



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2CVU / pdb_00002cvu
Title : Structures of Yeast Ribonucleotide Reductase I
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.
Deposited on : 2005-06-14
Resolution : 2.90 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 : 2022.3.0, CSD as543be (2022)
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

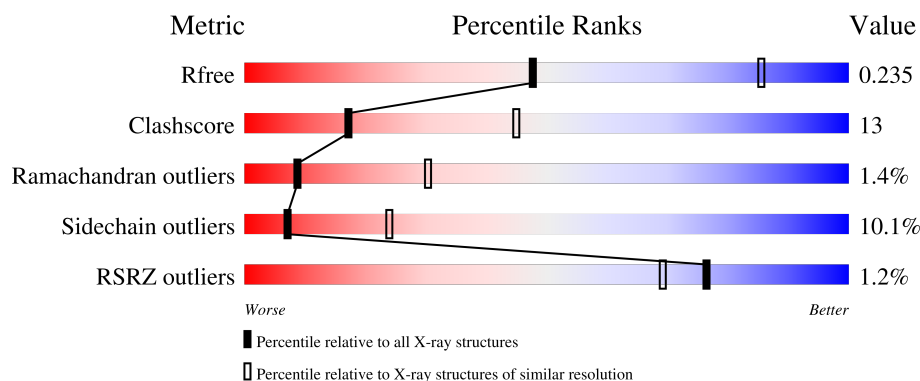
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	888	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5398 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.

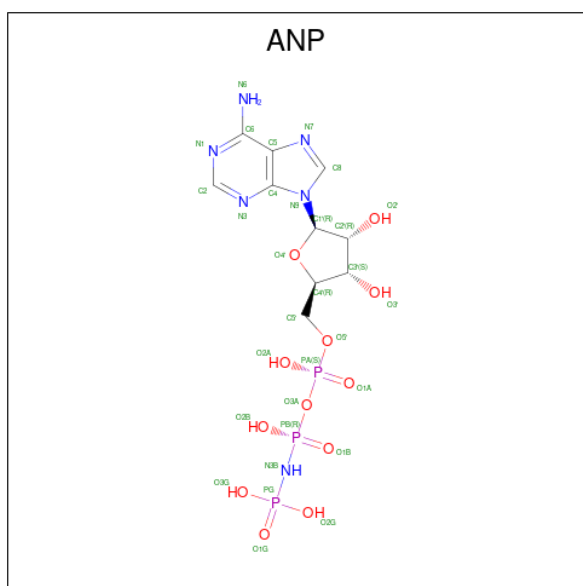
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5208	3317	883	977	31			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

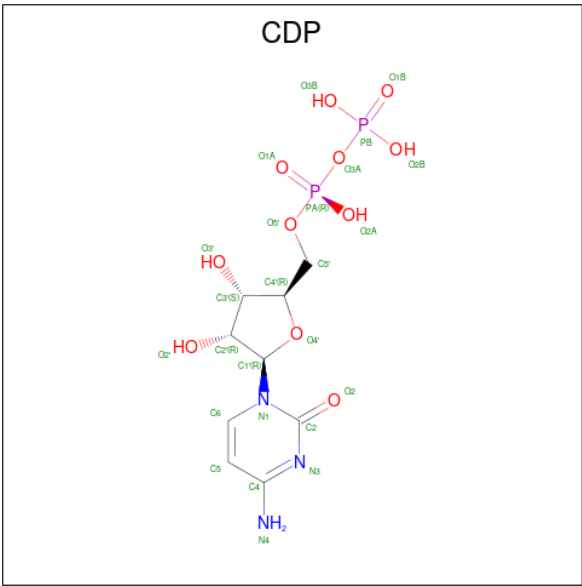
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is CYTIDINE-5'-DIPHOSPHATE (CCD ID: CDP) (formula: C₉H₁₅N₃O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

