



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 30, 2020 – 04:19 PM EDT

PDB ID : 7JUZ  
Title : Crystal Structure of KSR1:MEK1 in complex with AMP-PNP, and allosteric MEK inhibitor Selumetinib  
Authors : Khan, Z.M.; Dar, A.C.  
Deposited on : 2020-08-20  
Resolution : 3.21 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

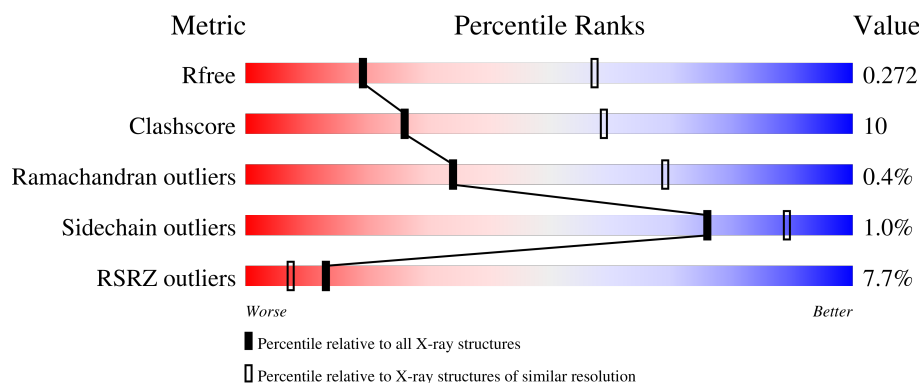
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	334	<div> <div></div> <div>65%</div> <div>17%</div> <div>18%</div> </div>
2	C	384	<div> <div>10%</div> <div>59%</div> <div>21%</div> <div>20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	3EW	C	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4717 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 Kinase suppressor of Ras 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2197	1408	383	393	13			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	MET	-	initiating methionine	UNP Q8IVT5
A	567	SER	-	expression tag	UNP Q8IVT5
A	568	TYR	-	expression tag	UNP Q8IVT5
A	569	TYR	-	expression tag	UNP Q8IVT5
A	570	HIS	-	expression tag	UNP Q8IVT5
A	571	HIS	-	expression tag	UNP Q8IVT5
A	572	HIS	-	expression tag	UNP Q8IVT5
A	573	HIS	-	expression tag	UNP Q8IVT5
A	574	HIS	-	expression tag	UNP Q8IVT5
A	575	HIS	-	expression tag	UNP Q8IVT5
A	576	ASP	-	expression tag	UNP Q8IVT5
A	577	TYR	-	expression tag	UNP Q8IVT5
A	578	ASP	-	expression tag	UNP Q8IVT5
A	579	ILE	-	expression tag	UNP Q8IVT5
A	580	PRO	-	expression tag	UNP Q8IVT5
A	581	THR	-	expression tag	UNP Q8IVT5
A	582	THR	-	expression tag	UNP Q8IVT5
A	583	GLU	-	expression tag	UNP Q8IVT5
A	584	ASN	-	expression tag	UNP Q8IVT5
A	585	LEU	-	expression tag	UNP Q8IVT5
A	586	TYR	-	expression tag	UNP Q8IVT5
A	587	PHE	-	expression tag	UNP Q8IVT5
A	588	GLN	-	expression tag	UNP Q8IVT5
A	589	GLY	-	expression tag	UNP Q8IVT5
A	590	ALA	-	expression tag	UNP Q8IVT5
A	898	GLU	ASP	conflict	UNP Q8IVT5

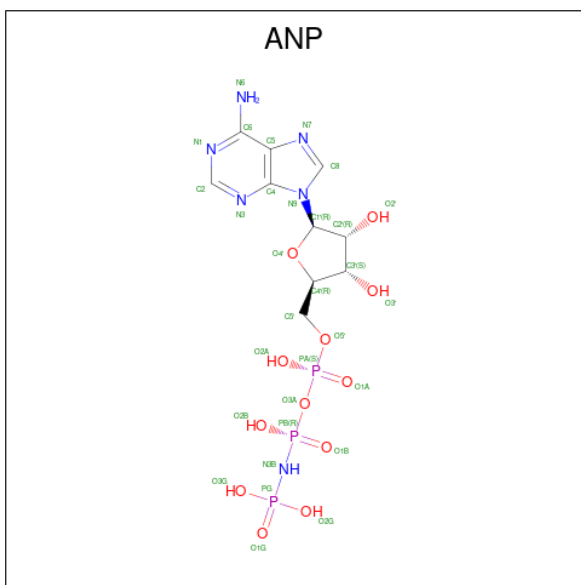
- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	308	Total	C	N	O	S	0	0	0
			2431	1554	413	448	16			

