

# Full wwPDB X-ray Structure Validation Report (i)

### May 15, 2020 – 06:41 am BST

PDB ID : 5DHQ

Title: Crystal structure of NAD kinase 1 from Listeria monocytogenes in complex

with a novel inhibitor

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Deposited on : 2015-08-31

Resolution : 2.29 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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)

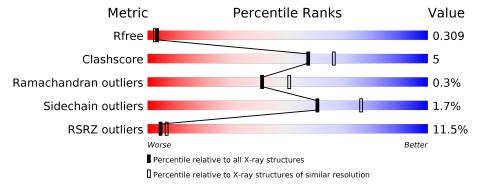
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.29 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=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	272	3% 87%	10% •
1	В	272	13% 79%	17% •
1	С	272	13% 83%	13% •
1	D	272	15% 79%	13% 7%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8483 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 NAD kinase 1.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Λ	263	Total	С	N	О	S	0	1	0
1	A	203	2070	1324	347	390	9	0	1	
1	В	260	Total	С	N	О	S	0	0	0
1	Ъ	200	2069	1328	347	385	9	0	0	
1	С	260	Total	С	N	О	S	0	0	0
1		200	2016	1294	339	374	9	0	U	
1	D	253	Total	С	N	О	S	0	0	0
1	ע	200	1966	1257	337	364	8		U	

There are 32 discrepancies between the modelled and reference sequences:

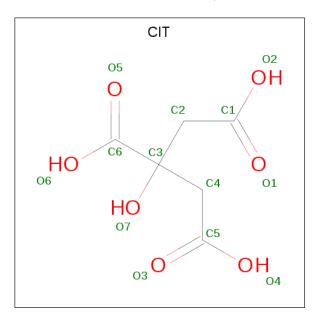
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
В	265	LEU	_	expression tag	UNP Q8Y8D7
В	266	GLU	-	expression tag	UNP Q8Y8D7
В	267	HIS	_	expression tag	UNP Q8Y8D7
В	268	HIS	_	expression tag	UNP Q8Y8D7
В	269	HIS	_	expression tag	UNP Q8Y8D7
В	270	HIS	_	expression tag	UNP Q8Y8D7
В	271	HIS	_	expression tag	UNP Q8Y8D7
В	272	HIS	_	expression tag	UNP Q8Y8D7
С	265	LEU	-	expression tag	UNP Q8Y8D7
С	266	GLU	-	expression tag	UNP Q8Y8D7
С	267	HIS	=	expression tag	UNP Q8Y8D7
С	268	HIS	-	expression tag	UNP Q8Y8D7
С	269	HIS	_	expression tag	UNP Q8Y8D7



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Chain	Residue	Modelled	Actual	Comment	Reference
С	270	HIS	-	expression tag	UNP Q8Y8D7
С	271	HIS	-	expression tag	UNP Q8Y8D7
С	272	HIS	_	expression tag	UNP Q8Y8D7
D	265	LEU	-	expression tag	UNP Q8Y8D7
D	266	GLU	_	expression tag	UNP Q8Y8D7
D	267	HIS	_	expression tag	UNP Q8Y8D7
D	268	HIS	_	expression tag	UNP Q8Y8D7
D	269	HIS	_	expression tag	UNP Q8Y8D7
D	270	HIS	_	expression tag	UNP Q8Y8D7
D	271	HIS	_	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

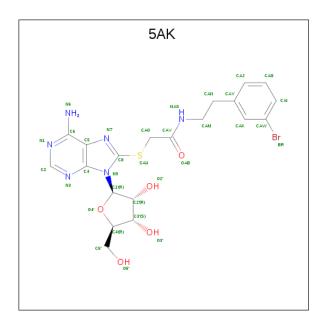
• Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	В	1	Total C O 13 6 7	0	0

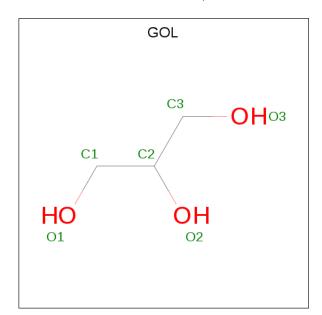
 $\bullet \ \ Molecule \ 3 \ is \ 8-[(2-\{[2-(3-bromophenyl)ethyl]amino\}-2-oxoethyl)sulfanyl]adenosine \ (three-letter code: 5AK) \ (formula: \ C_{20}H_{23}BrN_6O_5S).$ 





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
3	A	1	Total	Br	С	N	О	S	0	0	
	Λ	1	33	1	20	6	5	1	U	U	
3	В	1	Total	$\operatorname{Br}$	С	Ν	Ο	S	0	0	
	Ъ	1	33	1	20	6	5	1	0	U	
3	C	1	Total	$\operatorname{Br}$	С	Ν	О	S	0	0	
) 		1	33	1	20	6	5	1	0	0	
3	D	1	Total	$\operatorname{Br}$	С	N	О	S	0	0	
3		1	33	1	20	6	5	1			

 $\bullet$  Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total C O 6 3 3	0	0

