Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 06:32 PM EDT

PDB ID	:	3FHI
Title	:	Crystal structure of a complex between the catalytic and regulatory (RI{alpha}) subunits of PKA
Authors	:	Kim, C.
Deposited on	:	2008-12-09
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 (i) symbol.

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

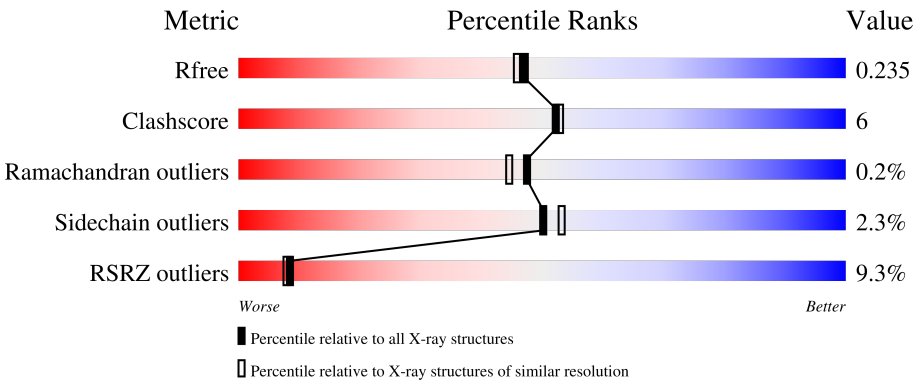
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	350	10% 87% 9% ·
2	B	154	7% 79% 16% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4034 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	338	2695	1751	454	481	2	7	0	0	0

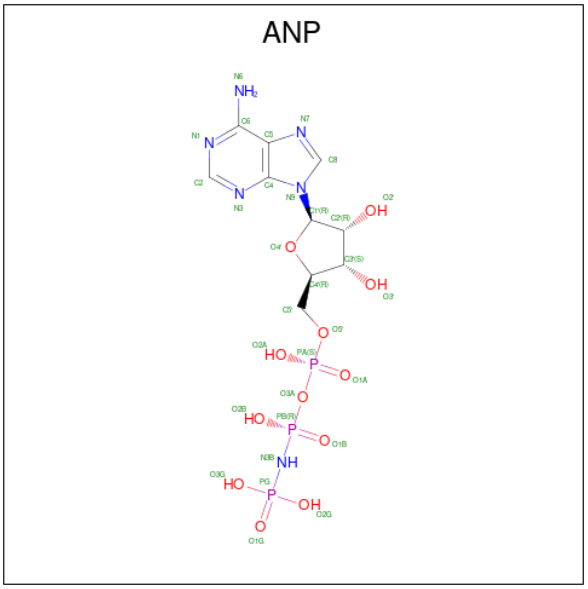
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	CYS	engineered mutation	UNP P05132

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	150	1147	724	197	222	4	0	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	2	2	2	0	0

- Molecule 5 is water.

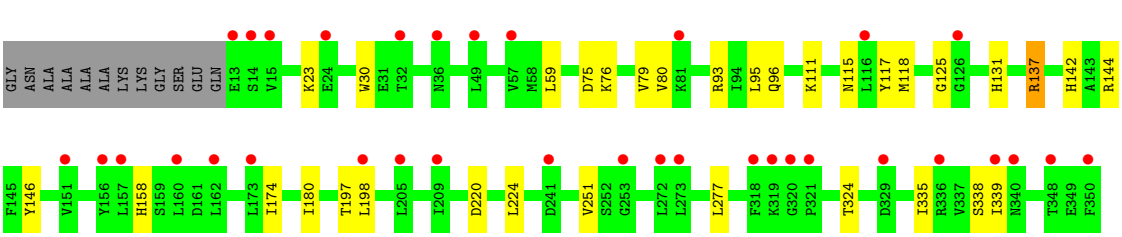
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	157	157	157	0	0
			Total	O		
5	B	2	2	2	0	0

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.