There are 25 discrepancies between the modelled and reference sequences:

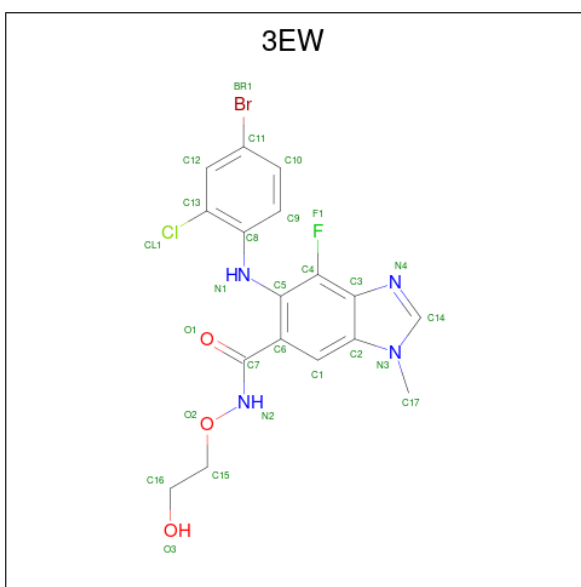
Chain	Residue	Modelled	Actual	Comment	Reference
C	10	MET	-	initiating methionine	UNP P29678
C	11	SER	-	expression tag	UNP P29678
C	12	TYR	-	expression tag	UNP P29678
C	13	TYR	-	expression tag	UNP P29678
C	14	HIS	-	expression tag	UNP P29678
C	15	HIS	-	expression tag	UNP P29678
C	16	HIS	-	expression tag	UNP P29678
C	17	HIS	-	expression tag	UNP P29678
C	18	HIS	-	expression tag	UNP P29678
C	19	HIS	-	expression tag	UNP P29678
C	20	ASP	-	expression tag	UNP P29678
C	21	TYR	-	expression tag	UNP P29678
C	22	ASP	-	expression tag	UNP P29678
C	23	ILE	-	expression tag	UNP P29678
C	24	PRO	-	expression tag	UNP P29678
C	25	THR	-	expression tag	UNP P29678
C	26	THR	-	expression tag	UNP P29678
C	27	GLU	-	expression tag	UNP P29678
C	28	ASN	-	expression tag	UNP P29678
C	29	LEU	-	expression tag	UNP P29678
C	30	TYR	-	expression tag	UNP P29678
C	31	PHE	-	expression tag	UNP P29678
C	32	GLN	-	expression tag	UNP P29678
C	33	GLY	-	expression tag	UNP P29678
C	34	ALA	-	expression tag	UNP P29678

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is 5-[(4-bromo-2-chlorophenyl)amino]-4-fluoro-N-(2-hydroxyethoxy)-1-methyl-1H-benzimidazole-6-carboxamide (three-letter code: 3EW) (formula:  $C_{17}H_{15}BrClFN_4O_3$ ) (labeled as "Ligand of Interest" by author).

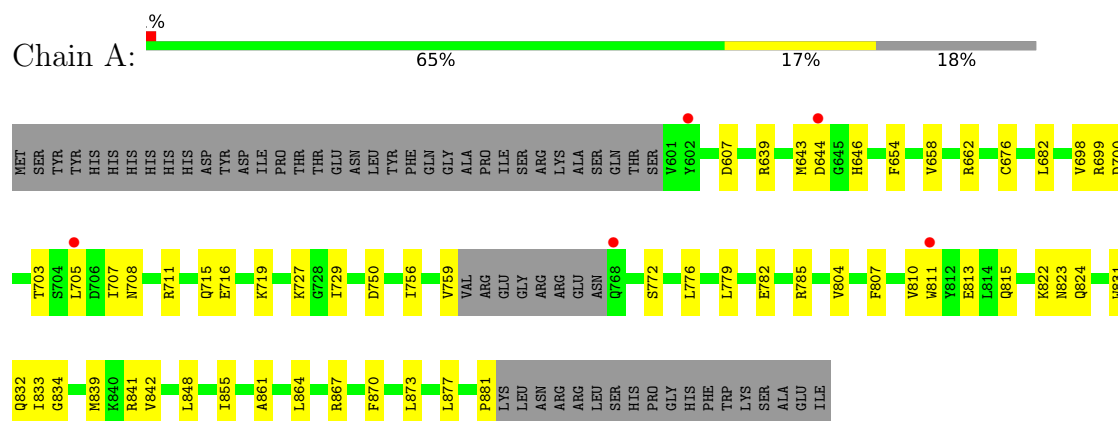


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	C	1	Total	Br	C	Cl	F	N	O	0	0
			27	1	17	1	1	4	3		

