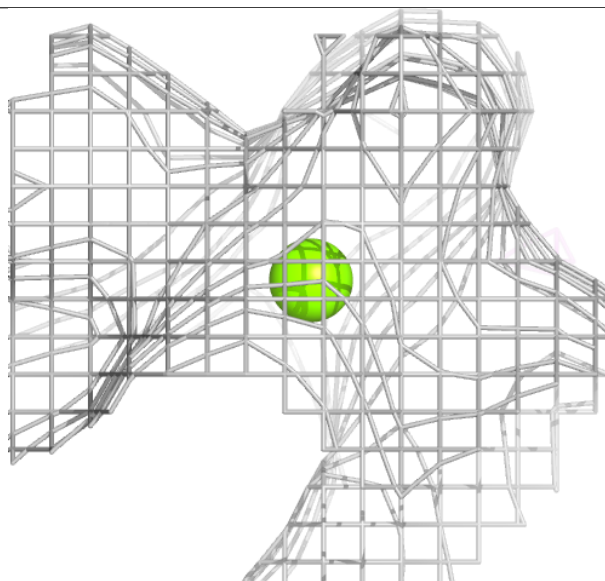
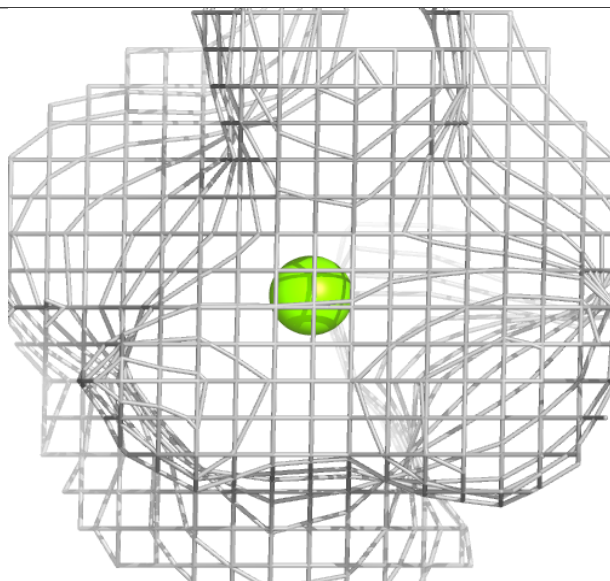
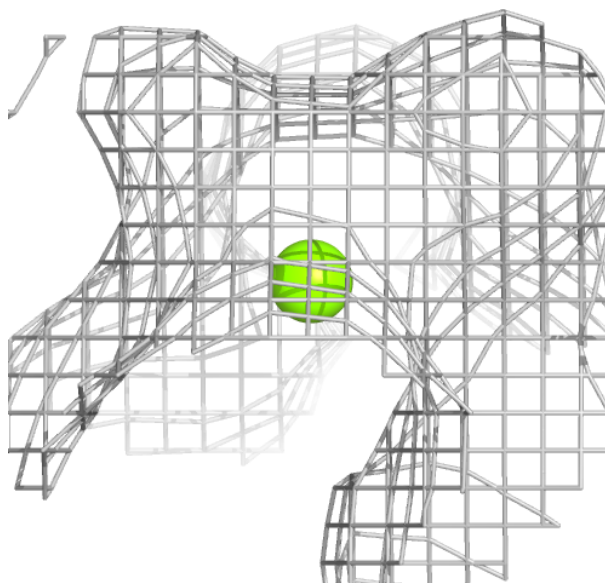
Electron density around ANP C 601:

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



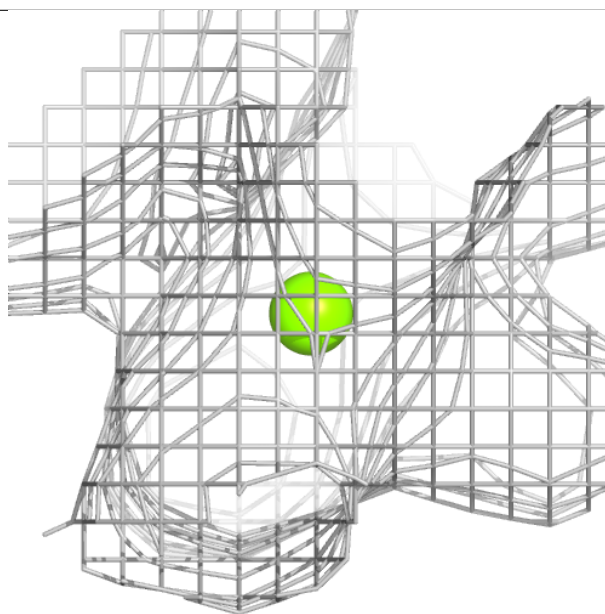
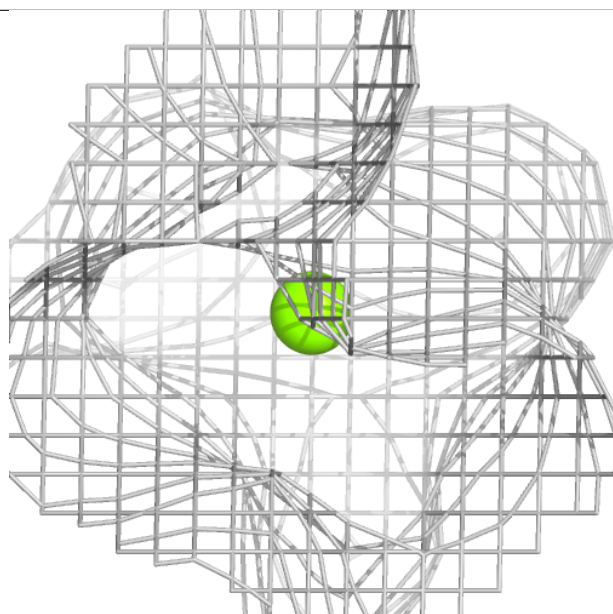
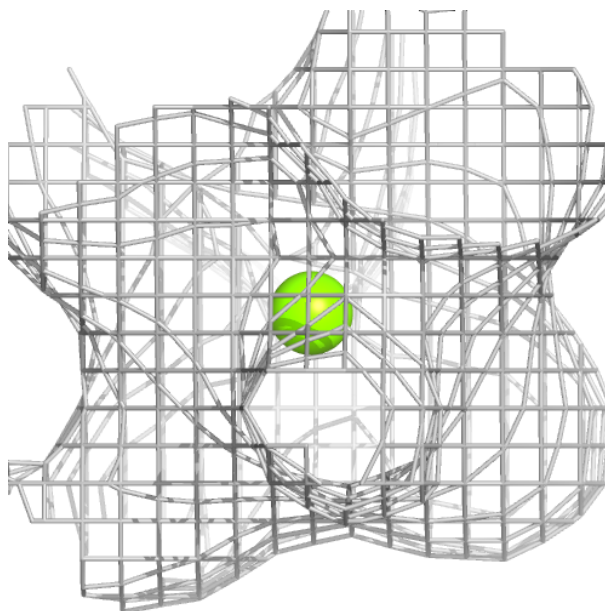
Electron density around MG A 602:

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



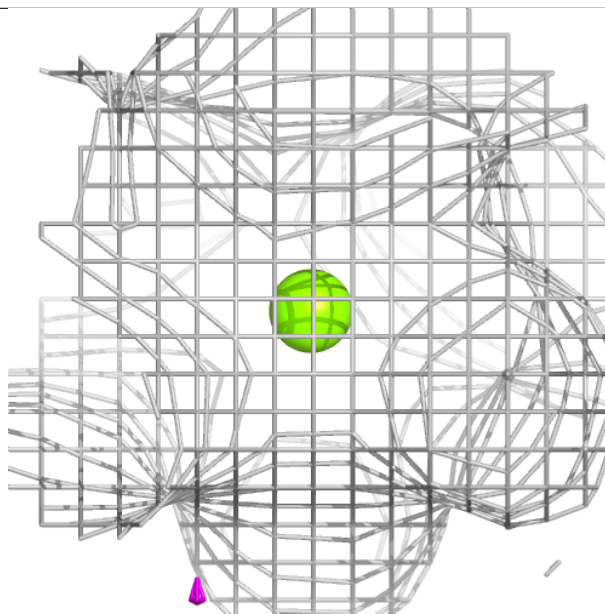
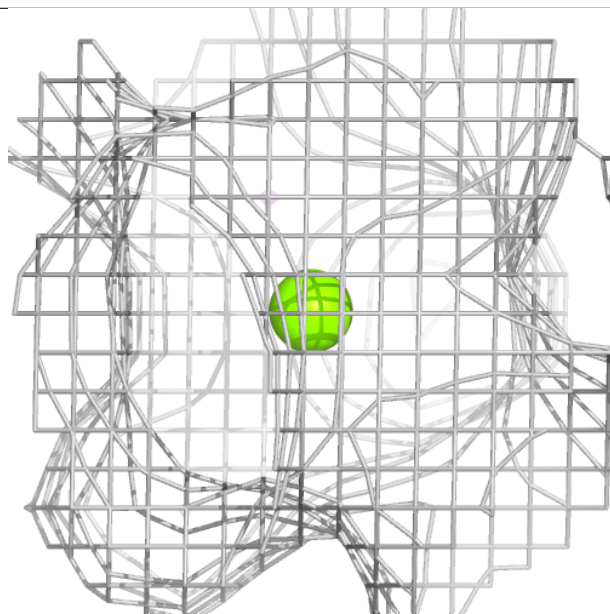
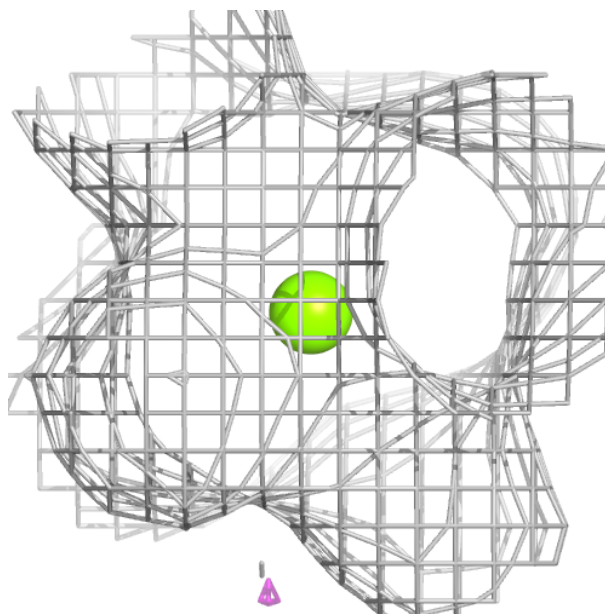
Electron density around MG C 602:

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and green (positive)



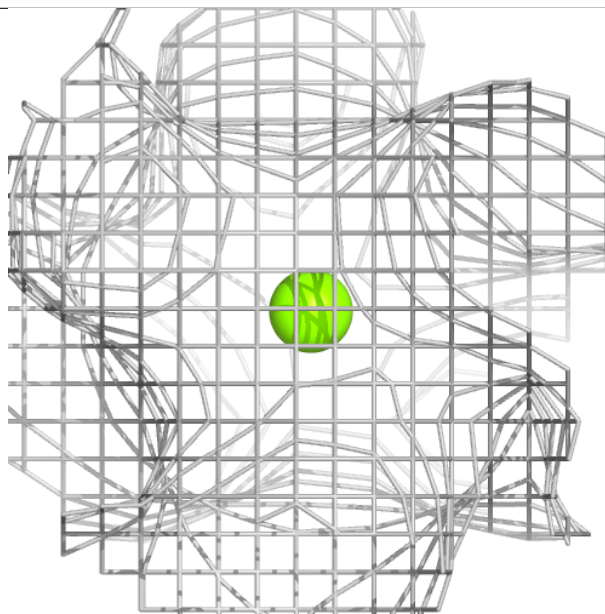
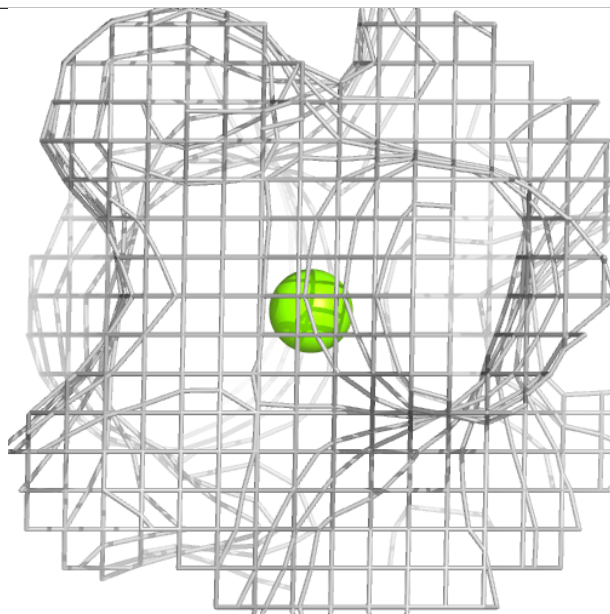
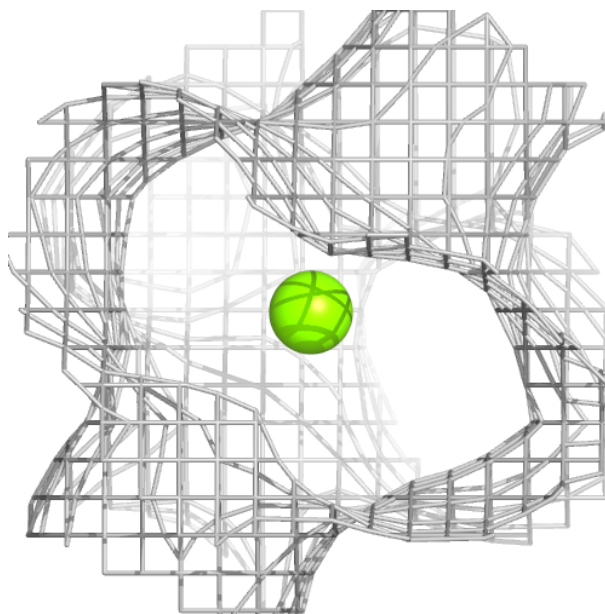
Electron density around MG B 601:

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



Electron density around MG D 601:

$2mF_o-DF_c$ (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.