



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:21 PM UTC

PDB ID : 5IDM / pdb_00005idm
Title : Bifunctional histidine kinase CckA (domain, CA) in complex with c-di-GMP and AMPPNP/Mg2+
Authors : Dubey, B.N.; Schirmer, T.
Deposited on : 2016-02-24
Resolution : 1.90 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

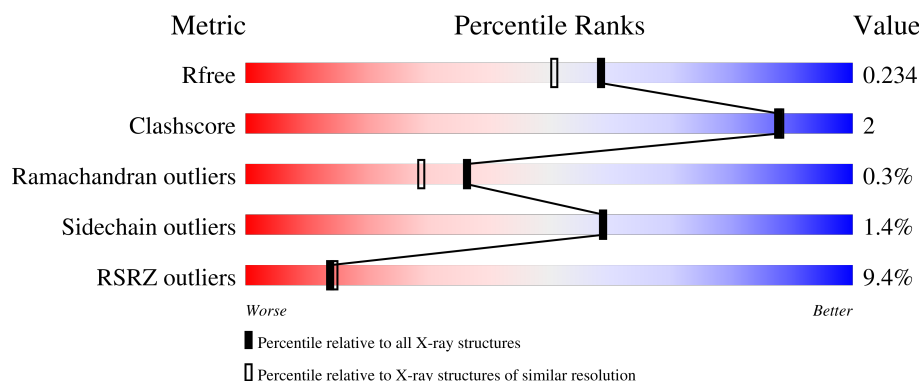
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	179	 4% 93% . ..
1	B	179	 14% 88% 10% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3251 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.

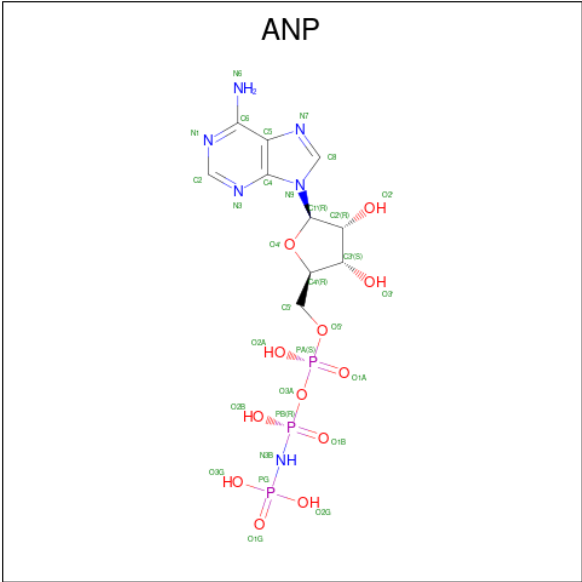
- Molecule 1 is a protein called Cell cycle histidine kinase CckA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	16	0	0
			1365	863	246	254	2			
1	B	177	Total	C	N	O	S	32	0	0
			1370	865	249	254	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	expression tag	UNP Q9X688
A	549	LEU	-	expression tag	UNP Q9X688
A	550	GLU	-	expression tag	UNP Q9X688
A	551	HIS	-	expression tag	UNP Q9X688
A	552	HIS	-	expression tag	UNP Q9X688
A	553	HIS	-	expression tag	UNP Q9X688
A	554	HIS	-	expression tag	UNP Q9X688
A	555	HIS	-	expression tag	UNP Q9X688
A	556	HIS	-	expression tag	UNP Q9X688
B	548	ALA	-	expression tag	UNP Q9X688
B	549	LEU	-	expression tag	UNP Q9X688
B	550	GLU	-	expression tag	UNP Q9X688
B	551	HIS	-	expression tag	UNP Q9X688
B	552	HIS	-	expression tag	UNP Q9X688
B	553	HIS	-	expression tag	UNP Q9X688
B	554	HIS	-	expression tag	UNP Q9X688
B	555	HIS	-	expression tag	UNP Q9X688
B	556	HIS	-	expression tag	UNP Q9X688

