Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 06:40 AM EST

PDB ID	:	2CVU
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 (i) 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 (i)) were used in the production of this report:

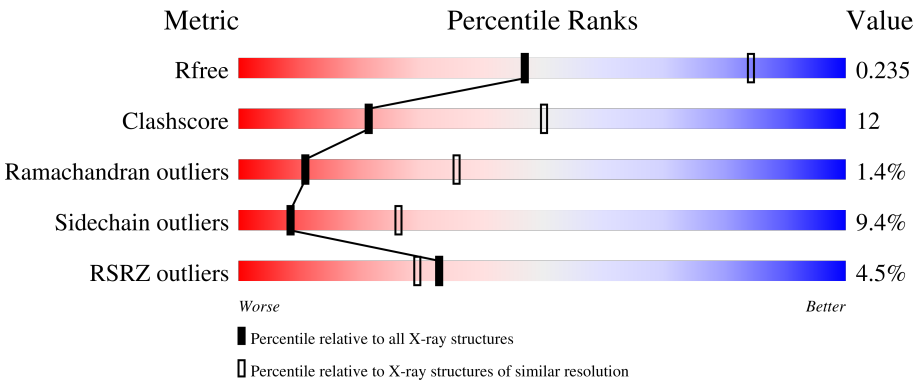
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	3% 50% 19% • 27%

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.

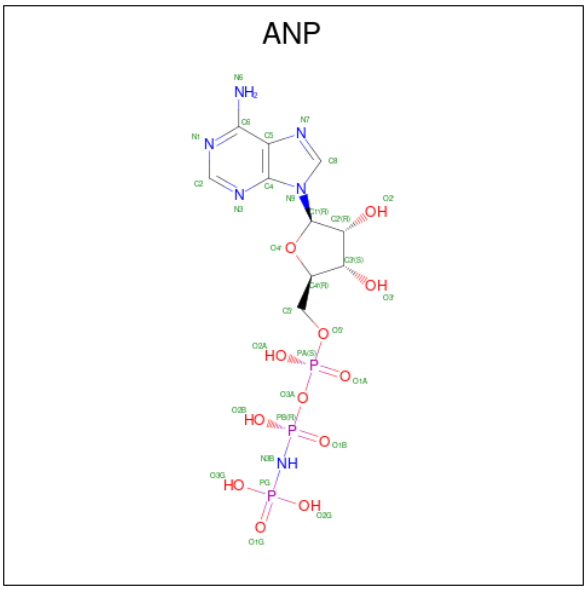
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

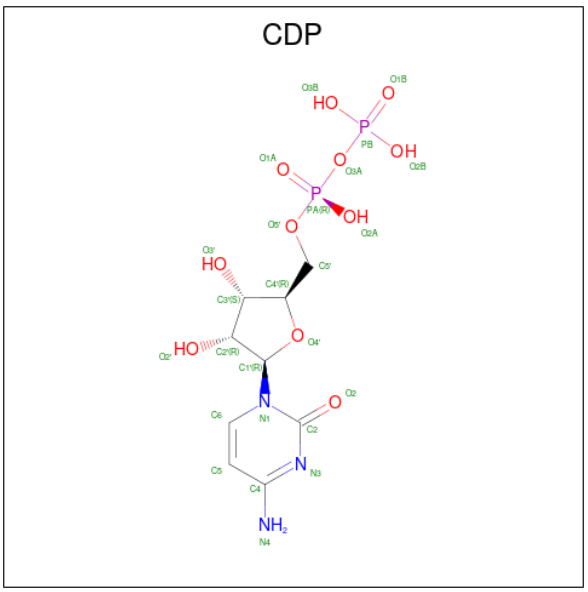
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

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

- Molecule 4 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



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

- Molecule 5 is water.

