



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:58 AM EDT

PDB ID : 2A19  
Title : PKR kinase domain- eIF2alpha- AMP-PNP complex.  
Authors : Dar, A.C.; Dever, T.E.; Sicheri, F.  
Deposited on : 2005-06-19  
Resolution : 2.50 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](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 : 2.23.2  
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

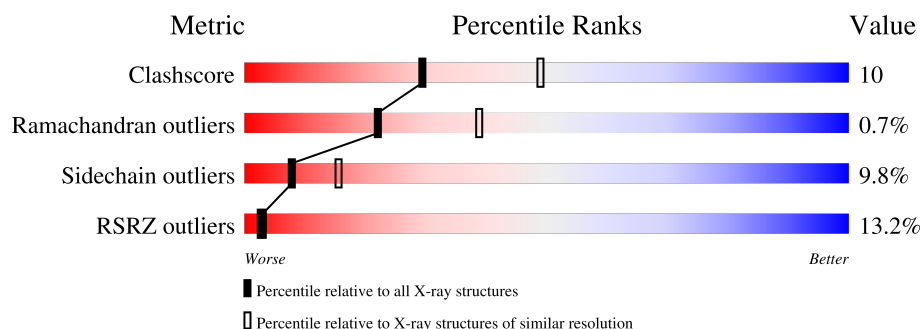
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	175	<div> <div>5%</div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div>
2	B	284	<div> <div>12%</div> <div>71%</div> <div>18%</div> <div>• 7%</div> </div>
2	C	284	<div> <div>14%</div> <div>49%</div> <div>19%</div> <div>• 29%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5216 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 Eukaryotic translation initiation factor 2 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1342	862	220	254	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P20459
A	2	SER	-	cloning artifact	UNP P20459

- Molecule 2 is a protein called Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	P	S	0	0
			2137	1363	366	400	1	7		
2	C	203	Total	C	N	O	S	0	0	0
			1594	1027	265	297	5			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	cloning artifact	UNP P19525
B	256	ALA	-	cloning artifact	UNP P19525
B	257	HIS	-	cloning artifact	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	LEU	deletion	UNP P19525
B	?	-	GLU	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	SER	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525

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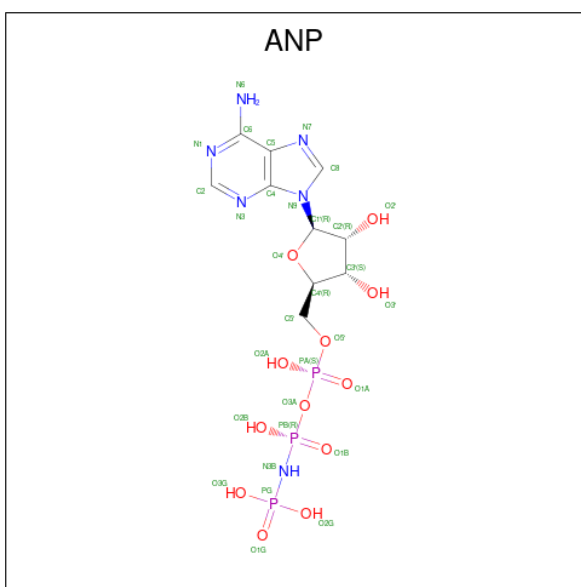
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P19525
B	?	-	ASP	deletion	UNP P19525
B	?	-	PRO	deletion	UNP P19525
B	?	-	GLU	deletion	UNP P19525
B	?	-	ASN	deletion	UNP P19525
B	412	ASN	HIS	engineered mutation	UNP P19525
B	446	TPO	THR	modified residue	UNP P19525
B	551	ALA	CYS	engineered mutation	UNP P19525
C	255	GLY	-	cloning artifact	UNP P19525
C	256	ALA	-	cloning artifact	UNP P19525
C	257	HIS	-	cloning artifact	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	LEU	deletion	UNP P19525
C	?	-	GLU	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	SER	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	TYR	deletion	UNP P19525
C	?	-	ASP	deletion	UNP P19525
C	?	-	PRO	deletion	UNP P19525
C	?	-	GLU	deletion	UNP P19525
C	?	-	ASN	deletion	UNP P19525
C	412	ASN	HIS	engineered mutation	UNP P19525
C	446	TPO	THR	modified residue	UNP P19525
C	551	ALA	CYS	engineered mutation	UNP P19525

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

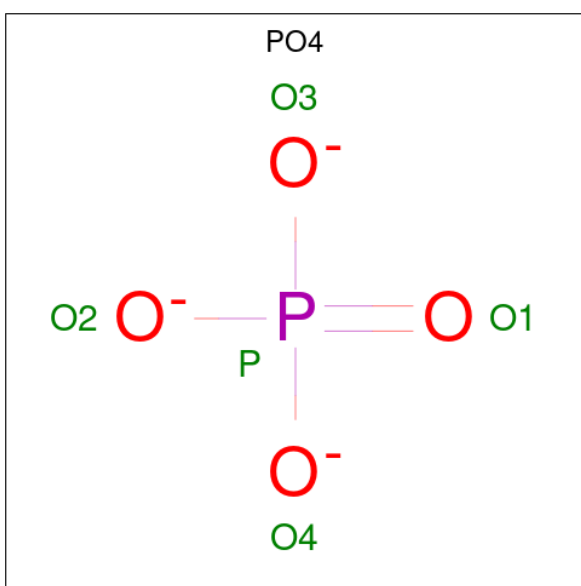
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 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>).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

