



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:59 AM UTC

PDB ID : 1ZY5 / pdb_00001zy5
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: R794G Hyperactivating Mutant Complexed with AMPPNP.
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.
Deposited on : 2005-06-09
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

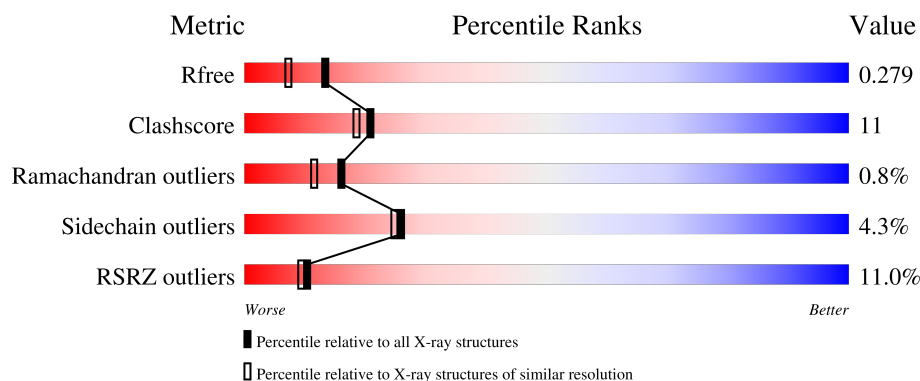
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	5% 72% 15% • 11%
1	B	303	14% 60% 19% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4590 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 Serine/threonine-protein kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	9	0	0
			2236	1434	390	403	9			
1	B	249	Total	C	N	O	S	0	0	0
			2059	1326	354	370	9			

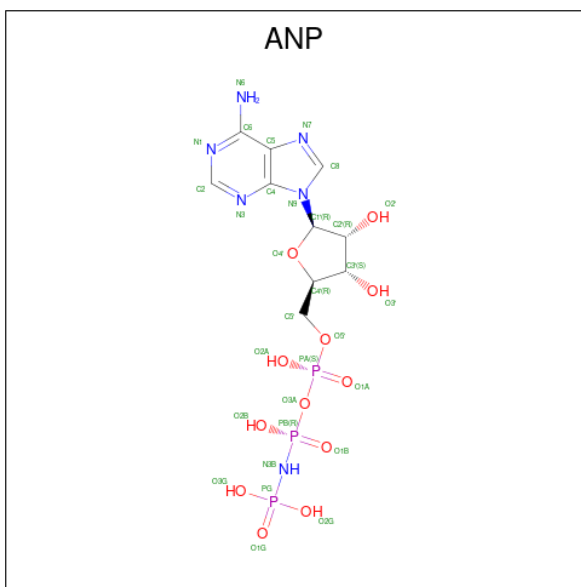
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	cloning artifact	UNP P15442
A	593	LEU	-	cloning artifact	UNP P15442
A	794	GLY	ARG	engineered mutation	UNP P15442
B	592	SER	-	cloning artifact	UNP P15442
B	593	LEU	-	cloning artifact	UNP P15442
B	794	GLY	ARG	engineered mutation	UNP P15442

- 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		
2	B	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 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

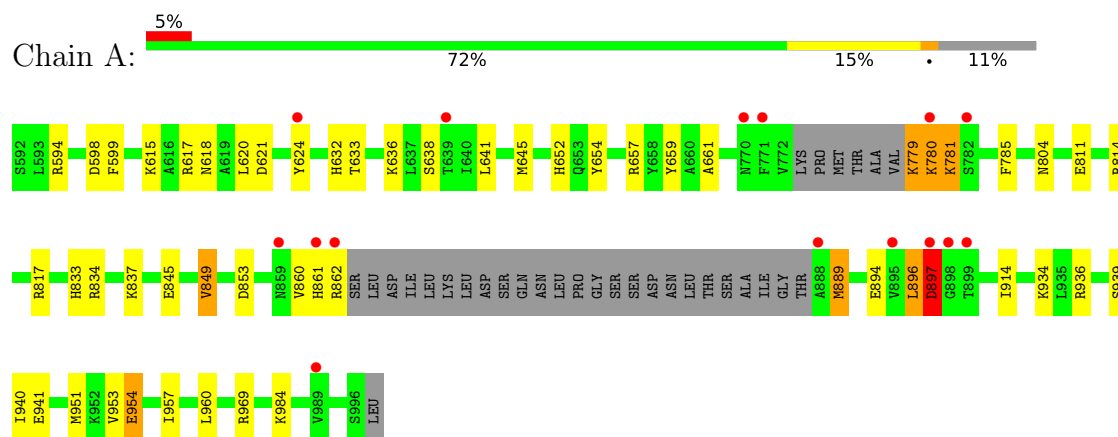
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	156	Total O 156 156	0	0
4	B	75	Total O 75 75	0	0