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

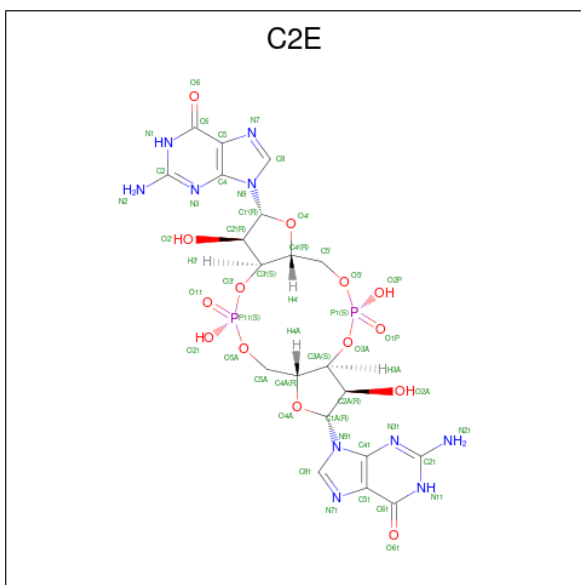


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	223	Total O 223 223	0	0
5	B	183	Total O 183 183	0	0

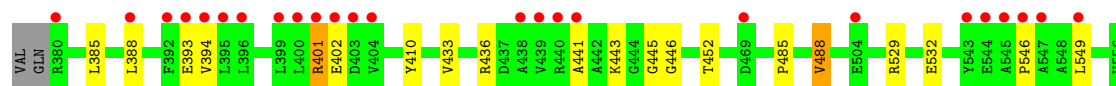
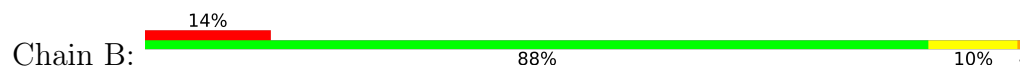
3 Residue-property plots [i](#)

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: Cell cycle histidine kinase CckA



- Molecule 1: Cell cycle histidine kinase CckA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.28Å 62.11Å 103.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.90) 99.0 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.229 0.200 , 0.234	Depositor DCC
R_{free} test set	1492 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3251	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1691e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: C2E, 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	0.77	2/1392 (0.1%)	0.96	4/1888 (0.2%)
1	B	1.22	4/1399 (0.3%)	1.06	6/1896 (0.3%)
All	All	1.02	6/2791 (0.2%)	1.01	10/3784 (0.3%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	ALA	C-N	-31.15	0.87	1.33
1	B	529	ARG	CB-CG	-20.84	0.90	1.52
1	A	532	GLU	CB-CG	-11.93	1.16	1.52
1	A	553	HIS	C-O	9.95	1.37	1.24
1	B	445	GLY	C-N	-8.07	1.22	1.33
1	B	532	GLU	CB-CG	-6.92	1.31	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ARG	CA-CB-CG	14.07	142.25	114.10
1	B	441	ALA	O-C-N	-12.80	106.53	122.27
1	A	532	GLU	CA-CB-CG	10.56	135.22	114.10
1	A	532	GLU	CB-CG-CD	-8.56	98.05	112.60
1	A	546	PRO	N-CA-CB	7.20	110.18	103.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	PRO	N-CA-CB	7.00	110.59	103.25
1	B	532	GLU	CB-CG-CD	6.42	123.52	112.60
1	B	446	GLY	N-CA-C	6.26	120.24	110.91
1	A	401	ARG	CA-CB-CG	-6.17	101.75	114.10
1	B	393	GLU	N-CA-C	5.51	118.00	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	553	HIS	Mainchain,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	1365	0	1357	7	4
1	B	1370	0	1353	7	4
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	46	0	22	0	0
5	A	223	0	0	2	0
5	B	183	0	0	1	0
All	All	3251	0	2758	11	4

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 2.