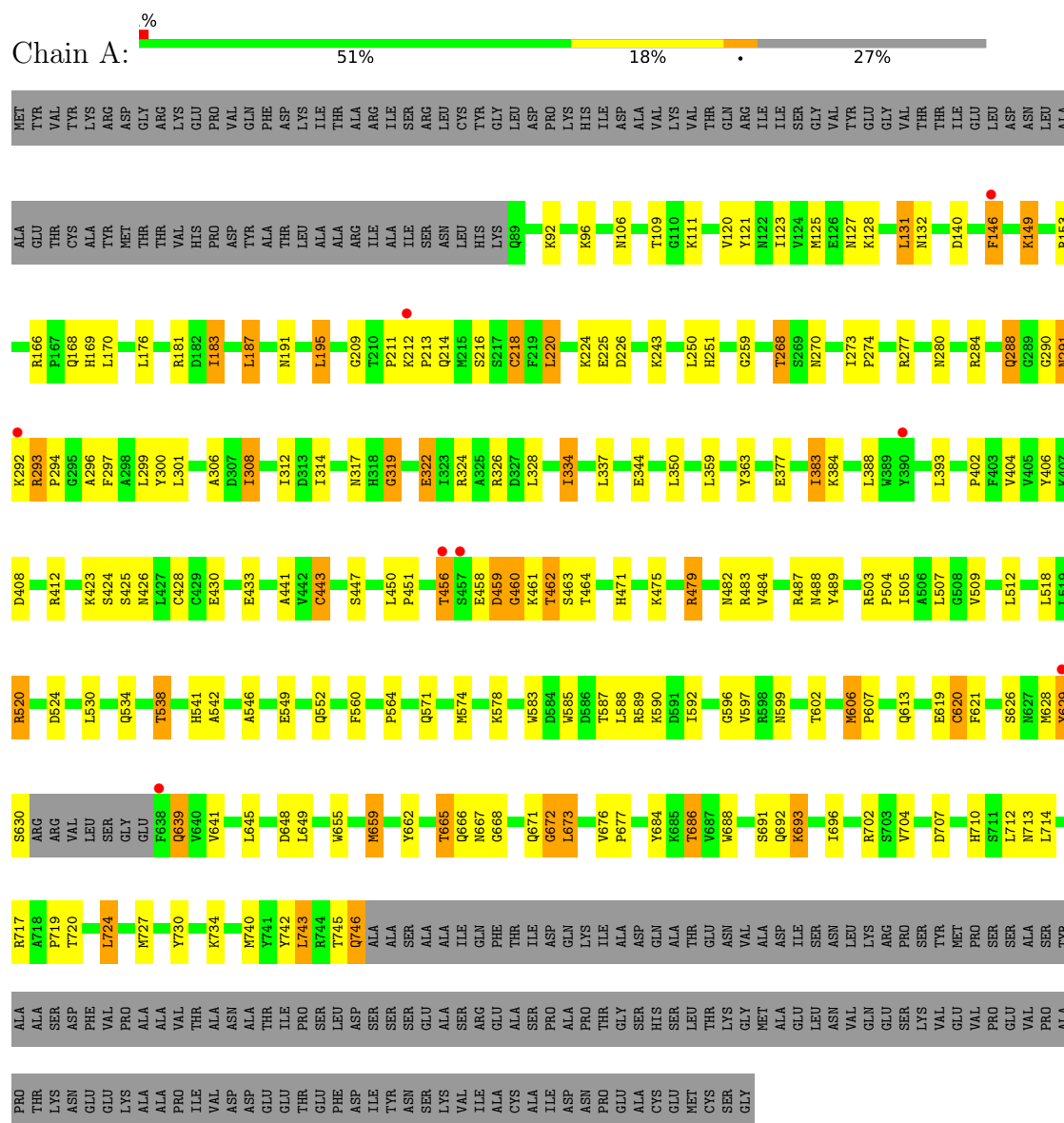
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total	O	0	0
			133	133		

3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large chain 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.76Å 117.51Å 64.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.90) 99.5 (50.00-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.177 , 0.236 0.178 , 0.235	Depositor DCC
R_{free} test set	2594 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5398	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: CDP, 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	0.80	0/5329	1.06	10/7214 (0.1%)

