



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:25 am BST

PDB ID : 1S9I  
Title : X-ray structure of the human mitogen-activated protein kinase kinase 2 (MEK2) in a complex with ligand and MgATP  
Authors : Ohren, J.F.; Chen, H.; Pavlovsky, A.; Whitehead, C.; Yan, C.; McConnell, P.; Delaney, A.; Dudley, D.T.; Sebolt-Leopold, J.; Hasemann, C.A.  
Deposited on : 2004-02-04  
Resolution : 3.20 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 : 2.11  
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) : 2.11

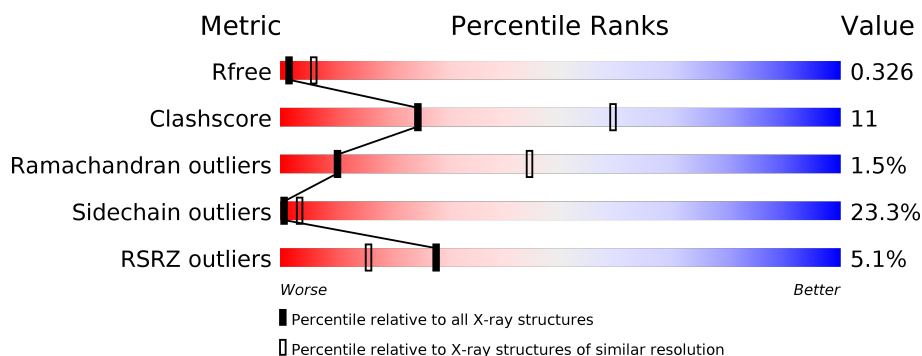
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	354	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>27%</div> <div>8%</div> <div>14%</div> </div> </div>
1	B	354	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div>5%</div> <div>18%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4812 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 Dual specificity mitogen-activated protein kinase kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2385	1518	416	437	14			
1	B	291	Total	C	N	O	S	0	0	0
			2301	1466	399	422	14			

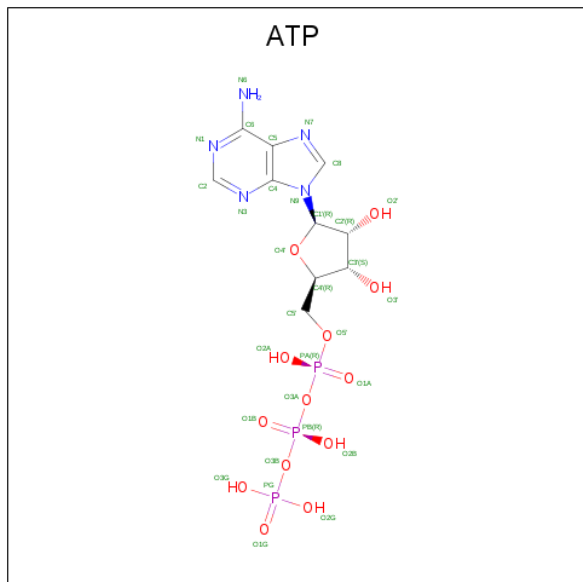
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LEU	-	CLONING ARTIFACT	UNP P36507
A	402	GLU	-	CLONING ARTIFACT	UNP P36507
A	403	HIS	-	EXPRESSION TAG	UNP P36507
A	404	HIS	-	EXPRESSION TAG	UNP P36507
A	405	HIS	-	EXPRESSION TAG	UNP P36507
A	406	HIS	-	EXPRESSION TAG	UNP P36507
A	407	HIS	-	EXPRESSION TAG	UNP P36507
A	408	HIS	-	EXPRESSION TAG	UNP P36507
B	401	LEU	-	CLONING ARTIFACT	UNP P36507
B	402	GLU	-	CLONING ARTIFACT	UNP P36507
B	403	HIS	-	EXPRESSION TAG	UNP P36507
B	404	HIS	-	EXPRESSION TAG	UNP P36507
B	405	HIS	-	EXPRESSION TAG	UNP P36507
B	406	HIS	-	EXPRESSION TAG	UNP P36507
B	407	HIS	-	EXPRESSION TAG	UNP P36507
B	408	HIS	-	EXPRESSION TAG	UNP P36507

