Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:29 am BST

PDB ID	:	2EUD
Title	:	Structures of Yeast Ribonucleotide Reductase I complexed with Ligands and Subunit Peptides
Authors	:	Dealwis, C.; Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.
Deposited on	:	2005-10-28
Resolution	:	2.30 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:

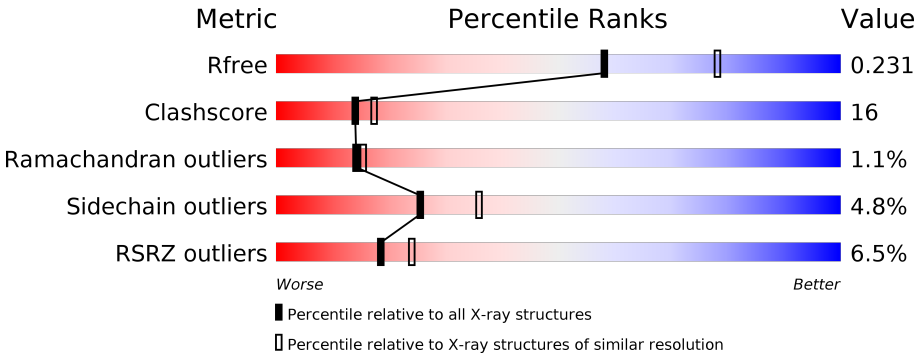
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	5% 51% 20% • 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5446 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.

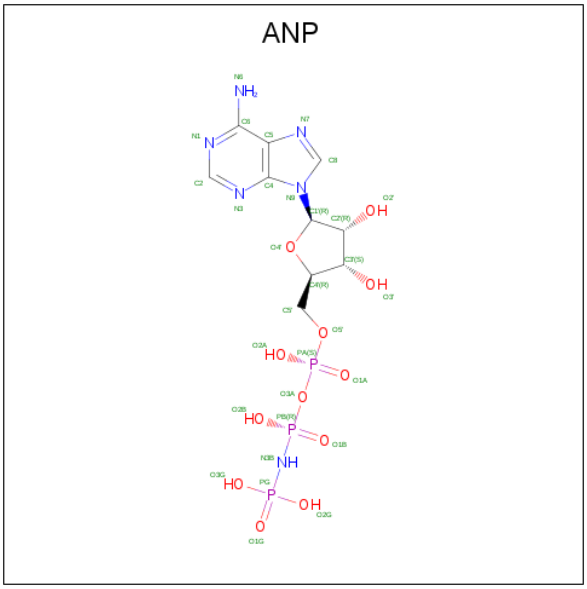
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	0	0
			5181	3300	879	971	31			

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

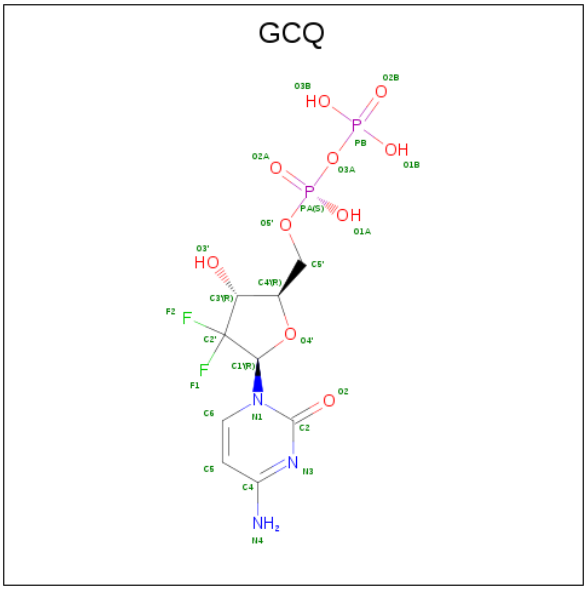
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 4 is GEMCITABINE DIPHOSPHATE (three-letter code: GCQ) (formula: $C_9H_{13}F_2N_3O_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	P	0	0
			26	9	2	3	10	2		