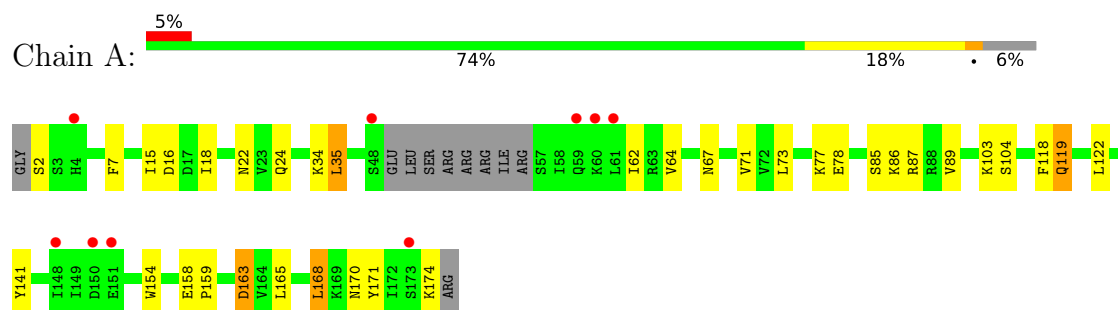
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	33	Total 33	O 33	0	0
6	C	7	Total 7	O 7	0	0

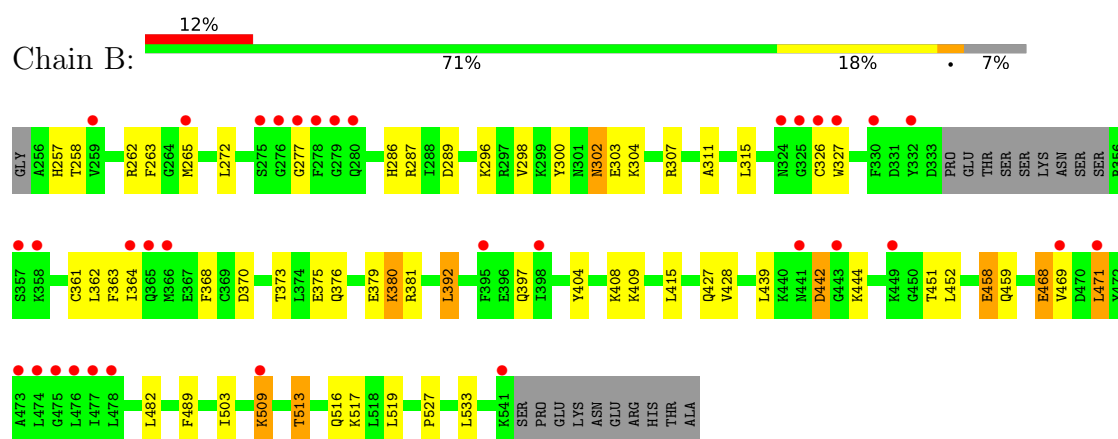
### 3 Residue-property plots [i](#)

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.

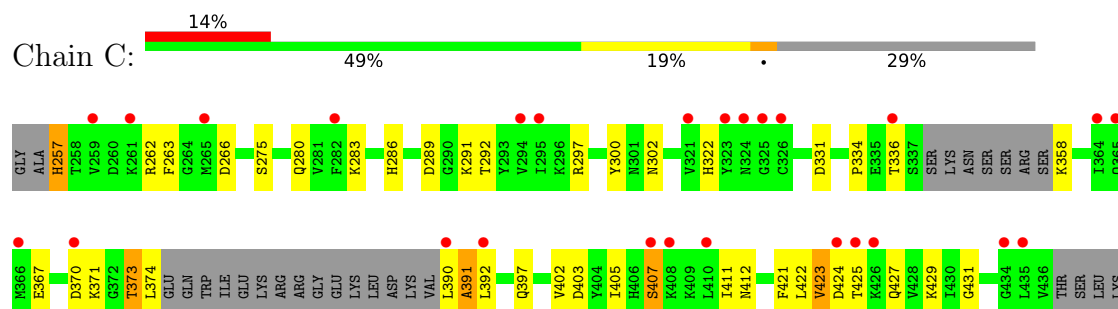
- Molecule 1: Eukaryotic translation initiation factor 2 alpha subunit

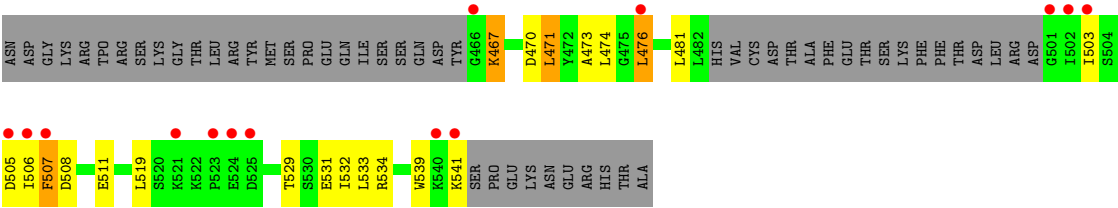


- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase



- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.66Å 48.75Å 133.43Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	27.33 – 2.50 27.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.33-2.50) 94.7 (27.33-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.228 , 0.286 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, ANP, TPO

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	0.59	0/1366	0.68	2/1839 (0.1%)
2	B	0.52	0/2161	0.64	0/2895
2	C	0.46	0/1618	0.59	0/2174
All	All	0.53	0/5145	0.64	2/6908 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	CA-CB-CG	7.49	132.52	115.30
1	A	168	LEU	CA-CB-CG	5.65	128.29	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1342	0	1350	23	0
2	B	2137	0	2160	33	0
2	C	1594	0	1588	37	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	B	31	0	13	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	31	0	13	0	0
5	C	5	0	0	0	0
6	A	32	0	0	0	0
6	B	33	0	0	1	0
6	C	7	0	0	0	0
All	All	5216	0	5124	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.