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	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	291	ASN	N-CA-C	12.35	126.27	108.86
1	A	334	ILE	N-CA-C	6.85	114.67	107.76
1	A	224	LYS	N-CA-C	5.42	117.94	111.71
1	A	727	MET	CB-CG-SD	5.40	128.91	112.70
1	A	589	ARG	N-CA-C	-5.35	105.45	111.28
1	A	456	THR	N-CA-C	-5.15	107.51	112.97
1	A	377	GLU	N-CA-C	5.11	119.27	113.19
1	A	308	ILE	N-CA-C	5.09	115.81	110.62
1	A	639	GLN	N-CA-C	5.08	121.61	110.80
1	A	406	TYR	N-CA-C	5.01	116.36	109.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	GLY	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	5208	0	5135	131	0
2	A	1	0	0	0	0
3	A	31	0	13	1	0
4	A	25	0	12	1	0
5	A	133	0	0	6	0
All	All	5398	0	5160	131	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 (131) 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:393:LEU:HD22	1:A:724:LEU:HD13	1.38	1.06
1:A:691:SER:HB2	1:A:693:LYS:HD2	1.63	0.81
1:A:665:THR:HG22	1:A:666:GLN:HE21	1.48	0.78
1:A:293:ARG:O	1:A:293:ARG:HG2	1.86	0.75
1:A:479:ARG:HH11	1:A:479:ARG:CG	2.01	0.73
1:A:483:ARG:HH22	1:A:487:ARG:HD2	1.54	0.72
1:A:288:GLN:O	1:A:291:ASN:ND2	2.23	0.71
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.05	0.71
1:A:665:THR:HG22	1:A:666:GLN:NE2	2.06	0.69
1:A:662:TYR:CZ	1:A:666:GLN:HG3	2.28	0.68
1:A:166:ARG:HB2	1:A:169:HIS:CE1	2.29	0.67
1:A:317:ASN:HB3	5:A:2074:HOH:O	1.95	0.66
1:A:665:THR:CG2	1:A:666:GLN:HE21	2.08	0.66
1:A:479:ARG:HH11	1:A:479:ARG:HG2	1.60	0.66
1:A:211:PRO:O	1:A:213:PRO:HD3	1.96	0.66
1:A:428:CYS:SG	4:A:1002:CDP:H3'	2.36	0.65
1:A:482:ASN:HD22	1:A:599:ASN:HD21	1.43	0.65
1:A:92:LYS:HG3	1:A:166:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG23	1:A:111:LYS:H	1.62	0.64
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.12	0.64
1:A:475:LYS:HD2	1:A:546:ALA:HB2	1.80	0.63
1:A:458:GLU:OE2	1:A:462:THR:HB	2.00	0.62
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.82	0.62
1:A:692:GLN:O	1:A:696:ILE:HG12	1.99	0.62
1:A:225:GLU:HG3	5:A:2124:HOH:O	1.99	0.61
1:A:740:MET:CE	1:A:743:LEU:HD23	2.32	0.59
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.83	0.59
1:A:659:MET:HE1	1:A:673:LEU:HD11	1.84	0.58
1:A:587:THR:O	1:A:590:LYS:HB3	2.04	0.58
1:A:251:HIS:HD2	5:A:2084:HOH:O	1.85	0.58
1:A:293:ARG:O	1:A:293:ARG:CG	2.52	0.58
1:A:671:GLN:O	1:A:672:GLY:C	2.47	0.58
1:A:123:ILE:HG12	1:A:181:ARG:HD3	1.87	0.57
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.86	0.57
1:A:746:GLN:HE21	1:A:746:GLN:CA	2.19	0.56
1:A:538:THR:HB	1:A:583:TRP:NE1	2.22	0.55
1:A:686:THR:HG23	1:A:688:TRP:H	1.71	0.55
1:A:120:VAL:HG21	1:A:209:GLY:HA2	1.89	0.54
1:A:226:ASP:O	3:A:1001:ANP:H5'2	2.08	0.54
1:A:628:MET:O	1:A:629:TYR:C	2.50	0.54
1:A:443:CYS:HA	5:A:2058:HOH:O	2.08	0.54
1:A:128:LYS:O	1:A:132:ASN:ND2	2.41	0.53
1:A:220:LEU:HB2	1:A:441:ALA:HB3	1.90	0.53
1:A:475:LYS:HG2	1:A:542:ALA:HB1	1.91	0.53
1:A:549:GLU:O	1:A:552:GLN:HB2	2.09	0.53
1:A:629:TYR:O	1:A:630:SER:HB3	2.08	0.53
1:A:213:PRO:HD2	1:A:489:TYR:HB3	1.92	0.52
1:A:319:GLY:HA3	1:A:324:ARG:HH12	1.73	0.52
1:A:447:SER:HB3	1:A:606:MET:HE3	1.90	0.52
1:A:588:LEU:O	1:A:592:ILE:HG13	2.09	0.52
1:A:713:ASN:ND2	1:A:742:TYR:H	2.07	0.52
1:A:745:THR:HG23	1:A:746:GLN:N	2.25	0.52
1:A:259:GLY:HA2	1:A:268:THR:HG23	1.92	0.51
1:A:746:GLN:NE2	1:A:746:GLN:HA	2.25	0.51
1:A:459:ASP:OD1	1:A:460:GLY:N	2.35	0.51
1:A:482:ASN:HD21	1:A:503:ARG:HH11	1.58	0.51
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.10	0.51
1:A:214:GLN:HE22	1:A:216:SER:H	1.57	0.51