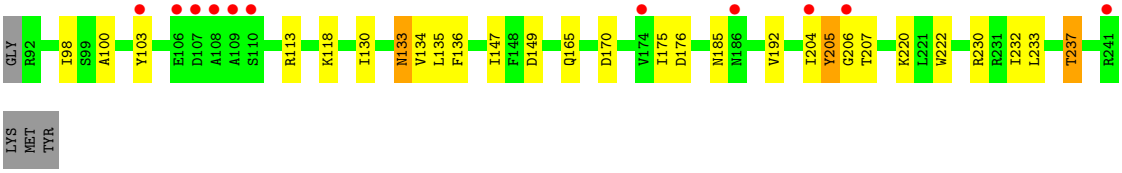
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain A:



• Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.45Å 93.02Å 122.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.00) 99.2 (19.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.226 0.216 , 0.235	Depositor DCC
R_{free} test set	2136 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4034	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: MN, ANP, TPO, SEP

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	0.55	0/2742	0.65	4/3710 (0.1%)
2	B	0.57	0/1167	0.74	0/1580
All	All	0.56	0/3909	0.68	4/5290 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	A	144	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	137	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	137	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	205	TYR	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	2695	0	2613	22	0
2	B	1147	0	1097	24	0
3	A	31	0	13	0	0
4	A	2	0	0	0	0
5	A	157	0	0	3	0
5	B	2	0	0	0	0
All	All	4034	0	3723	42	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 6.

All (42) 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:251:VAL:HG21	2:B:134:VAL:CG2	2.14	0.78
2:B:233:LEU:O	2:B:237:THR:HG23	1.92	0.70
1:A:174:ILE:HD13	1:A:180:ILE:HD13	1.77	0.66
1:A:76:LYS:O	1:A:80:VAL:HG23	1.97	0.65
1:A:198:LEU:HD13	2:B:204:ILE:HB	1.81	0.63
1:A:251:VAL:HG21	2:B:134:VAL:HG23	1.81	0.61
2:B:165:GLN:HE22	2:B:185:ASN:ND2	2.00	0.59
2:B:103:TYR:CZ	2:B:230:ARG:NH2	2.71	0.58
2:B:133:ASN:HD22	2:B:135:LEU:H	1.52	0.57
2:B:113:ARG:CD	2:B:232:ILE:HG12	2.34	0.57
5:A:460:HOH:O	2:B:100:ALA:HB3	2.05	0.55
2:B:98:ILE:HD13	2:B:205:TYR:CZ	2.43	0.54
1:A:174:ILE:HD13	1:A:180:ILE:CD1	2.37	0.53
1:A:125:GLY:O	1:A:131:HIS:HE1	1.91	0.53
1:A:59:LEU:HD22	1:A:324:THR:CG2	2.40	0.51
2:B:176:ASP:HB3	2:B:220:LYS:HG3	1.91	0.51
1:A:125:GLY:O	1:A:131:HIS:CE1	2.63	0.51
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.93	0.51
1:A:174:ILE:CD1	1:A:180:ILE:HD13	2.41	0.50
2:B:136:PHE:HE1	2:B:147:ILE:HG21	1.78	0.49
2:B:205:TYR:HB2	2:B:206:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TRP:CH2	1:A:93:ARG:HD3	2.48	0.49
2:B:165:GLN:HE22	2:B:185:ASN:HD22	1.61	0.48
2:B:130:ILE:HD12	2:B:136:PHE:HB3	1.94	0.48
2:B:175:ILE:HD12	2:B:192:VAL:HG12	1.95	0.48
2:B:98:ILE:HD13	2:B:205:TYR:CE1	2.49	0.48
1:A:174:ILE:CD1	1:A:180:ILE:CD1	2.92	0.47
1:A:142:HIS:HE1	1:A:146:TYR:OH	1.98	0.47
2:B:113:ARG:HH12	2:B:149:ASP:HB2	1.81	0.46
2:B:113:ARG:HD2	2:B:232:ILE:HG12	1.97	0.46
1:A:142:HIS:CE1	1:A:146:TYR:CE2	3.04	0.46
1:A:75:ASP:O	1:A:79:VAL:HG23	2.18	0.43
2:B:118:LYS:HE3	2:B:222:TRP:CZ3	2.53	0.42
2:B:133:ASN:ND2	2:B:135:LEU:H	2.16	0.42
1:A:158:HIS:HD2	5:A:360:HOH:O	2.02	0.42
1:A:93:ARG:O	1:A:96:GLN:HG3	2.19	0.42
1:A:95:LEU:HD23	1:A:118:MET:CE	2.51	0.41
1:A:251:VAL:HG21	2:B:134:VAL:HG21	1.99	0.41
2:B:133:ASN:HD22	2:B:133:ASN:C	2.24	0.41
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.56	0.40
1:A:142:HIS:HD2	5:A:359:HOH:O	2.03	0.40
2:B:205:TYR:HD2	2:B:207:THR:HG23	1.86	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	334/350 (95%)	323 (97%)	10 (3%)	1 (0%)	41 37
2	B	148/154 (96%)	148 (100%)	0	0	100 100
All	All	482/504 (96%)	471 (98%)	10 (2%)	1 (0%)	47 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ILE