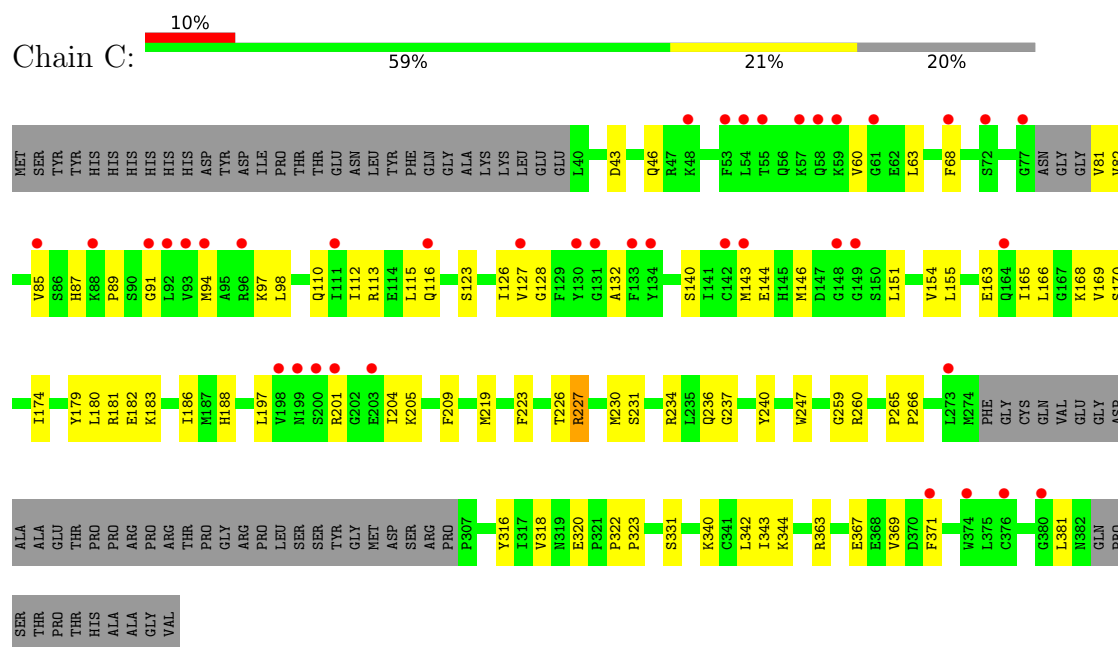
### 3 Residue-property plots [i](#)

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: Kinase suppressor of Ras 1



#### • Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.40Å 136.40Å 216.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 3.21 49.22 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.22-3.21) 99.1 (49.22-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14rc1_3177)	Depositor
R, $R_{free}$	0.254 , 0.272 0.254 , 0.272	Depositor DCC
$R_{free}$ test set	1047 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	128.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 76.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3EW, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/2250	0.46	0/3035
2	C	0.26	0/2477	0.47	0/3334
All	All	0.28	0/4727	0.46	0/6369

There are no bond length outliers.

There are no bond angle outliers.

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	2197	0	2178	35	0
2	C	2431	0	2473	63	0
3	A	31	0	13	0	0
3	C	31	0	13	2	0
4	C	27	0	15	9	0
All	All	4717	0	4692	98	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 10.

The worst 5 of 98 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)
2:C:143:MET:HE3	4:C:402:3EW:H6	1.44	0.97
2:C:127:VAL:HG21	2:C:143:MET:CE	2.14	0.78
2:C:143:MET:SD	4:C:402:3EW:CL1	2.80	0.76
2:C:127:VAL:HG11	2:C:197:LEU:HD12	1.66	0.74
2:C:60:VAL:HG23	2:C:87:HIS:CE1	2.24	0.72