All (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:507:PHE:H	2:C:507:PHE:HD1	1.04	1.01
4:B:1640:ANP:HNB1	4:B:1640:ANP:H5'2	1.33	0.93
2:B:373:THR:H	2:B:376:GLN:HE21	1.22	0.85
4:B:1640:ANP:HNB1	4:B:1640:ANP:C5'	1.90	0.83
4:B:1640:ANP:H5'2	4:B:1640:ANP:N3B	1.92	0.83
1:A:119:GLN:HE21	1:A:119:GLN:HA	1.44	0.81
4:B:1640:ANP:H8	4:B:1640:ANP:O5'	1.86	0.75
2:B:286:HIS:HD2	2:B:289:ASP:H	1.36	0.71
2:B:397:GLN:HE22	2:B:427:GLN:HA	1.56	0.71
1:A:15:ILE:O	1:A:16:ASP:HB2	1.96	0.65
2:C:507:PHE:CD1	2:C:507:PHE:N	2.55	0.64
2:C:507:PHE:HD1	2:C:507:PHE:N	1.85	0.64
2:C:322:HIS:HB3	2:C:367:GLU:HB3	1.80	0.63
2:B:300:TYR:HB2	2:B:362:LEU:HB2	1.79	0.62
2:B:381:ARG:HB3	6:B:59:HOH:O	1.99	0.61
2:B:503:ILE:HG13	2:B:516:GLN:HG2	1.83	0.61
2:C:424:ASP:OD1	2:C:425:THR:N	2.35	0.59
2:C:529:THR:HA	2:C:532:ILE:HD12	1.83	0.59
1:A:2:SER:N	1:A:122:LEU:H	2.01	0.59
2:B:509:LYS:O	2:B:513:THR:HG23	2.03	0.58
2:B:442:ASP:HB3	2:B:444:LYS:H	1.68	0.58
2:C:507:PHE:HB2	2:C:511:GLU:OE2	2.04	0.58
2:C:331:ASP:O	2:C:358:LYS:HA	2.03	0.57
2:B:262:ARG:HG2	2:B:327:TRP:CD1	2.40	0.56
2:C:390:LEU:HG	2:C:391:ALA:H	1.69	0.56
1:A:119:GLN:HE21	1:A:119:GLN:CA	2.17	0.56
2:C:397:GLN:HE22	2:C:427:GLN:HA	1.70	0.56
2:C:280:GLN:HE21	2:C:297:ARG:HH11	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:HIS:CD2	2:C:289:ASP:H	2.24	0.55
4:B:1640:ANP:C5'	4:B:1640:ANP:N3B	2.60	0.54
2:B:368:PHE:CE2	2:B:370:ASP:HB3	2.42	0.54
2:C:286:HIS:HD2	2:C:289:ASP:H	1.55	0.54
2:C:423:VAL:HG23	2:C:427:GLN:HB3	1.89	0.53
2:C:473:ALA:O	2:C:476:LEU:HB2	2.10	0.51
1:A:171:TYR:O	1:A:174:LYS:HG2	2.09	0.51
2:B:326:CYS:HA	2:B:363:PHE:O	2.10	0.51
1:A:154:TRP:HH2	1:A:168:LEU:HD11	1.75	0.51
2:B:517:LYS:HB3	2:B:527:PRO:HD3	1.93	0.51
1:A:22:ASN:HD22	1:A:67:ASN:ND2	2.09	0.50
2:B:409:LYS:HD2	2:B:439:LEU:HD23	1.93	0.50
2:B:392:LEU:HD13	2:B:482:LEU:HD21	1.93	0.50
2:B:397:GLN:NE2	2:B:428:VAL:H	2.10	0.49
2:B:404:TYR:O	2:B:408:LYS:HG2	2.12	0.49
1:A:18:ILE:HD13	1:A:71:VAL:HG22	1.94	0.49
2:C:402:VAL:HA	2:C:405:ILE:HD12	1.94	0.49
2:C:471:LEU:HA	2:C:474:LEU:HD12	1.95	0.49
2:C:291:LYS:HG2	2:C:292:THR:N	2.28	0.48
2:C:390:LEU:C	2:C:392:LEU:H	2.15	0.48
2:C:423:VAL:HG11	2:C:429:LYS:HD2	1.95	0.48
2:B:265:MET:O	2:B:287:ARG:HD2	2.13	0.48
2:B:257:HIS:CE1	2:B:272:LEU:HD22	2.48	0.48
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.22	0.48
2:C:291:LYS:HG2	2:C:292:THR:H	1.78	0.48
1:A:22:ASN:HD22	1:A:67:ASN:HD22	1.60	0.47
1:A:24:GLN:NE2	1:A:34:LYS:HD3	2.29	0.47
2:C:280:GLN:NE2	2:C:297:ARG:HH11	2.12	0.47
1:A:154:TRP:CH2	1:A:168:LEU:CD1	2.97	0.47
1:A:159:PRO:HG3	1:A:165:LEU:HB2	1.95	0.47
2:B:380:LYS:HA	2:B:380:LYS:HE3	1.97	0.47
2:C:297:ARG:HD3	2:C:334:PRO:HG3	1.97	0.47
2:C:411:ILE:HG13	2:C:411:ILE:O	2.15	0.47
1:A:154:TRP:CH2	1:A:168:LEU:HD11	2.50	0.46
2:B:458:GLU:CD	2:B:458:GLU:H	2.19	0.46
2:B:311:ALA:O	2:B:315:LEU:HG	2.16	0.46
2:B:302:ASN:O	2:B:304:LYS:N	2.49	0.46
2:B:302:ASN:HD22	2:B:302:ASN:N	2.14	0.46
2:C:286:HIS:HD2	2:C:289:ASP:N	2.13	0.45
1:A:103:LYS:HG2	1:A:141:TYR:CG	2.51	0.45
2:C:531:GLU:HA	2:C:534:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HG2	1:A:141:TYR:CD2	2.51	0.45
2:B:459:GLN:HB2	2:B:469:VAL:HG22	1.99	0.45
2:C:421:PHE:CE1	2:C:431:GLY:HA3	2.52	0.44
2:B:262:ARG:NH2	2:C:266:ASP:OD1	2.48	0.44
1:A:71:VAL:HG23	1:A:89:VAL:HG22	1.99	0.44
2:B:373:THR:H	2:B:376:GLN:NE2	2.02	0.44
4:B:1640:ANP:HNB1	4:B:1640:ANP:H5'1	1.79	0.43
2:C:257:HIS:O	2:C:297:ARG:NH2	2.35	0.43
1:A:15:ILE:O	1:A:16:ASP:CB	2.65	0.43
2:C:421:PHE:HE1	2:C:431:GLY:HA3	1.82	0.43
1:A:118:PHE:CE2	1:A:163:ASP:HB3	2.54	0.43
2:B:468:GLU:HA	2:B:471:LEU:HD22	2.01	0.43
1:A:86:LYS:O	1:A:87:ARG:C	2.55	0.43
2:B:262:ARG:HG2	2:B:327:TRP:NE1	2.33	0.43
2:B:468:GLU:CD	2:B:468:GLU:H	2.22	0.42
2:C:539:TRP:CD1	2:C:539:TRP:N	2.87	0.42
2:B:375:GLU:O	2:B:379:GLU:HG3	2.19	0.42
2:B:370:ASP:OD1	2:B:370:ASP:N	2.50	0.42
1:A:7:PHE:CD2	1:A:104:SER:HB3	2.55	0.42
1:A:73:LEU:HD11	1:A:85:SER:HB2	2.01	0.42
2:C:411:ILE:CG2	2:C:467:LYS:HB3	2.50	0.41
2:C:403:ASP:O	2:C:407:SER:HB2	2.20	0.41
2:C:467:LYS:HD3	2:C:467:LYS:H	1.85	0.41
2:B:302:ASN:HD22	2:B:302:ASN:H	1.68	0.41
2:C:373:THR:HG23	2:C:374:LEU:N	2.35	0.41
2:B:296:LYS:HB3	2:B:364:ILE:HB	2.02	0.41
2:C:412:ASN:O	2:C:470:ASP:OD1	2.39	0.41
2:C:373:THR:CG2	2:C:374:LEU:N	2.84	0.40
1:A:24:GLN:CD	1:A:34:LYS:HD3	2.42	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	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	B	259/284 (91%)	250 (96%)	7 (3%)	2 (1%)	19	35
2	C	193/284 (68%)	177 (92%)	14 (7%)	2 (1%)	15	28
All	All	613/743 (82%)	578 (94%)	31 (5%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	303	GLU
2	B	277	GLY
2	C	371	LYS
2	C	391	ALA