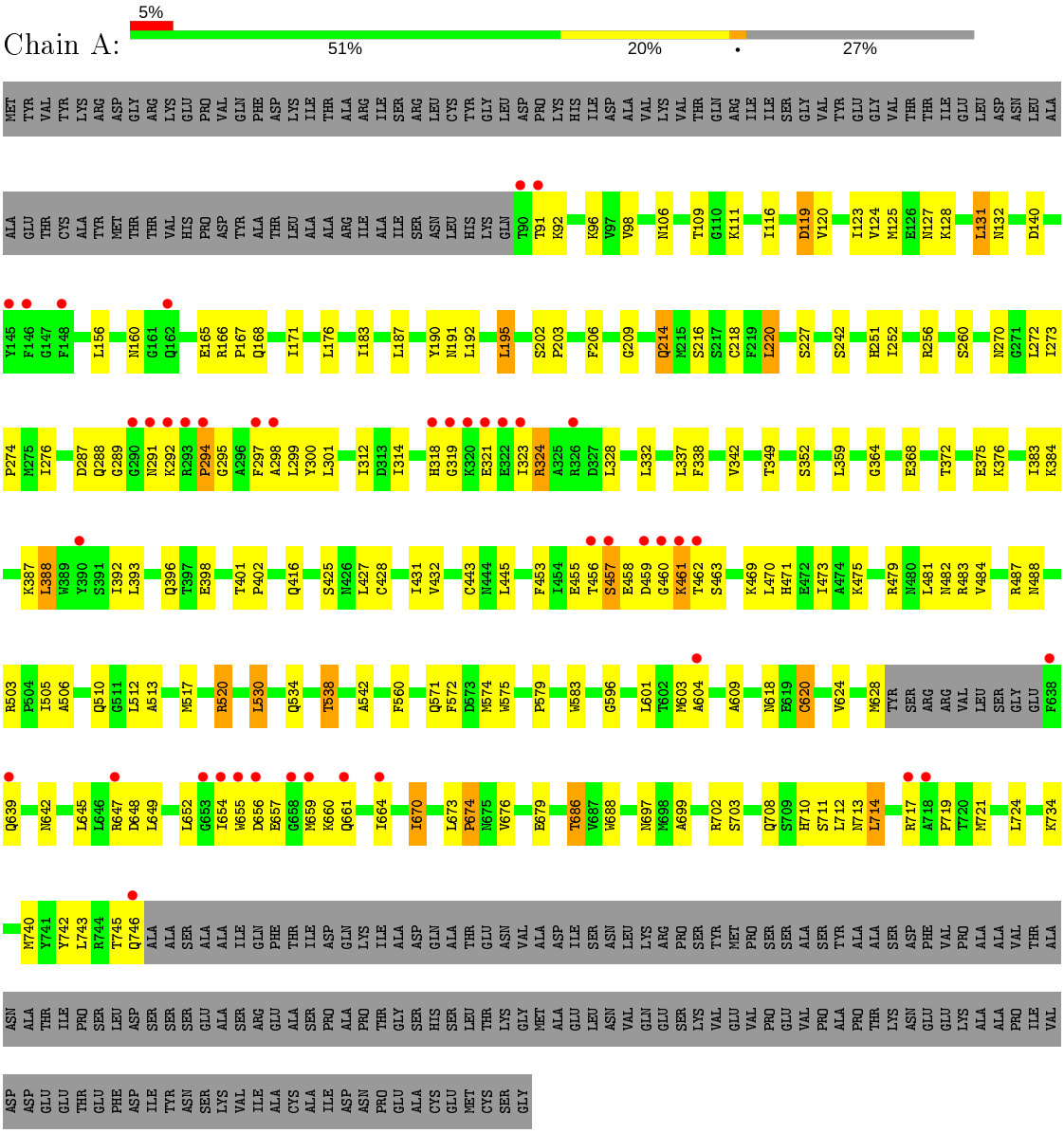
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total	O	0	0
			207	207		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.58Å 117.22Å 63.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.30) 93.9 (49.79-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.240 0.197 , 0.231	Depositor DCC
R_{free} test set	3569 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5446	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCQ, 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	0.35	0/5301	0.62	1/7176 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	SER	N-CA-C	-5.12	97.19	111.00

There are no chirality outliers.

There are no planarity outliers.

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	5181	0	5113	163	0
2	A	1	0	0	0	0
3	A	31	0	13	4	0
4	A	26	0	10	0	0
5	A	207	0	0	8	0
All	All	5446	0	5136	163	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 16.