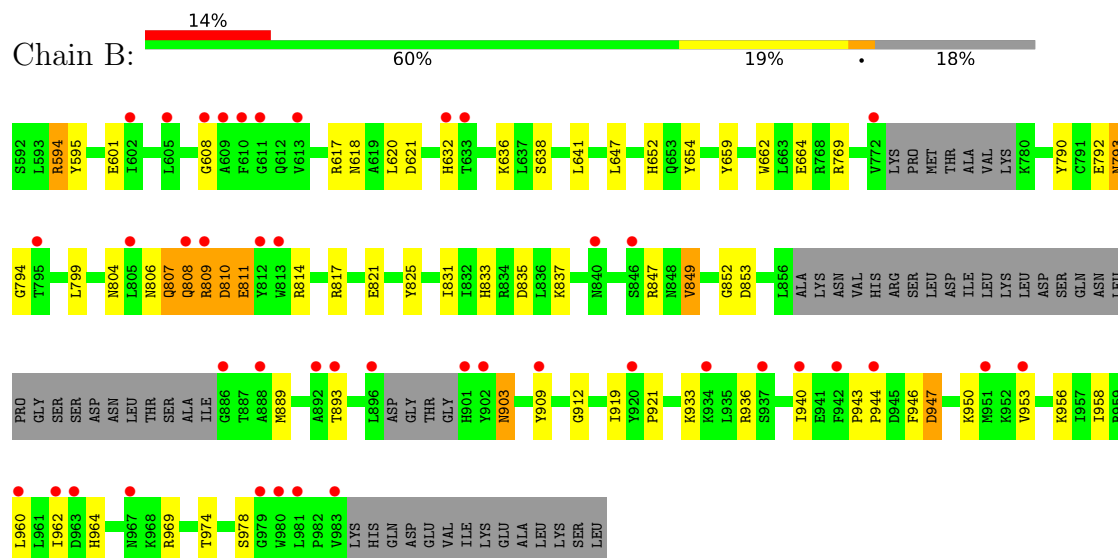
3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase GCN2



- Molecule 1: Serine/threonine-protein kinase GCN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.61Å 78.92Å 146.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.58 – 2.00 36.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (36.58-2.00) 94.4 (36.58-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	CNX 2000.1, REFMAC	Depositor
R, R_{free}	0.235 , 0.279 0.230 , 0.279	Depositor DCC
R_{free} test set	1222 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.9	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	0.93	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: ANP, MG

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	0.47	0/2281	0.94	7/3068 (0.2%)
1	B	0.38	0/2101	1.02	10/2828 (0.4%)
All	All	0.43	0/4382	0.98	17/5896 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	810	ASP	N-CA-C	-15.34	94.62	113.18
1	B	808	GLN	N-CA-C	11.40	127.12	111.74
1	B	809	ARG	N-CA-C	11.30	128.36	110.17
1	B	594	ARG	N-CA-C	7.56	120.18	111.11
1	A	781	LYS	N-CA-C	6.85	120.76	110.14
1	A	594	ARG	N-CA-C	6.66	119.10	111.11
1	A	659	TYR	N-CA-C	6.59	118.25	111.14
1	B	849	VAL	N-CA-C	6.44	117.07	110.05
1	A	598	ASP	N-CA-C	6.38	121.06	113.28
1	A	861	HIS	N-CA-C	-5.54	106.84	113.21
1	B	978	SER	N-CA-C	-5.53	107.18	114.04
1	B	808	GLN	CA-C-N	-5.36	113.53	122.64
1	B	808	GLN	C-N-CA	-5.36	113.53	122.64
1	A	599	PHE	N-CA-C	5.20	117.71	109.50
1	B	659	TYR	N-CA-C	5.16	117.69	111.40
1	B	793	ASN	N-CA-C	-5.15	103.81	110.19
1	A	849	VAL	N-CA-C	5.02	115.53	110.05

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	2236	0	2253	40	0
1	B	2059	0	2068	57	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	2	0
4	A	156	0	0	10	0
4	B	75	0	0	12	1
All	All	4590	0	4347	96	1

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 11.