### 5.3.2 Protein sidechains ⓘ

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	149/161 (92%)	140 (94%)	9 (6%)	19	37
2	B	232/254 (91%)	212 (91%)	20 (9%)	10	20
2	C	170/254 (67%)	145 (85%)	25 (15%)	3	5
All	All	551/669 (82%)	497 (90%)	54 (10%)	8	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	62	ILE
1	A	64	VAL
1	A	77	LYS
1	A	78	GLU
1	A	119	GLN
1	A	158	GLU
1	A	163	ASP
1	A	170	ASN

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Mol	Chain	Res	Type
2	B	258	THR
2	B	263	PHE
2	B	298	VAL
2	B	302	ASN
2	B	307	ARG
2	B	361	CYS
2	B	380	LYS
2	B	392	LEU
2	B	415	LEU
2	B	442	ASP
2	B	451	THR
2	B	452	LEU
2	B	458	GLU
2	B	468	GLU
2	B	471	LEU
2	B	489	PHE
2	B	509	LYS
2	B	513	THR
2	B	519	LEU
2	B	533	LEU
2	C	257	HIS
2	C	262	ARG
2	C	263	PHE
2	C	275	SER
2	C	283	LYS
2	C	300	TYR
2	C	302	ASN
2	C	336	THR
2	C	370	ASP
2	C	373	THR
2	C	407	SER
2	C	422	LEU
2	C	423	VAL
2	C	467	LYS
2	C	471	LEU
2	C	476	LEU
2	C	481	LEU
2	C	503	ILE
2	C	505	ASP
2	C	506	ILE
2	C	507	PHE
2	C	508	ASP