All (163) 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:218:CYS:HB2	1:A:443:CYS:SG	1.87	1.14
1:A:297:PHE:HB2	1:A:328:LEU:HD22	1.42	1.02
1:A:383:ILE:HD11	1:A:387:LYS:HD3	1.49	0.94
1:A:432:VAL:H	1:A:708:GLN:HE21	1.17	0.93
1:A:746:GLN:HE21	1:A:746:GLN:HA	1.35	0.92
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.54	0.90
1:A:227:SER:HA	3:A:890:ANP:H5'1	1.52	0.89
1:A:206:PHE:CD1	1:A:291:ASN:ND2	2.46	0.84
1:A:218:CYS:HB2	1:A:443:CYS:HG	1.43	0.82
1:A:534:GLN:O	1:A:538:THR:HG23	1.82	0.79
1:A:276:ILE:HD12	1:A:299:LEU:HD13	1.66	0.78
1:A:206:PHE:HD1	1:A:291:ASN:HD21	1.29	0.77
1:A:462:THR:HG22	1:A:463:SER:H	1.54	0.72
1:A:109:THR:HG23	1:A:111:LYS:H	1.53	0.72
1:A:432:VAL:H	1:A:708:GLN:NE2	1.87	0.71
1:A:256:ARG:HG2	1:A:260:SER:CB	2.21	0.71
1:A:673:LEU:HD22	1:A:676:VAL:HG23	1.72	0.70
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.75	0.69
1:A:746:GLN:NE2	1:A:746:GLN:HA	2.06	0.68
1:A:479:ARG:NH1	5:A:1080:HOH:O	2.25	0.68
1:A:106:ASN:OD1	1:A:109:THR:HG22	1.95	0.67
1:A:319:GLY:HA3	1:A:324:ARG:HD2	1.76	0.67
1:A:98:VAL:HG13	1:A:116:ILE:HD13	1.77	0.66
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.09	0.66
1:A:242:SER:O	1:A:292:LYS:HD2	1.97	0.65
1:A:686:THR:CG2	1:A:688:TRP:H	2.11	0.64
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.78	0.64
1:A:251:HIS:HD2	5:A:1052:HOH:O	1.81	0.63
1:A:218:CYS:CB	1:A:443:CYS:SG	2.78	0.63
1:A:647:ARG:HE	1:A:647:ARG:HA	1.65	0.61
1:A:401:THR:HB	1:A:402:PRO:HA	1.83	0.61
1:A:462:THR:HG22	1:A:463:SER:N	2.16	0.60
1:A:383:ILE:CD1	1:A:387:LYS:HD3	2.28	0.60
1:A:431:ILE:HG23	1:A:708:GLN:HE22	1.67	0.60
1:A:297:PHE:CB	1:A:328:LEU:HD22	2.25	0.59
1:A:392:ILE:O	1:A:396:GLN:HG3	2.03	0.58
1:A:167:PRO:O	1:A:171:ILE:HG13	2.04	0.58
1:A:276:ILE:HD12	1:A:299:LEU:CD1	2.32	0.58
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.36	0.58
1:A:660:LYS:HD3	1:A:660:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG2	1:A:260:SER:HB2	1.86	0.57
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.04	0.57
1:A:740:MET:SD	1:A:743:LEU:HB2	2.45	0.57
1:A:218:CYS:HB3	5:A:892:HOH:O	2.04	0.57
1:A:719:PRO:HG3	1:A:745:THR:HG21	1.86	0.56
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.20	0.56
1:A:300:TYR:OH	1:A:425:SER:HB3	2.05	0.56
1:A:686:THR:HG23	1:A:688:TRP:H	1.71	0.56
1:A:530:LEU:O	1:A:534:GLN:HG3	2.07	0.55
1:A:272:LEU:O	1:A:276:ILE:HG12	2.07	0.55
1:A:538:THR:HG22	1:A:583:TRP:HE1	1.71	0.55
1:A:349:THR:OG1	1:A:375:GLU:HG3	2.07	0.54
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.90	0.54
1:A:156:LEU:HD13	1:A:165:GLU:O	2.08	0.53
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.39	0.53
1:A:297:PHE:HB2	1:A:328:LEU:CD2	2.28	0.53
1:A:719:PRO:HG3	1:A:745:THR:CG2	2.39	0.53
1:A:652:LEU:HB2	1:A:654:ILE:HG12	1.91	0.53
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.74	0.52
1:A:513:ALA:O	1:A:517:MET:HG3	2.09	0.52
1:A:383:ILE:HG12	1:A:384:LYS:H	1.74	0.52
1:A:109:THR:HG23	1:A:111:LYS:N	2.23	0.52
1:A:242:SER:HB3	1:A:292:LYS:HE3	1.90	0.52
1:A:456:THR:O	1:A:458:GLU:HG3	2.09	0.52
1:A:481:LEU:CB	1:A:505:ILE:HD12	2.34	0.52
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.92	0.52
1:A:484:VAL:O	1:A:488:ASN:HB2	2.10	0.52
1:A:745:THR:CG2	1:A:746:GLN:N	2.73	0.52
1:A:657:GLU:C	1:A:659:MET:H	2.12	0.51
1:A:699:ALA:HA	1:A:702:ARG:NH1	2.26	0.51
1:A:91:THR:HG21	1:A:96:LYS:HD2	1.93	0.51
1:A:319:GLY:C	1:A:321:GLU:H	2.14	0.51
1:A:609:ALA:HB3	5:A:1089:HOH:O	2.10	0.51
1:A:319:GLY:HA3	1:A:324:ARG:NH1	2.26	0.51
1:A:300:TYR:CZ	1:A:425:SER:HB3	2.45	0.50
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.93	0.50
1:A:652:LEU:C	1:A:654:ILE:H	2.13	0.50
1:A:119:ASP:O	1:A:123:ILE:HG13	2.12	0.49
1:A:220:LEU:N	1:A:220:LEU:HD23	2.27	0.49
1:A:649:LEU:HB3	1:A:655:TRP:HB2	1.94	0.49
1:A:323:ILE:O	1:A:323:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:CE	1:A:743:LEU:HD23	2.42	0.49