All (96) 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:821:GLU:HB2	4:B:157:HOH:O	1.38	1.23
1:B:809:ARG:HB3	1:B:811:GLU:HB2	1.45	0.98
1:B:809:ARG:CB	1:B:811:GLU:HB2	2.02	0.90
1:A:953:VAL:HG12	4:A:35:HOH:O	1.70	0.90
1:B:654:TYR:HD1	4:B:157:HOH:O	1.59	0.85
1:B:809:ARG:HB3	1:B:811:GLU:H	1.41	0.85
1:B:790:TYR:CE2	1:B:792:GLU:HB3	2.13	0.82
1:B:889:MET:HE3	1:B:936:ARG:HD3	1.63	0.80
1:B:809:ARG:HG2	1:B:811:GLU:HB2	1.64	0.78
1:A:853:ASP:OD2	4:A:90:HOH:O	2.03	0.76
1:B:809:ARG:CG	1:B:811:GLU:HB2	2.16	0.75
1:B:833:HIS:HD2	1:B:835:ASP:H	1.33	0.75
1:B:809:ARG:HB3	1:B:811:GLU:CB	2.16	0.74
1:A:652:HIS:HD2	1:A:654:TYR:H	1.38	0.72
1:B:654:TYR:CD1	4:B:157:HOH:O	2.36	0.71
1:B:809:ARG:HB3	1:B:811:GLU:N	2.04	0.71
1:B:608:GLY:HA3	4:B:201:HOH:O	1.91	0.70
1:B:632:HIS:CE1	1:B:636:LYS:HD2	2.28	0.69
1:A:957:ILE:HG13	4:A:152:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:HIS:CD2	1:A:654:TYR:H	2.12	0.68
1:B:790:TYR:HE2	1:B:792:GLU:HB3	1.57	0.67
1:B:804:ASN:O	1:B:807:GLN:HB2	1.95	0.66
1:A:845:GLU:HG2	4:A:51:HOH:O	1.97	0.65
1:B:953:VAL:HG12	4:B:184:HOH:O	1.95	0.65
1:B:793:ASN:HB3	4:B:177:HOH:O	1.95	0.65
1:A:618:ASN:HD21	1:A:620:LEU:HB2	1.63	0.64
1:B:889:MET:HE3	1:B:936:ARG:CD	2.27	0.64
1:B:793:ASN:HB2	4:B:117:HOH:O	1.97	0.63
1:B:618:ASN:HD22	1:B:621:ASP:H	1.47	0.63
1:B:811:GLU:CD	1:B:847:ARG:HH12	2.06	0.62
1:A:633:THR:HG21	1:A:779:LYS:HB2	1.82	0.62
1:B:799:LEU:HD11	1:B:847:ARG:HH21	1.64	0.61
1:A:618:ASN:ND2	1:A:620:LEU:H	1.99	0.60
1:B:944:PRO:HD3	4:B:143:HOH:O	2.02	0.59
1:A:617:ARG:HG2	1:A:624:TYR:CE2	2.38	0.59
1:B:853:ASP:OD2	3:B:304:ANP:H5'2	2.02	0.59
1:B:889:MET:HE1	1:B:933:LYS:HG3	1.84	0.58
1:A:951:MET:HB3	1:A:954:GLU:HG2	1.86	0.58
1:B:833:HIS:HE1	1:B:852:GLY:O	1.85	0.58
1:A:618:ASN:HD22	1:A:621:ASP:H	1.53	0.57
1:B:806:ASN:CB	1:B:921:PRO:HD3	2.34	0.57
1:B:595:TYR:OH	1:B:601:GLU:HB3	2.05	0.57
1:B:618:ASN:HD21	1:B:620:LEU:HB2	1.70	0.56
1:B:853:ASP:OD2	3:B:304:ANP:H8	2.05	0.56
1:B:903:ASN:H	1:B:903:ASN:HD22	1.54	0.55
1:A:633:THR:CG2	1:A:779:LYS:HB2	2.36	0.55
1:A:889:MET:HE2	1:A:936:ARG:HD3	1.88	0.54
1:B:652:HIS:CD2	1:B:654:TYR:H	2.26	0.54
1:A:984:LYS:NZ	4:A:174:HOH:O	2.41	0.53
1:B:809:ARG:CB	1:B:811:GLU:H	2.19	0.52
1:B:618:ASN:HB3	1:B:621:ASP:OD2	2.10	0.52
1:B:664:GLU:HB3	1:B:769:ARG:HH12	1.75	0.52
1:A:617:ARG:HG2	1:A:624:TYR:CD2	2.45	0.52
1:B:652:HIS:HD2	1:B:654:TYR:H	1.57	0.52
1:A:845:GLU:CG	4:A:51:HOH:O	2.56	0.51
1:B:889:MET:CE	1:B:936:ARG:HD3	2.37	0.51
1:B:809:ARG:HB3	1:B:811:GLU:CA	2.41	0.50
1:B:944:PRO:HG2	4:B:81:HOH:O	2.11	0.50
1:B:638:SER:HA	1:B:641:LEU:HG	1.93	0.50
1:B:825:TYR:OH	4:B:70:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:HIS:CE1	1:B:852:GLY:O	2.65	0.49
1:B:958:ILE:O	1:B:962:ILE:HG12	2.11	0.49
1:B:647:LEU:HD23	1:B:831:ILE:HD13	1.94	0.49
1:B:806:ASN:HA	1:B:919:ILE:HA	1.94	0.49
1:A:853:ASP:OD2	4:A:205:HOH:O	2.18	0.48
1:B:809:ARG:C	1:B:811:GLU:N	2.66	0.48
1:A:837:LYS:HA	1:A:914:ILE:HD11	1.95	0.48
1:A:934:LYS:HB3	1:A:941:GLU:HB2	1.96	0.47
1:A:953:VAL:HG23	4:A:152:HOH:O	2.13	0.47
1:B:810:ASP:O	1:B:814:ARG:HB2	2.14	0.46
1:A:860:VAL:C	1:A:862:ARG:H	2.22	0.46
1:A:940:ILE:HG22	1:A:940:ILE:O	2.16	0.46
1:A:632:HIS:CE1	1:A:636:LYS:HG3	2.50	0.46
1:A:641:LEU:O	1:A:645:MET:HG2	2.16	0.45
1:A:657:ARG:HD3	4:A:107:HOH:O	2.15	0.45
1:A:645:MET:HE3	1:B:641:LEU:HD22	1.97	0.45
1:A:817:ARG:HD3	4:A:99:HOH:O	2.16	0.45
1:B:893:THR:HG21	1:B:964:HIS:CD2	2.51	0.45
1:A:780:LYS:HE2	1:A:781:LYS:N	2.32	0.45
1:B:594:ARG:HD3	1:B:662:TRP:CD2	2.53	0.44
1:B:793:ASN:CB	4:B:117:HOH:O	2.58	0.44
1:B:794:GLY:HA2	4:B:178:HOH:O	2.18	0.44
1:A:951:MET:HB3	1:A:954:GLU:CG	2.47	0.44
1:B:943:PRO:HG2	1:B:946:PHE:HB2	2.01	0.43
1:A:661:ALA:HA	1:A:785:PHE:O	2.18	0.42
1:A:638:SER:HA	1:A:641:LEU:HG	2.00	0.42
1:B:909:TYR:O	1:B:912:GLY:N	2.54	0.41
1:A:889:MET:HE3	1:A:889:MET:HA	2.03	0.41
1:A:811:GLU:CD	1:A:814:ARG:HH11	2.29	0.41
1:A:833:HIS:O	1:A:834:ARG:HB2	2.21	0.41
1:A:960:LEU:O	1:A:969:ARG:HG3	2.21	0.41
1:A:896:LEU:HB2	1:A:897:ASP:H	1.66	0.40
1:B:617:ARG:HH11	1:B:617:ARG:HG3	1.85	0.40
1:A:615:LYS:HE2	1:A:624:TYR:CD2	2.57	0.40
1:A:894:GLU:OE2	1:A:969:ARG:NH2	2.51	0.40
1:A:939:SER:O	1:A:940:ILE:C	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:GLU:OE1	4:B:218:HOH:O[3_545]	2.16	0.04