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	267/334 (80%)	255 (96%)	11 (4%)	1 (0%)	34	69
2	C	302/384 (79%)	291 (96%)	10 (3%)	1 (0%)	41	74
All	All	569/718 (79%)	546 (96%)	21 (4%)	2 (0%)	34	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	823	ASN
2	C	91	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/291 (81%)	233 (99%)	2 (1%)	78	90
2	C	270/333 (81%)	267 (99%)	3 (1%)	73	88
All	All	505/624 (81%)	500 (99%)	5 (1%)	76	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	CYS
1	A	772	SER
2	C	94	MET
2	C	201	ARG
2	C	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	832	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands 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
4	3EW	C	402	-	26,29,29	2.03	4 (15%)	29,41,41	1.11	3 (10%)
3	ANP	C	401	-	29,33,33	1.03	3 (10%)	31,52,52	1.09	5 (16%)
3	ANP	A	901	-	29,33,33	1.01	3 (10%)	31,52,52	1.08	3 (9%)

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	3EW	C	402	-	-	2/13/13/13	0/3/3/3
3	ANP	C	401	-	-	5/14/38/38	0/3/3/3
3	ANP	A	901	-	-	1/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	3EW	C7-N2	8.64	1.46	1.34
4	C	402	3EW	C8-N1	2.49	1.46	1.39
3	C	401	ANP	PG-N3B	2.48	1.69	1.63
3	A	901	ANP	PG-O1G	2.34	1.49	1.46
4	C	402	3EW	C13-CL1	2.32	1.79	1.73

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ANP	PA-O3A-PB	-2.81	122.73	132.62
3	A	901	ANP	O1G-PG-N3B	-2.59	107.96	111.77
3	C	401	ANP	PA-O3A-PB	-2.36	124.31	132.62
4	C	402	3EW	C6-C7-N2	2.35	119.41	114.91
4	C	402	3EW	C6-C5-C4	2.34	119.01	117.04

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

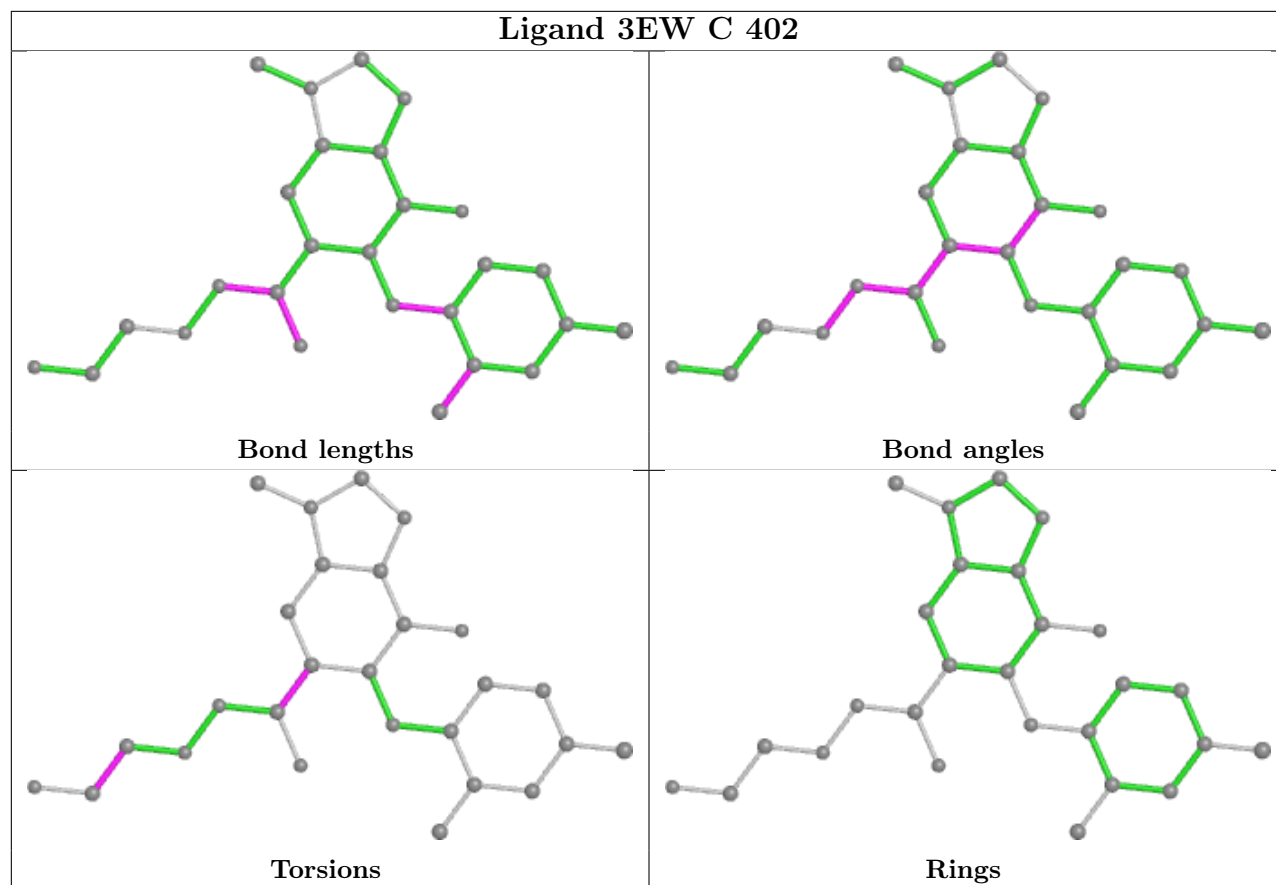
Mol	Chain	Res	Type	Atoms
4	C	402	3EW	O2-C15-C16-O3
3	C	401	ANP	PB-N3B-PG-O1G
3	C	401	ANP	PG-N3B-PB-O1B
3	C	401	ANP	PA-O3A-PB-O1B
3	C	401	ANP	PA-O3A-PB-O2B

