



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:47 AM BST

PDB ID : 6J9Q
Title : Crystal structure of Trypanosoma brucei gambiense glycerol kinase complex with AMP-PNP.
Authors : Balogun, E.O.; Chishima, T.; Ichinose, M.; Inaoka, D.K.; Kido, Y.; Ibrahim, B.; de Koning, H.; McKerrow, J.H.; Watanabe, Y.; Nozaki, T.; Michels, P.A.M.; Harada, S.; Kita, K.; Shiba, T.
Deposited on : 2019-01-24
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

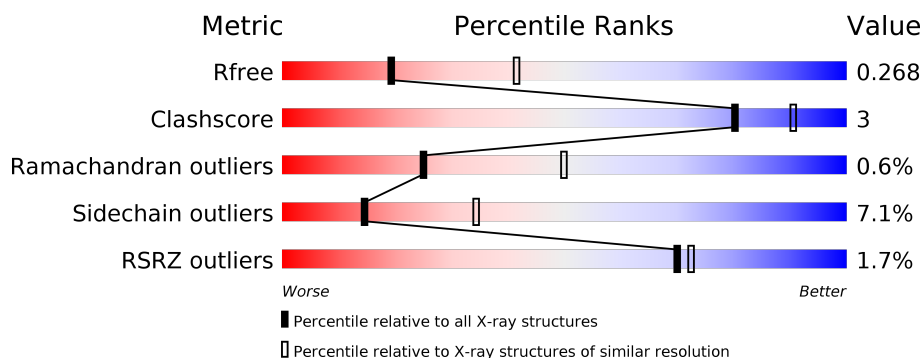
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	518	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	518	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	518	<div> <div></div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	D	518	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16007 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	B	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	C	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	D	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			

There are 24 discrepancies between the modelled and reference sequences:

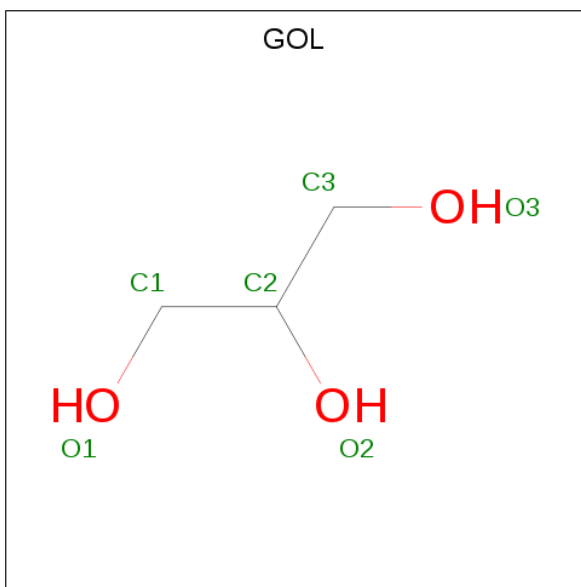
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-5	GLY	-	expression tag	UNP D3KVM3
C	-4	ILE	-	expression tag	UNP D3KVM3
C	-3	ASP	-	expression tag	UNP D3KVM3
C	-2	PRO	-	expression tag	UNP D3KVM3
C	-1	PHE	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-5	GLY	-	expression tag	UNP D3KVM3
D	-4	ILE	-	expression tag	UNP D3KVM3
D	-3	ASP	-	expression tag	UNP D3KVM3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

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

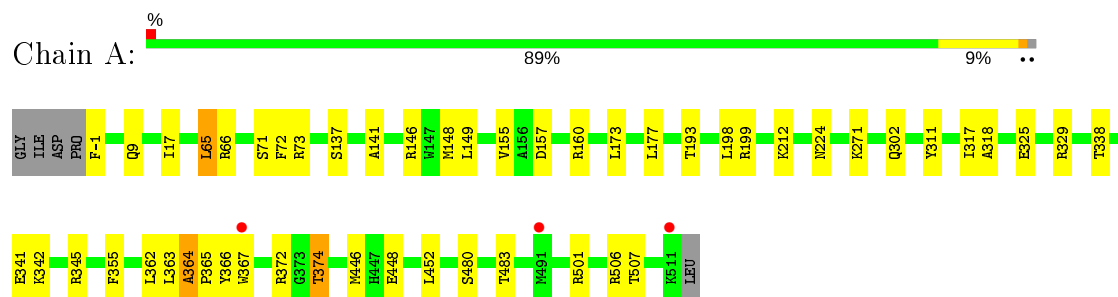
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	3	Total O 3 3	0	0
4	C	5	Total O 5 5	0	0
4	D	3	Total O 3 3	0	0

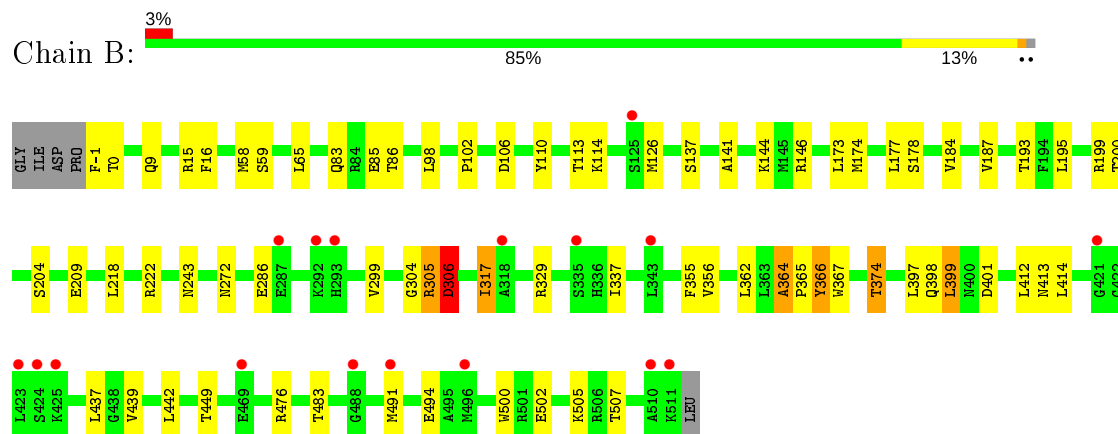
3 Residue-property plots [i](#)

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.