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	265/303 (88%)	253 (96%)	10 (4%)	2 (1%)	16	11
1	B	241/303 (80%)	224 (93%)	15 (6%)	2 (1%)	16	11
All	All	506/606 (84%)	477 (94%)	25 (5%)	4 (1%)	16	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	897	ASP
1	B	807	GLN
1	B	947	ASP
1	A	896	LEU

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	243/271 (90%)	236 (97%)	7 (3%)	37	40
1	B	224/271 (83%)	211 (94%)	13 (6%)	18	15
All	All	467/542 (86%)	447 (96%)	20 (4%)	26	25

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	779	LYS
1	A	780	LYS
1	A	804	ASN
1	A	849	VAL
1	A	889	MET
1	A	897	ASP
1	A	954	GLU
1	B	808	GLN
1	B	811	GLU
1	B	817	ARG
1	B	837	LYS
1	B	849	VAL
1	B	903	ASN
1	B	940	ILE
1	B	947	ASP
1	B	950	LYS
1	B	956	LYS
1	B	960	LEU
1	B	969	ARG
1	B	974	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	618	ASN
1	A	652	HIS
1	A	787	GLN
1	A	807	GLN
1	A	840	ASN
1	A	930	ASN
1	A	964	HIS
1	A	977	ASN
1	B	612	GLN
1	B	618	ASN
1	B	652	HIS
1	B	787	GLN
1	B	793	ASN
1	B	833	HIS
1	B	840	ASN
1	B	903	ASN
1	B	964	HIS

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Mol	Chain	Res	Type
1	B	977	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ANP	B	304	2	33,33,33	1.39	5 (15%)	45,52,52	1.89	12 (26%)
3	ANP	A	303	2	33,33,33	1.36	5 (15%)	45,52,52	1.81	11 (24%)