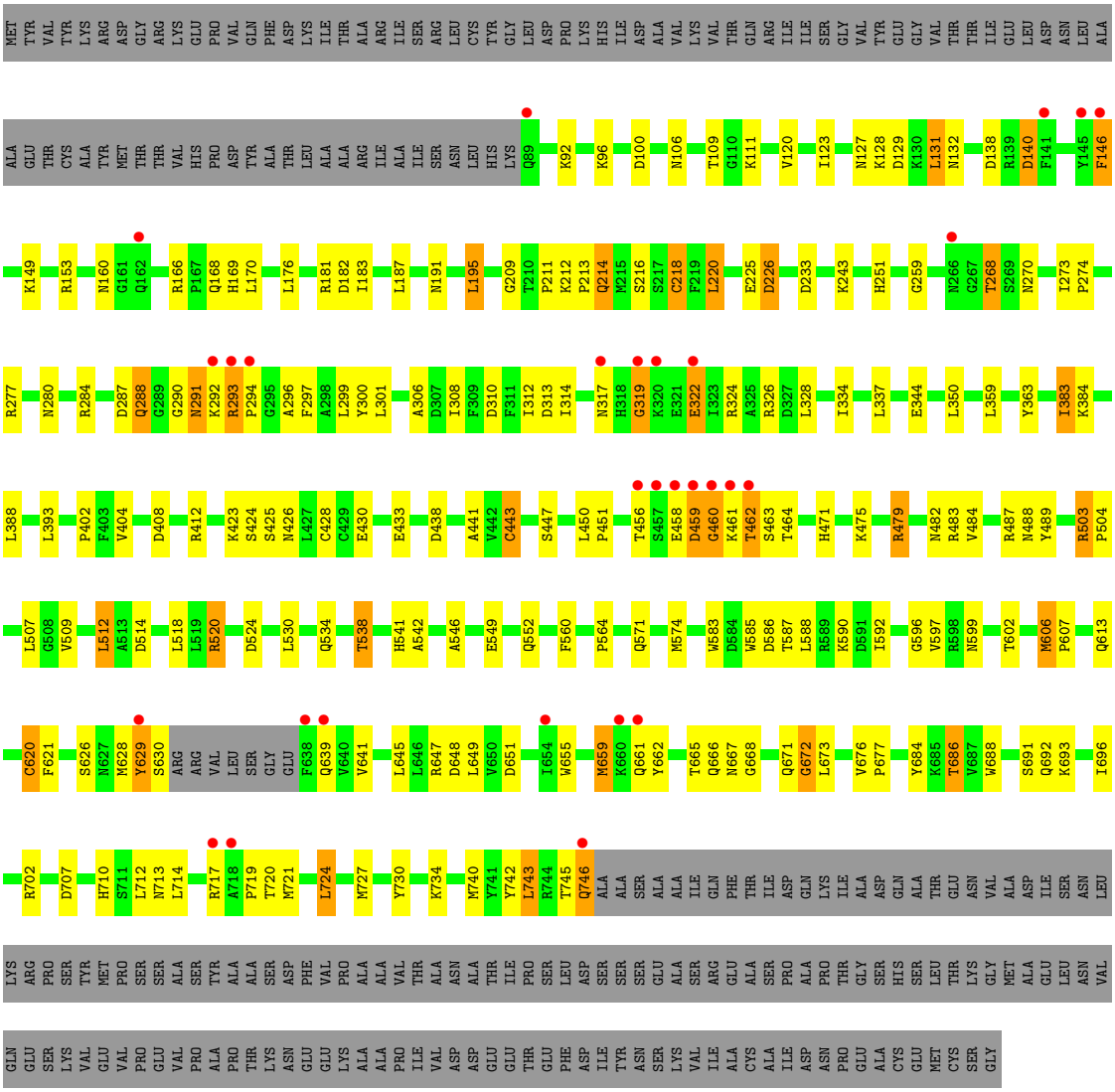
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	133	133	133	0	0

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: Ribonucleoside-diphosphate reductase large chain 1

Chain A:



4 Data and refinement statistics (i)

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 25.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.90) 99.7 (25.05-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [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 (10.07%)	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 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDP, 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	0.66	0/5329	0.87	17/7214 (0.2%)

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 (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	233	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	438	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	226	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	313	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	514	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	100	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	651	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	138	ASP	CB-CG-OD2	5.80	123.53	118.30
1	A	287	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	291	ASN	N-CA-C	5.66	126.27	111.00
1	A	727	MET	CB-CG-SD	5.50	128.91	112.40
1	A	129	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	586	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	512	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	310	ASP	CB-CG-OD2	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ASP	CB-CG-OD2	5.22	123.00	118.30

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 (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	5208	0	5135	125	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	125	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 12.