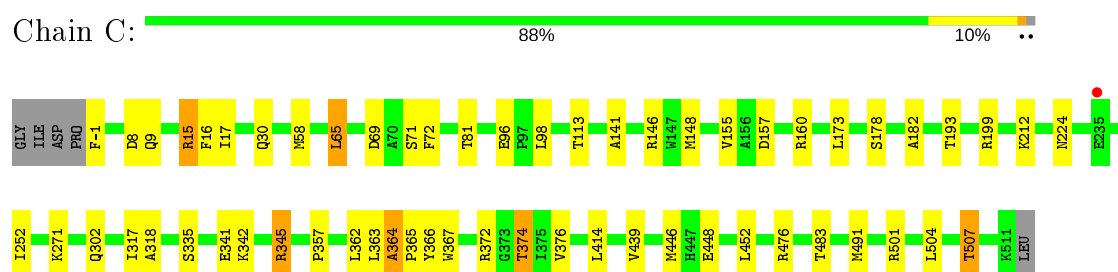
- Molecule 1: Glycerol kinase



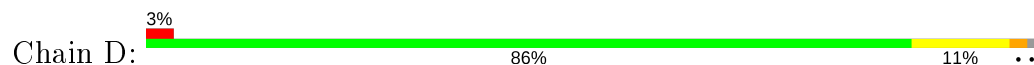
- Molecule 1: Glycerol kinase

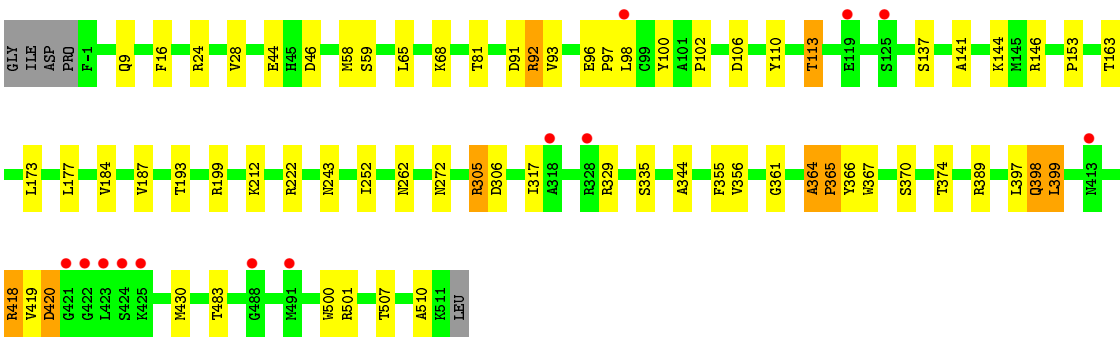


- Molecule 1: Glycerol kinase



- Molecule 1: Glycerol kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.60 Å 123.15 Å 154.22 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.70 19.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.88-2.70) 99.8 (19.88-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.71 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.191 , 0.269 0.196 , 0.268	Depositor DCC
R_{free} test set	3237 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16007	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.48	0/4039	0.73	1/5465 (0.0%)
1	B	0.47	0/4039	0.72	0/5465
1	C	0.48	0/4039	0.73	0/5465
1	D	0.47	0/4039	0.73	1/5465 (0.0%)
All	All	0.48	0/16156	0.73	2/21860 (0.0%)

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	506	ARG	NE-CZ-NH1	5.29	122.94	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	ASP	Peptide
1	D	306	ASP	Peptide

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	3957	0	3970	16	0
1	B	3957	0	3968	22	0
1	C	3957	0	3970	24	0
1	D	3957	0	3968	26	0
2	A	6	0	8	0	0
2	B	12	0	16	1	0
2	C	6	0	8	0	0
2	D	12	0	16	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
3	C	31	0	13	0	0
3	D	31	0	13	1	0
4	A	8	0	0	0	0
4	B	3	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
All	All	16007	0	15976	87	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 (87) 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:272:ASN:HD21	1:B:317:ILE:HD11	1.36	0.90
1:C:224:ASN:HD22	1:C:302:GLN:H	1.41	0.66
1:C:318:ALA:HB2	1:C:363:LEU:HD11	1.78	0.65
1:C:374:THR:HG21	1:C:507:THR:HA	1.77	0.65
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.28	0.63
1:A:364:ALA:HB1	1:A:365:PRO:CD	2.29	0.62
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.28	0.62
1:A:224:ASN:HD22	1:A:302:GLN:H	1.46	0.61
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.35	0.61
1:A:374:THR:HG21	1:A:507:THR:HA	1.83	0.58
1:C:446:MET:CE	1:C:452:LEU:HD22	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ALA:O	1:A:367:TRP:CZ3	2.58	0.57
1:C:372:ARG:O	1:C:374:THR:HG22	2.04	0.57
1:B:414:LEU:HD23	1:B:439:VAL:HG21	1.85	0.56
1:C:318:ALA:HB2	1:C:363:LEU:CD1	2.37	0.54
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.37	0.54
1:B:374:THR:OG1	1:B:507:THR:HG22	2.08	0.54
1:D:374:THR:OG1	1:D:507:THR:HG22	2.08	0.53
1:C:376:VAL:HA	1:D:374:THR:HG22	1.92	0.52
1:A:198:LEU:O	1:A:311:TYR:OH	2.23	0.52
1:D:419:VAL:HG21	1:D:430:MET:SD	2.50	0.52
1:A:141:ALA:HB3	1:A:193:THR:HA	1.92	0.52
1:C:17:ILE:HD13	1:C:448:GLU:HG2	1.92	0.52
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.45	0.51
1:A:318:ALA:HB2	1:A:363:LEU:HD11	1.91	0.51
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.93	0.51
1:D:370:SER:HA	1:D:510:ALA:HB3	1.93	0.51
1:D:356:VAL:HG11	1:D:507:THR:HG21	1.92	0.50
1:B:102:PRO:HB2	1:B:144:LYS:HD3	1.94	0.50