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	B	304	2	-	4/18/38/38	0/3/3/3
3	ANP	A	303	2	-	3/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	304	ANP	C2-N1	3.96	1.41	1.33
3	A	303	ANP	C2-N1	3.71	1.40	1.33
3	B	304	ANP	C2-N3	3.50	1.40	1.33
3	A	303	ANP	C2-N3	3.34	1.39	1.33
3	A	303	ANP	PA-O1A	-2.14	1.43	1.50
3	A	303	ANP	PG-O1G	2.05	1.49	1.46
3	A	303	ANP	C5-N7	-2.05	1.35	1.39
3	B	304	ANP	C5-N7	-2.04	1.35	1.39
3	B	304	ANP	C4-N3	2.03	1.38	1.34
3	B	304	ANP	PA-O3A	2.02	1.61	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	ANP	N3-C2-N1	-6.42	118.86	128.58
3	B	304	ANP	N3-C2-N1	-6.33	119.00	128.58
3	B	304	ANP	C5-C4-N3	-3.70	121.63	126.72
3	A	303	ANP	N9-C8-N7	-3.58	108.86	113.94
3	A	303	ANP	C5-C4-N3	-3.47	121.94	126.72
3	B	304	ANP	C2-N3-C4	3.35	120.01	111.83
3	B	304	ANP	N9-C8-N7	-3.30	109.25	113.94
3	B	304	ANP	O4'-C1'-N9	3.28	114.40	108.09
3	A	303	ANP	C2-N3-C4	3.27	119.81	111.83
3	B	304	ANP	N3-C4-N9	2.95	132.18	127.17
3	A	303	ANP	N3-C4-N9	2.88	132.07	127.17
3	B	304	ANP	C5-N7-C8	2.69	107.68	103.45
3	A	303	ANP	C5-N7-C8	2.67	107.64	103.45
3	B	304	ANP	C2'-C1'-N9	-2.56	106.95	113.30
3	A	303	ANP	O4'-C1'-N9	2.50	112.90	108.09
3	A	303	ANP	C4-N9-C8	2.49	108.35	105.74
3	B	304	ANP	C3'-C2'-C1'	2.30	105.81	101.46
3	B	304	ANP	O2G-PG-O1G	-2.19	107.95	113.45
3	B	304	ANP	C4-N9-C8	2.11	107.95	105.74
3	A	303	ANP	C2'-C1'-N9	-2.08	108.13	113.30
3	B	304	ANP	O1G-PG-N3B	-2.08	108.71	111.77
3	A	303	ANP	C5-C6-N6	-2.06	118.17	123.29
3	A	303	ANP	O2G-PG-O1G	-2.00	108.42	113.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