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	I	N	O	0	0
			31	20	3	1	5	2		
4	B	1	Total	C	F	I	N	O	0	0
			31	20	3	1	5	2		



HIS  
HIS  
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HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.89Å 161.89Å 122.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.40 – 3.20 14.41 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.40-3.20) 99.9 (14.41-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.96 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.290 , 0.364 0.267 , 0.326	Depositor DCC
$R_{free}$ test set	802 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	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	0.88	EDS
Total number of atoms	4812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MG, 5EA, ATP

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	0.35	0/2432	0.68	9/3282 (0.3%)
1	B	0.34	0/2345	0.64	9/3161 (0.3%)
All	All	0.35	0/4777	0.66	18/6443 (0.3%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	323	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	151	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	341	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	140	ASP	CB-CG-OD2	5.80	123.52	118.30

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	2385	0	2418	62	0
1	B	2301	0	2335	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	31	0	19	1	0
4	B	31	0	19	2	0
All	All	4812	0	4815	105	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 11.

The worst 5 of 105 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:313:ARG:HB3	1:A:314:PRO:CD	1.78	1.11
1:A:313:ARG:HB3	1:A:314:PRO:HD3	1.12	1.06
1:A:313:ARG:CB	1:A:314:PRO:HD3	2.01	0.88
1:A:108:LYS:N	1:A:109:PRO:HD3	2.02	0.75
1:B:92:ARG:HB3	1:B:93:PRO:HD3	1.76	0.66

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	297/354 (84%)	263 (89%)	28 (9%)	6 (2%)	7	38
1	B	285/354 (80%)	255 (90%)	27 (10%)	3 (1%)	14	51
All	All	582/708 (82%)	518 (89%)	55 (10%)	9 (2%)	10	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	284	VAL
1	A	109	PRO
1	A	106	GLU
1	B	110	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	262/305 (86%)	202 (77%)	60 (23%)	1	4
1	B	253/305 (83%)	193 (76%)	60 (24%)	1	3
All	All	515/610 (84%)	395 (77%)	120 (23%)	1	3

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	MET
1	B	97	ILE
1	B	353	ASN
1	A	367	THR
1	B	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	353	ASN
1	B	247	GLN
1	A	240	GLN
1	A	366	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ATP	B	537	2	26,33,33	1.02	1 (3%)	31,52,52	1.46	5 (16%)
4	5EA	A	1001	-	29,34,34	2.59	5 (17%)	37,47,47	2.29	14 (37%)
3	ATP	A	535	2	26,33,33	1.00	1 (3%)	31,52,52	1.49	5 (16%)
4	5EA	B	1002	-	29,34,34	2.65	5 (17%)	37,47,47	2.30	15 (40%)

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	ATP	B	537	2	-	2/18/38/38	0/3/3/3
4	5EA	A	1001	-	-	1/9/22/22	0/4/4/4
3	ATP	A	535	2	-	1/18/38/38	0/3/3/3
4	5EA	B	1002	-	-	0/9/22/22	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	5EA	C10-C15	8.20	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	5EA	C10-C15	8.13	1.49	1.38
4	B	1002	5EA	C2-C6	6.33	1.49	1.39
4	B	1002	5EA	C1-C2	6.31	1.49	1.41
4	A	1001	5EA	C1-C2	6.20	1.49	1.41

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	5EA	C28-N26-C27	7.85	126.51	108.83
4	A	1001	5EA	C28-N26-C27	7.85	126.50	108.83
4	B	1002	5EA	C30-O31-C29	4.10	123.58	109.89
4	A	1001	5EA	C30-O31-C29	4.09	123.56	109.89
4	B	1002	5EA	C19-C15-C10	-3.84	119.85	123.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	5EA	C22-C24-N26-C28
3	B	537	ATP	PB-O3A-PA-O5'
3	B	537	ATP	O4'-C4'-C5'-O5'
3	A	535	ATP	C5'-O5'-PA-O1A