All (11) 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:552:HIS:CD2	1:A:554:HIS:C	2.67	0.73
1:A:386:GLY:HA2	5:A:719:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:HIS:NE2	1:A:554:HIS:C	2.63	0.57
1:B:394:VAL:HG23	5:B:747:HOH:O	2.12	0.50
1:A:457:ARG:NH1	5:A:704:HOH:O	2.49	0.46
1:B:385:LEU:CD2	1:B:452:THR:OG1	2.66	0.44
1:B:433:VAL:HG13	1:B:436:ARG:NH2	2.33	0.44
1:B:485:PRO:HB2	1:B:488:VAL:HG13	2.00	0.44
1:A:554:HIS:HA	1:B:410:TYR:CE1	2.54	0.43
1:A:515:GLY:HA3	1:B:549:LEU:HG	2.02	0.41
1:A:554:HIS:HA	1:B:410:TYR:CD1	2.54	0.41

All (4) 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:A:529:ARG:NH2	1:B:402:GLU:CG[2_545]	1.70	0.50
1:A:529:ARG:NH2	1:B:401:ARG:O[2_545]	1.75	0.45
1:A:529:ARG:CZ	1:B:402:GLU:CG[2_545]	2.04	0.16
1:A:529:ARG:NE	1:B:402:GLU:CD[2_545]	2.05	0.15

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	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
1	B	175/179 (98%)	169 (97%)	5 (3%)	1 (1%)	21	13
All	All	350/358 (98%)	340 (97%)	9 (3%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	443	LYS

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	141/144 (98%)	140 (99%)	1 (1%)	76	78
1	B	141/144 (98%)	138 (98%)	3 (2%)	47	44
All	All	282/288 (98%)	278 (99%)	4 (1%)	59	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	GLU
1	B	388	LEU
1	B	401	ARG
1	B	488	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	519	GLN
1	B	525	HIS
1	B	527	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
2	ANP	A	601	3	33,33,33	1.99	11 (33%)	45,52,52	1.92	12 (26%)
2	ANP	B	600	3	33,33,33	1.85	10 (30%)	45,52,52	2.04	12 (26%)
4	C2E	A	603	-	52,52,52	1.13	5 (9%)	78,82,82	1.78	17 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	601	3	-	3/18/38/38	0/3/3/3
2	ANP	B	600	3	-	2/18/38/38	0/3/3/3
4	C2E	A	603	-	-	0/30/62/62	0/6/7/7