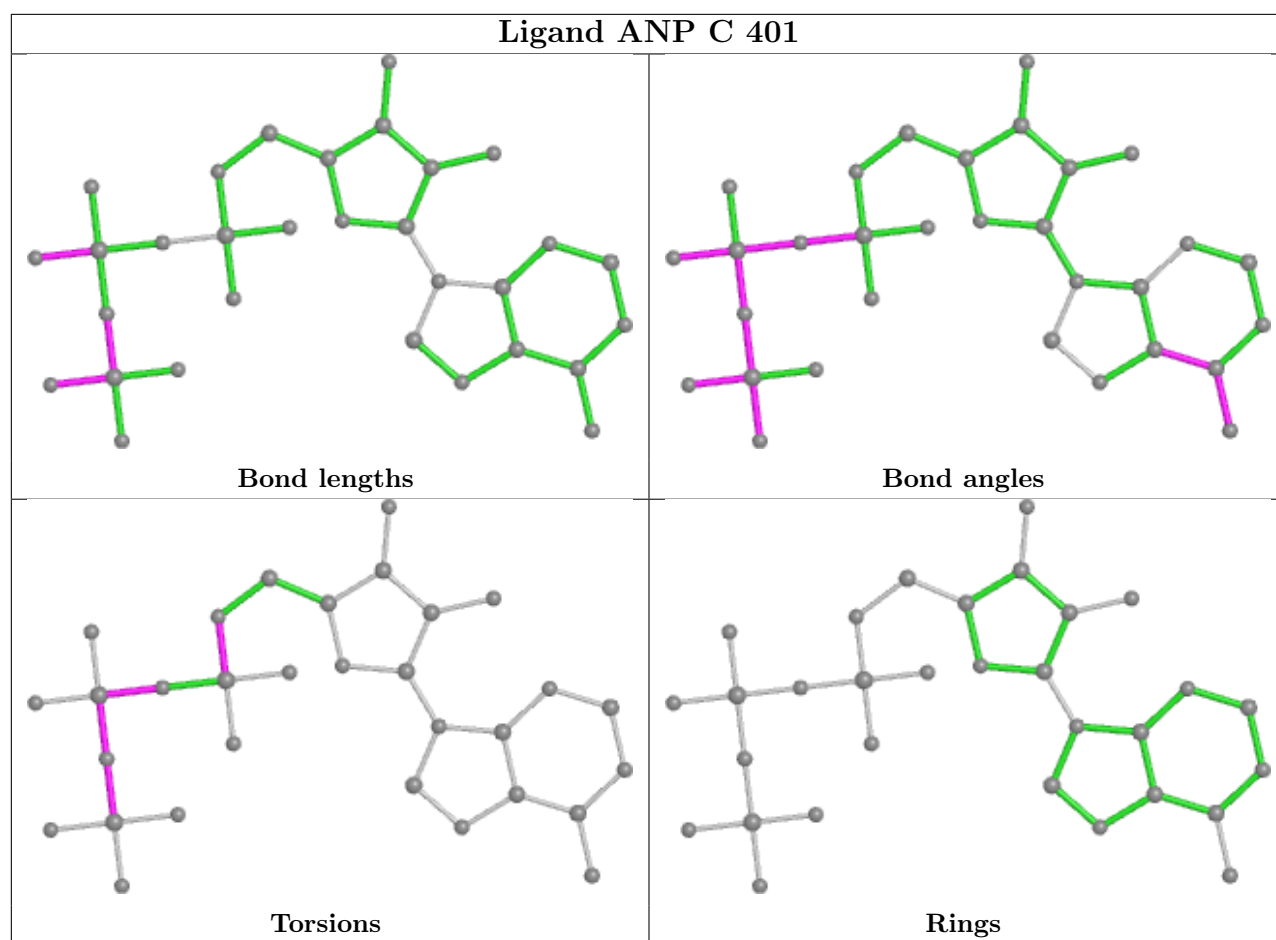
There are no ring outliers.