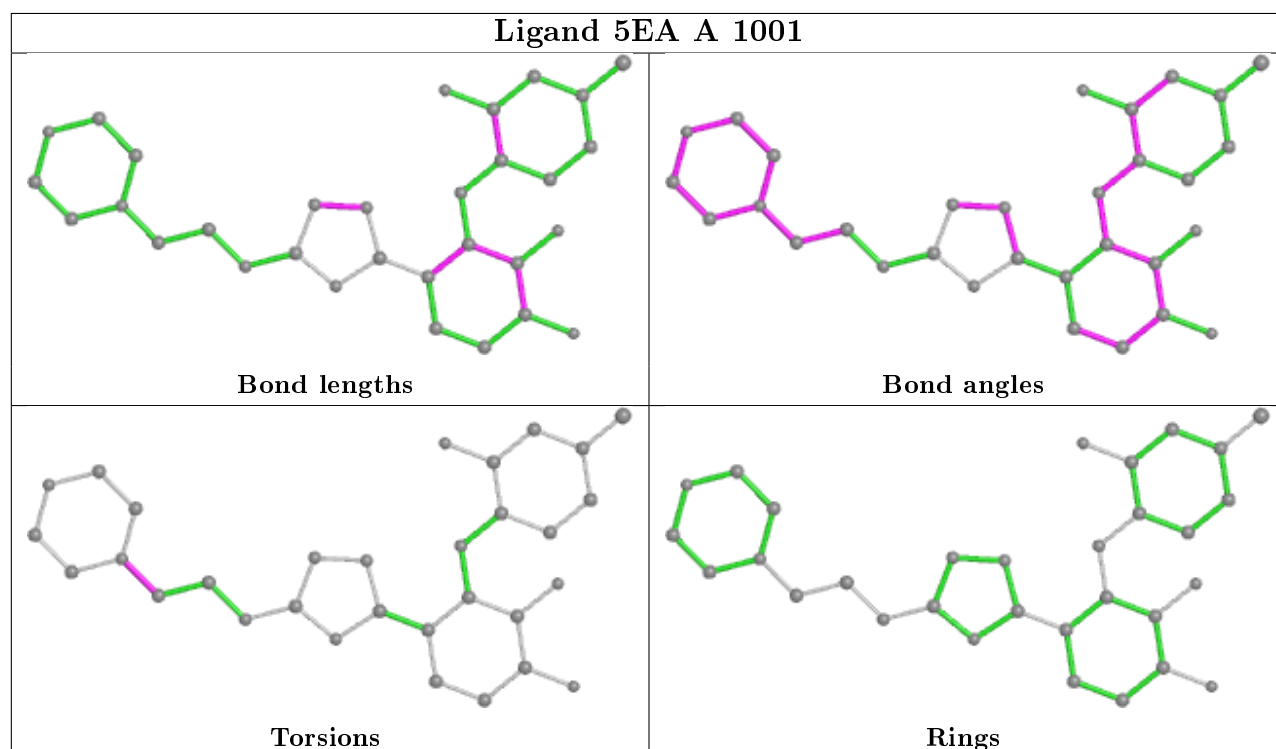
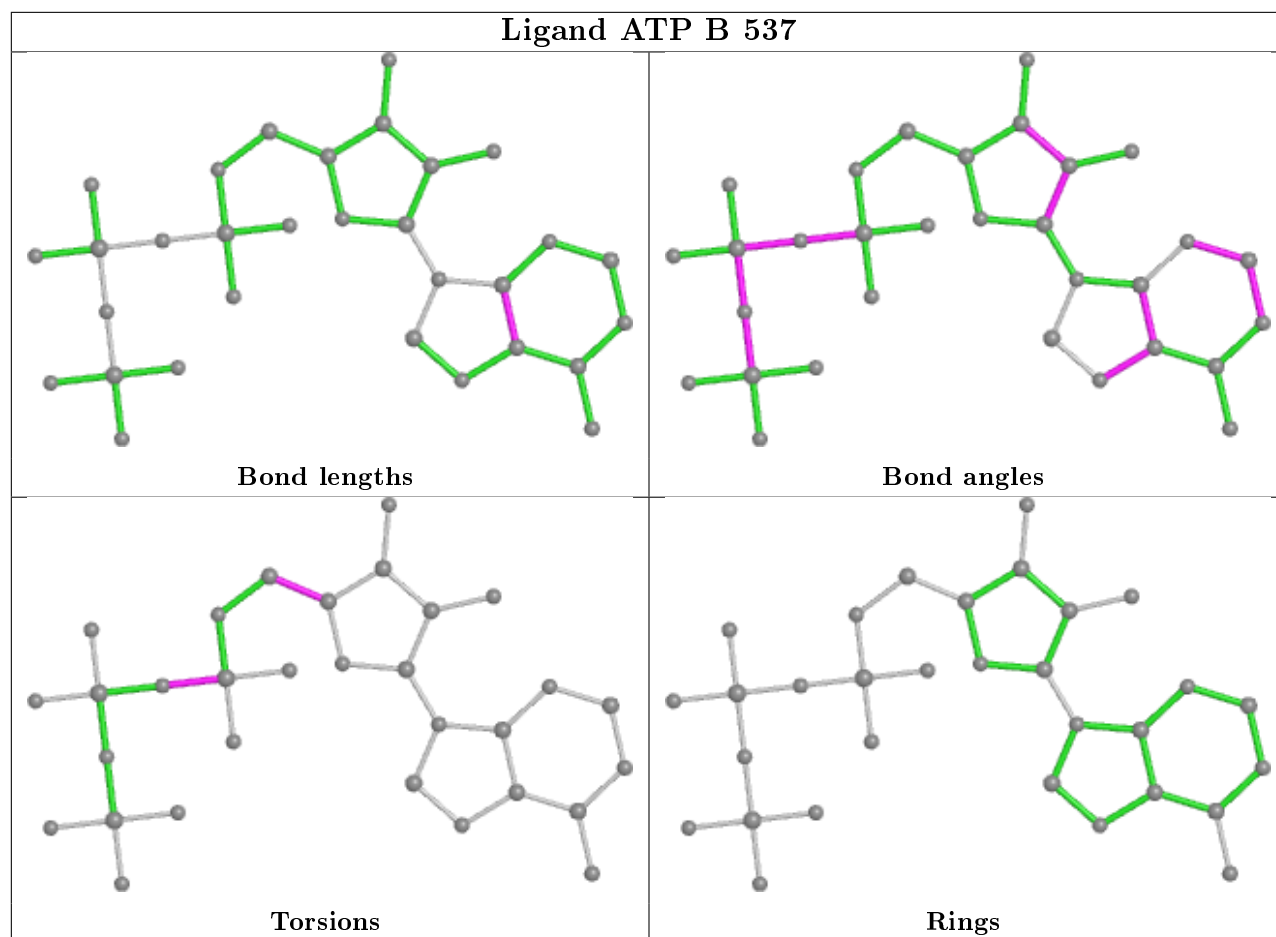
There are no ring outliers.