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Mol	Chain	Res	Type
2	C	519	LEU
2	C	533	LEU
2	C	541	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	67	ASN
1	A	119	GLN
2	B	286	HIS
2	B	302	ASN
2	B	319	ASN
2	B	322	HIS
2	B	376	GLN
2	B	397	GLN
2	B	463	GLN
2	C	280	GLN
2	C	286	HIS
2	C	301	ASN
2	C	302	ASN
2	C	319	ASN
2	C	397	GLN
2	C	528	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
2	TPO	B	446	2	8,10,11	0.84	0	10,14,16	1.15	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
2	TPO	B	446	2	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 7 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	PO4	C	901	-	4,4,4	0.85	0	6,6,6	0.56	0
4	ANP	C	2640	3	29,33,33	1.90	6 (20%)	31,52,52	1.69	6 (19%)
4	ANP	B	1640	3	29,33,33	1.87	8 (27%)	31,52,52	1.70	5 (16%)

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	2640	3	-	4/14/38/38	0/3/3/3
4	ANP	B	1640	3	-	3/14/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2640	ANP	PG-N3B	5.04	1.76	1.63
4	C	2640	ANP	PB-N3B	4.95	1.76	1.63
4	B	1640	ANP	PG-N3B	4.27	1.74	1.63
4	B	1640	ANP	PB-N3B	4.17	1.74	1.63
4	B	1640	ANP	PG-O1G	3.99	1.52	1.46
4	C	2640	ANP	PB-O1B	3.65	1.51	1.46
4	B	1640	ANP	PB-O1B	3.35	1.51	1.46
4	C	2640	ANP	PG-O1G	3.35	1.51	1.46
4	C	2640	ANP	C5-C4	2.47	1.47	1.40
4	B	1640	ANP	C2-N3	2.43	1.36	1.32
4	B	1640	ANP	C5-C4	2.30	1.47	1.40
4	B	1640	ANP	O4'-C1'	2.22	1.44	1.41
4	B	1640	ANP	PG-O2G	-2.04	1.51	1.56
4	C	2640	ANP	PG-O2G	-2.02	1.51	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1640	ANP	O2B-PB-O1B	5.12	120.65	109.92
4	C	2640	ANP	O2B-PB-O1B	3.95	118.20	109.92
4	C	2640	ANP	O1G-PG-N3B	-3.73	106.27	111.77
4	C	2640	ANP	N3-C2-N1	-3.62	123.02	128.68
4	B	1640	ANP	N3-C2-N1	-3.54	123.15	128.68
4	C	2640	ANP	PA-O3A-PB	-3.32	120.94	132.62
4	B	1640	ANP	O1G-PG-N3B	-3.26	106.97	111.77
4	B	1640	ANP	O3G-PG-O2G	3.00	115.61	107.64
4	B	1640	ANP	PA-O3A-PB	-2.35	124.34	132.62
4	C	2640	ANP	C4-C5-N7	-2.31	107.00	109.40
4	C	2640	ANP	C2-N1-C6	2.13	122.40	118.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

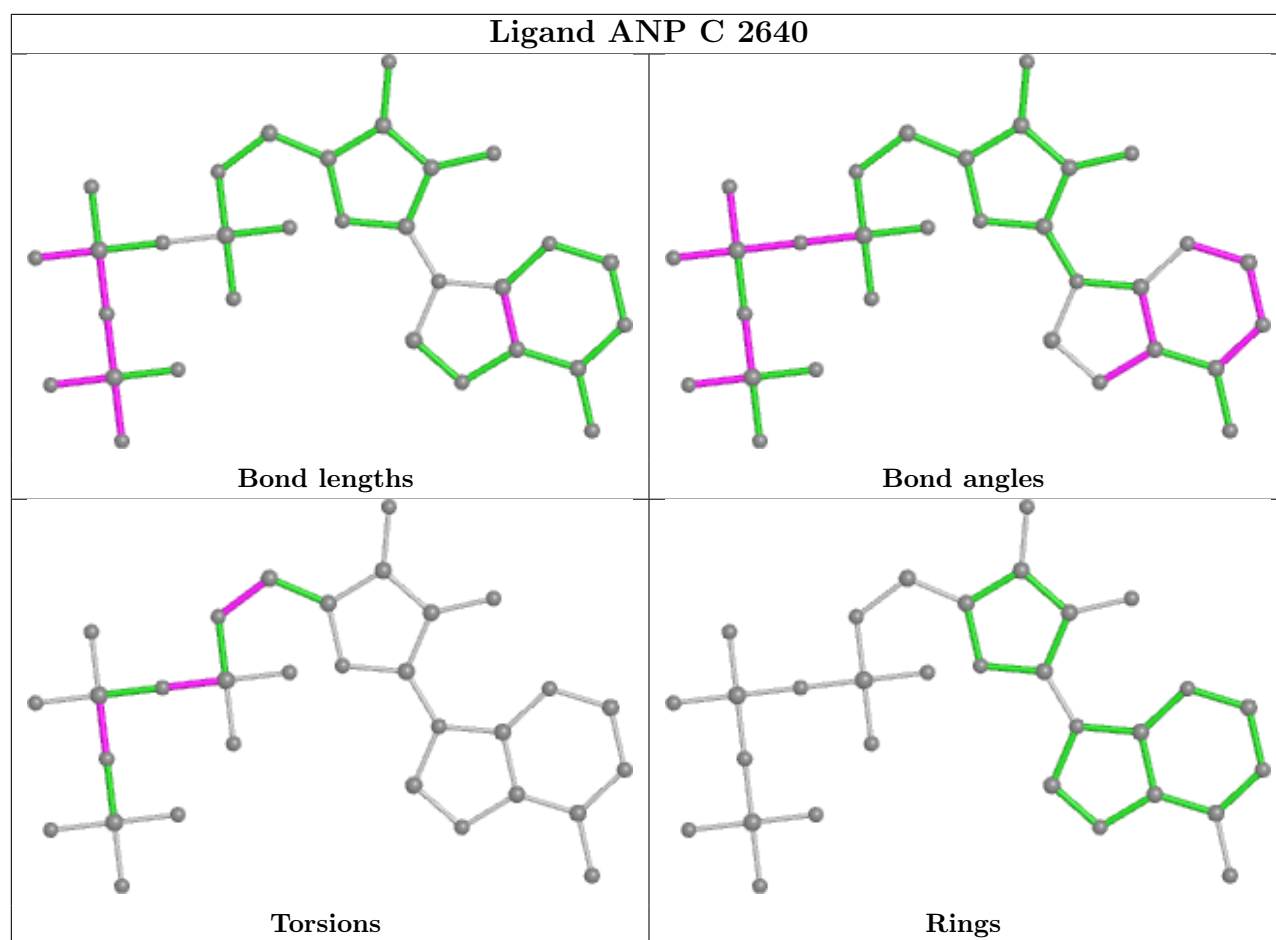
Mol	Chain	Res	Type	Atoms
4	B	1640	ANP	PB-N3B-PG-O1G
4	B	1640	ANP	PG-N3B-PB-O1B
4	B	1640	ANP	PA-O3A-PB-O1B
4	C	2640	ANP	PG-N3B-PB-O1B
4	C	2640	ANP	PG-N3B-PB-O3A
4	C	2640	ANP	PB-O3A-PA-O2A
4	C	2640	ANP	C4'-C5'-O5'-PA