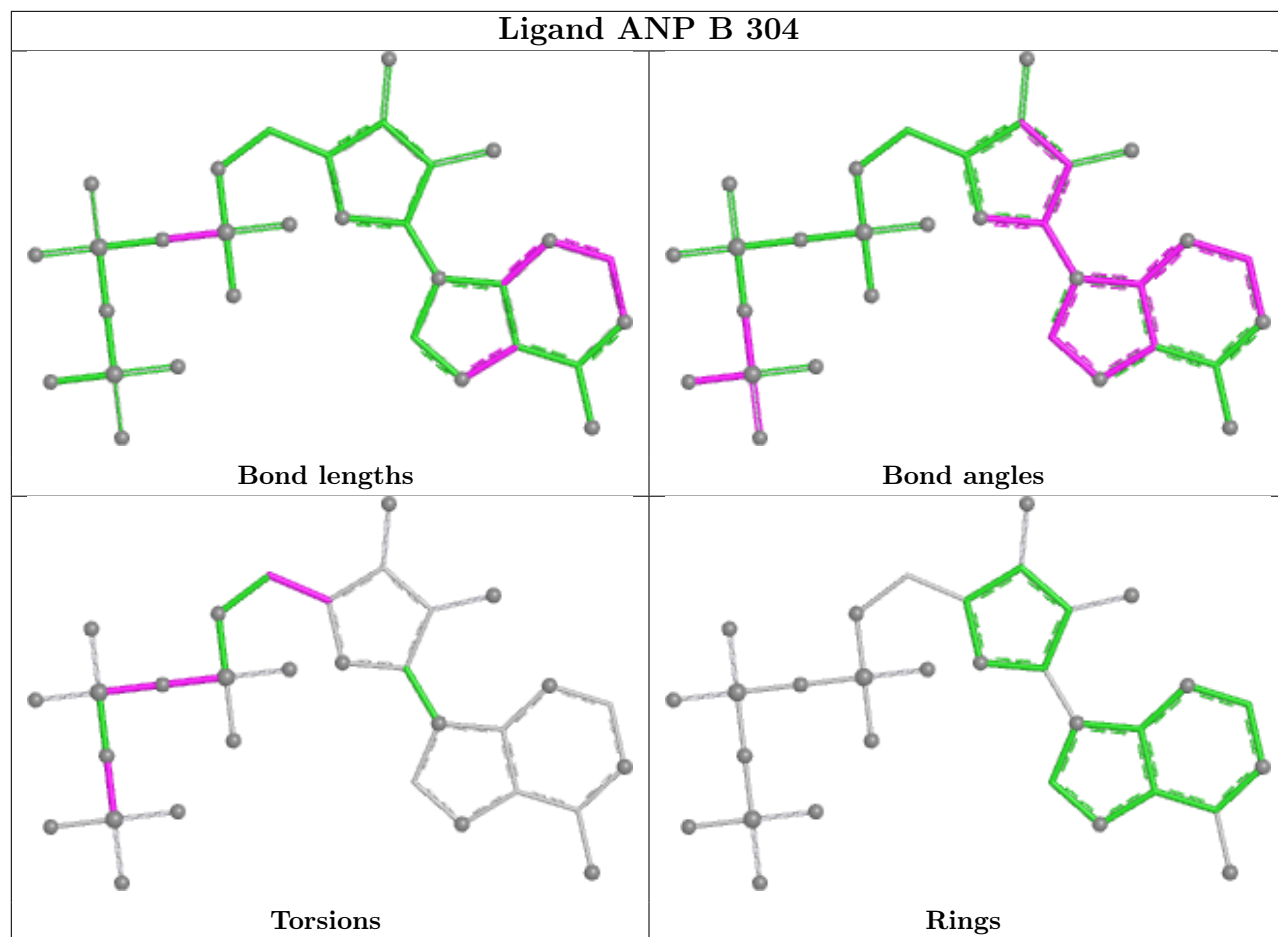
Mol	Chain	Res	Type	Atoms
3	A	303	ANP	PB-N3B-PG-O1G
3	B	304	ANP	PB-N3B-PG-O1G
3	A	303	ANP	C3'-C4'-C5'-O5'
3	B	304	ANP	C3'-C4'-C5'-O5'
3	B	304	ANP	PB-O3A-PA-O2A
3	A	303	ANP	PA-O3A-PB-O1B
3	B	304	ANP	PA-O3A-PB-O1B