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	272/302 (90%)	266 (98%)	6 (2%)	52	55
2	B	114/126 (90%)	111 (97%)	3 (3%)	46	48
All	All	386/428 (90%)	377 (98%)	9 (2%)	50	53

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	111	LYS
1	A	137	ARG
1	A	224	LEU
1	A	277	LEU
1	A	339	ILE
2	B	133	ASN
2	B	170	ASP
2	B	237	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	67	ASN
1	A	113	ASN
1	A	131	HIS
1	A	142	HIS
1	A	158	HIS
1	A	260	HIS

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Mol	Chain	Res	Type
1	A	271	ASN
1	A	307	GLN
2	B	133	ASN
2	B	185	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	TPO	A	197	1	8,10,11	1.11	1 (12%)	10,14,16	1.02	1 (10%)
1	SEP	A	338	1	8,9,10	0.66	0	8,12,14	2.55	1 (12%)

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
1	TPO	A	197	1	-	0/9/11/13	-
1	SEP	A	338	1	-	2/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	TPO	P-O1P	2.40	1.58	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-CB-CA	6.31	114.29	108.14
1	A	197	TPO	P-OG1-CB	-2.00	117.17	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	400	4	29,33,33	2.87	8 (27%)	31,52,52	2.12	11 (35%)

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	400	4	-	1/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ANP	PG-O1G	9.42	1.61	1.46
3	A	400	ANP	PB-O1B	7.98	1.58	1.46
3	A	400	ANP	C4-N3	4.69	1.42	1.35
3	A	400	ANP	PB-N3B	4.30	1.74	1.63
3	A	400	ANP	PG-N3B	3.48	1.72	1.63
3	A	400	ANP	PA-O1A	2.65	1.60	1.50
3	A	400	ANP	C2'-C1'	-2.33	1.50	1.53
3	A	400	ANP	PB-O3A	2.31	1.62	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	ANP	O1B-PB-N3B	-5.09	104.28	111.77
3	A	400	ANP	C3'-C2'-C1'	4.99	108.50	100.98
3	A	400	ANP	N3-C2-N1	-4.45	121.72	128.68
3	A	400	ANP	C4-C5-N7	-3.91	105.33	109.40
3	A	400	ANP	O1G-PG-N3B	-3.04	107.30	111.77
3	A	400	ANP	O3'-C3'-C4'	2.43	118.07	111.05
3	A	400	ANP	O2'-C2'-C1'	-2.42	101.90	110.85
3	A	400	ANP	O3G-PG-O1G	2.40	119.49	113.45
3	A	400	ANP	C2-N1-C6	2.40	122.85	118.75
3	A	400	ANP	O2B-PB-O3A	2.08	111.58	104.64
3	A	400	ANP	O3'-C3'-C2'	2.06	118.49	111.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	ANP	PG-N3B-PB-O1B