1:A:740:MET:HE2	1:A:743:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:C	1:A:170:LEU:HD23	2.36	0.51
1:A:214:GLN:HE21	1:A:488:ASN:HD21	1.60	0.50
1:A:571:GLN:HE21	1:A:571:GLN:HA	1.77	0.50
1:A:717:ARG:O	1:A:719:PRO:HD3	2.12	0.49
1:A:746:GLN:HE21	1:A:746:GLN:HA	1.77	0.49
1:A:383:ILE:HD12	1:A:384:LYS:H	1.79	0.48
1:A:482:ASN:ND2	1:A:503:ARG:NH1	2.61	0.48
1:A:191:ASN:O	1:A:195:LEU:HB2	2.14	0.48
1:A:299:LEU:HD11	1:A:328:LEU:HD13	1.96	0.48
1:A:655:TRP:HA	1:A:659:MET:HG3	1.96	0.48
1:A:308:ILE:O	1:A:312:ILE:HG12	2.14	0.47
1:A:740:MET:HE1	1:A:743:LEU:HD23	1.97	0.47
1:A:459:ASP:CG	1:A:460:GLY:H	2.23	0.47
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.62	0.47
1:A:482:ASN:HD21	1:A:503:ARG:NH1	2.13	0.47
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.97	0.47
1:A:447:SER:HB3	1:A:606:MET:CE	2.44	0.47
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.23	0.47
1:A:659:MET:HA	1:A:659:MET:CE	2.45	0.46
1:A:456:THR:HA	1:A:463:SER:HA	1.97	0.46
1:A:507:LEU:HD12	1:A:602:THR:O	2.15	0.46
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.34	0.46
1:A:213:PRO:HD2	1:A:489:TYR:CB	2.45	0.46
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.41	0.46
1:A:645:LEU:HD13	1:A:684:TYR:CD1	2.51	0.46
1:A:428:CYS:HB2	1:A:430:GLU:OE2	2.16	0.45
1:A:484:VAL:O	1:A:488:ASN:HB2	2.16	0.45
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.51	0.45
1:A:620:CYS:SG	1:A:621:PHE:N	2.87	0.45
1:A:277:ARG:HD2	1:A:322:GLU:HA	1.98	0.45
1:A:534:GLN:O	1:A:538:THR:CG2	2.65	0.45
1:A:602:THR:N	1:A:707:ASP:OD2	2.49	0.45
1:A:92:LYS:HG3	1:A:166:ARG:HH12	1.79	0.45
1:A:541:HIS:HB2	1:A:585:TRP:CZ2	2.51	0.45
1:A:509:VAL:O	1:A:620:CYS:HA	2.16	0.45
1:A:220:LEU:CD2	1:A:426:ASN:HB3	2.47	0.44
1:A:312:ILE:HG22	1:A:402:PRO:HG3	1.99	0.44
1:A:471:HIS:CD2	1:A:542:ALA:HB2	2.51	0.44
1:A:606:MET:HB2	1:A:607:PRO:CD	2.47	0.44
1:A:218:CYS:HB3	5:A:2006:HOH:O	2.17	0.44
1:A:564:PRO:HG2	1:A:574:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:TYR:O	1:A:734:LYS:HG2	2.17	0.44
1:A:280:ASN:O	1:A:284:ARG:HG3	2.18	0.44
1:A:482:ASN:ND2	1:A:503:ARG:HH11	2.15	0.44
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.99	0.44
1:A:475:LYS:O	1:A:479:ARG:HG3	2.18	0.44
1:A:475:LYS:NZ	1:A:549:GLU:OE1	2.50	0.44
1:A:319:GLY:HA3	1:A:324:ARG:NH1	2.33	0.43
1:A:149:LYS:O	1:A:153:ARG:HB3	2.18	0.43
1:A:214:GLN:NE2	1:A:216:SER:H	2.16	0.43
1:A:538:THR:HB	1:A:583:TRP:HE1	1.82	0.43
1:A:433:GLU:OE2	1:A:504:PRO:HB2	2.19	0.42
1:A:300:TYR:OH	1:A:425:SER:HB3	2.19	0.42
1:A:121:TYR:CE1	1:A:125:MET:HE3	2.54	0.42
1:A:456:THR:HG22	1:A:463:SER:OG	2.19	0.42
1:A:649:LEU:HB3	1:A:655:TRP:HB2	2.02	0.42
1:A:183:ILE:O	1:A:187:LEU:HB2	2.20	0.42
1:A:408:ASP:O	1:A:412:ARG:HB2	2.20	0.42
1:A:251:HIS:CE1	1:A:423:LYS:HB2	2.54	0.41
1:A:676:VAL:HA	1:A:677:PRO:HD3	1.88	0.41
1:A:626:SER:HB2	1:A:668:GLY:HA3	2.01	0.41
1:A:713:ASN:HD22	1:A:713:ASN:HA	1.70	0.41
1:A:106:ASN:HB3	1:A:109:THR:CG2	2.50	0.41
1:A:297:PHE:HB2	1:A:328:LEU:HD22	2.03	0.41
1:A:619:GLU:O	1:A:620:CYS:C	2.63	0.41
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.40
1:A:270:ASN:HB3	1:A:274:PRO:HG2	2.02	0.40
1:A:306:ALA:HA	1:A:350:LEU:HB3	2.02	0.40
1:A:106:ASN:OD1	1:A:109:THR:HG22	2.20	0.40
1:A:363:TYR:HB2	1:A:408:ASP:OD1	2.22	0.40
1:A:146:PHE:CD1	1:A:146:PHE:N	2.87	0.40
1:A:218:CYS:CB	5:A:2006:HOH:O	2.70	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	647/888 (73%)	586 (91%)	52 (8%)	9 (1%)	9	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO
1	A	296	ALA
1	A	319	GLY
1	A	459	ASP
1	A	629	TYR
1	A	460	GLY
1	A	672	GLY
1	A	344	GLU
1	A	620	CYS

