wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 06:51 PM EST

PDB ID	:	1JQH
Title	:	IGF-1 receptor kinase domain
Authors	:	Pautsch, A.; Zoephel, A.; Ahorn, H.; Spevak, W.; Hauptmann, R.; Nar, H.
Deposited on	:	2001-08-07
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

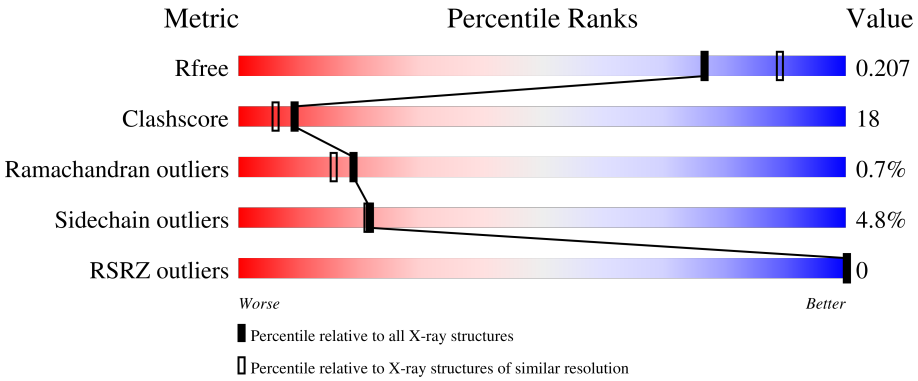
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	308	66% 27% • 6%
1	B	308	63% 27% • 7%
1	C	308	63% 28% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7292 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 IGF-1 receptor kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			
1	B	287	Total	C	N	O	S	0	0	0
			2291	1458	383	428	22			
1	C	291	Total	C	N	O	S	0	0	0
			2320	1477	387	434	22			

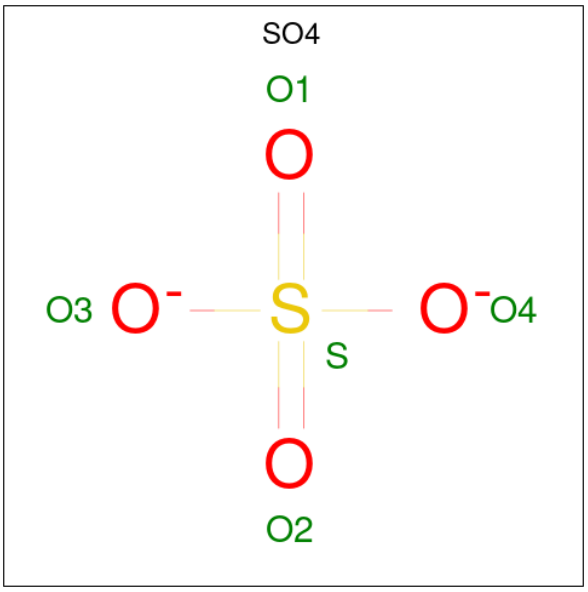
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	GLU	engineered mutation	UNP P08069
A	980	SER	TYR	engineered mutation	UNP P08069
B	979	GLY	GLU	engineered mutation	UNP P08069
B	980	SER	TYR	engineered mutation	UNP P08069
C	979	GLY	GLU	engineered mutation	UNP P08069
C	980	SER	TYR	engineered mutation	UNP P08069

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

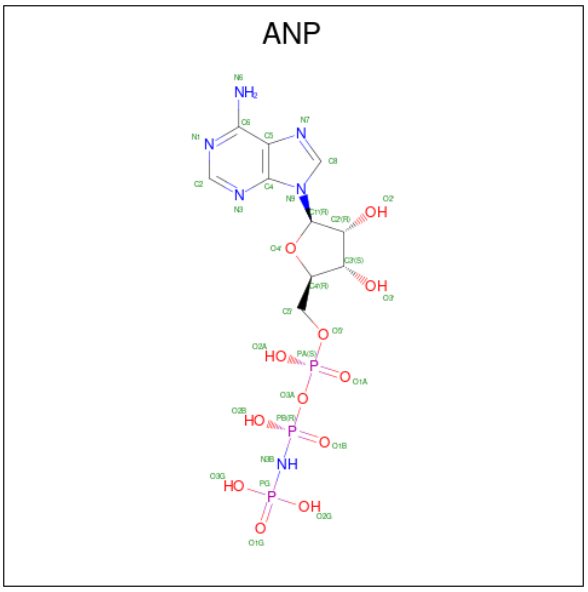
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is water.