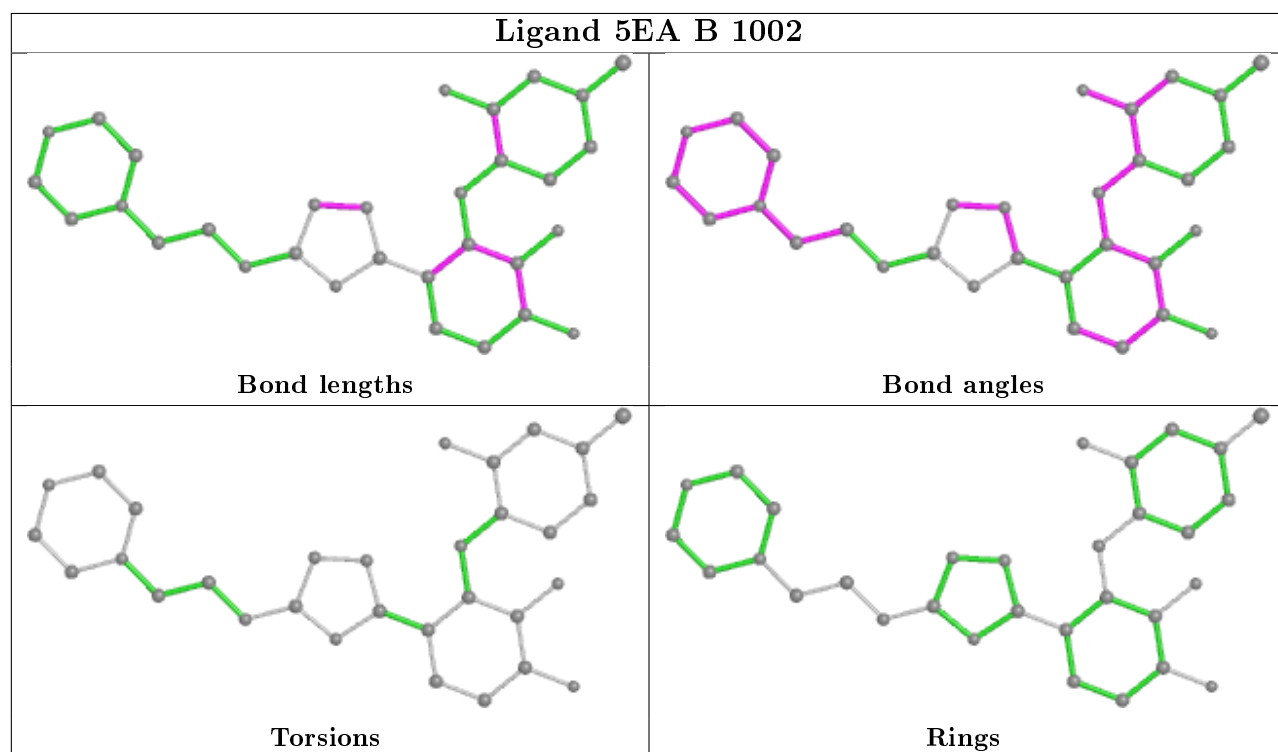
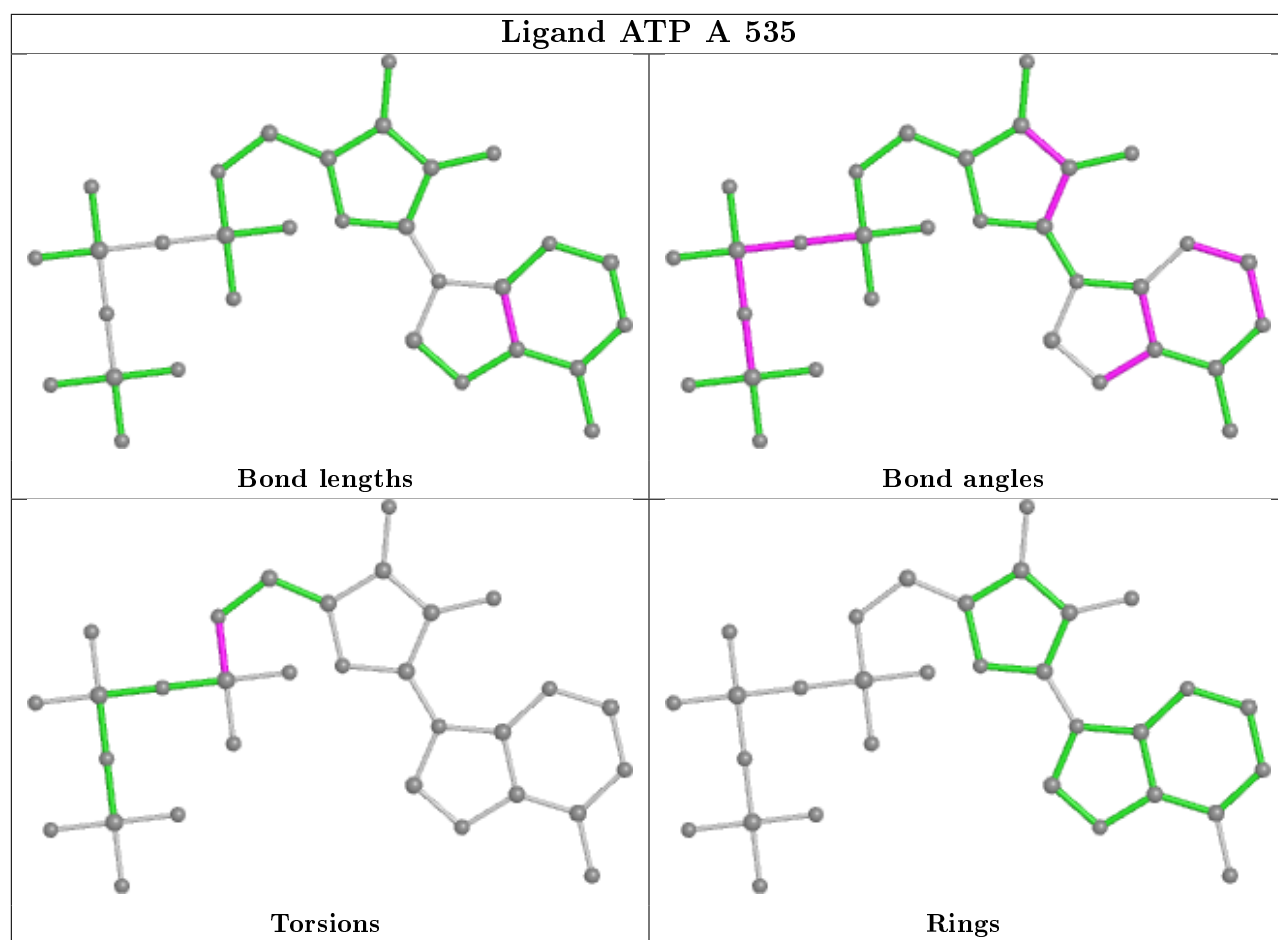
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	5EA	1	0
4	B	1002	5EA	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 [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, 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	303/354 (85%)	-0.01	11 (3%)	42 27	13, 34, 63, 68	2 (0%)
1	B	291/354 (82%)	0.18	19 (6%)	18 11	24, 46, 66, 68	2 (0%)
All	All	594/708 (83%)	0.08	30 (5%)	28 16	13, 40, 65, 68	4 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	ASP	5.2
1	B	109	PRO	4.7
1	A	392	PRO	4.6
1	B	82	ASN	3.9
1	B	140	ASP	3.7