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ANP	C5-C4	4.76	1.47	1.39
2	A	601	ANP	PB-N3B	4.24	1.74	1.63
2	A	601	ANP	C5-C4	4.21	1.46	1.39
2	A	601	ANP	PG-N3B	3.96	1.73	1.63
2	B	600	ANP	PG-N3B	3.82	1.73	1.63
2	B	600	ANP	PB-N3B	3.51	1.72	1.63
2	A	601	ANP	PG-O1G	3.47	1.51	1.46
2	A	601	ANP	PG-O3G	-3.29	1.48	1.56
2	B	600	ANP	PG-O1G	3.20	1.51	1.46
4	A	603	C2E	C51-C41	3.06	1.47	1.38
2	A	601	ANP	PB-O3A	2.93	1.62	1.59
2	B	600	ANP	PB-O1B	2.77	1.50	1.46
4	A	603	C2E	C5-C4	2.63	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ANP	C4-N9	-2.58	1.32	1.37
2	B	600	ANP	C5-N7	-2.55	1.34	1.39
2	A	601	ANP	C5-N7	-2.52	1.34	1.39
2	A	601	ANP	C4-N9	-2.47	1.32	1.37
2	A	601	ANP	PB-O2B	-2.43	1.50	1.56
4	A	603	C2E	C41-N91	-2.41	1.31	1.38
2	A	601	ANP	C5-C6	2.39	1.47	1.41
2	B	600	ANP	C5-C6	2.38	1.47	1.41
2	A	601	ANP	PB-O1B	2.32	1.49	1.46
2	B	600	ANP	PG-O3G	-2.18	1.51	1.56
2	B	600	ANP	C8-N7	2.17	1.35	1.31
4	A	603	C2E	C61-N11	-2.10	1.34	1.38
4	A	603	C2E	C51-N71	-2.05	1.35	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ANP	O1G-PG-N3B	-6.57	102.10	111.77
4	A	603	C2E	C5-C4-N3	-5.05	120.35	128.39
4	A	603	C2E	C51-C41-N31	-4.95	120.51	128.39
2	B	600	ANP	C5-C4-N3	-4.91	119.96	126.72
2	A	601	ANP	C5-C4-N3	-4.63	120.34	126.72
4	A	603	C2E	C2-N3-C4	4.61	120.23	112.30
2	A	601	ANP	N3-C2-N1	-4.51	121.76	128.58
4	A	603	C2E	N9-C4-N3	4.40	134.75	125.95
2	A	601	ANP	N3-C4-N9	4.27	134.43	127.17
4	A	603	C2E	C21-N31-C41	4.27	119.65	112.30
4	A	603	C2E	N91-C41-N31	4.04	134.02	125.95
2	B	600	ANP	N3-C4-N9	3.99	133.95	127.17
2	B	600	ANP	N3-C2-N1	-3.80	122.83	128.58
2	B	600	ANP	O2B-PB-O1B	3.76	117.93	109.87
2	A	601	ANP	O2B-PB-O1B	3.69	117.78	109.87
2	A	601	ANP	C4-N9-C8	3.59	109.51	105.74
2	A	601	ANP	C2-N3-C4	3.50	120.38	111.83
2	B	600	ANP	C2-N3-C4	3.41	120.17	111.83
4	A	603	C2E	C61-C51-N71	3.07	135.87	130.29
4	A	603	C2E	O4A-C1A-N91	-2.97	101.64	108.36
2	A	601	ANP	O1B-PB-N3B	-2.90	107.50	111.77
2	A	601	ANP	C4-C5-N7	-2.85	107.32	110.58
2	A	601	ANP	C2-N1-C6	2.85	123.41	118.73
4	A	603	C2E	O6-C6-C5	-2.83	119.07	126.53
2	B	600	ANP	C4-C5-N7	-2.76	107.42	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	C2E	C6-C5-N7	2.73	135.26	130.29
2	B	600	ANP	C2-N1-C6	2.70	123.17	118.73
2	B	600	ANP	C4-N9-C8	2.69	108.57	105.74
4	A	603	C2E	O61-C61-C51	-2.68	119.46	126.53
2	A	601	ANP	C5-N7-C8	2.50	107.38	103.45
4	A	603	C2E	C3A-C2A-C1A	2.43	105.23	99.89
2	A	601	ANP	N9-C8-N7	-2.37	110.57	113.94
2	B	600	ANP	C5-N7-C8	2.15	106.83	103.45
4	A	603	C2E	C8-N9-C4	2.13	110.02	106.03
2	A	601	ANP	C6-C5-N7	2.13	136.19	132.09
4	A	603	C2E	C2A-C1A-N91	2.10	119.10	113.25
2	B	600	ANP	C6-C5-N7	2.09	136.11	132.09
4	A	603	C2E	O2P-P1-O1P	2.03	121.89	112.44
4	A	603	C2E	C41-C51-N71	-2.02	107.47	110.67
4	A	603	C2E	C5-C6-N1	2.01	118.37	113.25
2	B	600	ANP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