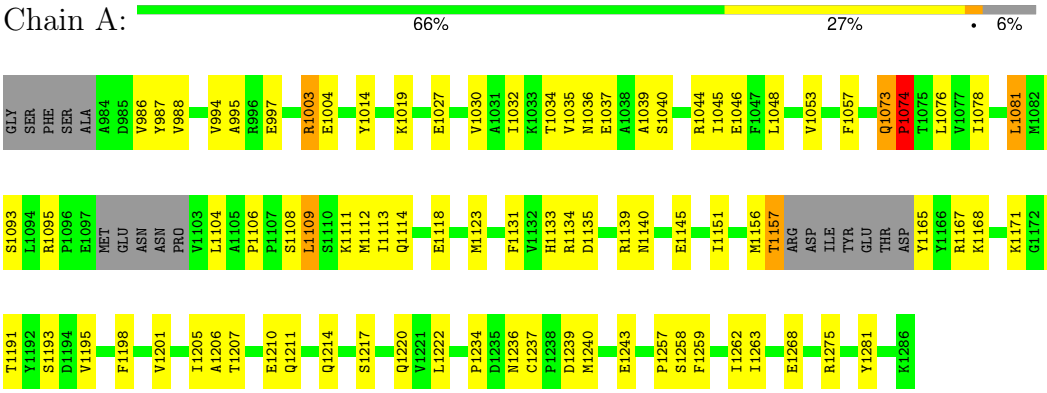
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	91	Total	O	0	0
			91	91		
5	C	77	Total	O	0	0
			77	77		

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.

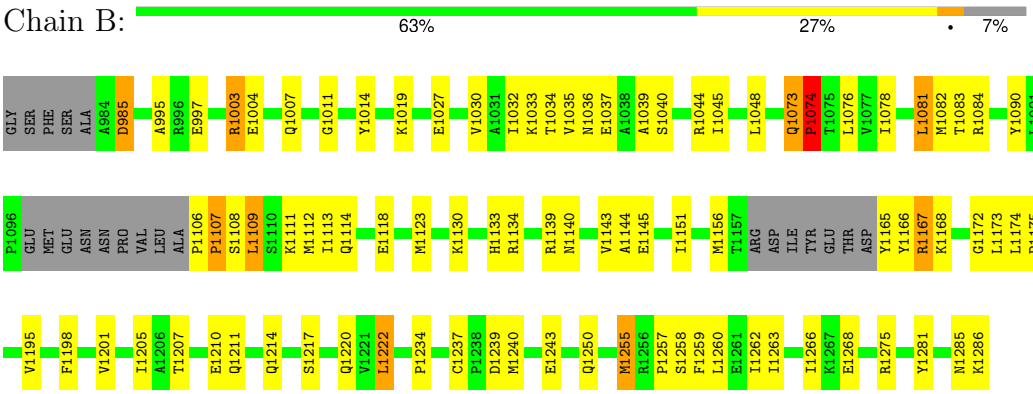
• Molecule 1: IGF-1 receptor kinase

Chain A:



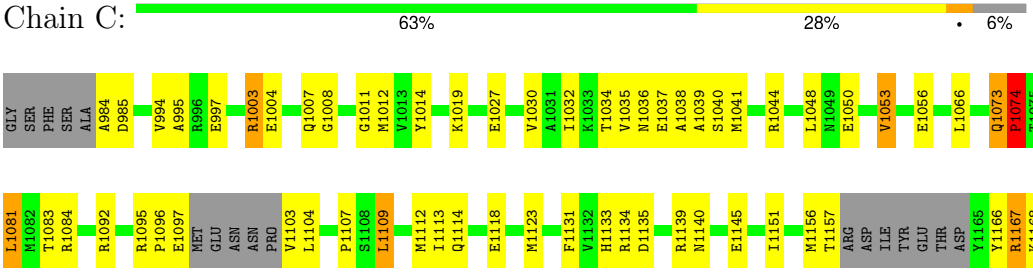
• Molecule 1: IGF-1 receptor kinase

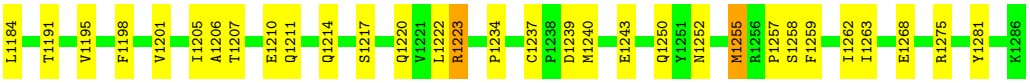
Chain B:



• Molecule 1: IGF-1 receptor kinase

Chain C:




L1184
T1191
V1195
F1198
V1201
I1205
A1206
T1207
E1210
Q1211
Q1214
S1217
Q1220
V1221
L1222
R1223
P1234
C1237
P1238
D1239
M1240
E1243
Q1250
Y1251
N1252
M1255
R1256
P1257
S1258
F1259
I1262
I1263
E1268
R1275
Y1281
K1286

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	85.96Å 85.96Å 132.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.10 19.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.85-2.10) 99.3 (19.85-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.01Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.195 , 0.219 0.190 , 0.207	Depositor DCC
R_{free} test set	3054 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.085 for -h,-k,l 0.288 for h,-h-k,-l 0.088 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: MG, ANP, SO4

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	0.41	0/2368	0.78	4/3190 (0.1%)
1	B	0.41	0/2339	0.76	3/3149 (0.1%)
1	C	0.41	0/2368	0.78	3/3190 (0.1%)
All	All	0.41	0/7075	0.77	10/9529 (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
1	C	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1073	GLN	C-N-CD	-20.49	75.52	120.60
1	C	1073	GLN	C-N-CD	-20.31	75.92	120.60
1	B	1073	GLN	C-N-CD	-20.04	76.52	120.60
1	A	1073	GLN	C-N-CA	10.14	164.60	122.00
1	C	1073	GLN	C-N-CA	9.81	163.19	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1223	ARG	Sidechain

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	2320	0	2295	84	0
1	B	2291	0	2265	88	0
1	C	2320	0	2295	93	1
2	A	1	0	0	0	0
3	A	5	0	0	0	1
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	1	0
5	A	84	0	0	6	0
5	B	91	0	0	2	0
5	C	77	0	0	0	0
All	All	7292	0	6894	249	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 18.

The worst 5 of 249 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:C:1053:VAL:HG12	1:C:1156:MET:CE	1.78	1.14
1:C:1092:ARG:HH21	1:C:1095:ARG:NE	1.48	1.11
1:C:1053:VAL:HG12	1:C:1156:MET:HE2	1.38	1.04
1:A:1157:THR:HG21	1:C:984:ALA:HA	1.37	1.02
1:B:1003:ARG:HG3	1:B:1003:ARG:HH11	1.28	0.93

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:C:1223:ARG:NH1	3:A:305:SO4:O3[1_545]	1.79	0.41

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	285/308 (92%)	273 (96%)	11 (4%)	1 (0%)	30 29
1	B	281/308 (91%)	268 (95%)	11 (4%)	2 (1%)	19 16
1	C	285/308 (92%)	273 (96%)	9 (3%)	3 (1%)	12 8
All	All	851/924 (92%)	814 (96%)	31 (4%)	6 (1%)	19 16

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1074	PRO
1	B	1074	PRO
1	B	1107	PRO
1	C	1074	PRO
1	C	985	ASP

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	253/268 (94%)	242 (96%)	11 (4%)	25 25
1	B	250/268 (93%)	239 (96%)	11 (4%)	24 24
1	C	253/268 (94%)	239 (94%)	14 (6%)	18 16
All	All	756/804 (94%)	720 (95%)	36 (5%)	21 21

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1103	VAL
1	C	1268	GLU
1	C	1109	LEU
1	C	1167	ARG
1	B	1003	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1007	GLN
1	C	1071	GLN
1	C	1214	GLN
1	B	1007	GLN
1	A	1214	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	SO4	C	306	-	4,4,4	0.50	0	6,6,6	0.14	0
4	ANP	B	302	-	29,33,33	2.10	8 (27%)	31,52,52	2.74	8 (25%)
4	ANP	C	303	-	29,33,33	2.12	8 (27%)	31,52,52	2.75	8 (25%)
4	ANP	A	301	2	29,33,33	2.29	10 (34%)	31,52,52	3.00	7 (22%)
3	SO4	A	305	-	4,4,4	0.43	0	6,6,6	0.16	0
3	SO4	B	307	-	4,4,4	0.29	0	6,6,6	0.10	0