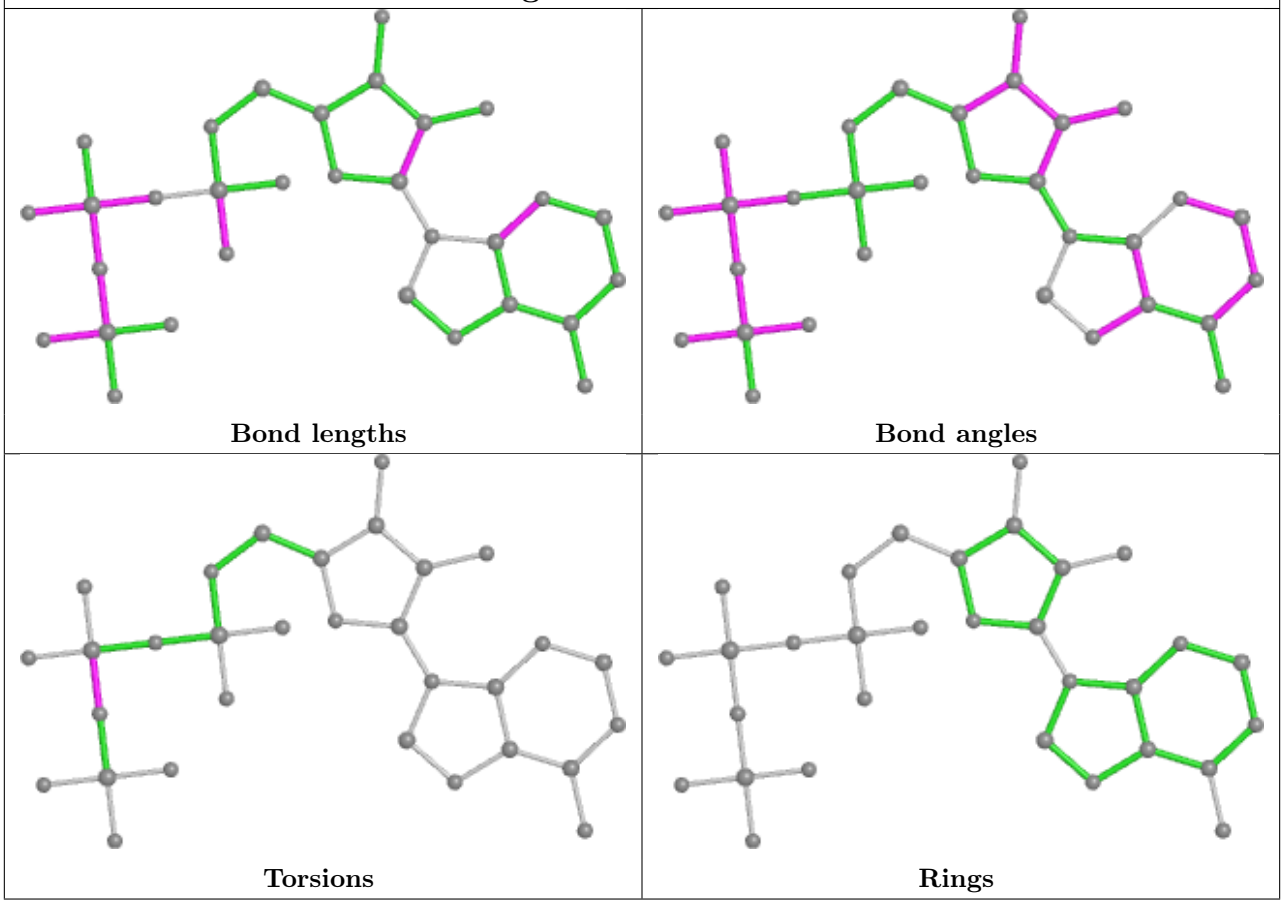
There are no ring outliers.