1:D:141:ALA:HB3	1:D:193:THR:HA	1.92	0.50
1:A:446:MET:CE	1:A:452:LEU:HD22	2.41	0.49
1:A:17:ILE:HD13	1:A:448:GLU:HG2	1.93	0.49
1:B:83:GLN:HA	2:B:601:GOL:H31	1.95	0.49
1:D:44:GLU:HG2	1:D:100:TYR:HB3	1.96	0.48
1:C:414:LEU:HD23	1:C:439:VAL:HG21	1.96	0.47
1:D:262:ASN:HB3	1:D:418:ARG:HG3	1.97	0.47
1:A:341:GLU:OE2	1:A:345:ARG:NH2	2.48	0.47
1:D:187:VAL:HG13	1:D:222:ARG:O	2.15	0.47
1:B:397:LEU:HD13	1:B:500:TRP:HB2	1.96	0.47
1:B:366:TYR:OH	1:B:401:ASP:OD1	2.32	0.47
1:B:304:GLY:O	1:B:306:ASP:N	2.48	0.47
1:B:141:ALA:HB3	1:B:193:THR:HA	1.96	0.46
1:D:96:GLU:HG3	1:D:97:PRO:HD2	1.98	0.46
1:B:110:TYR:O	1:B:113:THR:HG22	2.16	0.46
1:C:141:ALA:HB3	1:C:193:THR:HA	1.97	0.46
1:D:16:PHE:CD2	1:D:58:MET:HA	2.50	0.46
1:C:69:ASP:OD1	1:C:71:SER:OG	2.31	0.46
1:A:372:ARG:O	1:A:374:THR:HG22	2.16	0.45
1:D:317:ILE:HD11	1:D:399:LEU:HA	1.98	0.45
1:D:374:THR:HG21	1:D:507:THR:HA	1.99	0.45
1:C:364:ALA:CB	1:C:365:PRO:CD	2.94	0.45
1:B:364:ALA:CB	1:B:365:PRO:CD	2.94	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:SER:OG	1:C:182:ALA:HB3	2.17	0.44
1:D:102:PRO:HB2	1:D:144:LYS:HD3	1.98	0.44
1:A:318:ALA:HB2	1:A:363:LEU:CD1	2.47	0.44
1:D:397:LEU:HD13	1:D:500:TRP:HB2	2.00	0.44
1:B:187:VAL:HG13	1:B:222:ARG:O	2.18	0.44
1:D:364:ALA:CB	1:D:365:PRO:CD	2.95	0.44
1:A:364:ALA:CB	1:A:365:PRO:CD	2.95	0.43
1:C:81:THR:HA	1:C:252:ILE:O	2.18	0.43
1:A:149:LEU:HD23	1:A:155:VAL:HG12	2.00	0.43
1:C:16:PHE:CD2	1:C:58:MET:HA	2.53	0.43
1:C:341:GLU:OE2	1:C:345:ARG:NH2	2.51	0.43
1:B:502:GLU:OE2	1:B:505:LYS:NZ	2.49	0.43
1:D:272:ASN:HB3	1:D:419:VAL:HG12	2.00	0.43
1:D:81:THR:HA	1:D:252:ILE:O	2.18	0.43
1:A:148:MET:HB3	1:A:155:VAL:HG11	2.00	0.42
1:C:148:MET:HB3	1:C:155:VAL:HG11	2.00	0.42
1:D:344:ALA:O	1:D:389:ARG:NH1	2.51	0.42
1:D:24:ARG:NH1	3:D:602:ANP:O2G	2.52	0.42
1:B:-1:PHE:CE1	1:B:0:THR:HG22	2.54	0.42
1:C:8:ASP:HB3	1:C:15:ARG:HG2	2.02	0.41
1:C:362:LEU:HD21	1:C:504:LEU:HD22	2.02	0.41
1:B:85:GLU:O	1:B:86:THR:C	2.58	0.41
1:D:419:VAL:O	1:D:420:ASP:HB2	2.20	0.41
1:C:65:LEU:HD13	1:C:72:PHE:CD1	2.55	0.41
1:D:398:GLN:HB2	1:D:398:GLN:HE21	1.66	0.41
1:C:15:ARG:HD3	1:C:30:GLN:HE21	1.85	0.41
1:C:446:MET:HE1	1:C:452:LEU:HD22	2.02	0.41
1:D:110:TYR:O	1:D:113:THR:HG22	2.20	0.41
1:B:174:MET:O	1:B:178:SER:OG	2.30	0.41
1:D:92:ARG:HE	1:D:163:THR:HA	1.84	0.41
1:B:16:PHE:CD2	1:B:58:MET:HA	2.56	0.40
1:B:399:LEU:HD12	1:B:437:LEU:HD11	2.03	0.40
1:B:195:LEU:HD13	1:B:218:LEU:HD11	2.03	0.40
1:B:187:VAL:HG23	1:B:299:VAL:HG11	2.02	0.40
1:B:356:VAL:HG11	1:B:507:THR:HG21	2.04	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	511/518 (99%)	485 (95%)	25 (5%)	1 (0%)	47	73
1	B	511/518 (99%)	476 (93%)	31 (6%)	4 (1%)	19	43
1	C	511/518 (99%)	491 (96%)	19 (4%)	1 (0%)	47	73
1	D	511/518 (99%)	479 (94%)	25 (5%)	7 (1%)	11	28
All	All	2044/2072 (99%)	1931 (94%)	100 (5%)	13 (1%)	25	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA
1	C	364	ALA
1	D	361	GLY
1	D	364	ALA
1	B	305	ARG
1	D	305	ARG
1	B	243	ASN
1	D	243	ASN
1	D	420	ASP
1	B	126	MET
1	D	153	PRO
1	D	365	PRO