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
4	ANP	C	303	-	-	5/14/38/38	0/3/3/3
4	ANP	B	302	-	-	4/14/38/38	0/3/3/3
4	ANP	A	301	2	-	6/14/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	ANP	PB-O3A	6.16	1.66	1.59
4	C	303	ANP	PB-O3A	5.96	1.66	1.59
4	A	301	ANP	PB-O1B	5.47	1.54	1.46
4	C	303	ANP	PB-O2B	-5.29	1.42	1.56
4	A	301	ANP	PB-O3A	4.74	1.65	1.59

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	303	ANP	C4'-O4'-C1'	9.91	119.00	109.92
4	A	301	ANP	C4'-O4'-C1'	9.22	118.37	109.92
4	B	302	ANP	C4'-O4'-C1'	9.03	118.19	109.92
4	A	301	ANP	O1B-PB-N3B	-8.76	98.88	111.77
4	A	301	ANP	O4'-C1'-N9	7.01	118.05	108.75

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
4	A	301	ANP	PG-N3B-PB-O1B
4	A	301	ANP	PA-O3A-PB-O1B
4	A	301	ANP	PA-O3A-PB-O2B
4	B	302	ANP	PB-N3B-PG-O1G

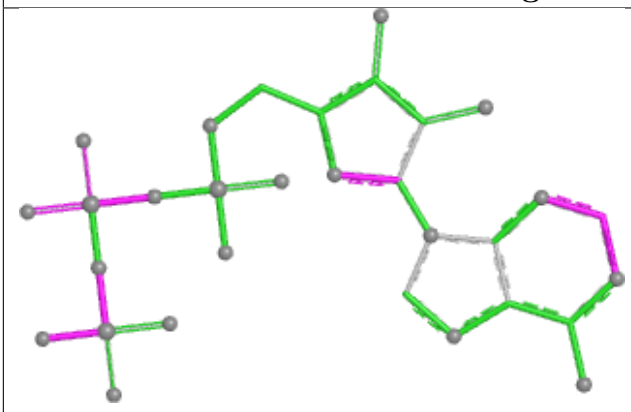
There are no ring outliers.

4 monomers are involved in 4 short contacts:

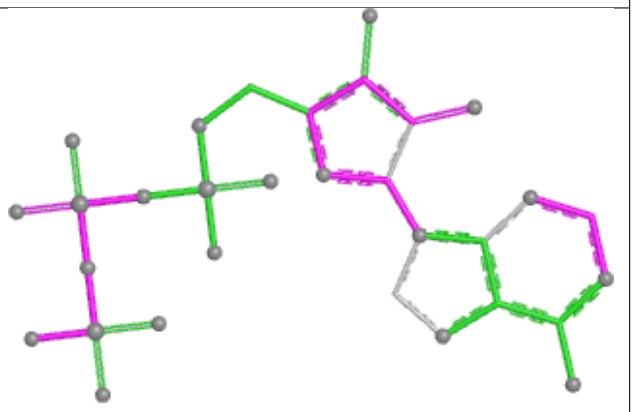
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	306	SO4	1	0
4	B	302	ANP	1	0
4	C	303	ANP	1	0
3	A	305	SO4	0	1

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.