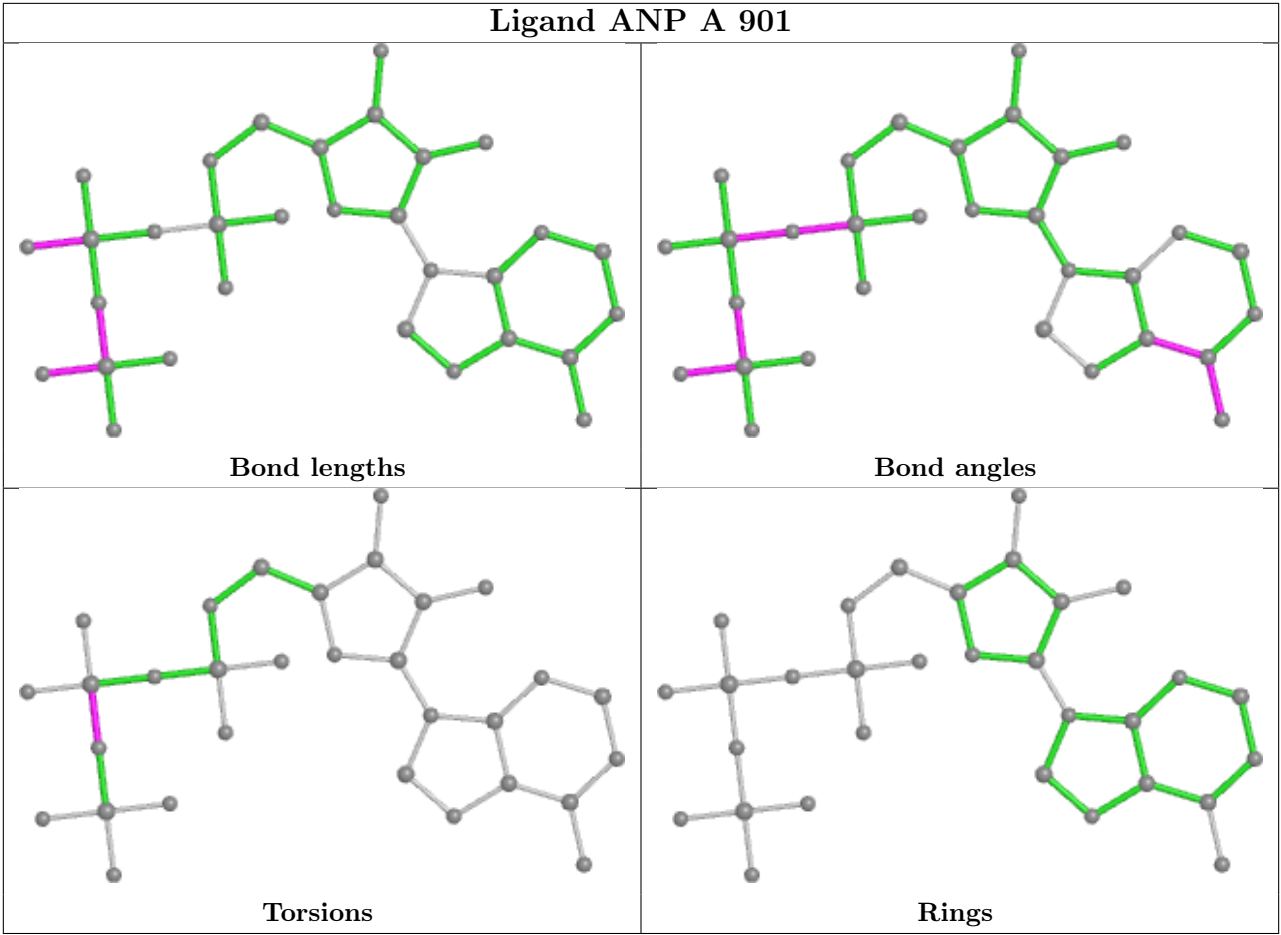
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	3EW	9	0
3	C	401	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 ⓘ