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	421/425 (99%)	394 (94%)	27 (6%)	17	39
1	B	421/425 (99%)	384 (91%)	37 (9%)	10	23
1	C	421/425 (99%)	394 (94%)	27 (6%)	17	39
1	D	421/425 (99%)	392 (93%)	29 (7%)	15	35
All	All	1684/1700 (99%)	1564 (93%)	120 (7%)	14	34

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	PHE
1	A	9	GLN
1	A	65	LEU
1	A	66	ARG
1	A	71	SER
1	A	73	ARG
1	A	137	SER
1	A	146	ARG
1	A	157	ASP
1	A	160	ARG
1	A	173	LEU
1	A	177	LEU
1	A	199	ARG
1	A	212	LYS
1	A	271	LYS
1	A	317	ILE
1	A	325	GLU
1	A	329	ARG
1	A	338	THR
1	A	342	LYS
1	A	355	PHE
1	A	362	LEU
1	A	366	TYR
1	A	374	THR
1	A	480	SER
1	A	483	THR
1	A	501	ARG
1	B	9	GLN
1	B	15	ARG
1	B	59	SER
1	B	65	LEU
1	B	98	LEU
1	B	106	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	114	LYS
1	B	137	SER
1	B	146	ARG
1	B	173	LEU
1	B	177	LEU
1	B	184	VAL
1	B	199	ARG
1	B	200	THR
1	B	204	SER
1	B	209	GLU
1	B	286	GLU
1	B	305	ARG
1	B	306	ASP
1	B	317	ILE
1	B	329	ARG
1	B	337	ILE
1	B	355	PHE
1	B	362	LEU
1	B	366	TYR
1	B	367	TRP
1	B	374	THR
1	B	398	GLN
1	B	399	LEU
1	B	412	LEU
1	B	413	ASN
1	B	442	LEU
1	B	449	THR
1	B	476	ARG
1	B	483	THR
1	B	491	MET
1	B	494	GLU
1	C	-1	PHE
1	C	9	GLN
1	C	15	ARG
1	C	65	LEU
1	C	96	GLU
1	C	98	LEU
1	C	113	THR
1	C	146	ARG
1	C	157	ASP
1	C	160	ARG
1	C	173	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	199	ARG
1	C	212	LYS
1	C	271	LYS
1	C	317	ILE
1	C	335	SER
1	C	342	LYS
1	C	345	ARG
1	C	357	PRO
1	C	366	TYR
1	C	367	TRP
1	C	374	THR
1	C	476	ARG
1	C	483	THR
1	C	491	MET
1	C	501	ARG
1	C	507	THR
1	D	9	GLN
1	D	28	VAL
1	D	59	SER
1	D	65	LEU
1	D	68	LYS
1	D	91	ASP
1	D	92	ARG
1	D	93	VAL
1	D	98	LEU
1	D	106	ASP
1	D	113	THR
1	D	137	SER
1	D	146	ARG
1	D	173	LEU
1	D	177	LEU
1	D	184	VAL
1	D	199	ARG
1	D	212	LYS
1	D	305	ARG
1	D	329	ARG
1	D	335	SER
1	D	355	PHE
1	D	366	TYR
1	D	367	TRP
1	D	398	GLN
1	D	399	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	418	ARG
1	D	483	THR
1	D	501	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	30	GLN
1	A	224	ASN
1	A	272	ASN
1	A	302	GLN
1	A	413	ASN
1	B	23	GLN
1	B	272	ASN
1	B	293	HIS
1	B	413	ASN
1	C	23	GLN
1	C	29	HIS
1	C	30	GLN
1	C	224	ASN
1	C	272	ASN
1	C	302	GLN
1	C	413	ASN
1	D	23	GLN
1	D	36	HIS
1	D	224	ASN
1	D	293	HIS
1	D	398	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	602	-	5,5,5	0.45	0	5,5,5	0.60	0
2	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.70	0
3	ANP	A	602	-	29,33,33	1.98	7 (24%)	31,52,52	2.05	8 (25%)
3	ANP	D	602	-	29,33,33	1.83	8 (27%)	31,52,52	1.71	6 (19%)
2	GOL	C	601	-	5,5,5	0.40	0	5,5,5	0.89	0
2	GOL	A	601	-	5,5,5	0.41	0	5,5,5	0.55	0
2	GOL	D	601	-	5,5,5	0.28	0	5,5,5	0.41	0
3	ANP	C	602	-	29,33,33	2.04	7 (24%)	31,52,52	1.84	6 (19%)
3	ANP	B	603	-	29,33,33	1.84	6 (20%)	31,52,52	1.70	7 (22%)
2	GOL	D	603	-	5,5,5	0.50	0	5,5,5	0.26	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
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
3	ANP	A	602	-	-	2/14/38/38	0/3/3/3
3	ANP	D	602	-	-	7/14/38/38	0/3/3/3
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	3/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	602	-	-	4/14/38/38	0/3/3/3
3	ANP	B	603	-	-	0/14/38/38	0/3/3/3
2	GOL	D	603	-	-	4/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	ANP	PG-N3B	5.11	1.76	1.63
3	C	602	ANP	PB-N3B	5.05	1.76	1.63
3	A	602	ANP	PG-N3B	5.04	1.76	1.63
3	B	603	ANP	PG-N3B	5.01	1.76	1.63
3	A	602	ANP	PB-N3B	4.90	1.76	1.63
3	D	602	ANP	PG-N3B	4.62	1.75	1.63
3	B	603	ANP	PB-N3B	4.52	1.75	1.63
3	D	602	ANP	PB-N3B	4.40	1.74	1.63
3	C	602	ANP	PG-O1G	3.85	1.52	1.46
3	A	602	ANP	PB-O1B	3.61	1.51	1.46
3	A	602	ANP	PG-O1G	3.60	1.51	1.46
3	C	602	ANP	PB-O1B	3.42	1.51	1.46
3	B	603	ANP	PG-O1G	3.25	1.51	1.46
3	D	602	ANP	PG-O1G	3.22	1.51	1.46
3	B	603	ANP	PB-O1B	3.17	1.51	1.46
3	D	602	ANP	PB-O1B	3.04	1.51	1.46
3	C	602	ANP	C5-C4	2.91	1.48	1.40
3	A	602	ANP	C5-C4	2.74	1.48	1.40
3	D	602	ANP	C5-C4	2.50	1.47	1.40
3	B	603	ANP	C5-C4	2.42	1.47	1.40
3	D	602	ANP	PG-O3G	-2.32	1.50	1.56
3	C	602	ANP	C2-N3	2.26	1.35	1.32
3	D	602	ANP	PG-O2G	-2.21	1.50	1.56
3	C	602	ANP	PB-O3A	2.18	1.61	1.59
3	A	602	ANP	C2-N3	2.14	1.35	1.32
3	D	602	ANP	C2'-C1'	-2.06	1.50	1.53
3	A	602	ANP	PB-O2B	-2.04	1.51	1.56
3	B	603	ANP	PG-O3G	-2.02	1.51	1.56

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ANP	O1G-PG-N3B	-7.15	101.25	111.77
3	C	602	ANP	O1G-PG-N3B	-4.93	104.50	111.77
3	D	602	ANP	O1G-PG-N3B	-4.60	105.00	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ANP	N3-C2-N1	-4.22	122.08	128.68
3	C	602	ANP	O2B-PB-O1B	4.05	118.41	109.92
3	D	602	ANP	N3-C2-N1	-4.01	122.41	128.68
3	C	602	ANP	N3-C2-N1	-4.00	122.42	128.68
3	A	602	ANP	O2B-PB-O1B	3.82	117.93	109.92
3	A	602	ANP	N3-C2-N1	-3.82	122.71	128.68
3	B	603	ANP	O1G-PG-N3B	-3.77	106.22	111.77
3	D	602	ANP	O2B-PB-O1B	3.71	117.70	109.92
3	B	603	ANP	PA-O3A-PB	-3.70	119.60	132.62
3	C	602	ANP	C3'-C2'-C1'	3.54	106.30	100.98
3	D	602	ANP	PA-O3A-PB	-3.18	121.43	132.62
3	A	602	ANP	C3'-C2'-C1'	3.14	105.71	100.98
3	A	602	ANP	PA-O3A-PB	-2.83	122.63	132.62
3	B	603	ANP	O3G-PG-O2G	2.72	114.89	107.64
3	C	602	ANP	PA-O3A-PB	-2.64	123.32	132.62
3	B	603	ANP	O2B-PB-O1B	2.63	115.44	109.92
3	B	603	ANP	N6-C6-N1	2.58	123.93	118.57
3	A	602	ANP	C4-C5-N7	-2.35	106.95	109.40
3	D	602	ANP	N6-C6-N1	2.29	123.33	118.57
3	A	602	ANP	O3G-PG-O2G	2.28	113.71	107.64
3	C	602	ANP	C2-N1-C6	2.27	122.63	118.75
3	D	602	ANP	C2-N1-C6	2.22	122.55	118.75
3	B	603	ANP	C2-N1-C6	2.19	122.50	118.75
3	A	602	ANP	C2-N1-C6	2.06	122.27	118.75

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ANP	PG-N3B-PB-O1B
3	D	602	ANP	PB-N3B-PG-O1G
3	D	602	ANP	PG-N3B-PB-O1B
3	D	602	ANP	PA-O3A-PB-O1B
3	D	602	ANP	PA-O3A-PB-O2B
3	D	602	ANP	C5'-O5'-PA-O1A
2	C	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	D	601	GOL	C1-C2-C3-O3
3	C	602	ANP	PB-N3B-PG-O1G
3	C	602	ANP	PA-O3A-PB-O1B
3	C	602	ANP	PA-O3A-PB-O2B
3	C	602	ANP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