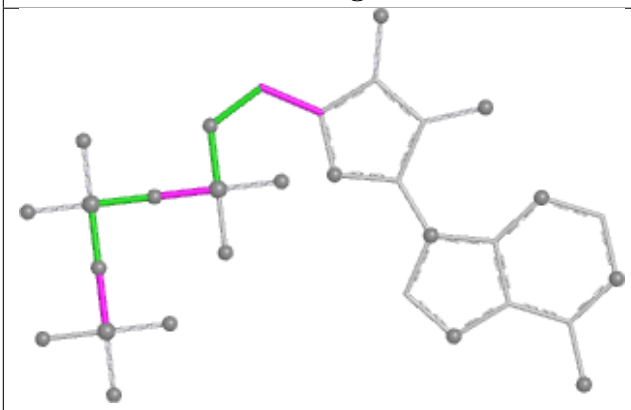
Ligand ANP B 302



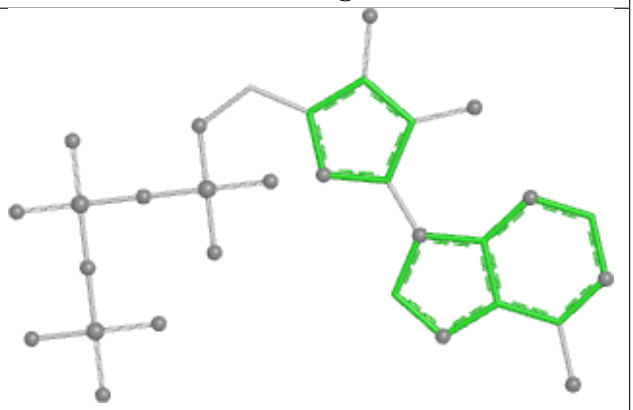
Bond lengths



Bond angles

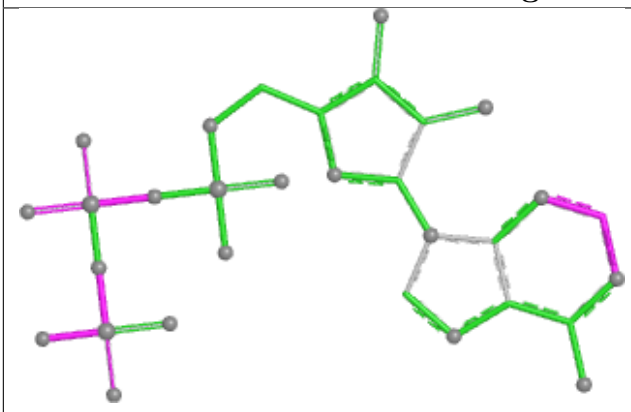


Torsions

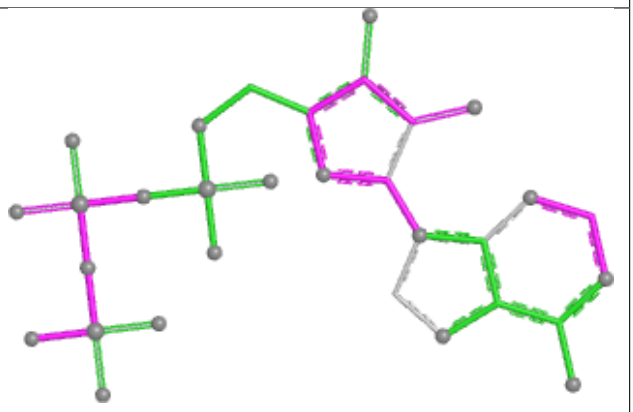


Rings

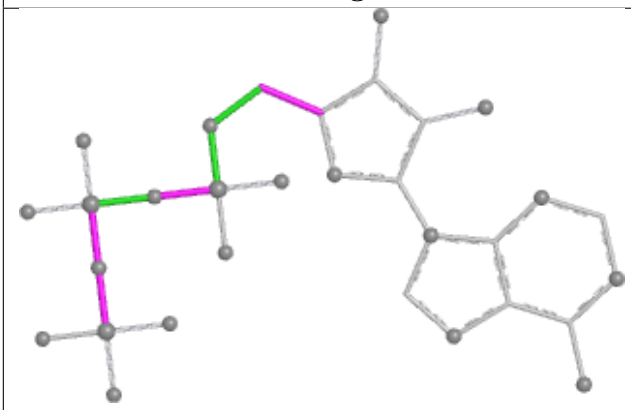
Ligand ANP C 303



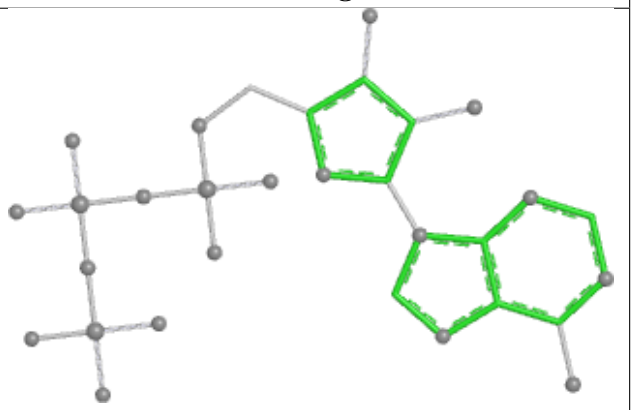
Bond lengths



Bond angles

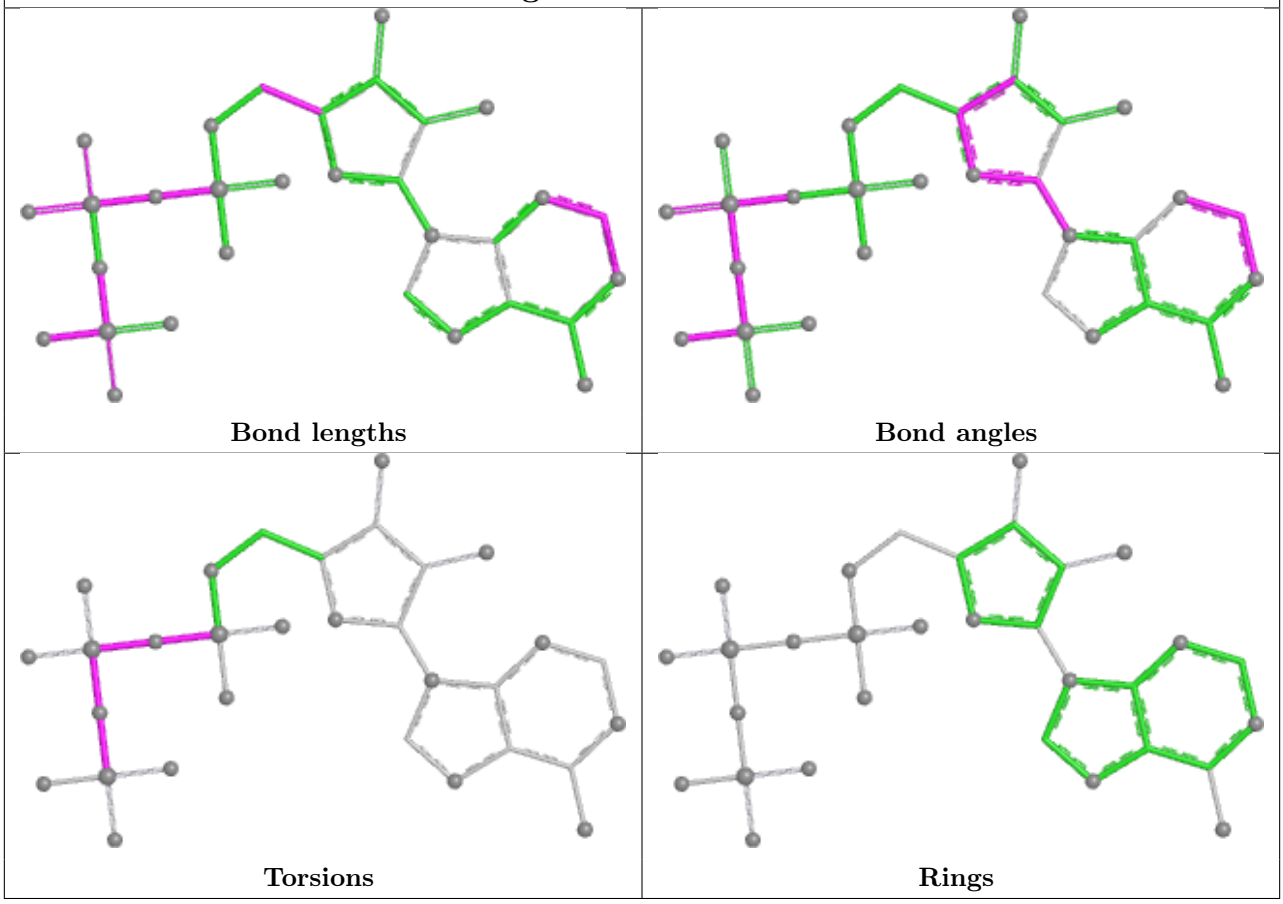


Torsions



Rings