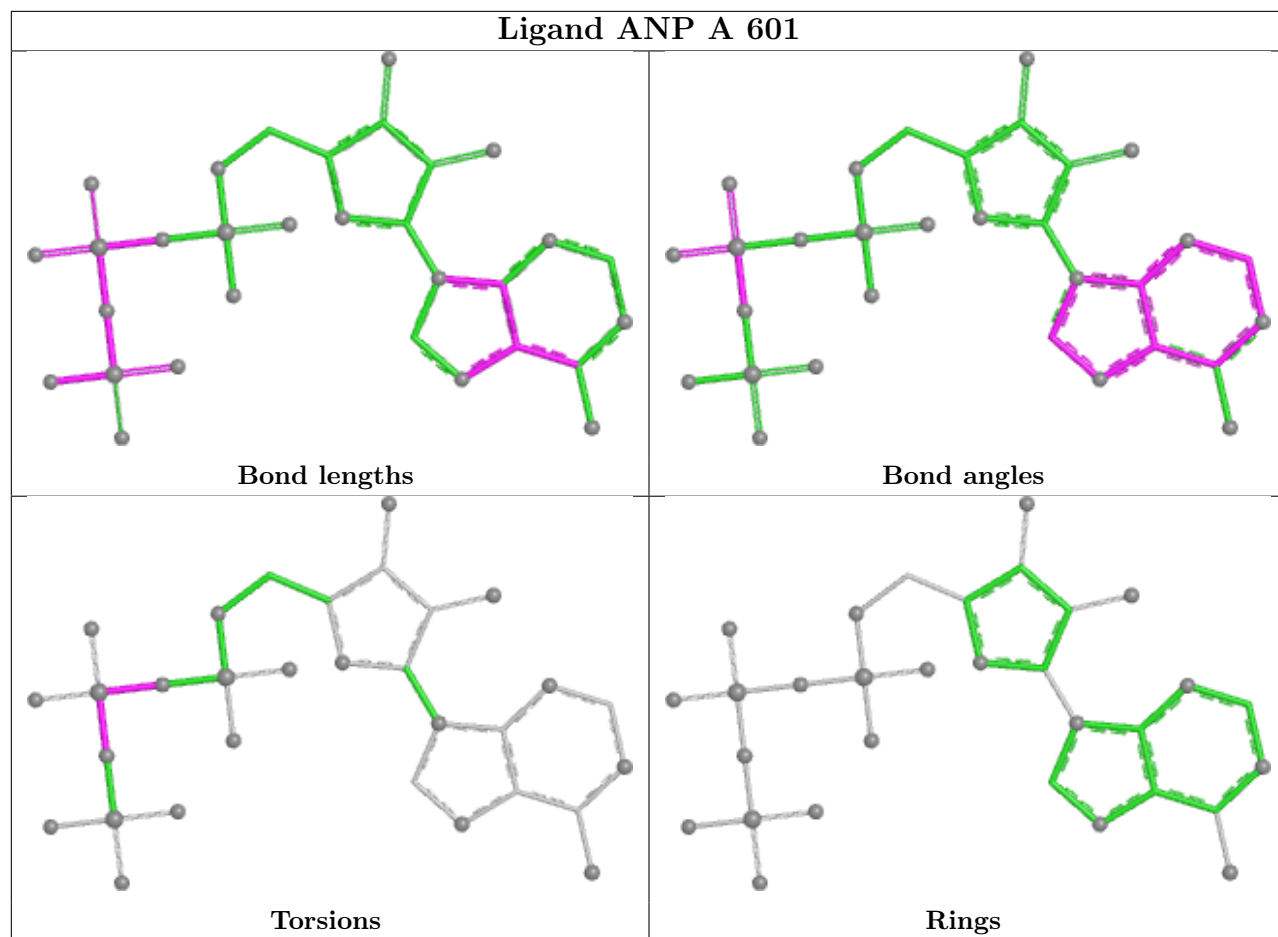
All (5) torsion outliers are listed below:

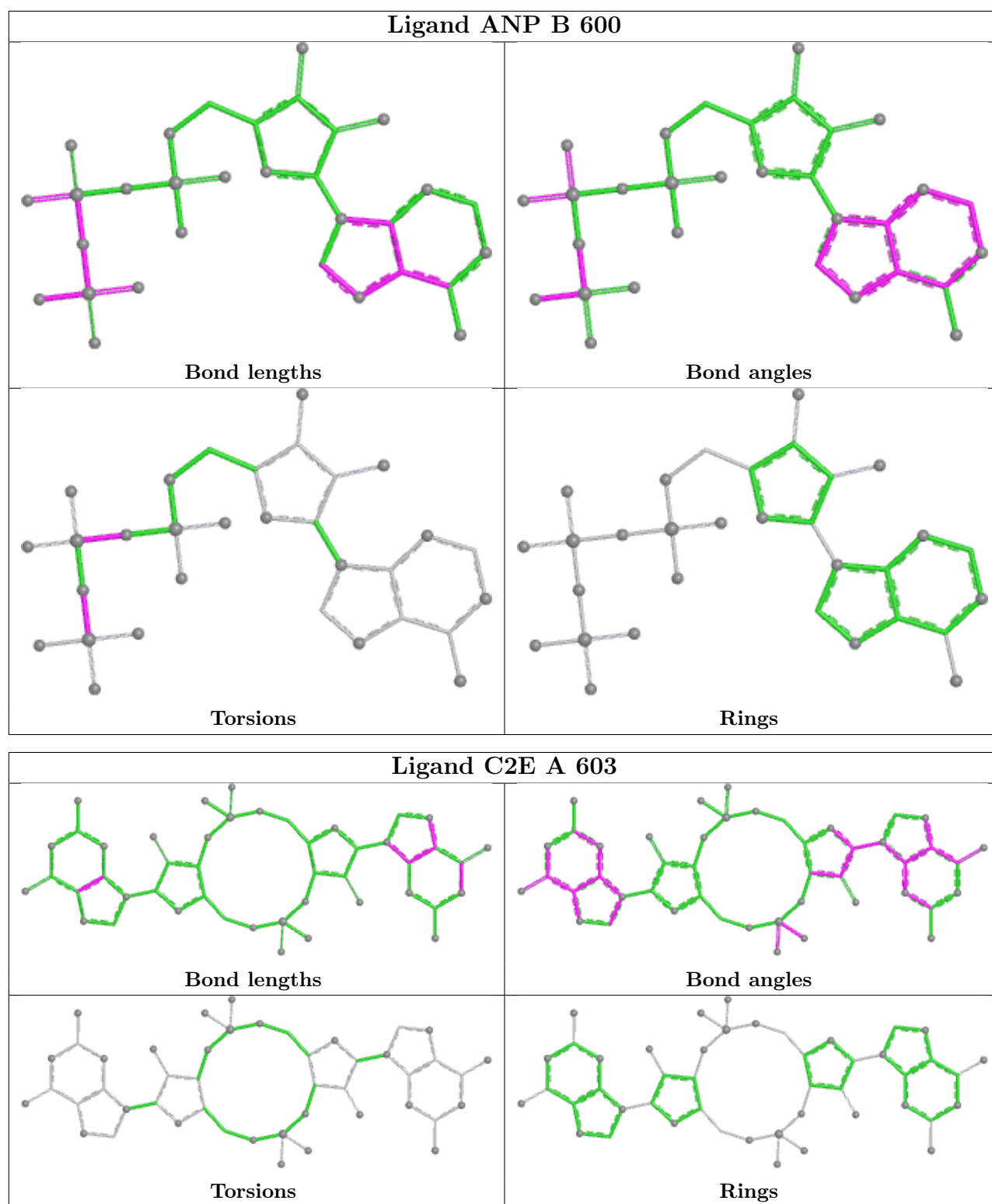
Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
2	B	600	ANP	PB-N3B-PG-O1G
2	B	600	ANP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	441:ALA	C	442:ALA	N	0.87