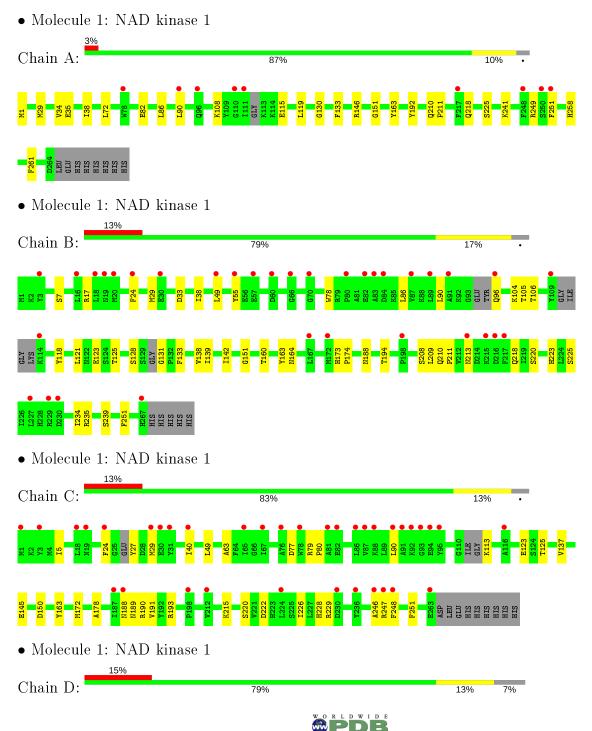
## $\bullet$ Molecule 5 is water.

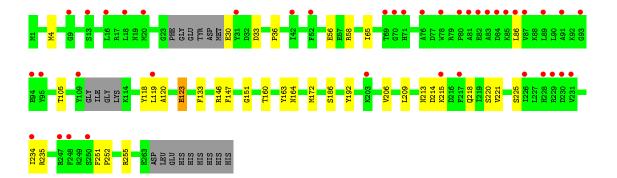
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	В	36	Total O 36 36	0	0
5	С	63	Total O 63 63	0	0
5	D	43	Total O 43 43	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.79Å 119.18Å 67.21Å	Domositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.91^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.29 - 2.29	Depositor
Resolution (A)	44.29 - 2.29	EDS
% Data completeness	89.9 (44.29-2.29)	Depositor
(in resolution range)	90.1 (44.29-2.29)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$< I/\sigma(I) > 1$	3.56 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.260 , 0.311	Depositor
$R, R_{free}$	0.262 , $0.309$	DCC
$R_{free}$ test set	1273 reflections $(3.03\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.28, 56.5	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: GOL, 5AK, CIT

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		
MIOI	Chain	RMSZ   # Z  > 5		RMSZ	# Z  > 5	
1	A	0.20	0/2125	0.35	0/2876	
1	В	0.21	0/2117	0.35	0/2858	
1	С	0.20	0/2065	0.35	0/2795	
1	D	0.21	0/2013	0.36	0/2728	
All	All	0.21	0/8320	0.35	0/11257	

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 (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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2070	0	1990	12	0
1	В	2069	0	2022	24	0
1	С	2016	0	1923	20	0
1	D	1966	0	1876	19	0
2	A	13	0	5	0	0
2	В	13	0	5	0	0
3	A	33	0	0	2	0
3	В	33	0	0	2	0
3	С	33	0	0	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	33	0	0	4	0
4	С	6	0	8	0	0
5	A	56	0	0	0	0
5	В	36	0	0	1	0
5	С	63	0	0	4	0
5	D	43	0	0	1	0
All	All	8483	0	7829	79	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 5.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1 4 00 H D HD 10	1 4 00 1 511 115 00	distance (Å)	overlap (Å)
1:A:38:ILE:HD13	1:A:90:LEU:HD22	1.77	0.67
1:D:160:THR:HG21	1:D:172:MET:HG2	1.81	0.62
1:C:188:ASN:ND2	5:C:401:HOH:O	2.35	0.59
1:C:125:THR:OG1	1:C:220:SER:OG	2.19	0.59
1:B:24:PHE:HD1	1:B:29:MET:HG3	1.69	0.58
1:D:30:GLU:N	5:D:402:HOH:O	2.36	0.58
1:D:218:GLN:OE1	1:D:225:SER:OG	2.20	0.57
1:C:24:PHE:HB3	1:C:29:MET:HB2	1.87	0.57
1:B:125:THR:OG1	1:B:220:SER:OG	2.22	0.56
1:B:38:ILE:HD13	1:B:90:LEU:HD22	1.85	0.56
1:D:65:ILE:HG21	1:D:86:LEU:HD21	1.88	0.56
3:B:302:5AK:SAU	3:B:302:5AK:C2'	2.93	0.55
1:D:213:ASN:O	1:D:215:LYS:N	2.39	0.55
1:D:36:PRO:HD2	1:D:58:ARG:HE	1.74	0.53
1:B:138:VAL:HB	1:B:208:SER:HB3	1.91	0.52
1:B:104:LYS:HB2	1:B:239:SER:HB2	1.92	0.52
1:A:108:LYS:NZ	1:A:115:GLU:OE1	2.42	0.52
1:C:79:ARG:HG3	1:C:80:PRO:HD2	1.92	0.51
1:A:261:PHE:O	1:C:193:ARG:NH2	2.43	0.51
1:D:252:PRO:HD2	1:D:255:ARG:HD3	1.93	0.50
1:B:96:GLN:N	5:B:407:HOH:O	2.45	0.49
1:B:209:LEU:HB2	1:B:234:ILE:HB	1.95	0.49
1:B:33:ASP:O	1:B:55:TYR:OH	2.27	0.49
1:C:215:LYS:NZ	5:C:404:HOH:O	2.40	0.49
1:D:4:MET:HG3	1:D:33:ASP:HA	1.95	0.49
1:C:229:ARG:NH2	5:C:407:HOH:O	2.46	0.48
1:B:49:LEU:HD23	1:B:121:LEU:HD23	1.95	0.48