All (125) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:740:MET:HE2	1:A:743:LEU:HD23	1.79	0.64
1:A:92:LYS:HG3	1:A:166:ARG:NH1	2.12	0.64
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:106:ASN:HB3	1:A:109:THR:HG22	1.83	0.59
1:A:740:MET:CE	1:A:743:LEU:HD23	2.32	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:564:PRO:HG2	1:A:574:MET:HE1	1.86	0.57
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: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:671:GLN:O	1:A:672:GLY:C	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:628:MET:O	1:A:629:TYR:C	2.50	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: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:170:LEU:C	1:A:170:LEU:HD23	2.36	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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 (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	647/888 (73%)	586 (91%)	52 (8%)	9 (1%)	11 36

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 (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	565/761 (74%)	512 (91%)	53 (9%)	8 26

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	131	LEU

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Mol	Chain	Res	Type
1	A	146	PHE
1	A	160	ASN
1	A	176	LEU
1	A	195	LEU
1	A	212	LYS
1	A	214	GLN
1	A	218	CYS
1	A	220	LEU
1	A	243	LYS
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	503	ARG
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	597	VAL
1	A	606	MET
1	A	613	GLN
1	A	639	GLN
1	A	641	VAL
1	A	647	ARG
1	A	659	MET
1	A	661	GLN

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Mol	Chain	Res	Type
1	A	667	ASN
1	A	686	THR
1	A	712	LEU
1	A	714	LEU
1	A	720	THR
1	A	721	MET
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
3	ANP	A	1001	2	29,33,33	1.57	5 (17%)	31,52,52	2.38	11 (35%)
4	CDP	A	1002	-	24,26,26	0.83	0	37,40,40	1.24	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1001	2	-	2/14/38/38	0/3/3/3
4	CDP	A	1002	-	-	7/16/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ANP	PG-O1G	3.91	1.52	1.46
3	A	1001	ANP	PB-O1B	3.32	1.51	1.46
3	A	1001	ANP	C5-C4	3.10	1.49	1.40
3	A	1001	ANP	PB-O3A	2.17	1.61	1.59
3	A	1001	ANP	C2'-C1'	-2.16	1.50	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	ANP	O1G-PG-N3B	-6.75	101.83	111.77
3	A	1001	ANP	O2B-PB-O1B	5.32	121.08	109.92
3	A	1001	ANP	C3'-C2'-C1'	4.05	107.08	100.98
3	A	1001	ANP	O1B-PB-N3B	-4.03	105.83	111.77
3	A	1001	ANP	PB-O3A-PA	-3.16	121.49	132.62
3	A	1001	ANP	C4-C5-N7	-3.13	106.14	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	ANP	O4'-C1'-C2'	-2.93	102.64	106.93
4	A	1002	CDP	O2B-PB-O3B	2.78	118.25	107.64
4	A	1002	CDP	C3'-C2'-C1'	2.45	106.08	101.43
3	A	1001	ANP	N3-C2-N1	-2.45	124.85	128.68
3	A	1001	ANP	O2A-PA-O1A	2.17	122.95	112.24
4	A	1002	CDP	N4-C4-N3	2.11	121.66	117.97
3	A	1001	ANP	C2-N1-C6	2.08	122.31	118.75
3	A	1001	ANP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