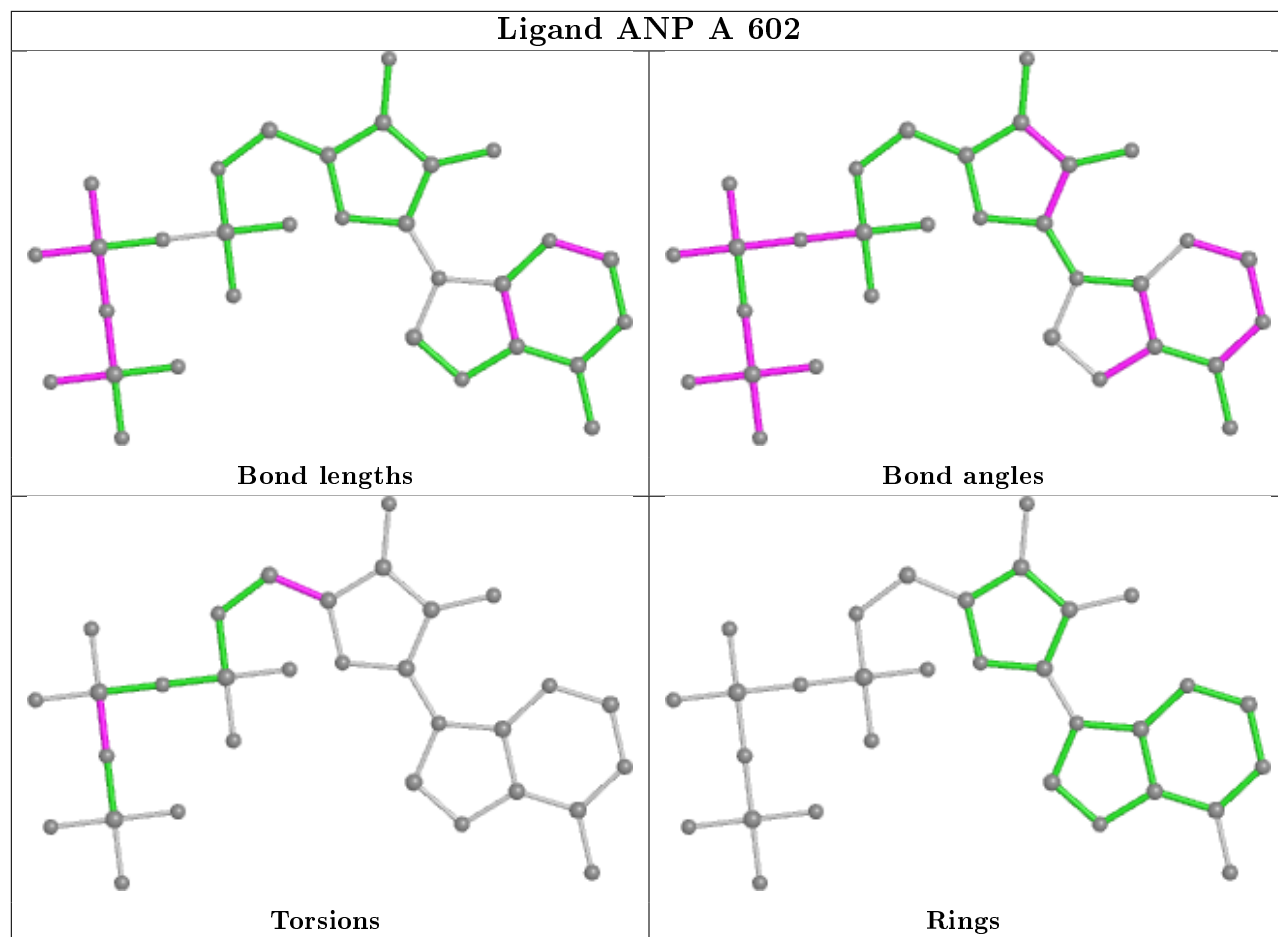
Mol	Chain	Res	Type	Atoms
2	D	603	GOL	C1-C2-C3-O3
2	D	603	GOL	O2-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-C3
2	D	603	GOL	O1-C1-C2-C3
2	C	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3
2	D	601	GOL	O2-C2-C3-O3
2	D	603	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
3	D	602	ANP	C5'-O5'-PA-O3A
3	D	602	ANP	C5'-O5'-PA-O2A
3	A	602	ANP	O4'-C4'-C5'-O5'

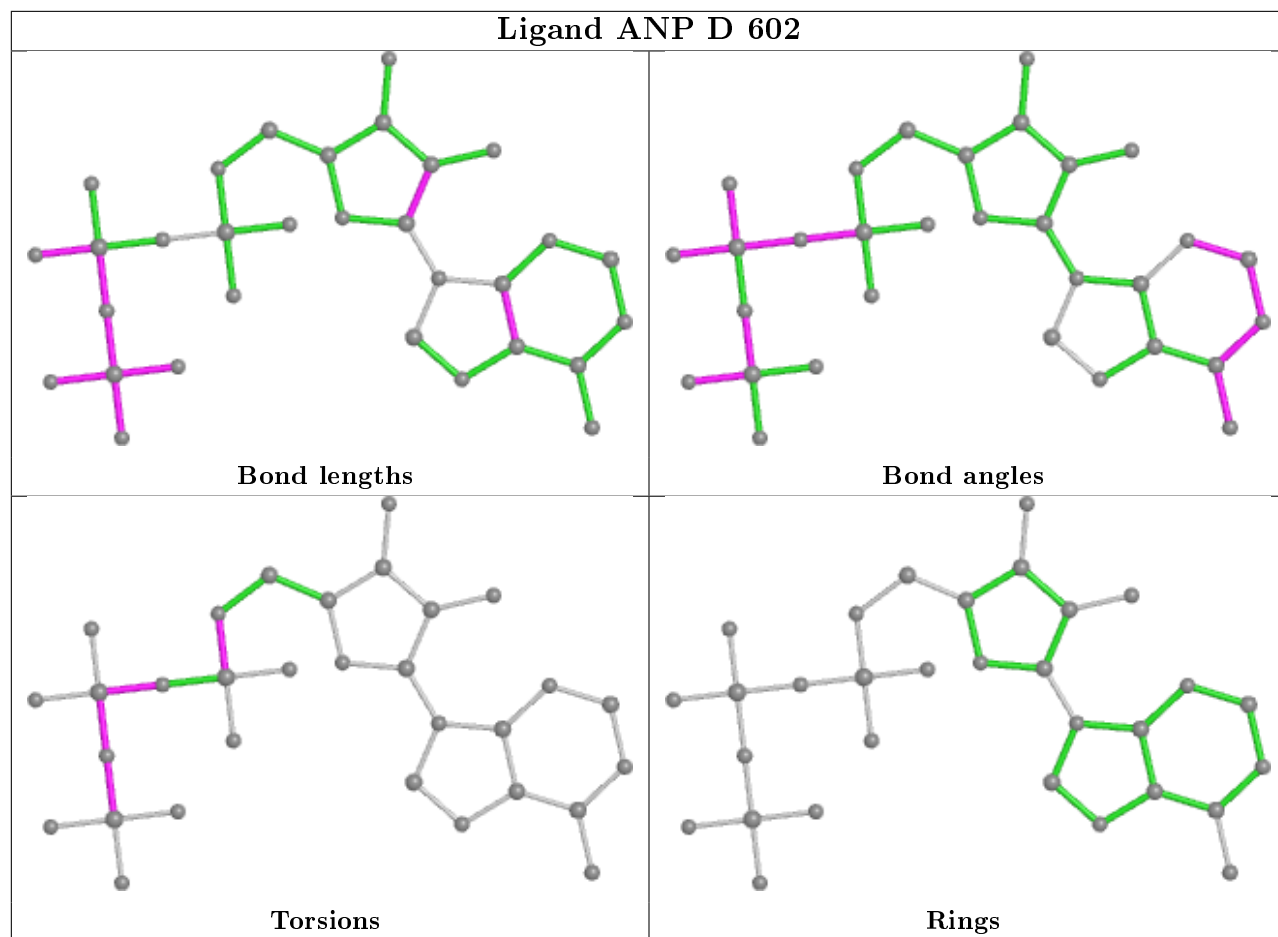
There are no ring outliers.