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Continuea from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:C:172:MET:HE1	1:C:178:ALA:HB3	1.96	0.48
1:D:123:GLU:OE2	3:D:301:5AK:O2'	2.32	0.47
1:A:82:GLU:OE1	1:A:249:ARG:NH2	2.47	0.47
1:B:218:GLN:NE2	1:B:225:SER:OG	2.30	0.47
1:C:5:ILE:HG12	1:C:40:ILE:HB	1.96	0.47
1:D:209:LEU:HB2	1:D:234:ILE:HB	1.97	0.46
1:A:34:VAL:HG12	1:A:35:GLU:HG3	1.96	0.46
1:D:56:GLU:HB3	1:D:119:LEU:HD12	1.97	0.46
1:D:120:ALA:HB2	1:D:221:VAL:HG13	1.97	0.46
1:B:218:GLN:HE21	1:B:225:SER:HG	1.61	0.45
1:B:106:THR:HB	1:B:235:ARG:HB2	1.97	0.45
1:A:210:GLN:HA	1:A:211:PRO:HD3	1.84	0.45
1:B:173:HIS:HA	1:B:174:PRO:HD3	1.85	0.44
1:D:160:THR:HA	1:D:164:ASN:HB3	1.99	0.44
1:C:189:ASN:C	1:C:191:VAL:H	2.21	0.44
1:A:218:GLN:NE2	1:A:225:SER:OG	2.37	0.44
1:C:27:TYR:N	5:C:410:HOH:O	2.51	0.44
1:B:133:PHE:CD2	1:B:151:GLY:HA2	2.53	0.43
1:C:49:LEU:HD23	1:C:222:ASP:HB3	1.99	0.43
1:B:160:THR:HA	1:B:164:ASN:HB3	2.00	0.43
1:C:226:ILE:HG13	1:C:228:HIS:CE1	2.53	0.43
1:D:146:ARG:HG2	1:D:192:TYR:HD1	1.83	0.43
1:B:7:SER:HB2	1:B:17:ARG:HD2	2.00	0.42
1:D:206:VAL:HG11	1:D:235:ARG:NH2	2.34	0.42
1:A:133:PHE:CD2	1:A:151:GLY:HA2	2.54	0.42
1:B:188:ASN:OD1	1:B:194:THR:N	2.47	0.42
1:D:220:SER:HA	1:D:225:SER:HA	2.01	0.42
3:D:301:5AK:C2'	3:D:301:5AK:SAU	3.08	0.42
3:A:302:5AK:NAS	3:A:302:5AK:CAJ	2.76	0.42
3:A:302:5AK:N6	1:C:150:ASP:OD1	2.53	0.42
1:A:146:ARG:HG2	1:A:192:TYR:HD1	1.84	0.42
1:C:63:ALA:HB1	1:C:246:ALA:HB2	2.01	0.42
3:D:301:5AK:CAV	3:D:301:5AK:CAJ	2.97	0.42
1:A:119:LEU:HD11	1:A:241:LYS:HD2	2.01	0.42
1:C:137:VAL:HB	1:C:145:GLU:HG2	2.02	0.42
1:D:147:PHE:CE2	1:D:186:SER:HB2	2.55	0.42
1:C:77:ASP:OD2	1:C:247:ARG:NH1	2.53	0.41
1:B:210:GLN:HA	1:B:211:PRO:HD3	1.84	0.41
1:B:105:THR:HB	1:B:118:TYR:HB2	2.01	0.41
1:B:128:SER:HB3	1:B:133:PHE:HB2	2.03	0.41
1:C:90:LEU:HB3	1:C:248:PHE:HZ	1.86	0.41



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Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:D:105:THR:HB	1:D:118:TYR:HB2	2.03	0.41
1:B:123:GLU:OE1	3:B:302:5AK:O2'	2.38	0.41
1:B:78:TRP:CD2	1:B:86:LEU:HD21	2.56	0.41
1:B:128:SER:OG	1:B:131:GLY:O	2.31	0.41
1:C:189:ASN:O	1:C:191:VAL:N	2.51	0.41
1:A:146:ARG:HG2	1:A:192:TYR:CD1	2.56	0.41
1:B:139:ILE:O	1:B:142:ILE:HG22	2.20	0.41
1:D:133:PHE:CD2	1:D:151:GLY:HA2	2.56	0.41
1:A:1:MET:HB2	1:A:29:MET:SD	2.61	0.40
1:C:123:GLU:OE1	3:C:301:5AK:O2'	2.39	0.40
3:D:301:5AK:CAJ	3:D:301:5AK:NAS	2.83	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	Perce	ntiles
1	A	260/272~(96%)	247 (95%)	12 (5%)	1 (0%)	34	42
1	В	$252/272 \ (93\%)$	233 (92%)	19 (8%)	0	100	100
1	С	$254/272 \ (93\%)$	232 (91%)	21 (8%)	1 (0%)	34	42
1	D	247/272 (91%)	231 (94%)	15 (6%)	1 (0%)	34	42
All	All	1013/1088 (93%)	943 (93%)	67 (7%)	3 (0%)	41	50