1:A:92:LYS:HG3	1:A:166:ARG:NH1	2.28	0.49
1:A:740:MET:HE2	1:A:743:LEU:HD23	1.94	0.48
1:A:673:LEU:HD22	1:A:676:VAL:CG2	2.42	0.48
1:A:453:PHE:CE2	1:A:470:LEU:HA	2.49	0.48
1:A:318:HIS:HE1	1:A:398:GLU:OE1	1.97	0.48
1:A:372:THR:HG22	1:A:376:LYS:HE3	1.96	0.48
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.48	0.48
1:A:697:ASN:OD1	1:A:734:LYS:HE3	2.13	0.48
1:A:461:LYS:HE2	1:A:461:LYS:HA	1.96	0.48
1:A:383:ILE:HD11	1:A:387:LYS:CD	2.33	0.47
1:A:745:THR:HG22	1:A:746:GLN:N	2.28	0.47
1:A:710:HIS:HD2	5:A:908:HOH:O	1.96	0.47
1:A:661:GLN:HA	1:A:664:ILE:HD11	1.97	0.47
1:A:686:THR:HG22	1:A:688:TRP:H	1.79	0.47
1:A:647:ARG:HE	1:A:647:ARG:CA	2.28	0.47
1:A:227:SER:CB	3:A:890:ANP:O2A	2.63	0.47
1:A:460:GLY:O	1:A:462:THR:N	2.43	0.47
1:A:538:THR:CG2	1:A:583:TRP:HE1	2.28	0.47
1:A:214:GLN:NE2	1:A:216:SER:H	2.14	0.46
1:A:475:LYS:O	1:A:479:ARG:HG3	2.16	0.46
1:A:456:THR:O	1:A:458:GLU:N	2.49	0.46
1:A:713:ASN:ND2	1:A:742:TYR:H	2.13	0.46
1:A:520:ARG:NH1	1:A:679:GLU:OE2	2.49	0.46
1:A:242:SER:CB	1:A:292:LYS:HE3	2.46	0.46
1:A:670:ILE:HD13	5:A:995:HOH:O	2.17	0.45
1:A:713:ASN:HD22	1:A:742:TYR:H	1.63	0.45
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.99	0.45
1:A:120:VAL:HG21	1:A:209:GLY:HA2	1.99	0.45
1:A:388:LEU:O	1:A:392:ILE:HG12	2.17	0.45
1:A:192:LEU:HD13	1:A:473:ILE:HD12	1.99	0.45
1:A:202:SER:HB2	1:A:203:PRO:HD3	1.98	0.45
1:A:431:ILE:HG13	1:A:443:CYS:SG	2.57	0.45
1:A:120:VAL:O	1:A:124:VAL:HG23	2.16	0.45
1:A:458:GLU:OE1	1:A:462:THR:HB	2.17	0.45
1:A:396:GLN:HA	1:A:401:THR:O	2.17	0.44
1:A:746:GLN:CA	1:A:746:GLN:NE2	2.74	0.44
1:A:227:SER:HA	3:A:890:ANP:O2A	2.18	0.44
1:A:416:GLN:HG3	1:A:601:LEU:HD11	1.99	0.44
1:A:645:LEU:O	1:A:649:LEU:HG	2.17	0.44
1:A:191:ASN:O	1:A:195:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ASN:HD21	1:A:624:VAL:HA	1.82	0.44
1:A:227:SER:HB2	3:A:890:ANP:O2A	2.17	0.44
1:A:270:ASN:HB2	5:A:916:HOH:O	2.18	0.44
1:A:572:PHE:CE2	1:A:579:PRO:HD3	2.52	0.43
1:A:183:ILE:O	1:A:187:LEU:HD23	2.18	0.43
1:A:670:ILE:HD13	1:A:670:ILE:H	1.83	0.43
1:A:289:GLY:O	1:A:291:ASN:N	2.50	0.43
1:A:109:THR:OG1	1:A:111:LYS:HD2	2.19	0.42
1:A:657:GLU:C	1:A:659:MET:N	2.72	0.42
1:A:298:ALA:HB2	1:A:427:LEU:HA	2.01	0.42
1:A:338:PHE:O	1:A:342:VAL:HG23	2.18	0.42
1:A:455:GLU:HG3	1:A:457:SER:HB2	2.01	0.42
1:A:471:HIS:CD2	1:A:542:ALA:HB2	2.54	0.42
1:A:393:LEU:HD22	1:A:724:LEU:HG	2.02	0.42
1:A:214:GLN:HE22	1:A:216:SER:H	1.68	0.42
1:A:628:MET:CE	1:A:664:ILE:HG23	2.49	0.42
1:A:256:ARG:HG2	1:A:260:SER:HB3	2.01	0.42
1:A:443:CYS:HB3	1:A:445:LEU:CD1	2.50	0.42
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.53	0.42
1:A:673:LEU:HA	1:A:674:PRO:HD3	1.90	0.41
1:A:575:TRP:CZ2	1:A:703:SER:HB3	2.55	0.41
1:A:714:LEU:HB2	1:A:740:MET:HE2	2.02	0.41
1:A:312:ILE:HG21	1:A:392:ILE:CD1	2.50	0.41
1:A:717:ARG:O	1:A:719:PRO:HD3	2.20	0.41
1:A:383:ILE:HG12	1:A:384:LYS:N	2.36	0.41
1:A:503:ARG:HB3	1:A:503:ARG:HH11	1.86	0.41
1:A:603:MET:O	1:A:708:GLN:HG3	2.20	0.41
1:A:639:GLN:N	1:A:639:GLN:CD	2.74	0.41
1:A:618:ASN:ND2	1:A:624:VAL:HA	2.36	0.41
1:A:206:PHE:CD1	1:A:291:ASN:CG	2.93	0.41
1:A:453:PHE:HD2	1:A:469:LYS:HB3	1.86	0.41
1:A:510:GLN:HA	1:A:620:CYS:HA	2.03	0.40
1:A:642:ASN:HB3	1:A:645:LEU:HB3	2.03	0.40
1:A:125:MET:O	1:A:128:LYS:HE3	2.21	0.40
1:A:128:LYS:O	1:A:132:ASN:ND2	2.54	0.40
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.90	0.40
1:A:364:GLY:O	1:A:368:GLU:HG3	2.21	0.40
1:A:746:GLN:HG3	1:A:746:GLN:O	2.22	0.40
1:A:252:ILE:CD1	1:A:276:ILE:HD11	2.52	0.40
1:A:428:CYS:HB2	5:A:1034:HOH:O	2.21	0.40
1:A:571:GLN:HA	1:A:574:MET:HE3	2.04	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	644/888 (72%)	594 (92%)	43 (7%)	7 (1%)	14 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO
1	A	457	SER
1	A	711	SER
1	A	288	GLN
1	A	620	CYS
1	A	674	PRO
1	A	295	GLY