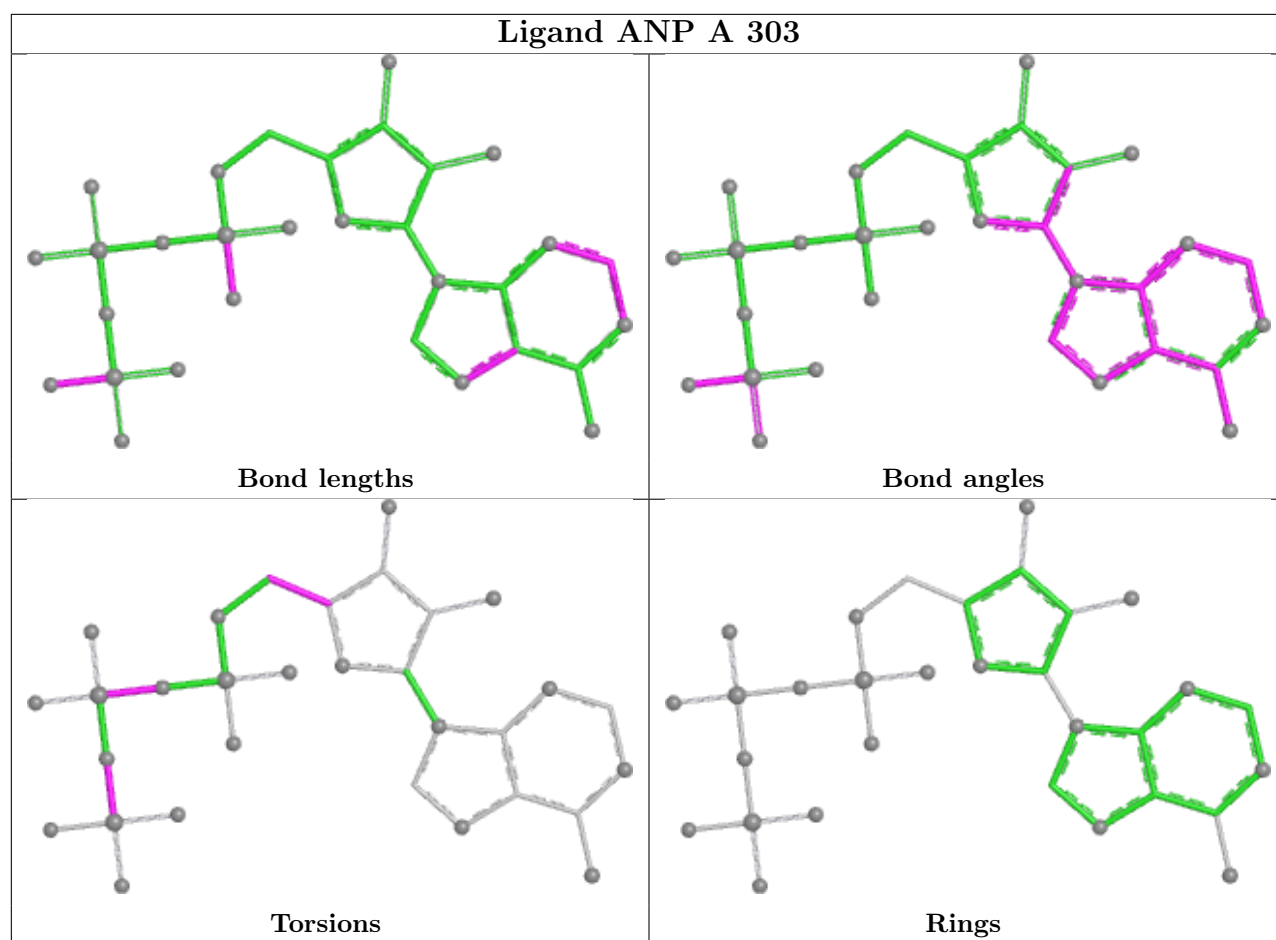
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	ANP	2	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	271/303 (89%)	0.43	15 (5%) 30 29	21, 42, 75, 101	2 (0%)
1	B	249/303 (82%)	1.13	42 (16%) 4 4	27, 59, 92, 104	0
All	All	520/606 (85%)	0.77	57 (10%) 10 9	21, 51, 90, 104	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	602	ILE	5.0
1	B	605	LEU	4.2
1	B	886	GLY	3.6
1	A	861	HIS	3.3
1	B	953	VAL	3.3
1	A	898	GLY	3.2
1	B	979	GLY	3.1
1	B	909	TYR	3.0
1	B	772	VAL	2.9
1	A	771	PHE	2.9
1	A	888	ALA	2.8
1	B	609	ALA	2.8
1	B	888	ALA	2.8
1	B	805	LEU	2.7
1	B	812	TYR	2.7
1	A	780	LYS	2.7
1	B	893	THR	2.6
1	B	940	ILE	2.6
1	B	980	TRP	2.6
1	B	902	TYR	2.6
1	B	611	GLY	2.6
1	B	951	MET	2.6
1	B	967	ASN	2.6
1	B	963	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	840	ASN	2.5
1	B	610	PHE	2.5
1	B	942	PHE	2.5
1	B	960	LEU	2.5
1	B	813	TRP	2.5
1	A	624	TYR	2.4
1	A	639	THR	2.4
1	B	808	GLN	2.4
1	B	937	SER	2.4
1	B	981	LEU	2.4
1	B	608	GLY	2.3
1	B	795	THR	2.3
1	B	892	ALA	2.3
1	B	920	TYR	2.3
1	B	983	VAL	2.3
1	A	862	ARG	2.3
1	B	809	ARG	2.3
1	A	895	VAL	2.2
1	B	613	VAL	2.2
1	B	944	PRO	2.2
1	B	633	THR	2.2
1	A	989	VAL	2.1
1	B	632	HIS	2.1
1	A	899	THR	2.1
1	B	962	ILE	2.1
1	A	897	ASP	2.1
1	B	934	LYS	2.1
1	B	896	LEU	2.0
1	A	859	ASN	2.0
1	B	901	HIS	2.0
1	A	782	SER	2.0
1	B	846	SER	2.0
1	A	770	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](#)