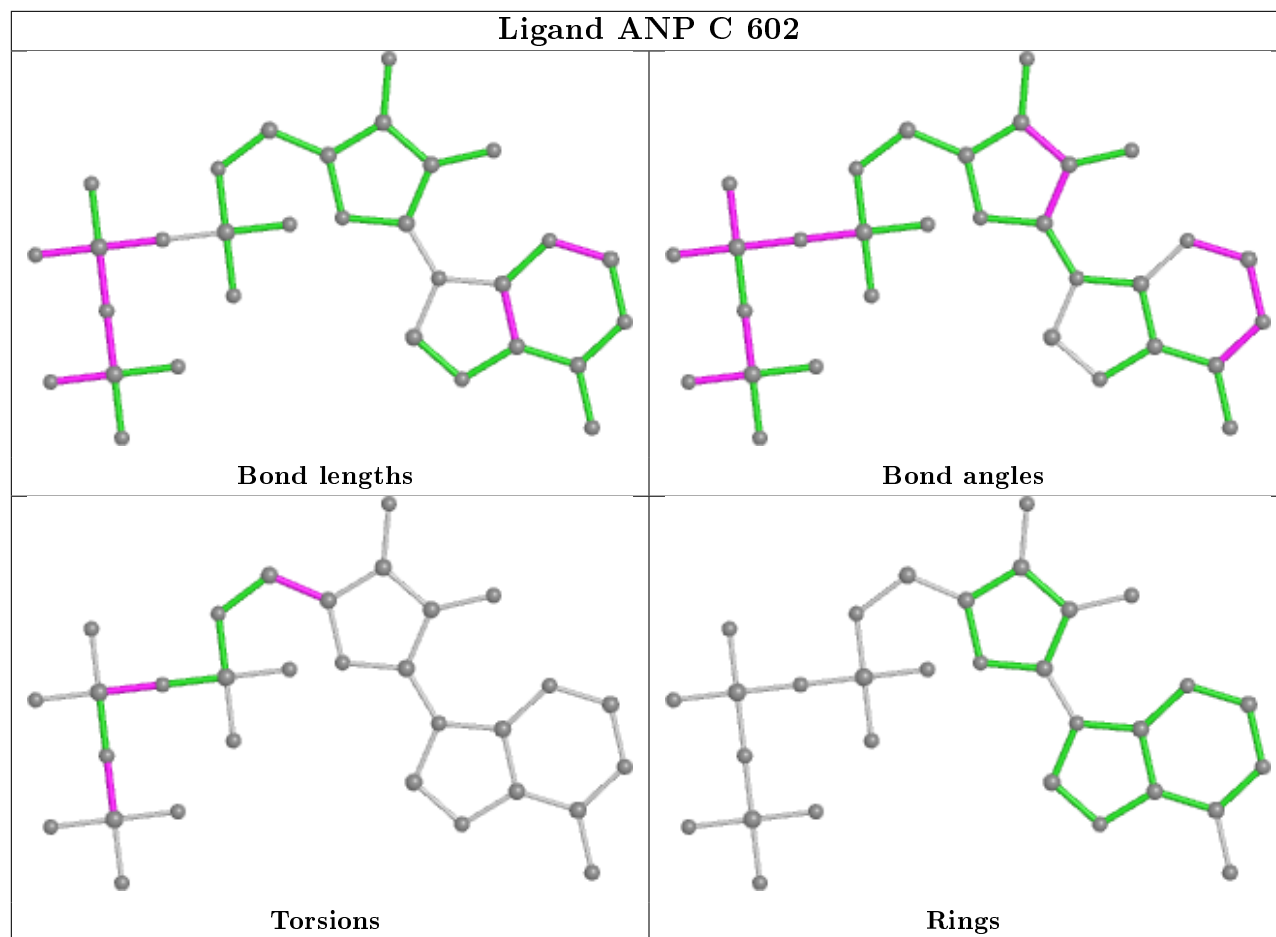
2 monomers are involved in 2 short contacts:

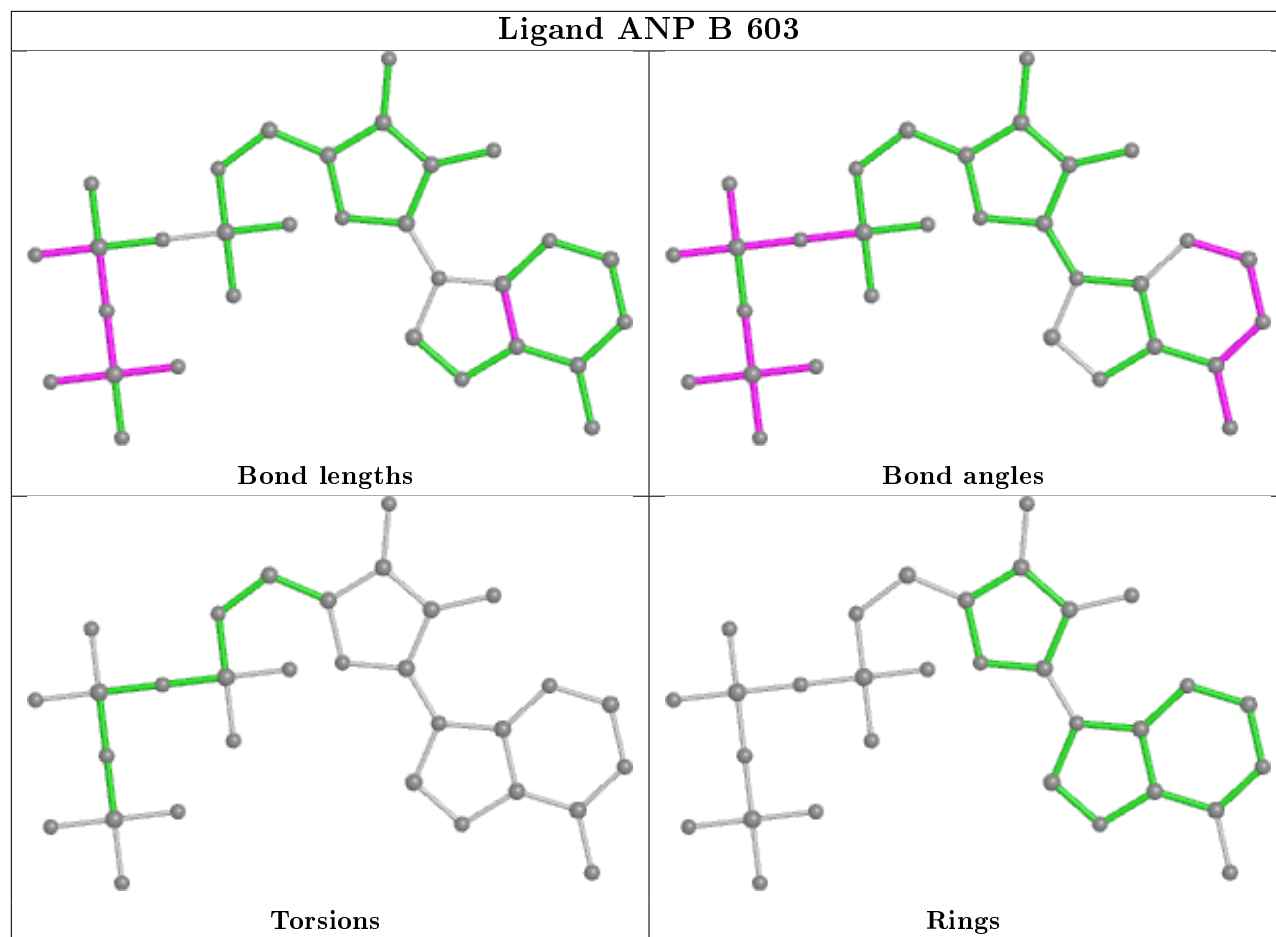
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	1	0
3	D	602	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	513/518 (99%)	-0.01	3 (0%) 89 91	42, 62, 87, 112	0
1	B	513/518 (99%)	0.26	17 (3%) 46 46	46, 75, 109, 162	0
1	C	513/518 (99%)	-0.03	1 (0%) 95 96	41, 62, 86, 127	0
1	D	513/518 (99%)	0.26	13 (2%) 57 59	44, 75, 109, 156	0
All	All	2052/2072 (99%)	0.12	34 (1%) 70 72	41, 68, 104, 162	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	GLY	7.2
1	B	491	MET	7.1
1	D	423	LEU	6.5
1	D	488	GLY	5.7
1	B	423	LEU	5.6
1	D	422	GLY	5.1
1	B	511	LYS	5.0
1	D	424	SER	4.8
1	B	421	GLY	4.5
1	B	425	LYS	4.4
1	D	491	MET	3.4
1	B	424	SER	3.2
1	D	425	LYS	3.1
1	B	335	SER	3.0
1	B	469	GLU	2.8
1	B	510	ALA	2.8
1	D	125	SER	2.7
1	D	413	ASN	2.7
1	D	328	ARG	2.6
1	A	511	LYS	2.5
1	A	367	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	292	LYS	2.4
1	D	119	GLU	2.3
1	D	98	LEU	2.2
1	C	235	GLU	2.2
1	B	125	SER	2.1
1	A	491	MET	2.1
1	B	496	MET	2.1
1	D	318	ALA	2.1
1	B	343	LEU	2.1
1	B	287	GLU	2.1
1	B	488	GLY	2.0
1	B	293	HIS	2.0
1	B	318	ALA	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](#)