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 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 400



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	336/350 (96%)	0.65	34 (10%) 7 6	31, 44, 56, 67	0
2	B	150/154 (97%)	0.58	11 (7%) 15 14	36, 44, 59, 64	1 (0%)
All	All	486/504 (96%)	0.63	45 (9%) 8 8	31, 44, 58, 67	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	109	ALA	8.6
1	A	57	VAL	4.6
1	A	320	GLY	4.4
1	A	15	VAL	4.2
1	A	340	ASN	3.9
1	A	14	SER	3.8
2	B	110	SER	3.7
1	A	49	LEU	3.4
1	A	198	LEU	3.3
2	B	204	ILE	3.3
1	A	321	PRO	3.3
1	A	205	LEU	3.3
2	B	186	ASN	3.1
2	B	106	GLU	3.1
1	A	32	THR	3.0
1	A	339	ILE	2.9
1	A	318	PHE	2.9
1	A	348	THR	2.8
1	A	272	LEU	2.8
1	A	241	ASP	2.8
2	B	103	TYR	2.8
1	A	160	LEU	2.7
1	A	36	ASN	2.7
2	B	107	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	2.6
1	A	173	LEU	2.6
2	B	206	GLY	2.5
1	A	329	ASP	2.5
1	A	156	TYR	2.5
2	B	241	ARG	2.5
1	A	273	LEU	2.4
1	A	319	LYS	2.4
1	A	209	ILE	2.4
1	A	151	VAL	2.4
1	A	253	GLY	2.3
2	B	108	ALA	2.3
2	B	174	VAL	2.3
1	A	126	GLY	2.3
1	A	24	GLU	2.3
1	A	350	PHE	2.3
1	A	162	LEU	2.2
1	A	81	LYS	2.2
1	A	157	LEU	2.1
1	A	336	ARG	2.1
1	A	13	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	A	338	10/11	0.93	0.20	46,47,49,49	0
1	TPO	A	197	11/12	0.96	0.16	39,42,44,44	0

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,

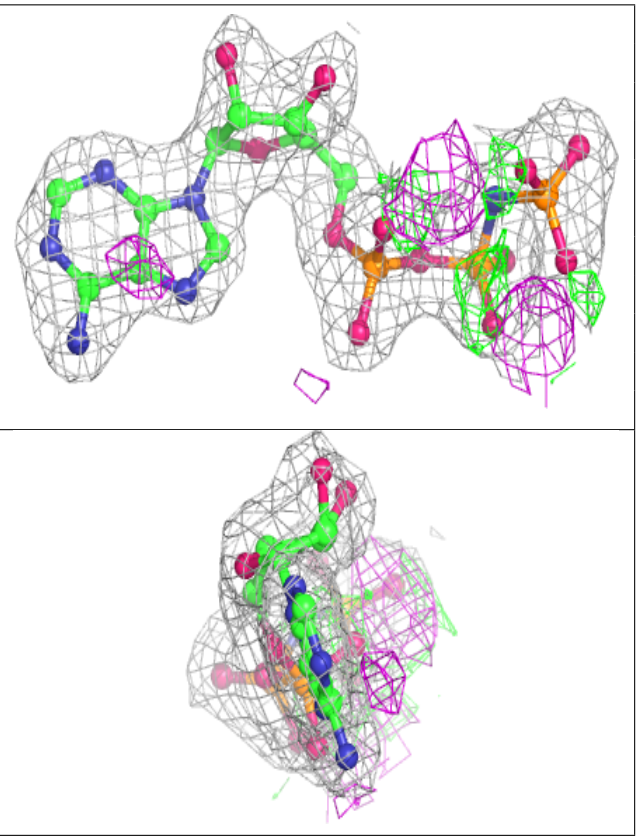
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANP	A	400	31/31	0.96	0.17	14,21,24,26	0
4	MN	A	402	1/1	0.98	0.08	2,2,2,2	0
4	MN	A	401	1/1	0.99	0.07	2,2,2,2	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 400:

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.