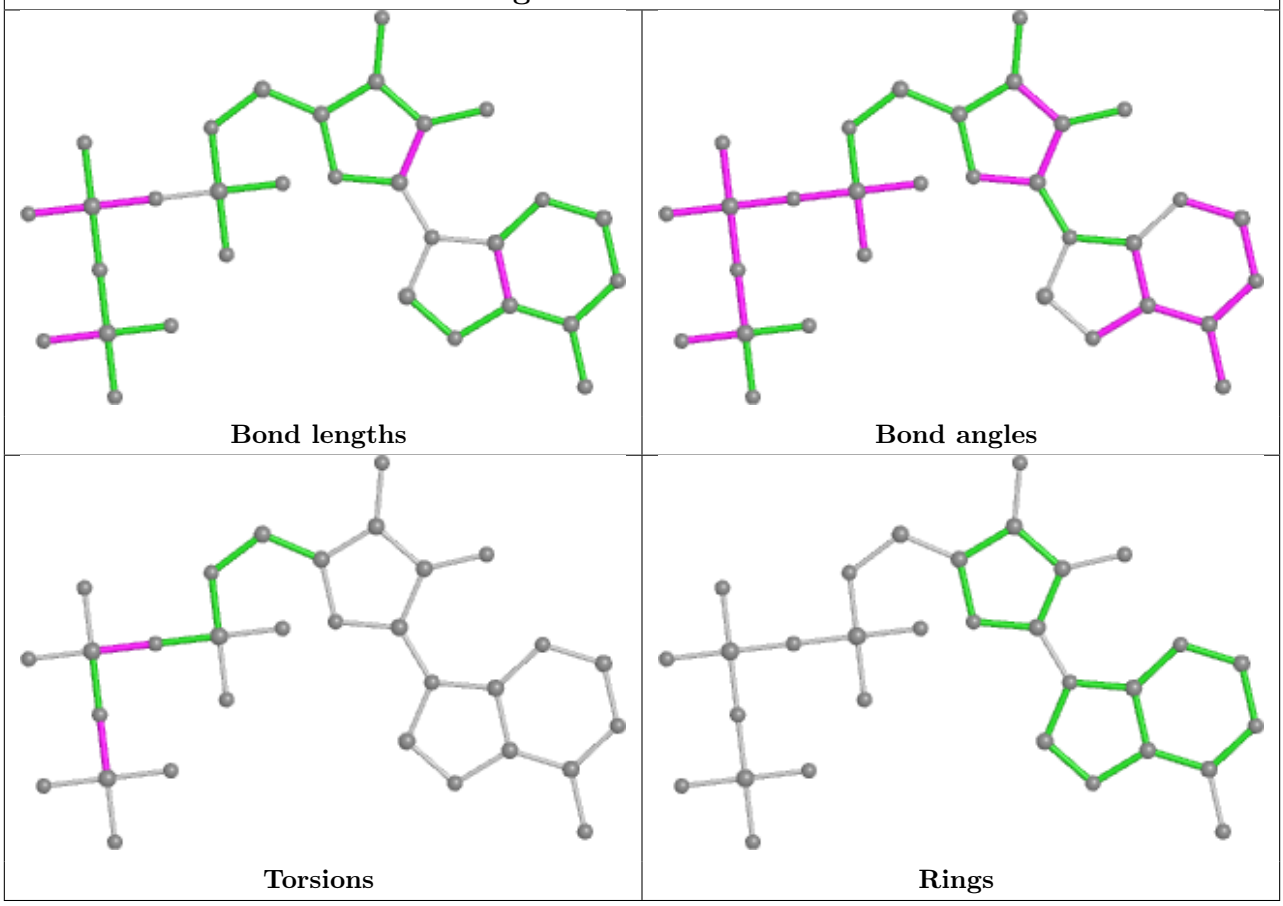
There are no ring outliers.

2 monomers are involved in 2 short contacts:

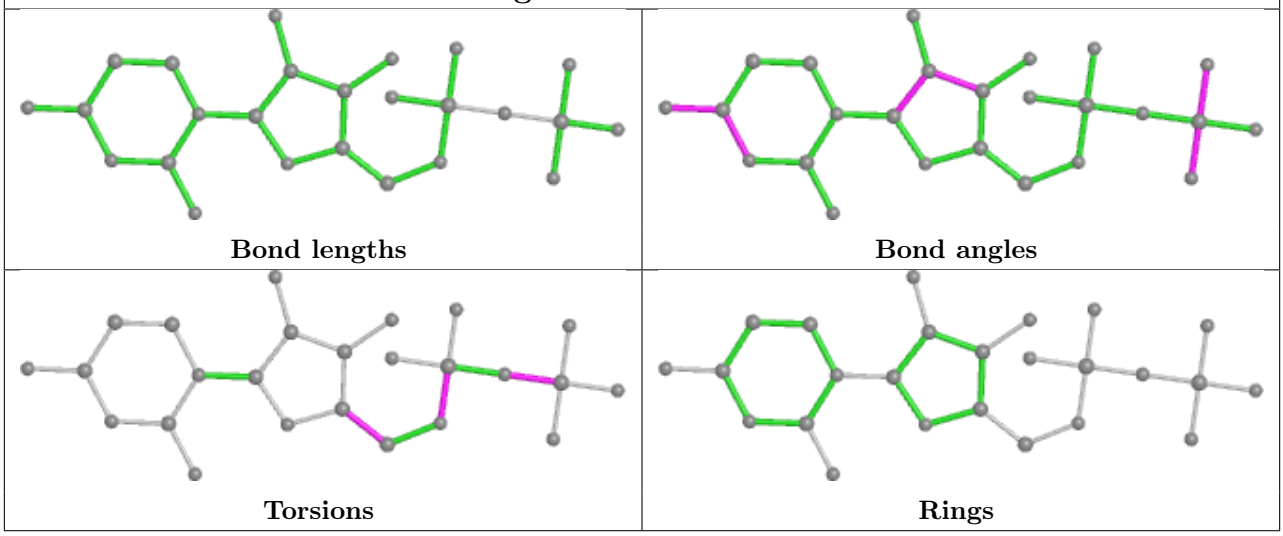
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	ANP	1	0
4	A	1002	CDP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ANP A 1001