Ligand ANP A 301



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, 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	291/308 (94%)	-1.42	0	100	100	24, 42, 66, 84	0
1	B	287/308 (93%)	-1.45	0	100	100	24, 40, 65, 85	0
1	C	291/308 (94%)	-1.45	0	100	100	22, 39, 66, 83	0
All	All	869/924 (94%)	-1.44	0	100	100	22, 41, 66, 85	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
2	MG	A	304	1/1	0.98	0.04	54,54,54,54	0
3	SO4	B	307	5/5	0.98	0.04	19,19,19,19	5
3	SO4	C	306	5/5	0.99	0.04	20,20,20,20	5
4	ANP	A	301	31/31	0.99	0.03	39,53,71,72	0
4	ANP	B	302	31/31	0.99	0.03	28,46,76,79	0

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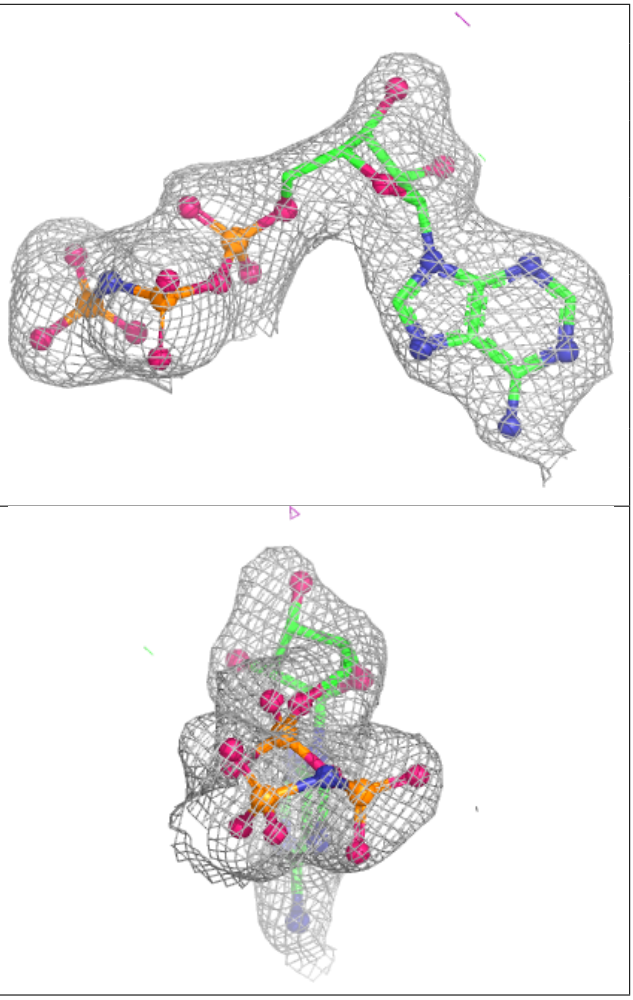
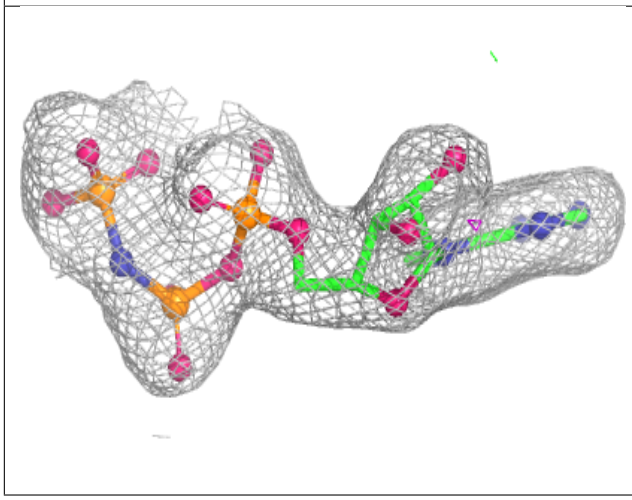
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ANP	C	303	31/31	0.99	0.03	45,54,72,74	0
3	SO4	A	305	5/5	1.00	0.07	20,20,20,20	5