### All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	190	ARG
1	D	214	ASP
1	A	130	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	$221/237 \ (93\%)$	216 (98%)	5 (2%)	50 67
1	В	224/237 (94%)	220 (98%)	4 (2%)	59 75
1	С	210/237 (89%)	207 (99%)	3 (1%)	67 81
1	D	205/237~(86%)	202 (98%)	3 (2%)	65 79
All	All	860/948 (91%)	845 (98%)	15 (2%)	60 76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	Type
1	A	72	LEU
1	A	86	LEU
1	A	163	TYR
1	A	251	PHE
1	A	258	HIS
1	В	163	TYR
1	В	213	ASN
1	В	223	HIS
1	В	251	PHE
1	С	113	LYS
1	С	163	TYR
1	С	251	PHE
1	D	123	GLU
1	D	163	TYR
1	D	251	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

7 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	В	ond leng	$\operatorname{gths}$	Bond angles			
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	5AK	A	302	_	34,36,36	2.55	7 (20%)	35,51,51	2.18	4 (11%)
3	5AK	В	302	-	34,36,36	3.62	16 (47%)	35,51,51	2.66	9 (25%)
3	5AK	D	301	-	34,36,36	2.86	16 (47%)	35,51,51	2.64	8 (22%)
2	CIT	A	301	-	3,12,12	1.29	0	3,17,17	1.64	1 (33%)
2	CIT	В	301	-	3,12,12	1.45	0	3,17,17	2.34	2 (66%)
4	GOL	С	302	_	5,5,5	0.37	0	5,5,5	0.27	0
3	5AK	С	301	_	34,36,36	3.24	14 (41%)	35,51,51	2.80	6 (17%)

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	5AK	A	302	-	-	5/11/45/45	0/4/4/4
3	5AK	В	302	-	-	3/11/45/45	0/4/4/4
3	5AK	D	301	-	-	2/11/45/45	0/4/4/4
2	CIT	A	301	-	-	2/6/16/16	_
2	CIT	В	301	-	-	3/6/16/16	_



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	$\operatorname{GOL}$	С	302	_	-	2/4/4/4	-
3	5AK	С	301	_	-	3/11/45/45	0/4/4/4

All (53) bond length outliers are listed below:

3 3	В	0.00			$\mathbf{Z}$	$oxed{\mathbf{Observed}}(\mathbf{\mathring{A}})$	$Ideal(A)$
		302	5AK	BR-CAW	-10.15	1.69	1.90
3	Α	302	5AK	C2-N3	10.11	1.48	1.32
, ,	В	302	5AK	C8-SAU	-9.31	1.50	1.75
3	С	301	5AK	C8-SAU	-8.29	1.53	1.75
3	D	301	5AK	C2-N3	8.13	1.45	1.32
3	В	302	5AK	C2-N3	7.95	1.44	1.32
3	A	302	5AK	C2-N1	7.75	1.48	1.33
3	С	301	5AK	BR-CAW	-7.52	1.75	1.90
3	С	301	5AK	C2-N3	7.28	1.43	1.32
3	D	301	5AK	C2-N1	6.51	1.46	1.33
3	В	302	5AK	C2-N1	6.16	1.45	1.33
3	С	301	5AK	C8-N9	-6.16	1.30	1.36
3	D	301	5AK	BR-CAW	-6.10	1.78	1.90
3	В	302	5AK	C8-N9	-5.89	1.30	1.36
3	С	301	5AK	CAN-CAY	-5.26	1.36	1.51
3	С	301	5AK	C2-N1	5.20	1.43	1.33
3	В	302	5AK	CAN-CAY	-4.96	1.37	1.51
3	В	302	5AK	C2'-C1'	-4.80	1.46	1.53
3	D	301	5AK	C8-N9	-4.64	1.31	1.36
3	D	301	5AK	CAN-CAY	-4.44	1.38	1.51
3	A	302	5AK	CAN-CAY	-4.25	1.39	1.51
3	С	301	5AK	C5-C4	-3.87	1.30	1.40
3	A	302	5AK	C8-N9	-3.65	1.32	1.36
3	В	302	5AK	C5-C4	-3.60	1.31	1.40
3	D	301	5AK	C5-C4	-3.39	1.32	1.40
3	В	302	5AK	C6-C5	-3.15	1.31	1.43
3	С	301	5AK	O4'-C4'	-3.10	1.38	1.45
3	D	301	5AK	C6-C5	-3.06	1.31	1.43
3	D	301	5AK	C2'-C1'	-3.03	1.49	1.53
3	С	301	5AK	C6-C5	-3.02	1.32	1.43
3	D	301	5AK	C2'-C3'	-2.95	1.45	1.53
3	D	301	5AK	C8-SAU	-2.93	1.67	1.75
3	D	301	5AK	C3'-C4'	-2.90	1.45	1.53
3	С	301	5AK	C4-N3	-2.79	1.31	1.35
3	В	302	5AK	C2'-C3'	-2.71	1.45	1.53
3	С	301	5AK	C2'-C1'	-2.67	1.49	1.53