### 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](#)

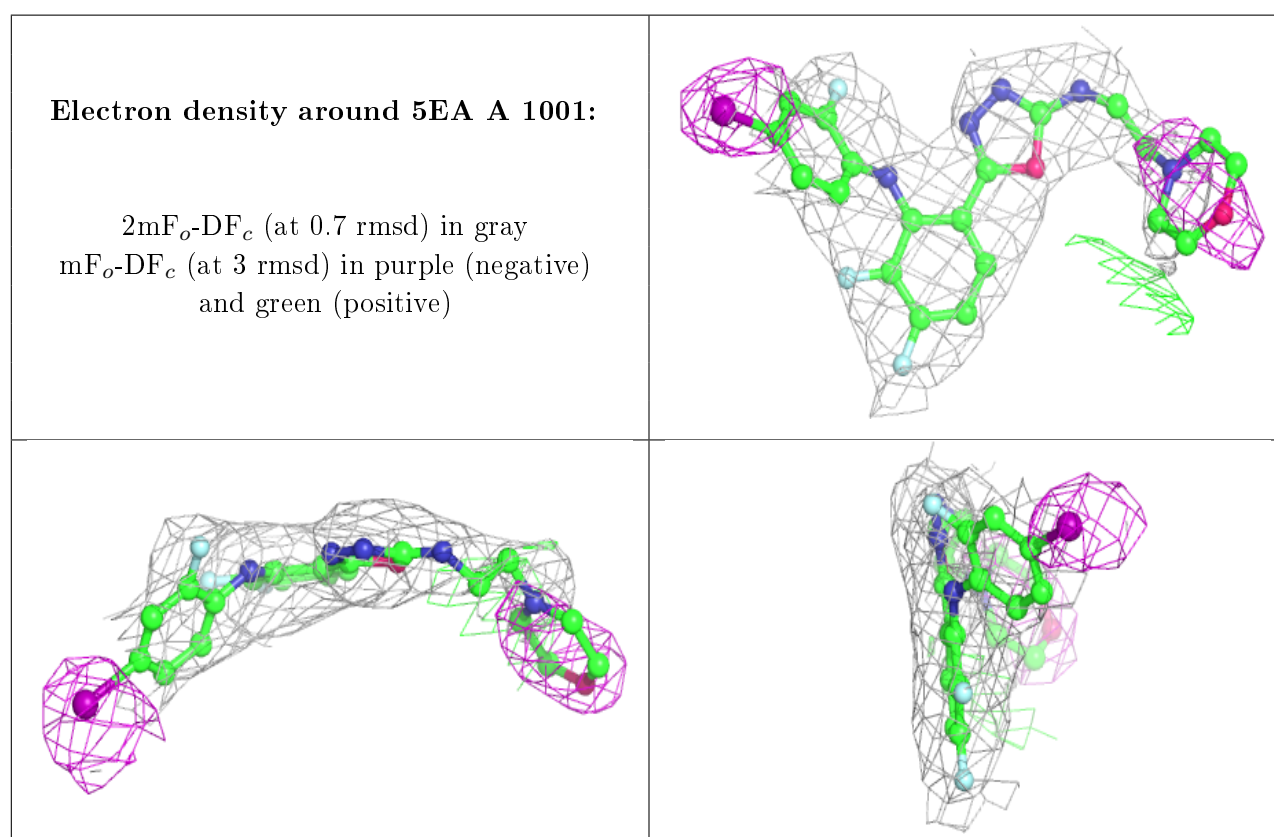
There are no carbohydrates in this entry.