Ligand CDP A 1002



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%)	-0.21	29 (4%) 33 29	20, 34, 66, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	SER	6.5
1	A	292	LYS	5.1
1	A	293	ARG	4.7
1	A	458	GLU	4.6
1	A	146	PHE	4.4
1	A	145	TYR	4.4
1	A	456	THR	4.3
1	A	459	ASP	4.2
1	A	89	GLN	4.1
1	A	638	PHE	3.7
1	A	294	PRO	3.6
1	A	460	GLY	3.1
1	A	322	GLU	2.9
1	A	718	ALA	2.9
1	A	320	LYS	2.7
1	A	462	THR	2.6
1	A	319	GLY	2.5
1	A	629	TYR	2.5
1	A	654	ILE	2.3
1	A	162	GLN	2.3
1	A	639	GLN	2.3
1	A	746	GLN	2.3
1	A	717	ARG	2.2
1	A	661	GLN	2.2
1	A	266	ASN	2.1
1	A	461	LYS	2.0
1	A	660	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	141	PHE	2.0
1	A	317	ASN	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)

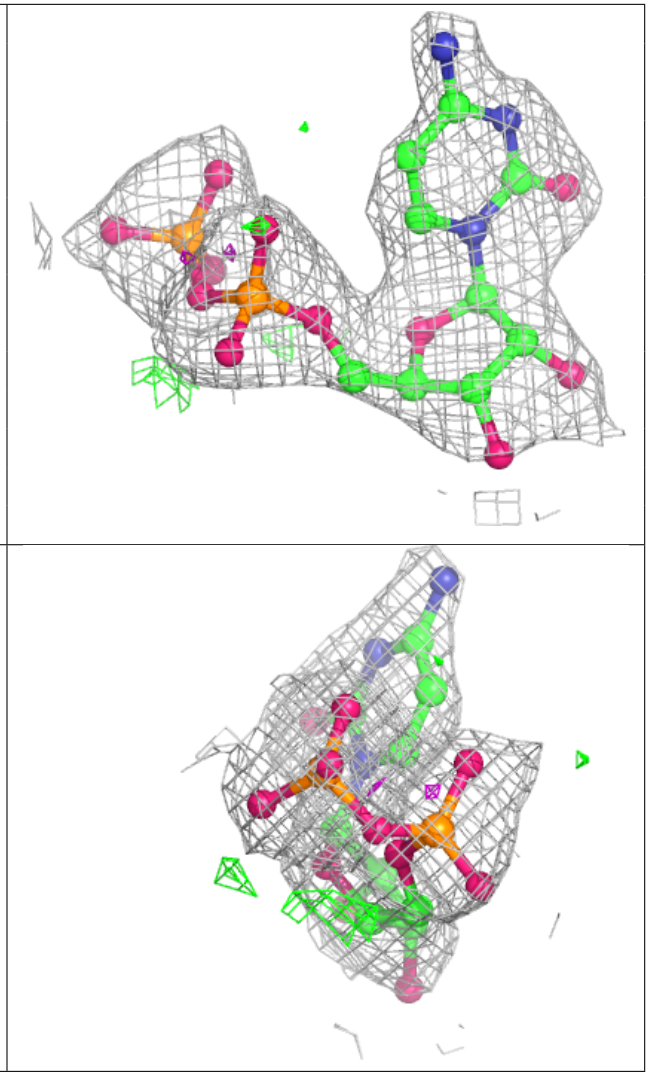
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	2001	1/1	0.87	0.11	34,34,34,34	0
4	CDP	A	1002	25/25	0.95	0.19	47,50,52,53	0
3	ANP	A	1001	31/31	0.96	0.12	24,26,31,35	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.