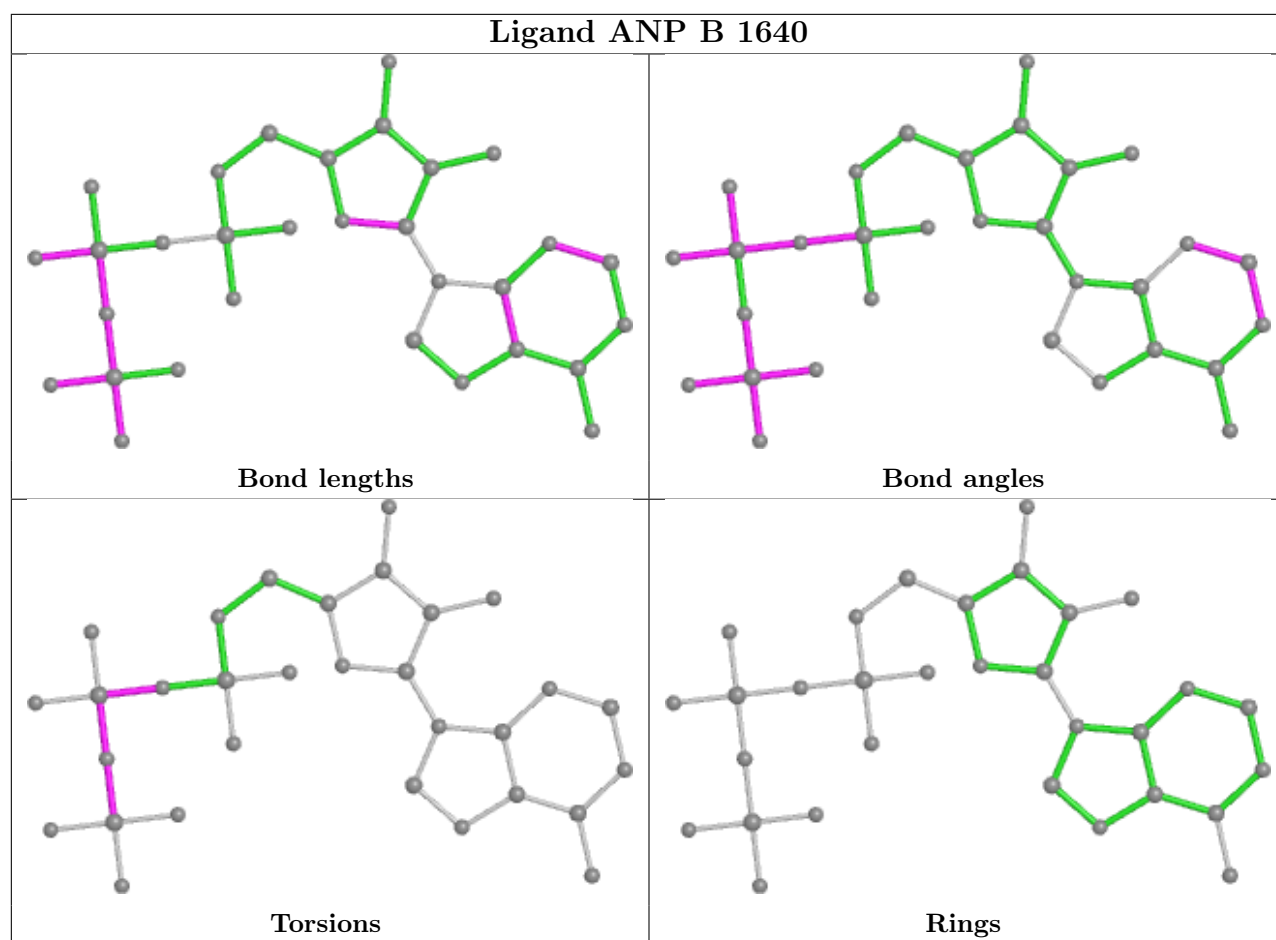
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1640	ANP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	165/175 (94%)	0.16	9 (5%)	25 26	43, 51, 65, 71	0
2	B	263/284 (92%)	0.53	34 (12%)	3 3	45, 57, 77, 86	0
2	C	203/284 (71%)	0.99	40 (19%)	1 1	52, 67, 79, 82	0
All	All	631/743 (84%)	0.58	83 (13%)	3 3	43, 59, 77, 86	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	PHE	9.1
2	C	523	PRO	8.0
2	C	502	ILE	7.6
2	C	506	ILE	6.7
2	B	279	GLY	5.8
2	C	425	THR	5.8
2	C	466	GLY	5.5
2	B	332	TYR	4.9
2	B	277	GLY	4.3
2	B	473	ALA	4.0
2	C	261	LYS	3.8
1	A	59	GLN	3.8
2	C	541	LYS	3.6
2	B	326	CYS	3.6
2	C	505	ASP	3.6
2	B	325	GLY	3.6
2	B	330	PHE	3.5
2	C	325	GLY	3.5
2	C	521	LYS	3.5
2	C	295	ILE	3.5
2	B	365	GLN	3.5
2	C	265	MET	3.5
2	C	501	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	3.3
2	C	503	ILE	3.3
2	C	540	LYS	3.2
2	B	477	ILE	3.2
1	A	60	LYS	3.2
2	B	449	LYS	3.2
2	C	507	PHE	3.0
2	B	474	LEU	3.0
2	B	509	LYS	2.9
2	C	407	SER	2.8
1	A	173	SER	2.8
2	C	321	VAL	2.8
2	B	475	GLY	2.8
2	C	294	VAL	2.7
2	B	259	VAL	2.7
2	B	276	GLY	2.7
2	C	524	GLU	2.6
2	C	366	MET	2.6
2	C	426	LYS	2.6
2	B	476	LEU	2.6
1	A	151	GLU	2.6
1	A	48	SER	2.6
2	B	357	SER	2.6
2	C	365	GLN	2.6
2	C	434	GLY	2.6
2	C	336	THR	2.6
2	B	275	SER	2.5
2	C	410	LEU	2.5
2	B	327	TRP	2.5
2	C	435	LEU	2.4
2	B	265	MET	2.4
2	B	441	ASN	2.4
1	A	150	ASP	2.4
2	C	525	ASP	2.4
1	A	4	HIS	2.4
2	B	364	ILE	2.3
2	B	358	LYS	2.3
2	B	443	GLY	2.3
2	C	324	ASN	2.3
2	C	364	ILE	2.3
2	B	478	LEU	2.3
2	C	390	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	408	LYS	2.2
2	B	395	PHE	2.2
2	C	323	TYR	2.2
2	B	280	GLN	2.2
2	B	471	LEU	2.2
2	B	324	ASN	2.2
2	C	259	VAL	2.2
2	B	366	MET	2.2
2	C	370	ASP	2.2
2	B	398	ILE	2.2
1	A	148	ILE	2.1
2	C	424	ASP	2.1
2	C	282	PHE	2.1
2	C	476	LEU	2.1
2	B	469	VAL	2.0
2	C	392	LEU	2.0
2	B	541	LYS	2.0
2	C	326	CYS	2.0