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Mol	Chain	${f Res}$	Type	${f Atoms}$	$\mathbf{Z}$	${ m Observed}({ m \AA})$	$oxed{Ideal(A)}$
3	A	302	5AK	C6-C5	-2.65	1.33	1.43
3	С	301	5AK	C2'-C3'	-2.65	1.46	1.53
3	A	302	5AK	C5-C4	-2.57	1.34	1.40
3	С	301	5AK	O2'-C2'	-2.53	1.37	1.43
3	D	301	5AK	O4'-C4'	-2.46	1.39	1.45
3	В	302	5AK	O3'-C3'	-2.36	1.37	1.43
3	D	301	5AK	C4-N3	-2.34	1.32	1.35
3	В	302	5AK	C4-N3	-2.33	1.32	1.35
3	В	302	5AK	O4'-C4'	-2.27	1.39	1.45
3	В	302	5AK	O2'-C2'	-2.24	1.37	1.43
3	D	301	5AK	O4'-C1'	-2.20	1.38	1.41
3	D	301	5AK	O3'-C3'	-2.19	1.37	1.43
3	С	301	5AK	O3'-C3'	-2.16	1.37	1.43
3	D	301	5AK	C1'-N9	-2.06	1.43	1.49
3	A	302	5AK	O4'-C1'	2.06	1.43	1.41
3	В	302	5AK	C1'-N9	-2.05	1.43	1.49
3	В	302	5AK	CAO-CAV	-2.03	1.49	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
3	С	301	5AK	N3-C2-N1	-13.28	107.92	128.68
3	В	302	5AK	N3-C2-N1	-12.83	108.63	128.68
3	D	301	5AK	N3-C2-N1	-12.83	108.63	128.68
3	A	302	5AK	N3-C2-N1	-11.15	111.25	128.68
3	С	301	5AK	O4'-C4'-C5'	-5.07	98.26	109.21
3	С	301	5AK	C1'-N9-C4	-3.93	119.82	126.71
3	D	301	5AK	O4'-C4'-C3'	-3.33	98.53	105.11
3	В	302	5AK	O4'-C1'-C2'	-3.32	102.07	106.93
3	В	302	5AK	C5'-C4'-C3'	-3.13	107.54	115.09
3	D	301	5AK	C1'-N9-C4	-3.03	121.40	126.71
3	С	301	5AK	C3'-C2'-C1'	3.02	105.52	100.98
3	В	302	5AK	O3'-C3'-C2'	-2.97	102.20	111.82
3	A	302	5AK	C5-C6-N6	-2.94	115.88	120.35
3	С	301	5AK	C2-N1-C6	2.90	123.72	118.75
2	В	301	CIT	C3-C4-C5	-2.89	110.36	114.98
2	В	301	CIT	C3-C2-C1	-2.80	110.50	114.98
3	D	301	5AK	C2-N1-C6	2.66	123.30	118.75
3	В	302	5AK	C5-C6-N6	-2.63	116.35	120.35
3	С	301	5AK	C5'-C4'-C3'	-2.61	108.78	115.09
3	D	301	5AK	O4'-C1'-C2'	-2.59	103.14	106.93
3	D	301	5AK	O2'-C2'-C3'	-2.58	103.47	111.82



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Mol	Chain	${f Res}$	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	301	CIT	C3-C4-C5	-2.57	110.86	114.98
3	В	302	5AK	C1'-N9-C4	-2.47	122.38	126.71
3	В	302	5AK	C3'-C2'-C1'	2.47	104.69	100.98
3	В	302	5AK	O2'-C2'-C3'	-2.46	103.88	111.82
3	D	301	5AK	C2'-C3'-C4'	-2.38	98.02	102.64
3	В	302	5AK	C2-N1-C6	2.38	122.82	118.75
3	A	302	5AK	C5'-C4'-C3'	-2.32	109.50	115.09
3	D	301	5AK	C5-C6-N6	-2.29	116.87	120.35
3	A	302	5AK	C3'-C2'-C1'	2.07	104.10	100.98

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	301	CIT	C2-C3-C4-C5
3	С	301	5AK	O4'-C4'-C5'-O5'
3	С	301	5AK	C3'-C4'-C5'-O5'
3	A	302	5AK	O4'-C4'-C5'-O5'
3	A	302	5AK	C3'-C4'-C5'-O5'
3	D	301	5AK	NAS-CAM-CAN-CAY
4	С	302	GOL	O1-C1-C2-C3
2	A	301	CIT	C1-C2-C3-O7
4	С	302	GOL	O1-C1-C2-O2
2	В	301	CIT	O7-C3-C4-C5
3	A	302	5AK	NAS-CAM-CAN-CAY
3	С	301	5AK	NAS-CAM-CAN-CAY
2	В	301	CIT	C6-C3-C4-C5
2	A	301	CIT	C1-C2-C3-C4
3	D	301	5AK	C3'-C4'-C5'-O5'
3	В	302	5AK	NAS-CAM-CAN-CAY
3	A	302	5AK	CAM-CAN-CAY-CAJ
3	В	302	5AK	CAM-CAN-CAY-CAJ
3	В	302	5AK	CAM-CAN-CAY-CAK
3	A	302	5AK	CAM-CAN-CAY-CAK

There are no ring outliers.