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	632:TRP	C	633:HIS	N	5.91



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/334 (81%)	0.16	5 (1%) 68 56	80, 109, 157, 191	0
2	C	308/384 (80%)	0.73	40 (12%) 3 2	95, 165, 203, 209	0
All	All	581/718 (80%)	0.46	45 (7%) 13 7	80, 131, 198, 209	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	93	VAL	5.6
2	C	77	GLY	5.4
2	C	148	GLY	5.3
2	C	57	LYS	4.8
2	C	198	VAL	4.8

### 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](#)

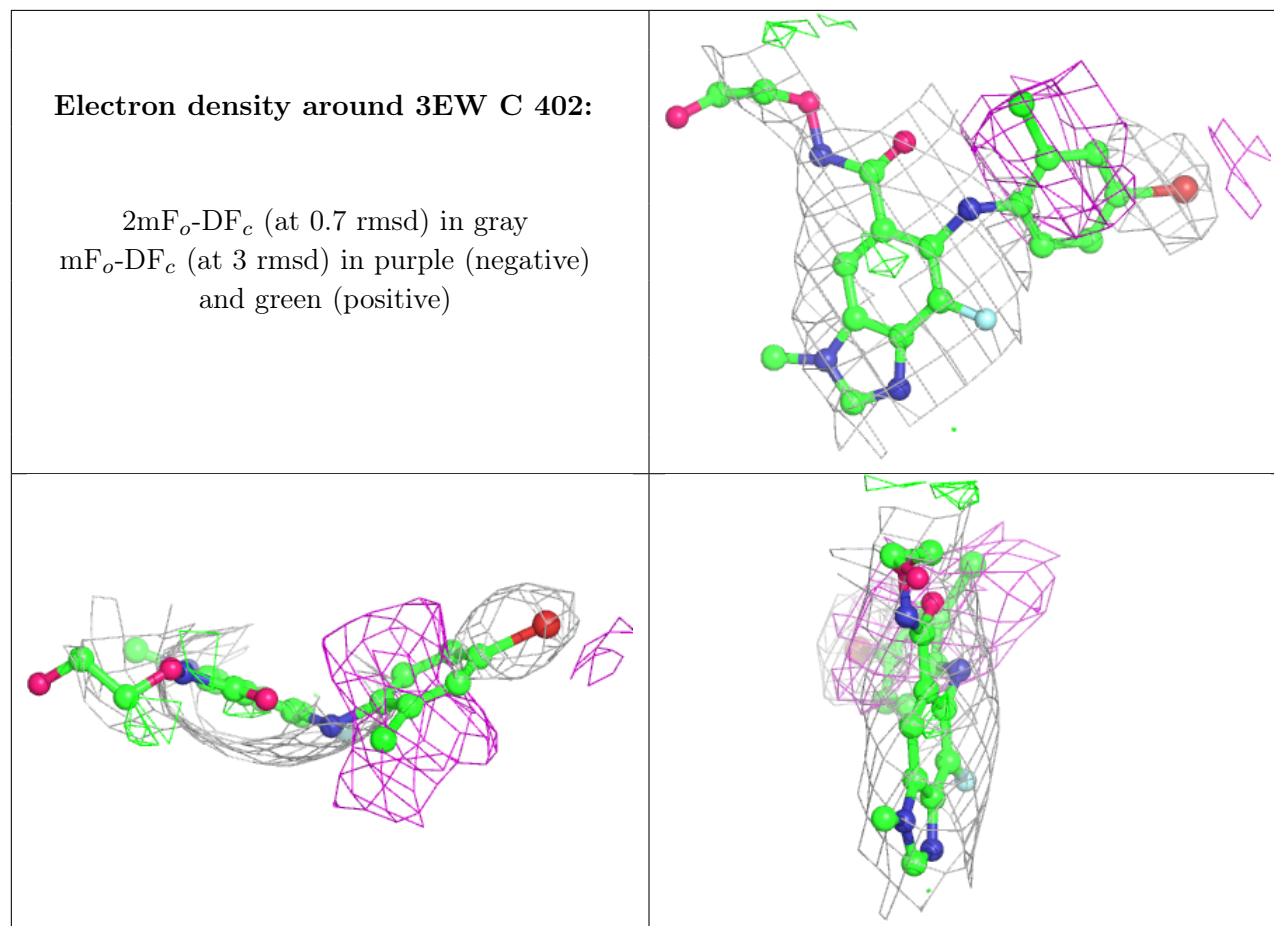
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