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	565/761 (74%)	508 (90%)	57 (10%)	7	24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	131	LEU
1	A	146	PHE
1	A	149	LYS
1	A	176	LEU
1	A	183	ILE
1	A	187	LEU
1	A	195	LEU
1	A	212	LYS
1	A	218	CYS

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	243	LYS
1	A	250	LEU
1	A	268	THR
1	A	273	ILE
1	A	288	GLN
1	A	292	LYS
1	A	293	ARG
1	A	301	LEU
1	A	314	ILE
1	A	322	GLU
1	A	326	ARG
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE
1	A	388	LEU
1	A	443	CYS
1	A	461	LYS
1	A	462	THR
1	A	464	THR
1	A	479	ARG
1	A	505	ILE
1	A	512	LEU
1	A	518	LEU
1	A	520	ARG
1	A	524	ASP
1	A	530	LEU
1	A	538	THR
1	A	578	LYS
1	A	597	VAL
1	A	606	MET
1	A	613	GLN
1	A	639	GLN
1	A	641	VAL
1	A	659	MET
1	A	665	THR
1	A	667	ASN
1	A	673	LEU
1	A	686	THR
1	A	693	LYS
1	A	704	VAL
1	A	712	LEU

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Mol	Chain	Res	Type
1	A	714	LEU
1	A	720	THR
1	A	724	LEU
1	A	743	LEU
1	A	746	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	345	ASN
1	A	482	ASN
1	A	552	GLN
1	A	639	GLN
1	A	666	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN
1	A	746	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	CDP	A	1002	-	25,26,26	1.01	1 (4%)	38,40,40	1.34	5 (13%)
3	ANP	A	1001	2	33,33,33	1.84	7 (21%)	45,52,52	2.29	14 (31%)