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	562/761 (74%)	535 (95%)	27 (5%)	25 36

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASP

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Mol	Chain	Res	Type
1	A	131	LEU
1	A	160	ASN
1	A	176	LEU
1	A	195	LEU
1	A	214	GLN
1	A	220	LEU
1	A	287	ASP
1	A	294	PRO
1	A	301	LEU
1	A	314	ILE
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	459	ASP
1	A	461	LYS
1	A	512	LEU
1	A	520	ARG
1	A	530	LEU
1	A	538	THR
1	A	656	ASP
1	A	670	ILE
1	A	686	THR
1	A	712	LEU
1	A	714	LEU
1	A	721	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	160	ASN
1	A	162	GLN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	318	HIS
1	A	345	ASN
1	A	552	GLN
1	A	595	HIS

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Mol	Chain	Res	Type
1	A	613	GLN
1	A	618	ASN
1	A	639	GLN
1	A	692	GLN
1	A	708	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 carbohydrates 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	890	2	29,33,33	1.87	9 (31%)	31,52,52	1.71	6 (19%)
4	GCQ	A	891	-	21,27,27	1.31	2 (9%)	27,43,43	1.80	5 (18%)

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	890	2	-	3/14/38/38	0/3/3/3
4	GCQ	A	891	-	-	4/13/36/36	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	ANP	PB-O3A	-4.17	1.53	1.59
3	A	890	ANP	C2-N1	3.45	1.40	1.33
3	A	890	ANP	PB-O2B	-3.32	1.47	1.56
3	A	890	ANP	PG-O3G	-3.31	1.47	1.56
3	A	890	ANP	C8-N7	-3.31	1.28	1.34
4	A	891	GCQ	C6-N1	2.61	1.39	1.35
4	A	891	GCQ	F1-C2'	2.56	1.43	1.37
3	A	890	ANP	C4-N3	2.54	1.39	1.35
3	A	890	ANP	PG-O2G	-2.43	1.50	1.56
3	A	890	ANP	C5-N7	-2.05	1.32	1.39
3	A	890	ANP	O2'-C2'	2.05	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	891	GCQ	C2-N3-C4	5.46	121.87	116.34
3	A	890	ANP	O3A-PB-N3B	-4.52	94.05	106.59
4	A	891	GCQ	O4'-C4'-C3'	4.18	108.99	104.42
3	A	890	ANP	C4-C5-N7	3.26	112.80	109.40
3	A	890	ANP	C5-C6-N6	3.26	125.30	120.35
4	A	891	GCQ	N4-C4-N3	2.54	120.50	116.49
3	A	890	ANP	C2'-C3'-C4'	-2.52	97.75	102.64
3	A	890	ANP	O3G-PG-O1G	-2.40	107.43	113.45
4	A	891	GCQ	O1B-PB-O3B	2.11	115.69	107.64
3	A	890	ANP	O3'-C3'-C2'	2.10	118.61	111.82
4	A	891	GCQ	O3'-C3'-C4'	-2.07	107.50	112.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	890	ANP	C5'-O5'-PA-O1A
4	A	891	GCQ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	891	GCQ	O4'-C4'-C5'-O5'
3	A	890	ANP	PB-O3A-PA-O1A
4	A	891	GCQ	PA-O3A-PB-O2B
4	A	891	GCQ	PA-O3A-PB-O3B
3	A	890	ANP	PB-O3A-PA-O2A