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	177/179 (98%)	0.26	8 (4%) 38 40	6, 13, 26, 49	3 (1%)
1	B	173/179 (96%)	0.51	25 (14%) 6 6	7, 14, 36, 52	2 (1%)
All	All	350/358 (97%)	0.39	33 (9%) 14 14	6, 14, 34, 52	5 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	VAL	6.9
1	B	547	ALA	6.5
1	A	554	HIS	5.0
1	B	403	ASP	4.8
1	B	402	GLU	4.3
1	B	439	VAL	4.0
1	B	394	VAL	4.0
1	B	392	PHE	3.9
1	B	543	TYR	3.6
1	B	544	GLU	3.0
1	B	546	PRO	2.9
1	B	441	ALA	2.9
1	B	399	LEU	2.8
1	B	400	LEU	2.8
1	A	531	ASN	2.7
1	B	545	ALA	2.7
1	B	395	LEU	2.6
1	B	388	LEU	2.5
1	B	549	LEU	2.5
1	B	401	ARG	2.5
1	B	469	ASP	2.5
1	B	380	ARG	2.4
1	A	552	HIS	2.3
1	A	440	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	440	ARG	2.2
1	B	396	LEU	2.2
1	A	553	HIS	2.2
1	A	394	VAL	2.2
1	A	410	TYR	2.1
1	B	393	GLU	2.1
1	B	504	GLU	2.0
1	B	404	VAL	2.0
1	B	438	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

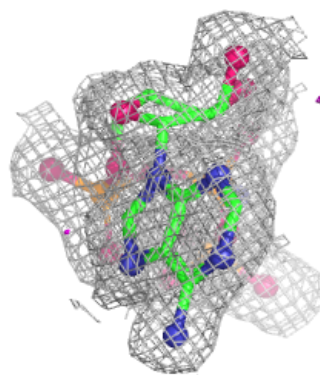
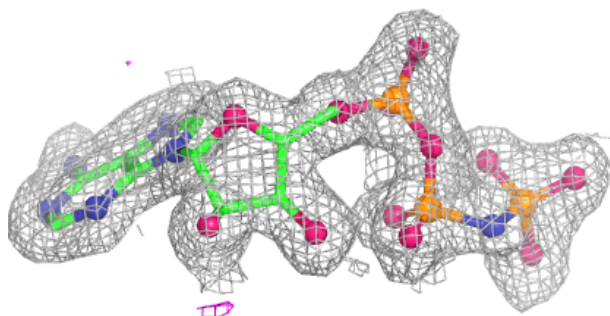
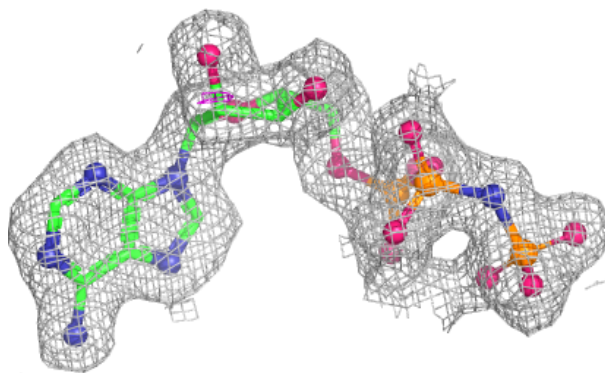
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	A	602	1/1	0.97	0.03	8,8,8,8	0
2	ANP	B	600	31/31	0.98	0.04	7,8,12,12	0
2	ANP	A	601	31/31	0.98	0.04	6,7,11,11	0
3	MG	B	601	1/1	0.98	0.02	12,12,12,12	0
4	C2E	A	603	46/46	0.98	0.04	6,7,7,8	0