## 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, 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(Å <sup>2</sup> )	Q<0.9
2	TPO	B	446	11/12	0.96	0.10	51,54,57,57	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

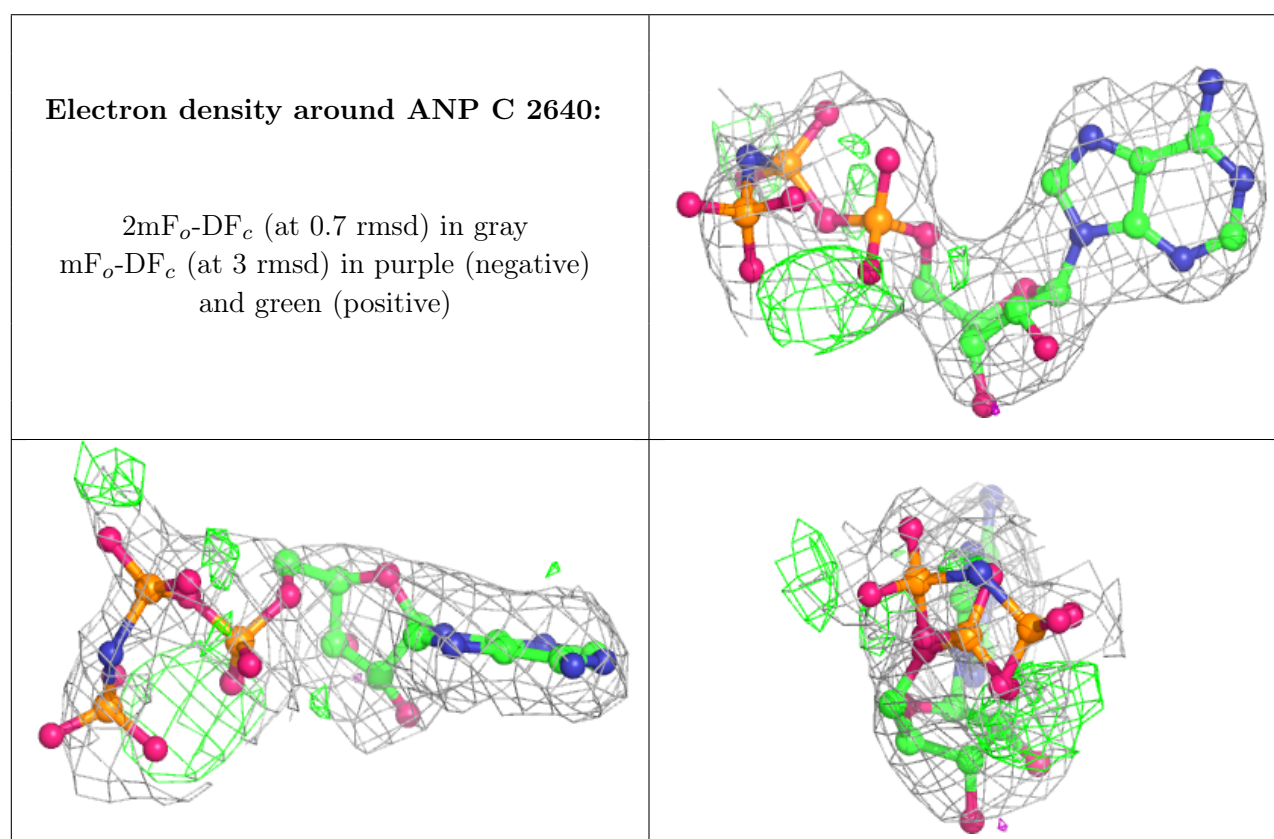
## 6.4 Ligands [i](#)