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 301:

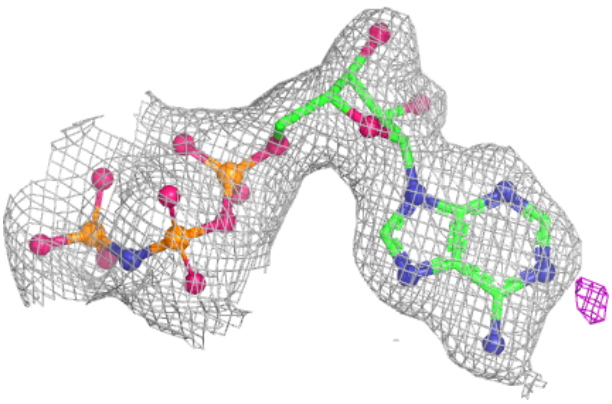
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

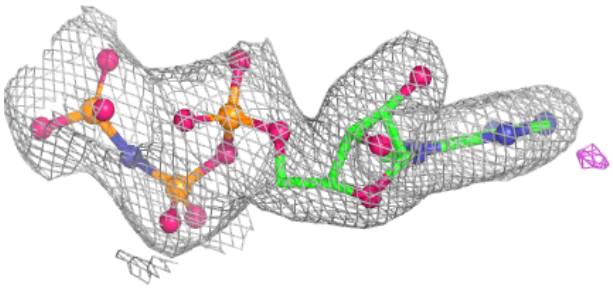


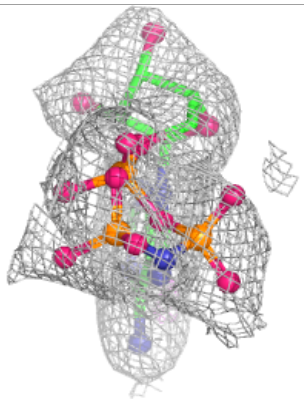


Electron density around ANP B 302:

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

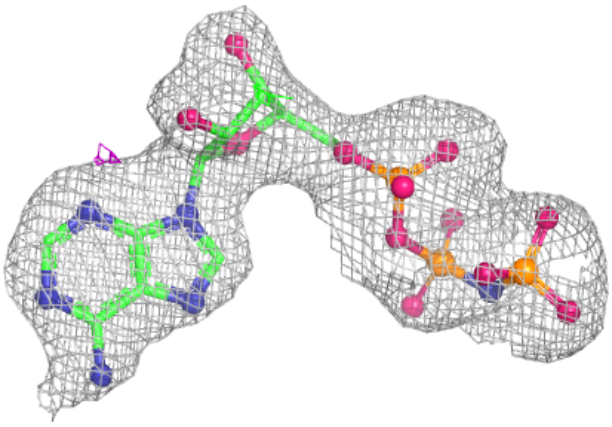


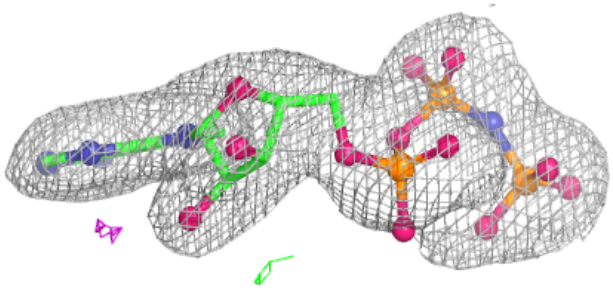


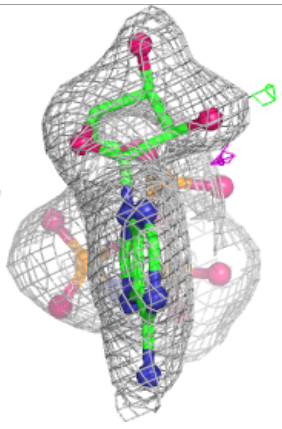


Electron density around ANP C 303:

$2mF_o$-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.