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
4	CDP	A	1002	-	-	7/16/32/32	0/2/2/2
3	ANP	A	1001	2	-	1/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ANP	C5-C4	5.63	1.49	1.39
3	A	1001	ANP	PG-O1G	4.08	1.52	1.46
3	A	1001	ANP	PB-O1B	3.46	1.51	1.46
3	A	1001	ANP	C5-C6	3.37	1.50	1.41
4	A	1002	CDP	PA-O3A	3.01	1.62	1.59
3	A	1001	ANP	C8-N7	2.58	1.36	1.31
3	A	1001	ANP	PB-O3A	2.19	1.61	1.59
3	A	1001	ANP	PB-O2B	-2.02	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ANP	O1G-PG-N3B	-6.75	101.83	111.77
3	A	1001	ANP	C5-C4-N3	-5.48	119.17	126.72
3	A	1001	ANP	O2B-PB-O1B	5.22	121.08	109.87
3	A	1001	ANP	N3-C4-N9	4.11	134.16	127.17
3	A	1001	ANP	O1B-PB-N3B	-4.03	105.83	111.77
3	A	1001	ANP	C4-C5-N7	-3.89	106.14	110.58
3	A	1001	ANP	C2-N3-C4	3.18	119.61	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ANP	C3'-C2'-C1'	2.97	107.08	101.46
4	A	1002	CDP	O2B-PB-O3B	2.79	118.25	107.80
4	A	1002	CDP	O2A-PA-O3A	2.68	114.52	107.27
3	A	1001	ANP	C6-C5-N7	2.47	136.84	132.09
3	A	1001	ANP	N3-C2-N1	-2.46	124.85	128.58
4	A	1002	CDP	C3'-C2'-C1'	2.44	106.08	101.46
3	A	1001	ANP	C5-N7-C8	2.42	107.26	103.45
3	A	1001	ANP	C4-N9-C8	2.36	108.22	105.74
3	A	1001	ANP	O2A-PA-O1A	2.26	122.95	112.44
4	A	1002	CDP	O3A-PA-O1A	-2.20	104.09	110.70
3	A	1001	ANP	C2-N1-C6	2.18	122.31	118.73
4	A	1002	CDP	N4-C4-N3	2.10	121.66	117.91

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	ANP	PB-N3B-PG-O1G
4	A	1002	CDP	PA-O3A-PB-O2B
4	A	1002	CDP	C5'-O5'-PA-O3A
4	A	1002	CDP	C5'-O5'-PA-O1A
4	A	1002	CDP	C5'-O5'-PA-O2A
4	A	1002	CDP	O4'-C4'-C5'-O5'
4	A	1002	CDP	C3'-C4'-C5'-O5'
4	A	1002	CDP	PA-O3A-PB-O1B