4 monomers are involved in 9 short contacts:

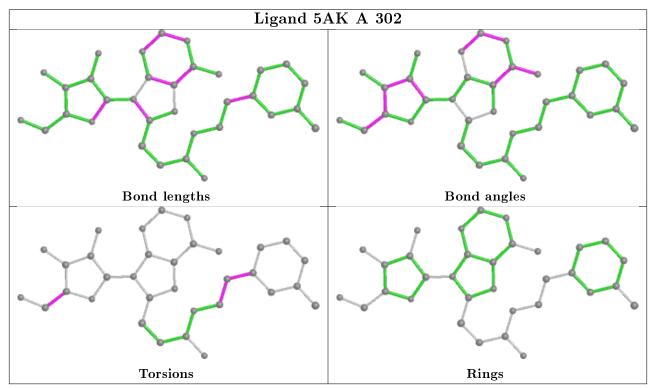
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	5AK	2	0
3	В	302	5AK	2	0



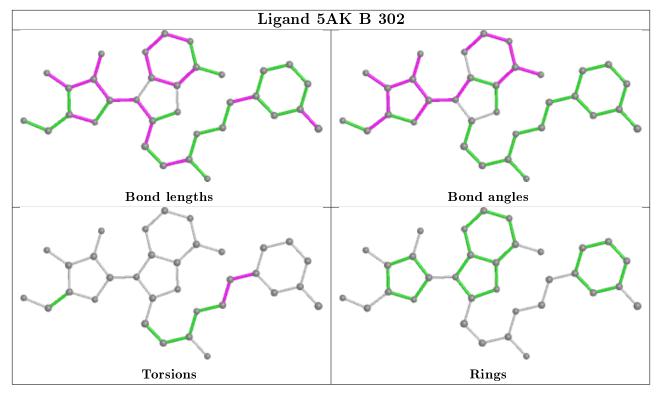
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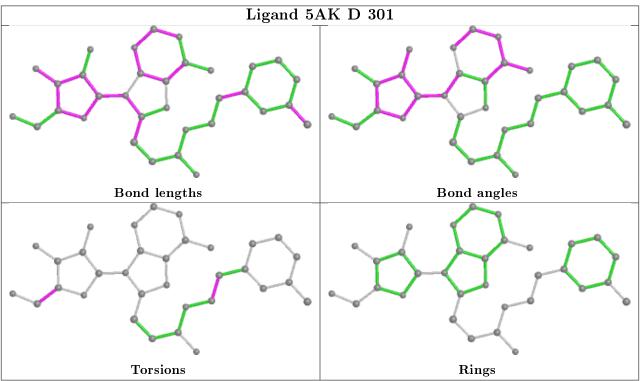
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	5AK	4	0
3	С	301	5AK	1	0

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 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.

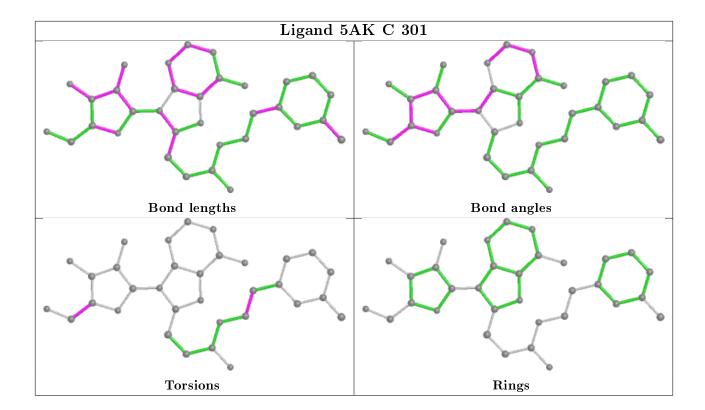












## 5.7 Other polymers (i)

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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	#RSRZ	Z>2	2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	$263/272 \; (96\%)$	0.30	9 (3%) 45		52	25, 50, 90, 128	37 (14%)
1	В	$260/272 \; (95\%)$	0.96	34 (13%)	3	4	29, 71, 114, 137	40 (15%)
1	С	$260/272 \; (95\%)$	0.85	36 (13%)	2	4	27, 62, 114, 147	36 (13%)
1	D	253/272 (93%)	0.99	40 (15%)	2	2	35, 71, 128, 163	30 (11%)
All	All	1036/1088 (95%)	0.77	119 (11%)	4	7	25, 62, 117, 163	143 (13%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	90	LEU	6.6
1	В	20	MET	6.4
1	D	86	LEU	6.2
1	D	83	ALA	5.6
1	С	248	PHE	5.6
1	D	93	GLY	5.4
1	D	91	ALA	5.4
1	D	89	LEU	5.3
1	D	94	GLU	5.3
1	С	31	TYR	5.2
1	В	216	ASP	5.0
1	D	70	GLY	4.8
1	D	9	GLY	4.8
1	D	248	PHE	4.6
1	D	247	ARG	4.5
1	С	3	TYR	4.5
1	С	29	MET	4.4
1	A	248	PHE	4.3
1	В	70	GLY	4.1
1	В	230	ASP	4.0
1	D	217	PHE	4.0