### 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.

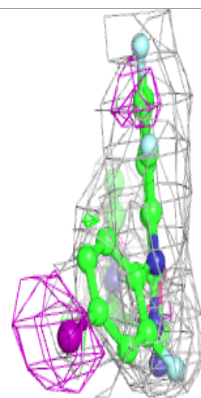
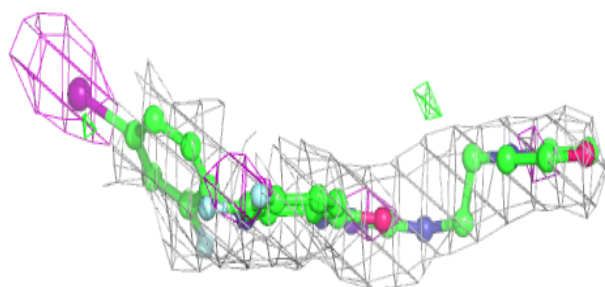
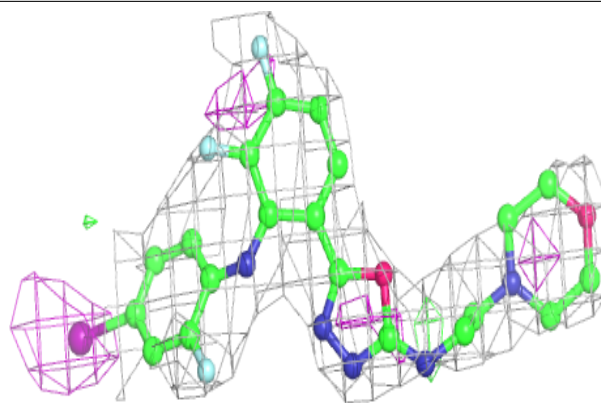
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	538	1/1	0.87	0.20	32,32,32,32	0
4	5EA	A	1001	31/31	0.92	0.20	28,31,34,38	0
4	5EA	B	1002	31/31	0.93	0.19	33,33,40,46	0
3	ATP	B	537	31/31	0.94	0.17	50,51,52,52	0
3	ATP	A	535	31/31	0.94	0.20	46,47,48,49	0
2	MG	A	536	1/1	0.96	0.21	18,18,18,18	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.

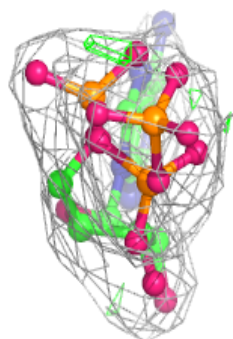
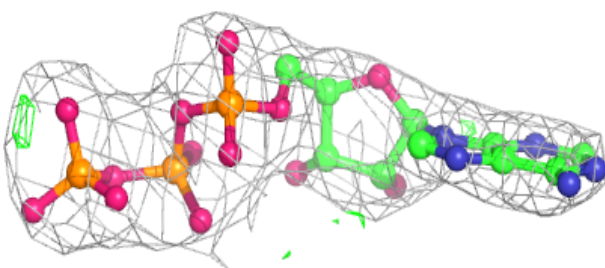
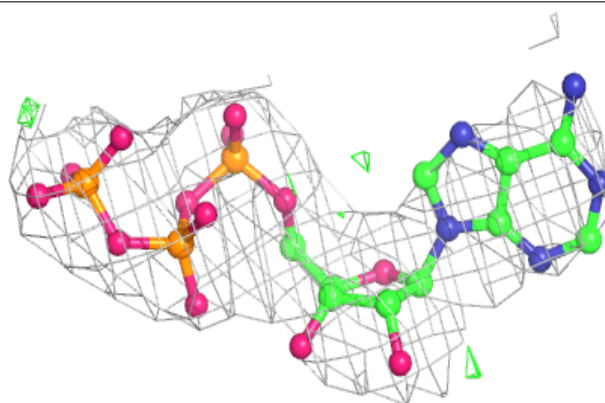