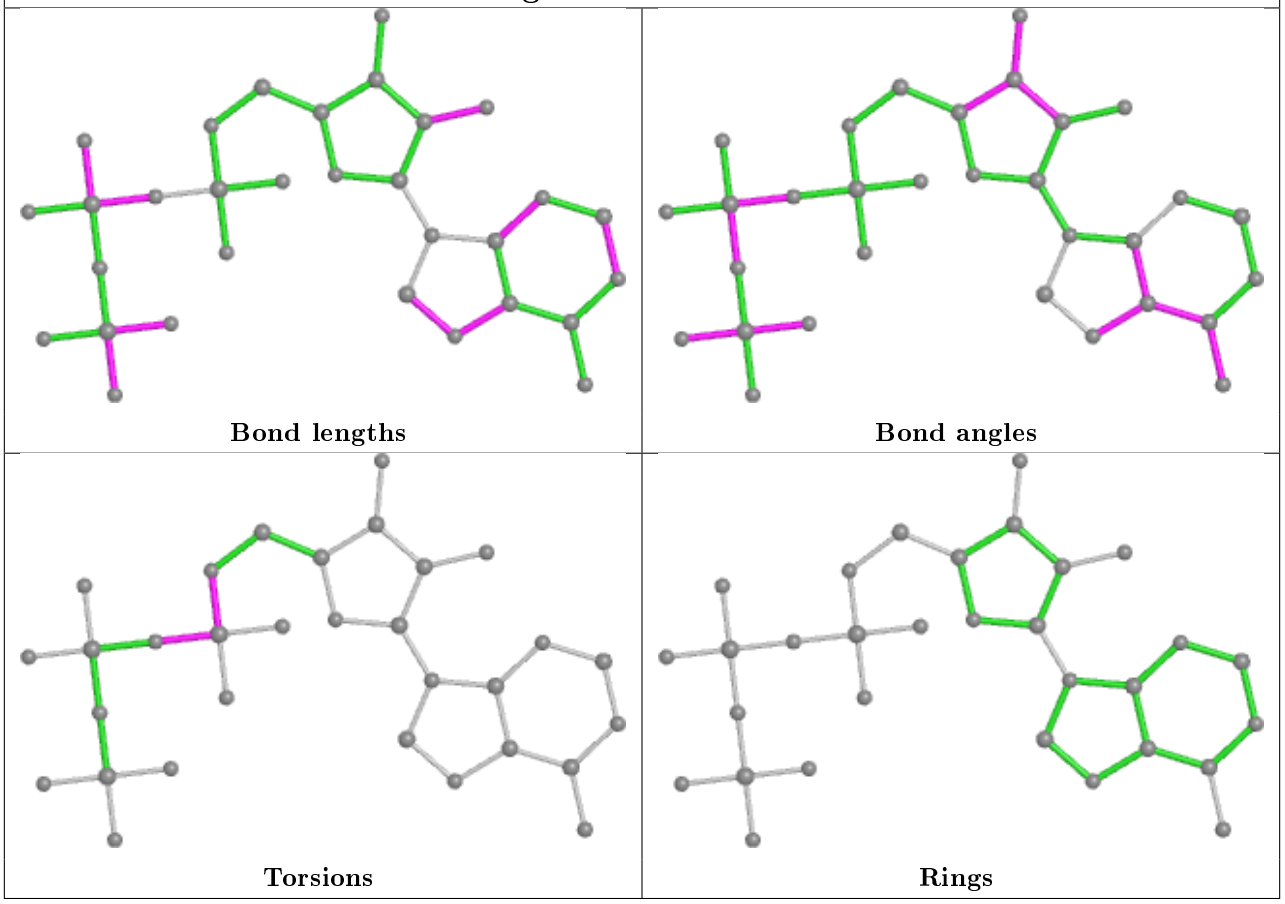
There are no ring outliers.