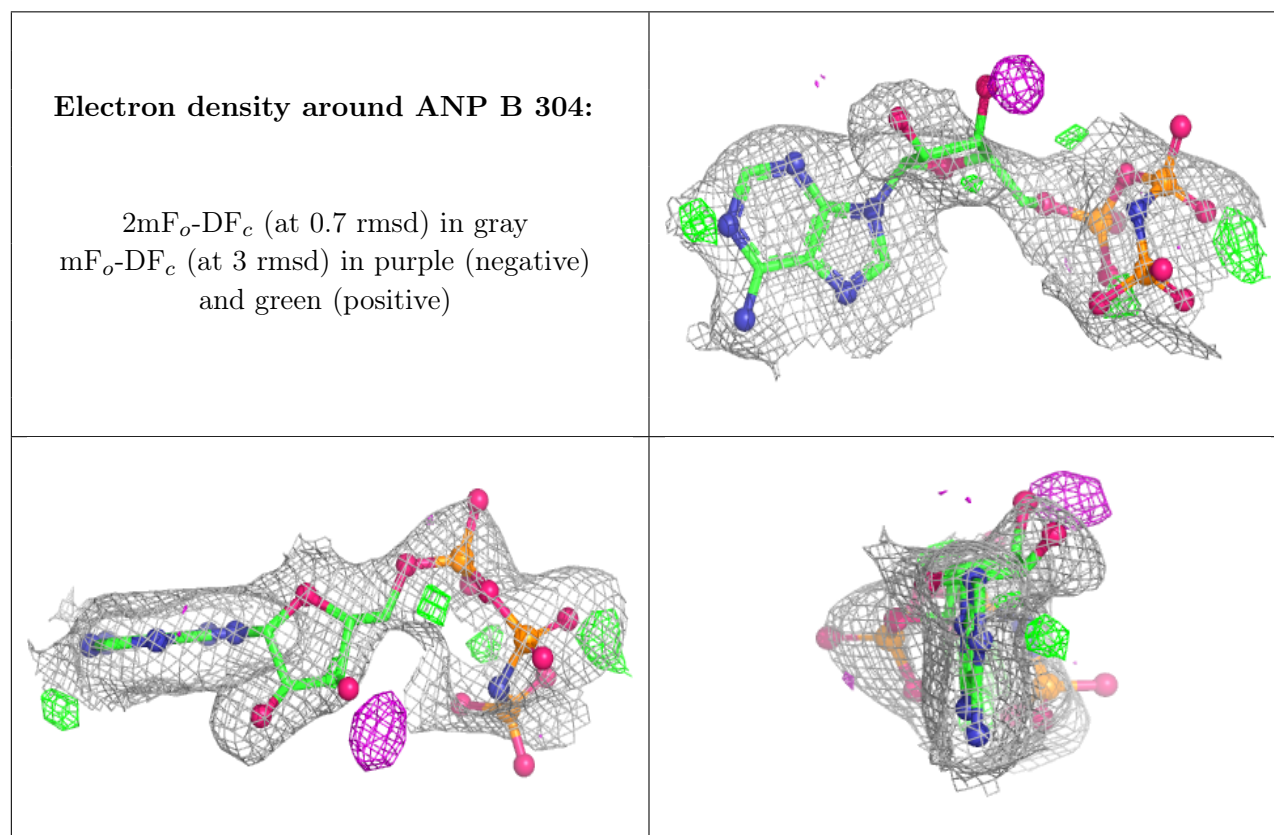
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

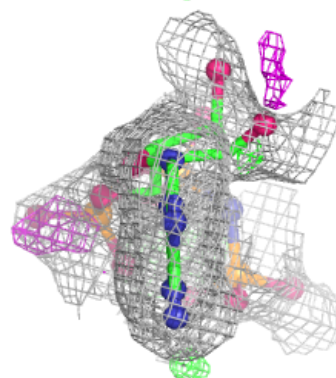
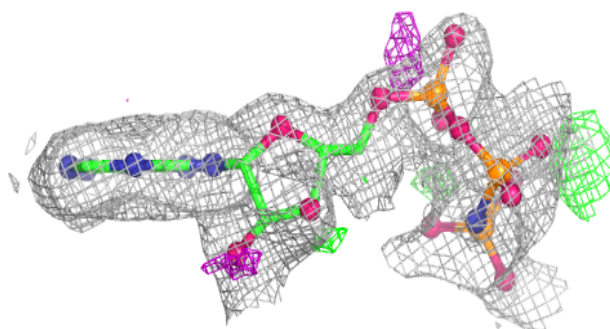
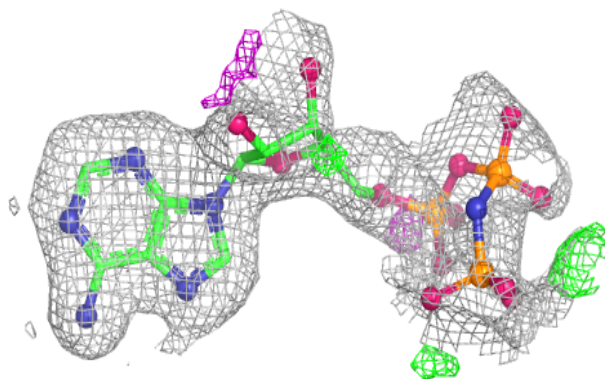
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	B	304	31/31	0.84	0.13	42,74,110,115	0
2	MG	A	305	1/1	0.86	0.10	98,98,98,98	0
2	MG	B	306	1/1	0.87	0.20	94,94,94,94	0
3	ANP	A	303	31/31	0.90	0.11	22,52,92,97	0

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 303:

$2mF_o-DF_c$ (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.