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Mol	Chain	Res	Type	RSRZ			
1	D	95	TYR	4.0			
1	С	92	LYS	3.7			
1	D	18	LEU	3.7			
1	С	24	PHE	3.6			
1	С	65	ILE	3.6			
1	A	110	GLY	3.5			
1	С	95	TYR	3.5			
1	D	78	TRP	3.5			
1	В	217	PHE	3.4			
1	В	89	LEU	3.4			
1	С	88	LYS	3.4			
1	D	109	TYR	3.3			
1	В	91	ALA	3.3			
1	D	13	SER	3.3			
1	D	119	LEU	3.3			
1	A	251	PHE	3.2			
1	A	111	ILE	3.1			
1	D	16	LEU	3.1			
1	С	81	ALA	3.0			
1	С	187	ILE	3.0			
1	В	82	GLU	3.0			
1	D	82	GLU	3.0			
1	В	80	PRO	3.0			
1	С	40	ILE	2.9			
1	С	1	MET	2.9			
1	A	250	SER	2.8			
1	С	263	GLU	2.8			
1	D	250	SER	2.8			
1	В	3	TYR	2.8			
1	В	55	TYR	2.8			
1	В	109	TYR	2.8			
1	D	80	PRO	2.8			
1	В	213	ASN	2.8			
1	С	212	VAL	2.7			
1	D	81	ALA	2.7			
1	С	19	ASN	2.7			
1	С	93	GLY	2.7			
1	С	18	LEU	2.7			
1	С	78	TRP	2.7			
1	В	83	ALA	2.6			
1	В	84	ASP	2.6			
1	D	20	MET	2.6			
	I	1	L				



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Mol	nued fron Chain	Res	Type	RSRZ
1	D	76	ALA	2.6
1	В	60	ASP	2.6
1	В	16	LEU	2.6
1	D	231	VAL	2.6
1	D	228	HIS	2.6
1	В	18	LEU	2.5
1	A	78	TRP	2.5
1	D	42	ILE	2.5
1	В	19	ASN	2.5
1	D	215	LYS	2.5
1	D	52	PHE	2.5
1	A	96	GLN	2.5
1	С	30	GLU	2.5
1	С	86	LEU	2.5
1	D	84	ASP	2.5
1	В	87	VAL	2.4
1	D	31	TYR	2.4
1	В	267	HIS	2.4
1	D	69	THR	2.4
1	A	217	PHE	2.4
1	С	188	ASN	2.4
1	D	87	VAL	2.4
1	D	234	ILE	2.3
1	С	94	GLU	2.3
1	С	82	GLU	2.3
1	С	246	ALA	2.3
1	В	198	PRO	2.3
1	A	90	LEU	2.3
1	В	229	ARG	2.3
1	В	30	GLU	2.3
1	D	85	LYS	2.3
1	С	87	VAL	2.3
1	С	230	ASP	2.3
1	C	116	ALA	2.3
1	В	215	LYS	2.2
1	D	230	ASP	2.2
1	В	66	GLY	2.2
1	С	76	ALA	2.2
1	С	91	ALA	2.2
1	D	203	LYS	2.2
1	С	67	ILE	2.2
1	С	224	LEU	2.2



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Mol	Chain	Res	Type	RSRZ
1	D	226	ILE	2.1
1	В	227	LEU	2.1
1	В	24	PHE	2.1
1	С	247	ARG	2.1
1	D	229	ARG	2.1
1	С	198	PRO	2.1
1	В	114	LYS	2.1
1	В	167	LEU	2.1
1	С	236	TYR	2.1
1	D	71	HIS	2.0
1	В	49	LEU	2.0
1	В	57	GLU	2.0
1	В	96	GLN	2.0
1	В	172	MET	2.0