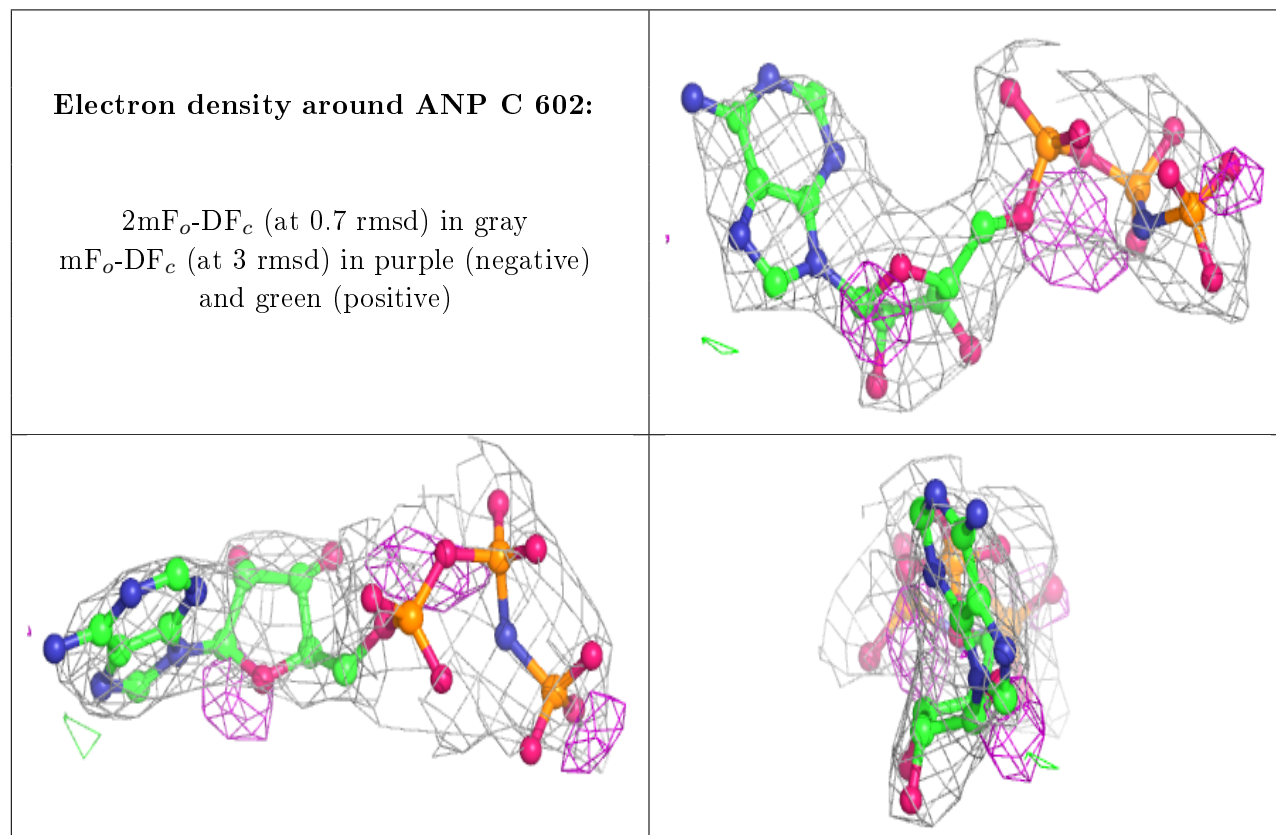
There are no monosaccharides in this entry.

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, 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.