1 monomer is involved in 4 short contacts:

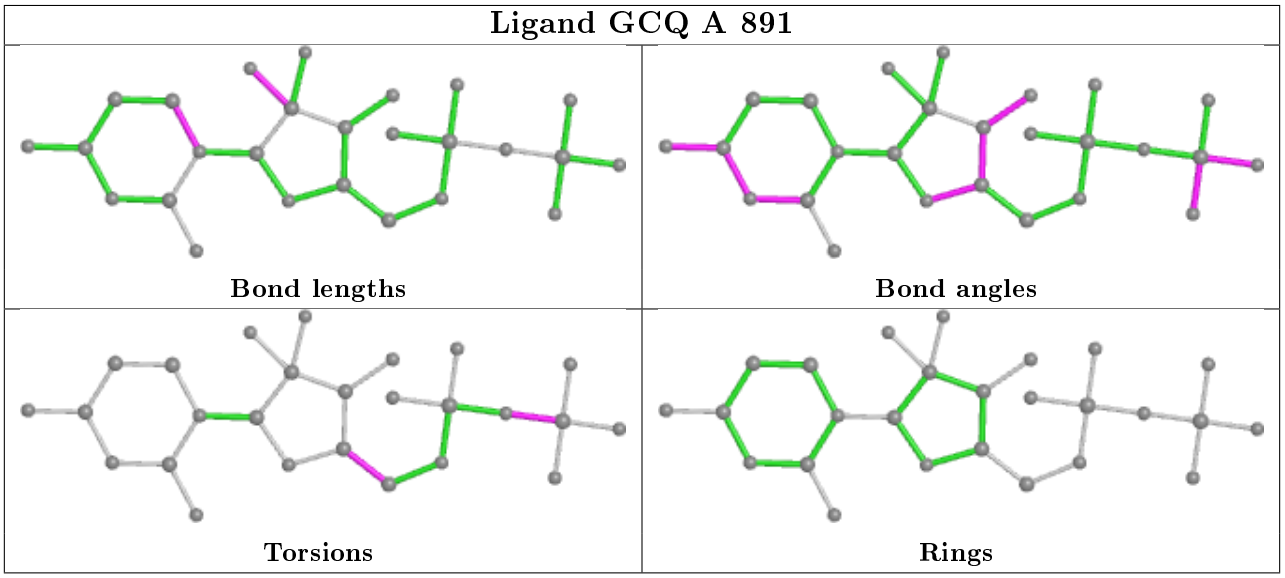
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	890	ANP	4	0

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 890



Ligand GCQ A 891



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	648/888 (72%)	0.20	42 (6%)	18	24	16, 30, 72, 96	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	PHE	8.7
1	A	457	SER	8.0
1	A	460	GLY	6.8
1	A	461	LYS	6.8
1	A	291	ASN	6.3
1	A	462	THR	5.8
1	A	654	ILE	5.4
1	A	661	GLN	5.3
1	A	639	GLN	5.2
1	A	318	HIS	4.7
1	A	659	MET	4.5
1	A	294	PRO	4.4
1	A	145	TYR	4.1
1	A	290	GLY	4.0
1	A	319	GLY	3.7
1	A	320	LYS	3.6
1	A	456	THR	3.4
1	A	321	GLU	3.1
1	A	292	LYS	3.1
1	A	658	GLY	3.0
1	A	459	ASP	3.0
1	A	146	PHE	3.0
1	A	390	TYR	2.9
1	A	664	ILE	2.8
1	A	293	ARG	2.8
1	A	297	PHE	2.8
1	A	653	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	322	GLU	2.6
1	A	90	THR	2.5
1	A	326	ARG	2.5
1	A	162	GLN	2.4
1	A	655	TRP	2.3
1	A	647	ARG	2.3
1	A	148	PHE	2.3
1	A	656	ASP	2.2
1	A	323	ILE	2.2
1	A	91	THR	2.1
1	A	718	ALA	2.1
1	A	717	ARG	2.1
1	A	298	ALA	2.1
1	A	746	GLN	2.0
1	A	604	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 carbohydrates in this entry.

6.4 Ligands (i)

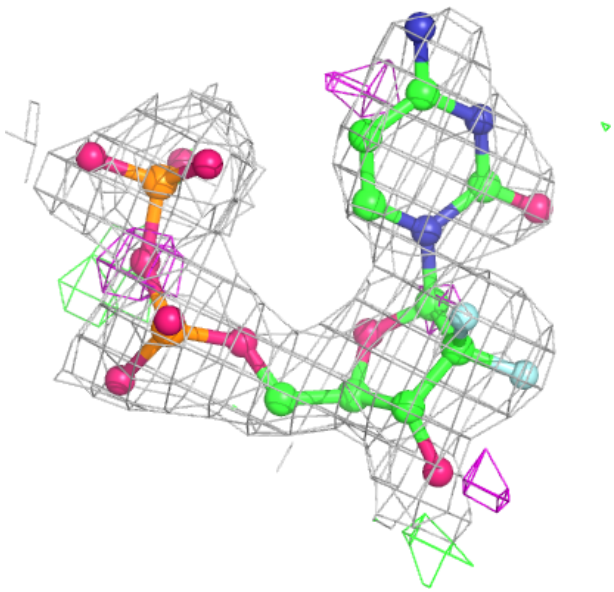
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