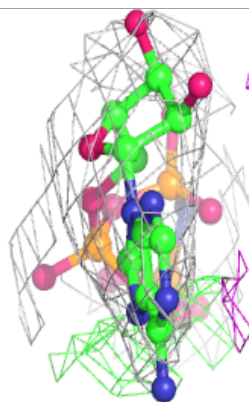
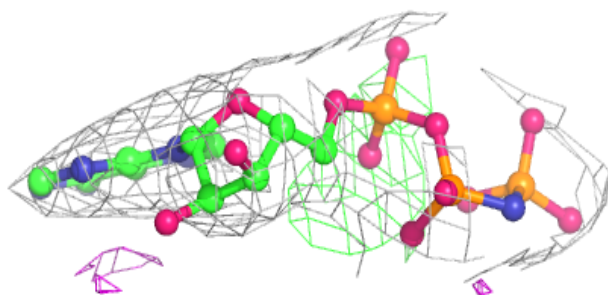
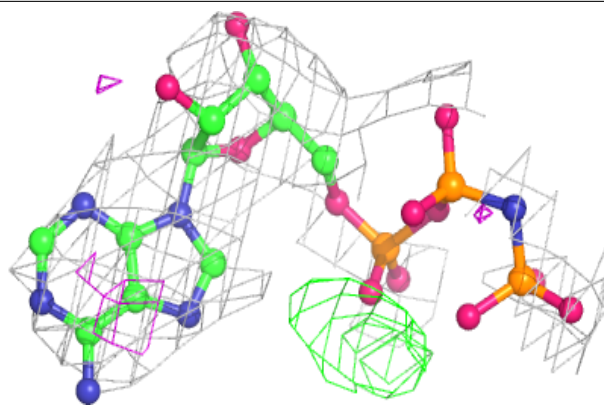
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	3EW	C	402	27/27	0.67	0.39	139,158,184,272	0
3	ANP	C	401	31/31	0.80	0.29	158,172,180,185	0
3	ANP	A	901	31/31	0.93	0.25	84,97,119,126	0

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.

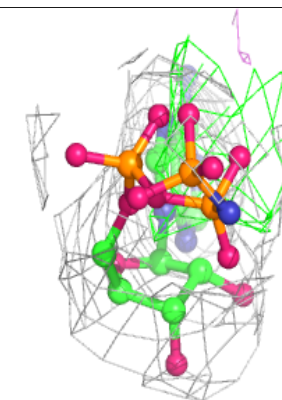
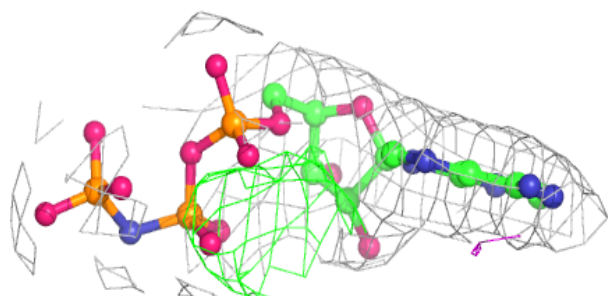
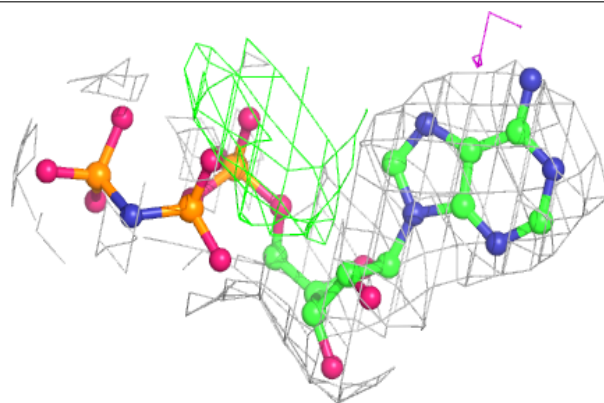


**Electron density around ANP C 401:**

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

**Electron density around ANP A 901:**

$2mF_o-DF_c$  (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.