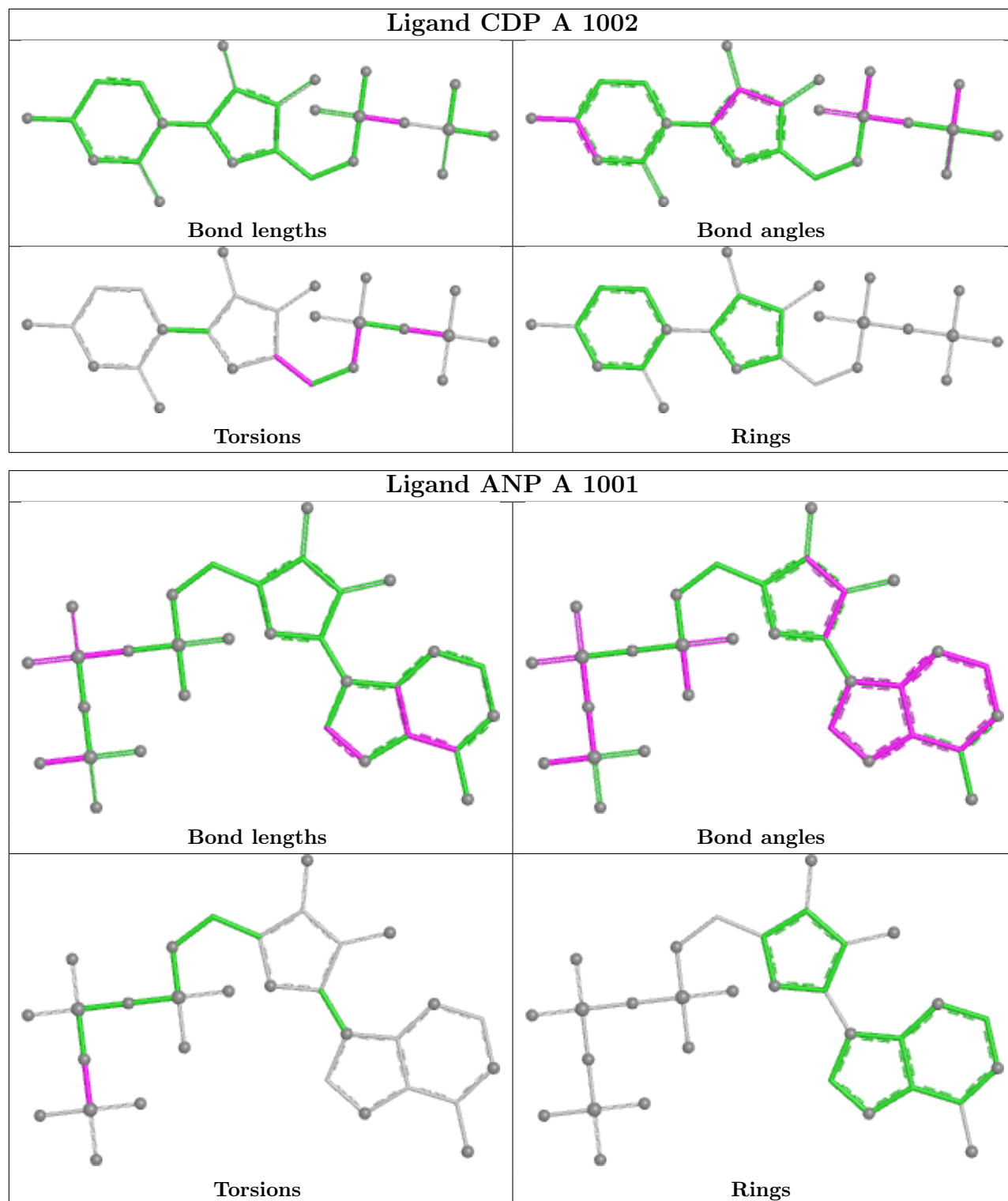
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	CDP	1	0
3	A	1001	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 [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	651/888 (73%)	-0.42	8 (1%) 76 69	20, 34, 66, 83	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	2.5
1	A	457	SER	2.5
1	A	629	TYR	2.4
1	A	456	THR	2.2
1	A	638	PHE	2.1
1	A	212	LYS	2.0
1	A	292	LYS	2.0
1	A	390	TYR	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](#)

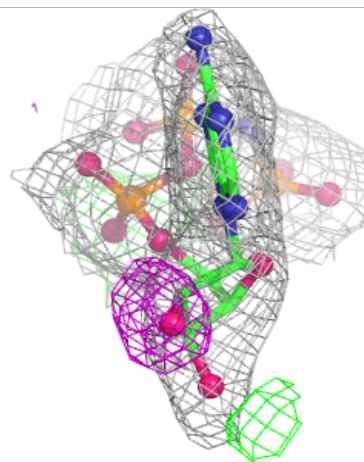
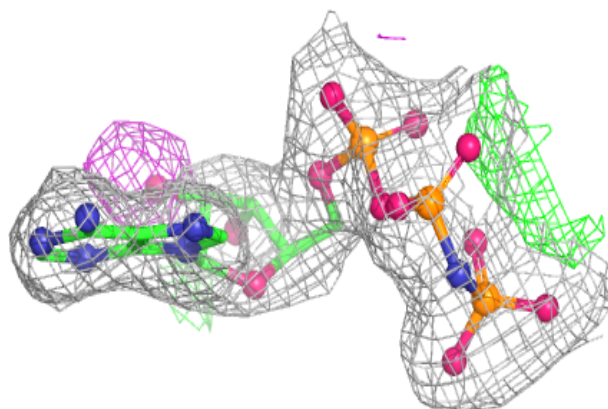
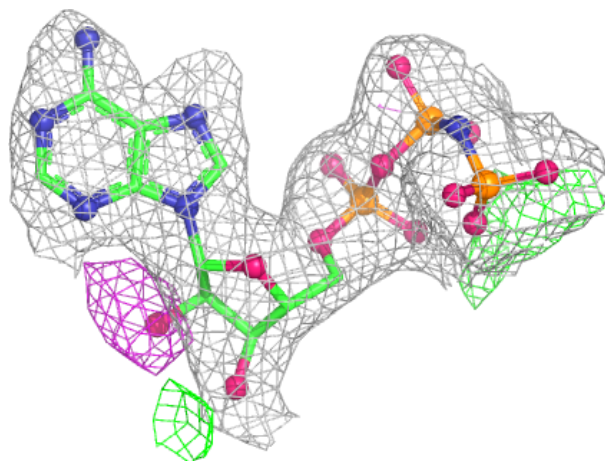
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	2001	1/1	0.79	0.21	34,34,34,34	0
3	ANP	A	1001	31/31	0.96	0.07	24,26,31,35	0
4	CDP	A	1002	25/25	0.96	0.07	47,50,52,53	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.