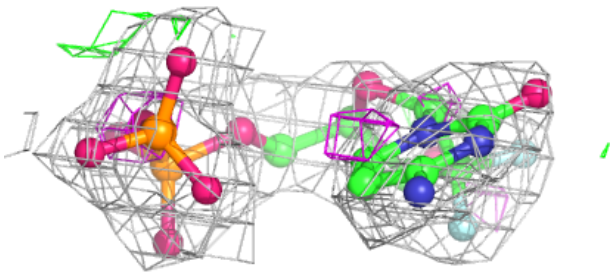
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GCQ	A	891	26/26	0.92	0.18	45,57,60,60	0
2	MG	A	889	1/1	0.94	0.25	31,31,31,31	0
3	ANP	A	890	31/31	0.96	0.14	24,28,35,38	0

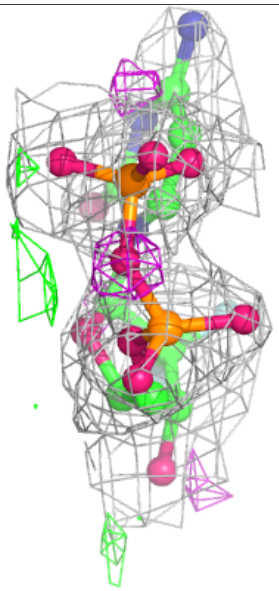
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCQ A 891:

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

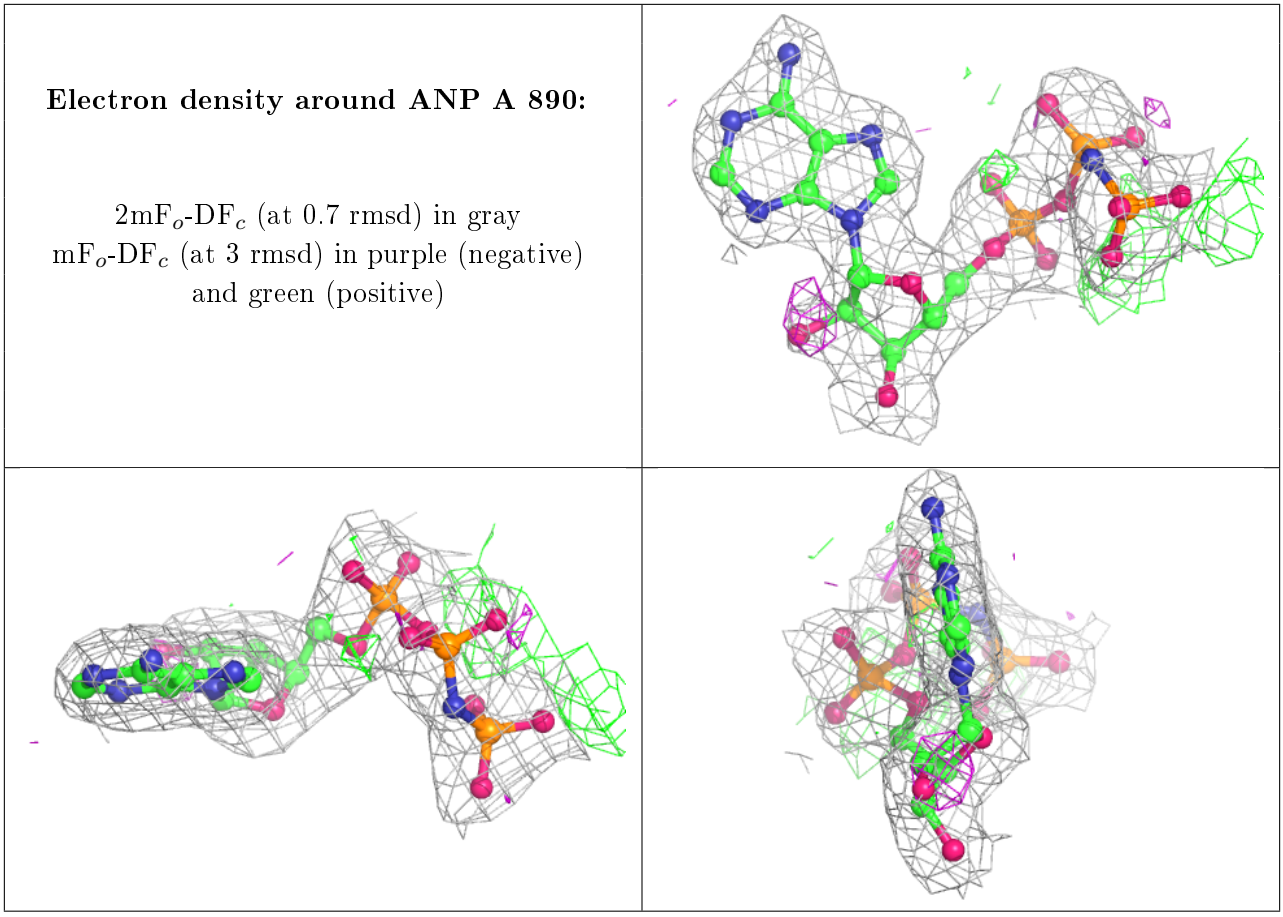






Electron density around ANP A 890:

$2mF_o$-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.