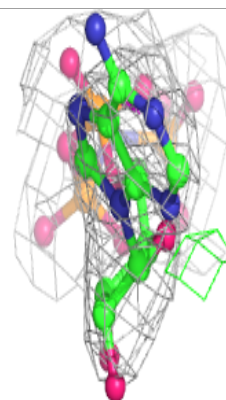
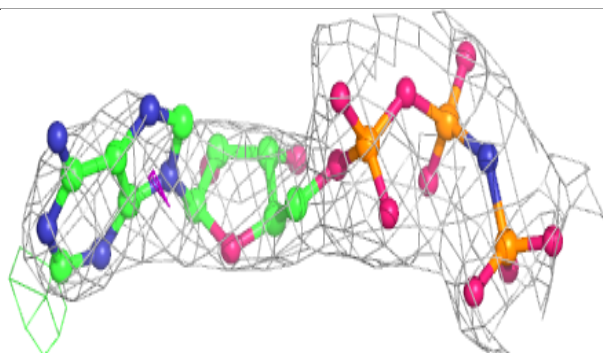
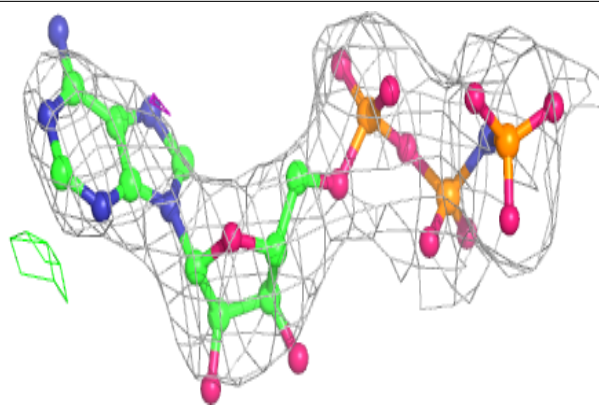
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	601	6/6	0.88	0.32	62,68,73,76	0
3	ANP	C	602	31/31	0.88	0.24	88,99,131,139	0
2	GOL	D	603	6/6	0.88	0.19	66,68,69,71	0
2	GOL	C	601	6/6	0.90	0.26	65,66,66,69	0
3	ANP	A	602	31/31	0.91	0.18	89,101,127,134	0
2	GOL	A	601	6/6	0.93	0.16	61,65,68,68	0
2	GOL	B	602	6/6	0.94	0.17	62,68,70,71	0
3	ANP	D	602	31/31	0.95	0.16	53,62,91,107	0
2	GOL	D	601	6/6	0.95	0.26	57,60,64,64	0
3	ANP	B	603	31/31	0.96	0.17	51,62,83,83	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.



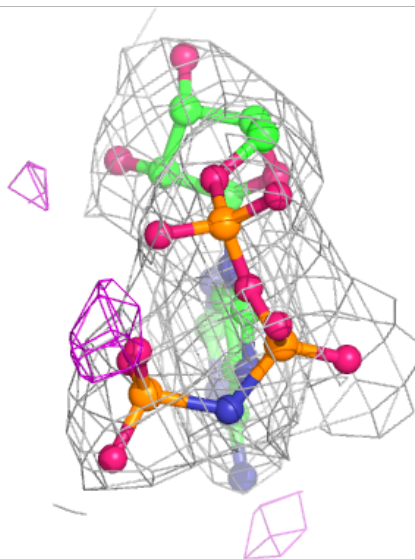
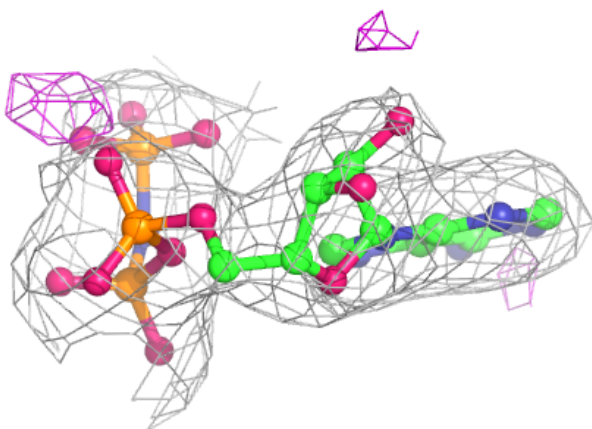
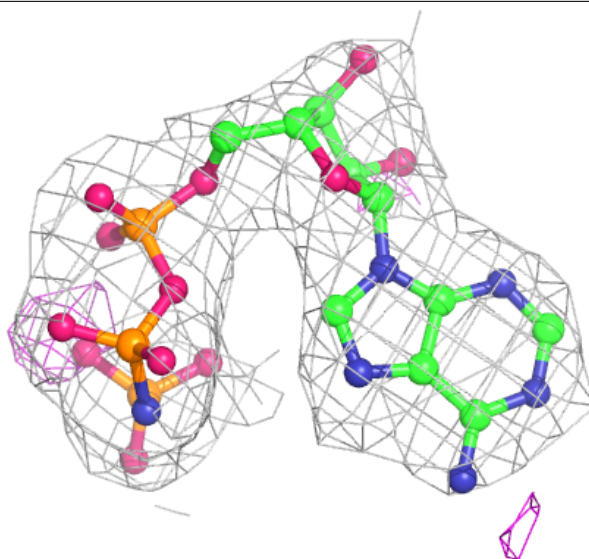
Electron density around ANP A 602:

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



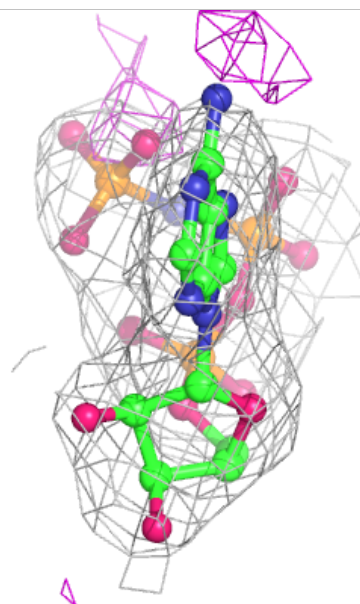
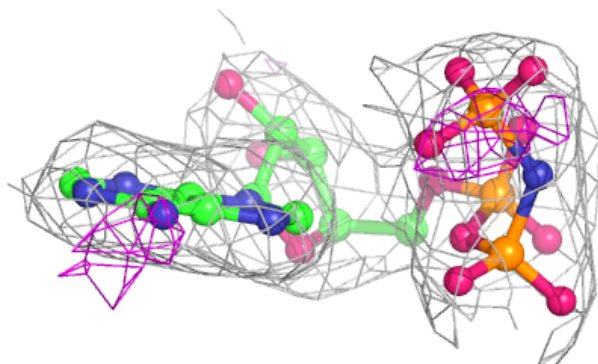
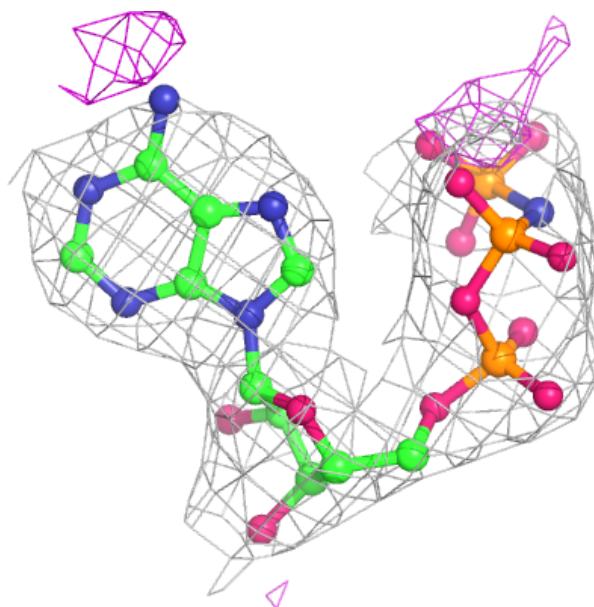
Electron density around ANP D 602:

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



Electron density around ANP B 603:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.