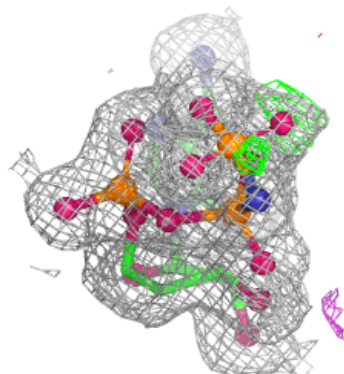
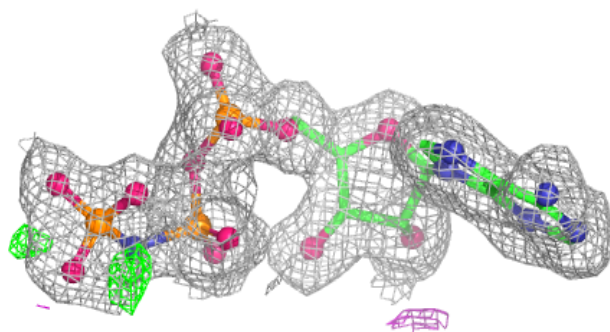
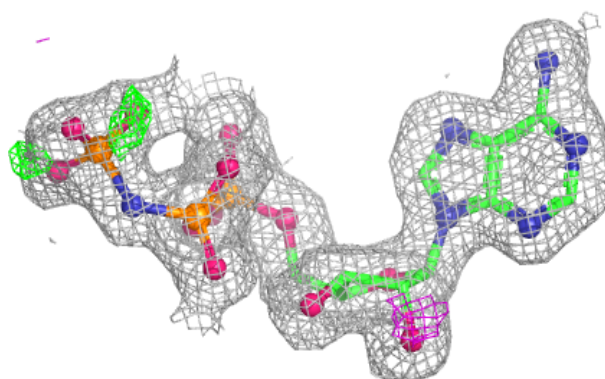
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 600:

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

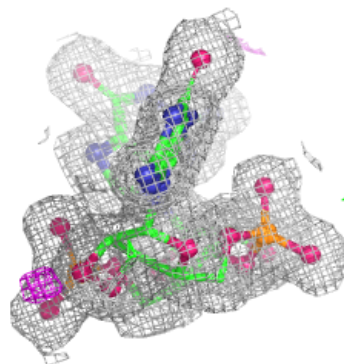
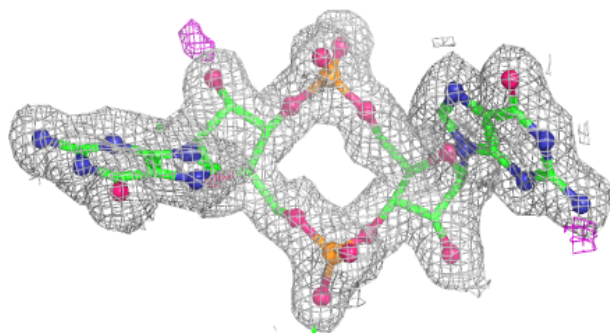
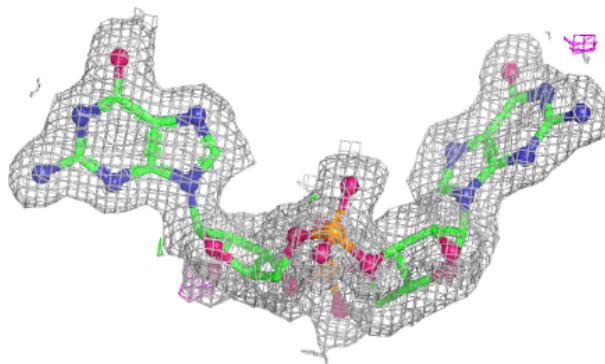
**Electron density around ANP A 601:**

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



Electron density around C2E A 603:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.