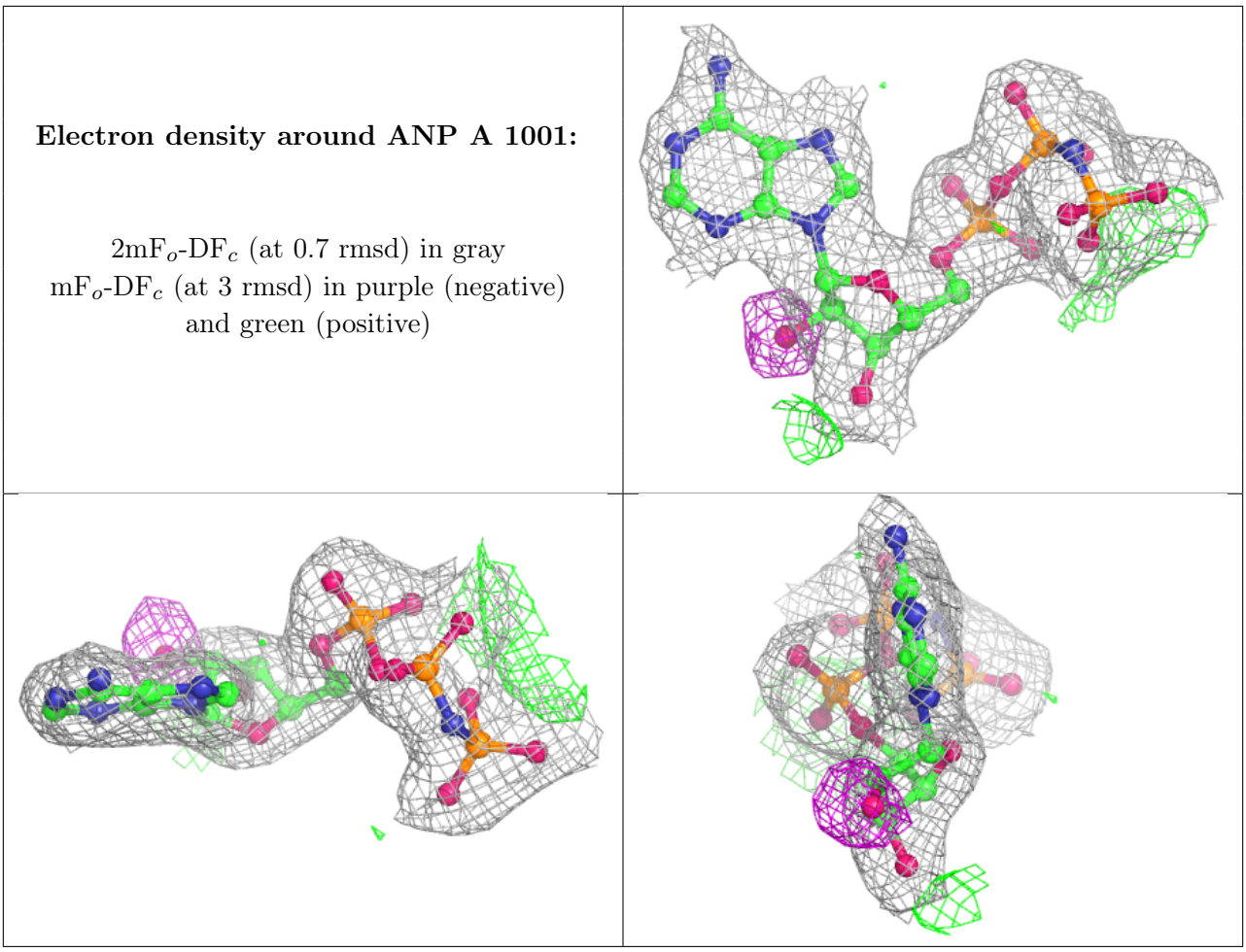
Electron density around CDP A 1002:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.