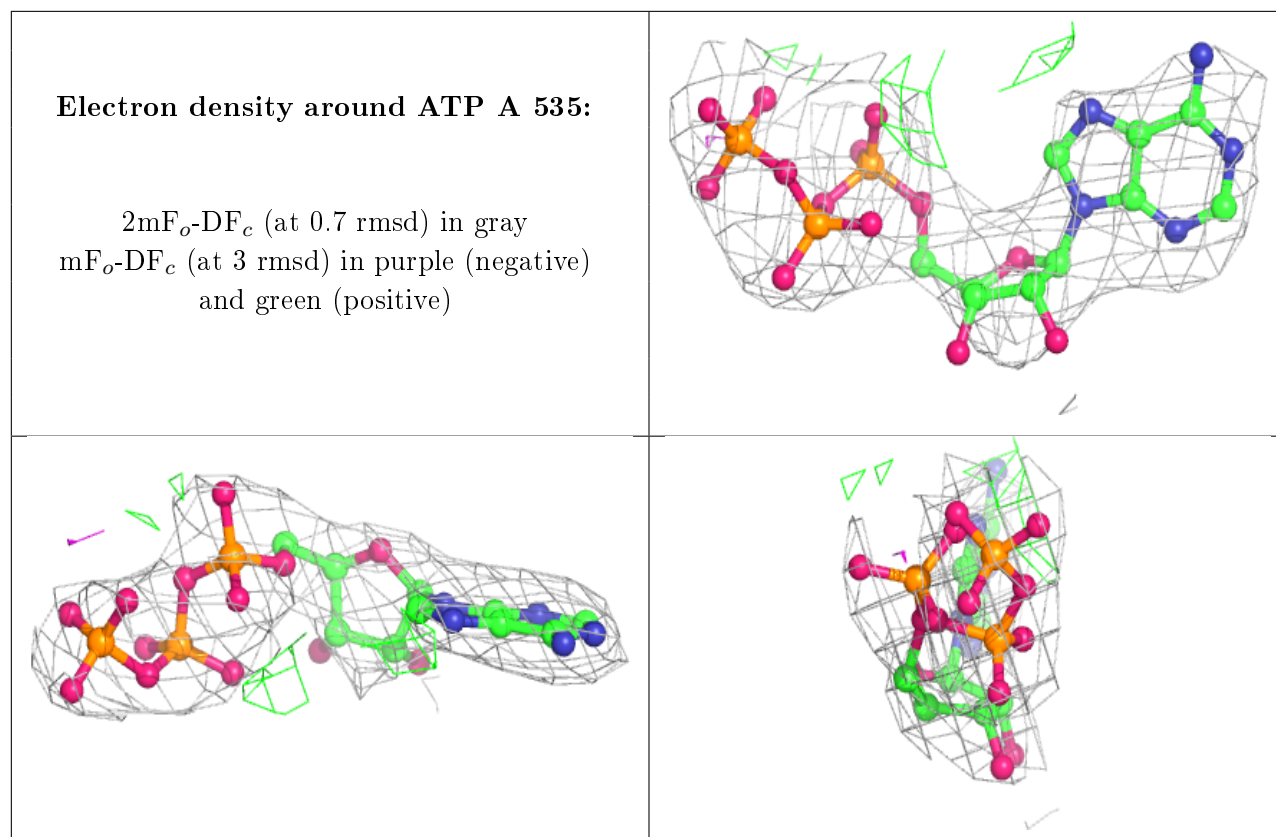
**Electron density around 5EA B 1002:**

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

**Electron density around ATP B 537:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.