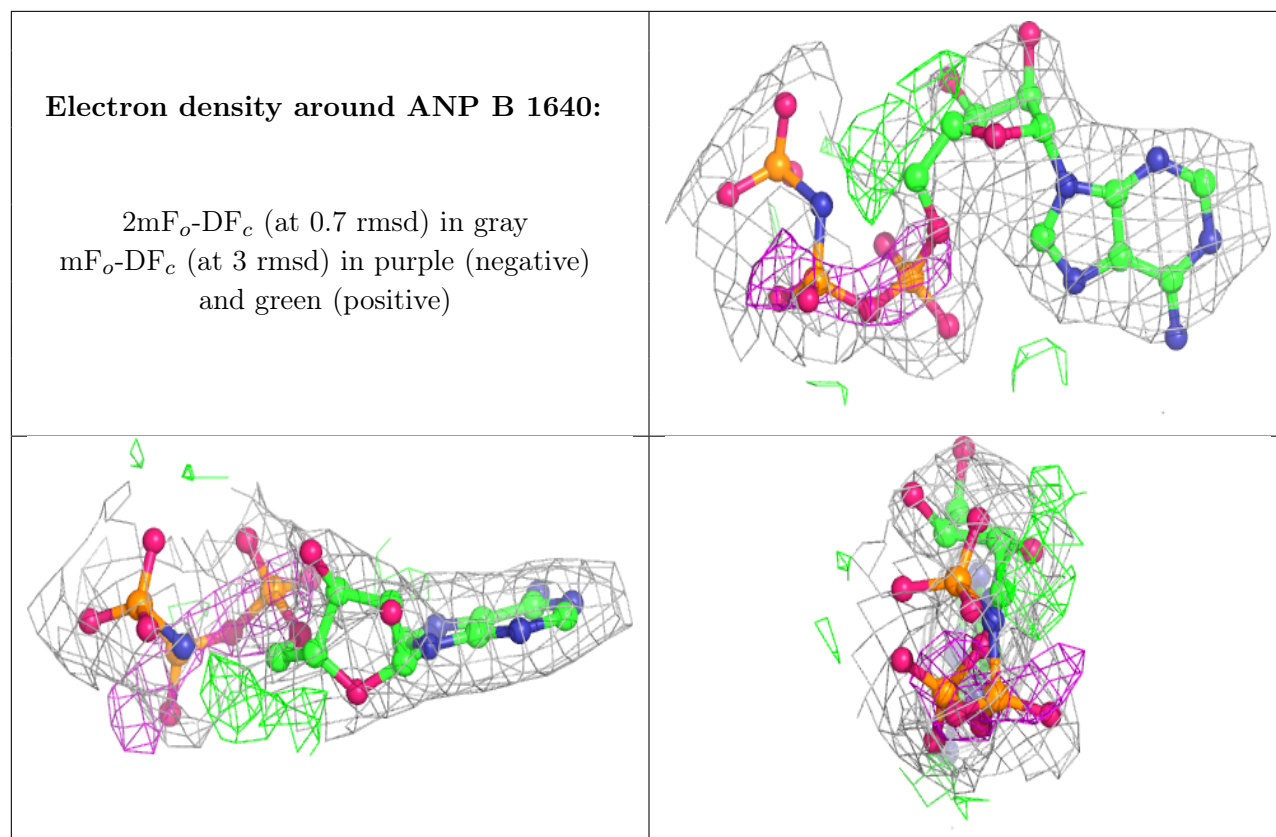
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	ANP	C	2640	31/31	0.79	0.19	75,77,79,80	12
4	ANP	B	1640	31/31	0.89	0.16	70,76,90,91	0
3	MG	C	2642	1/1	0.89	0.09	79,79,79,79	0
5	PO4	C	901	5/5	0.89	0.15	108,108,108,108	0
3	MG	B	1642	1/1	0.90	0.13	44,44,44,44	0
3	MG	B	1641	1/1	0.93	0.17	63,63,63,63	0
3	MG	C	2641	1/1	0.96	0.07	75,75,75,75	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.