### 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)

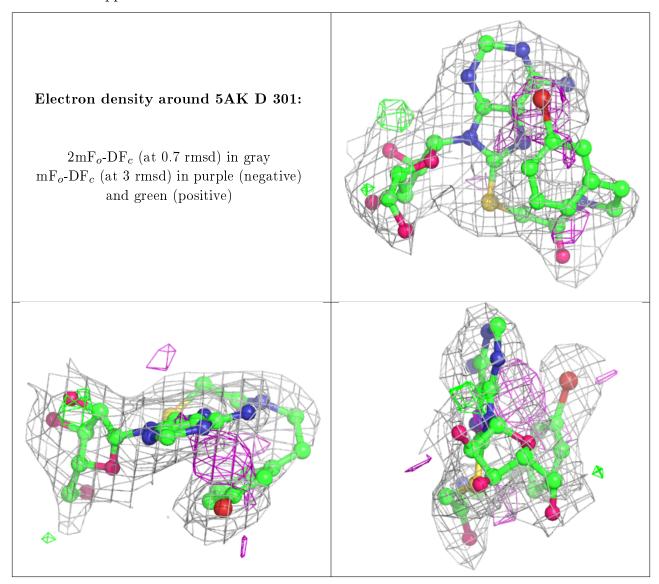
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	CIT	A	301	13/13	0.79	0.30	37,42,48,49	13
3	5AK	D	301	33/33	0.87	0.17	40,62,81,128	0
2	CIT	В	301	13/13	0.87	0.22	49,59,65,66	13
4	GOL	С	302	6/6	0.87	0.33	59,63,70,79	0
3	5AK	С	301	33/33	0.91	0.12	27,38,69,112	0
3	5AK	В	302	33/33	0.95	0.11	41,59,73,77	1
3	5AK	A	302	33/33	0.95	0.13	17,38,57,70	0

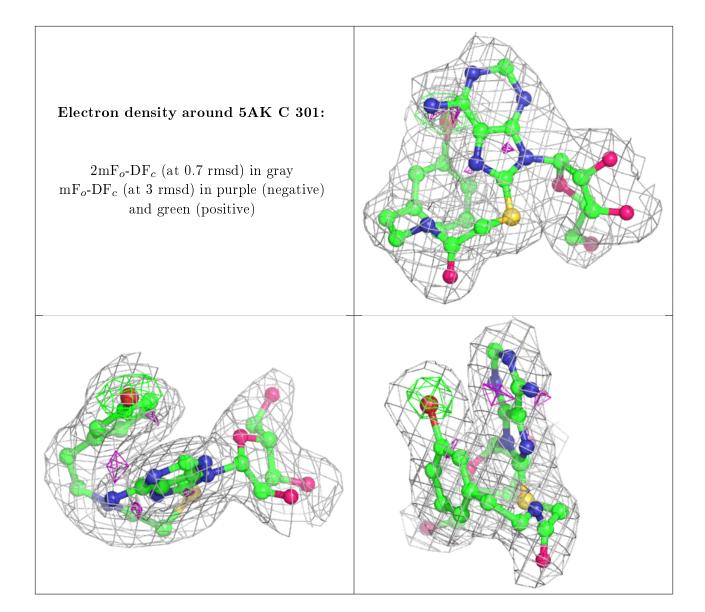
The following is a graphical depiction of the model fit to experimental electron density of all



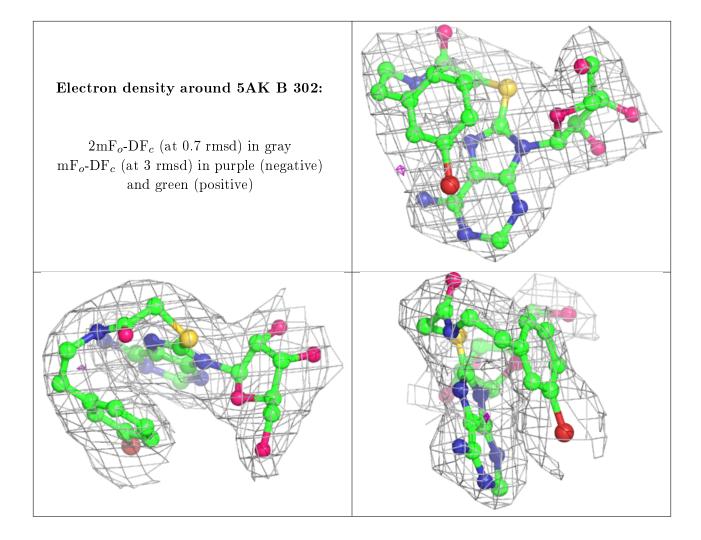
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



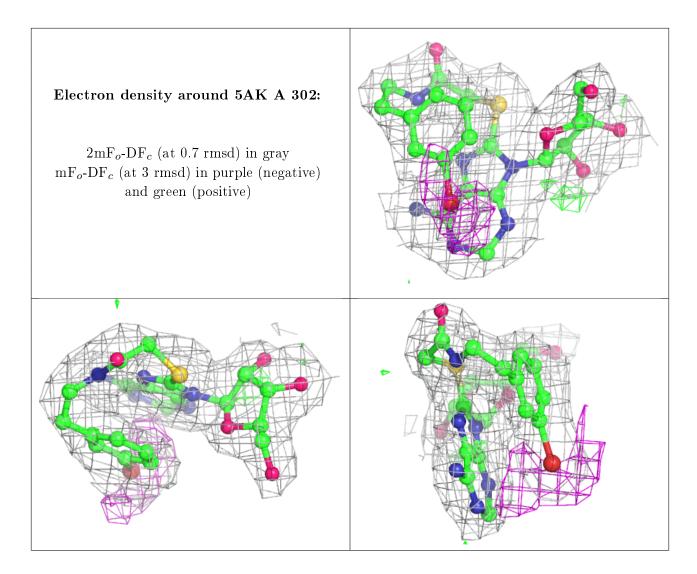












# 6.5 Other polymers (i)

There are no such residues in this entry.