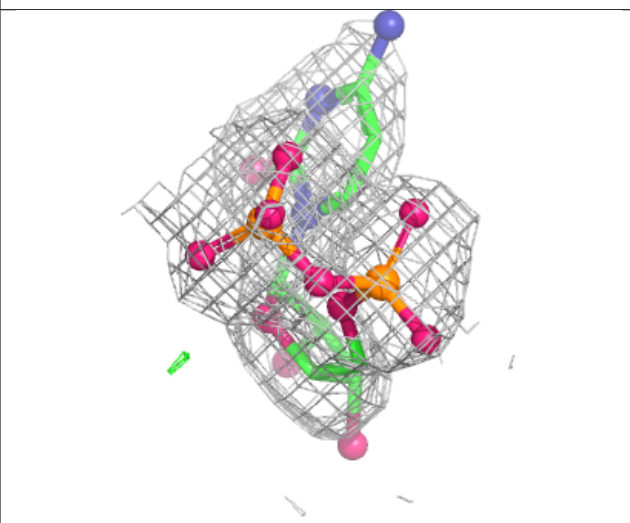
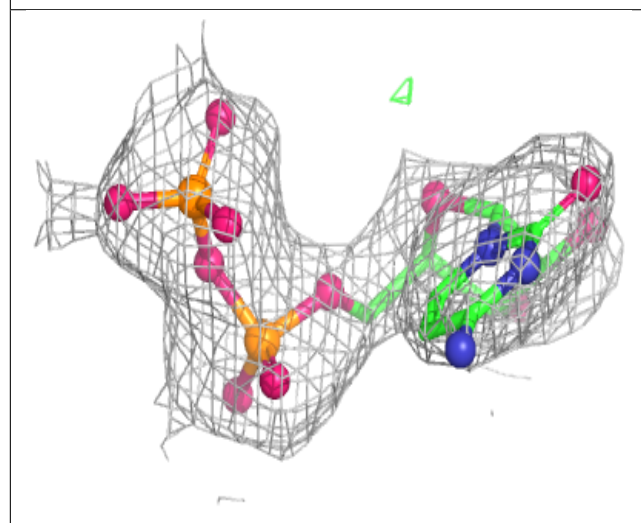
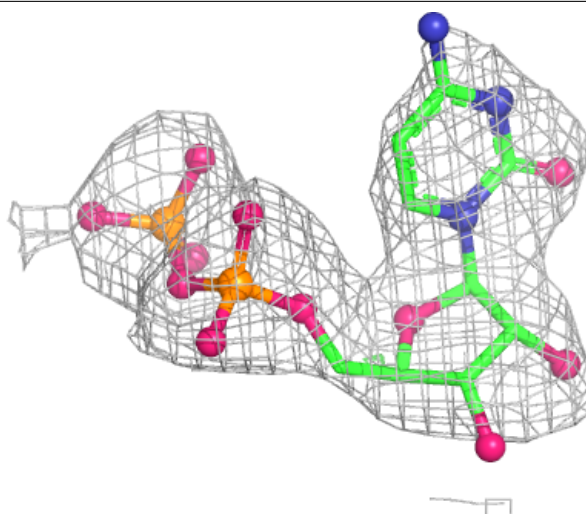
Electron density around ANP A 1001:

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 CDP A 1002:

$2mF_o-DF_c$ (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.