



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:16 PM BST

PDB ID : 5DHS  
Title : Crystal structure of NAD kinase 1 from *Listeria monocytogenes* in complex with a novel inhibitor  
Authors : Gelin, M.; Paoletti, J.; Assairi, L.; Huteau, V.; Pochet, S.; Labesse, G.  
Deposited on : 2015-08-31  
Resolution : 2.62 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 : 2.13.1  
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) : 2.13.1

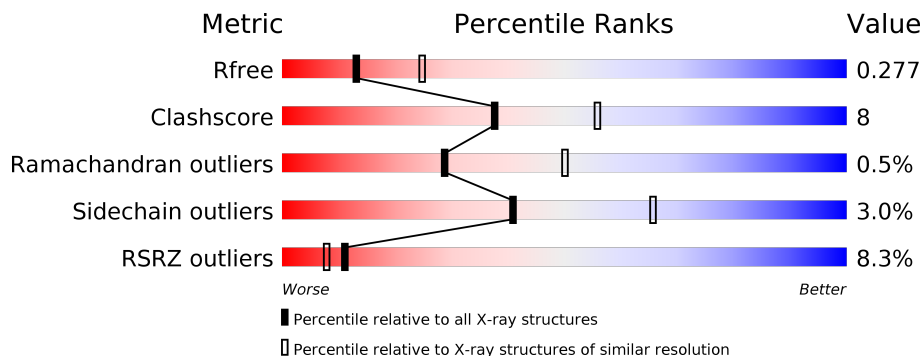
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	272	 3% 79% 17% •
1	B	272	 9% 77% 18% ••
1	C	272	 9% 76% 19% •
1	D	272	 11% 71% 18% • 10%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8421 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	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	Total 2065	C 1323	N 345	O 388	S 9	0	1	0
1	B	262	Total 2080	C 1332	N 348	O 391	S 9	0	0	0
1	C	260	Total 2026	C 1298	N 342	O 377	S 9	0	0	0
1	D	245	Total 1901	C 1218	N 327	O 349	S 7	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

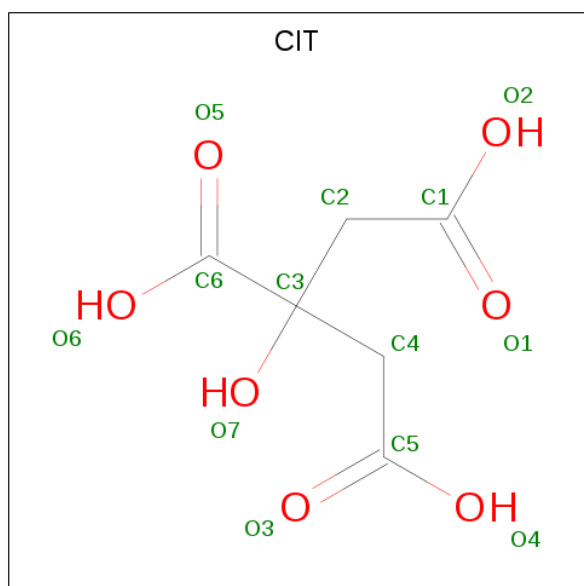
Chain	Residue	Modelled	Actual	Comment	Reference
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	265	LEU	-	expression tag	UNP Q8Y8D7
B	266	GLU	-	expression tag	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	265	LEU	-	expression tag	UNP Q8Y8D7
C	266	GLU	-	expression tag	UNP Q8Y8D7
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	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<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			36	22	9	4	1		
4	D	1	Total	C	N	O	S	0	0
			36	22	9	4	1		

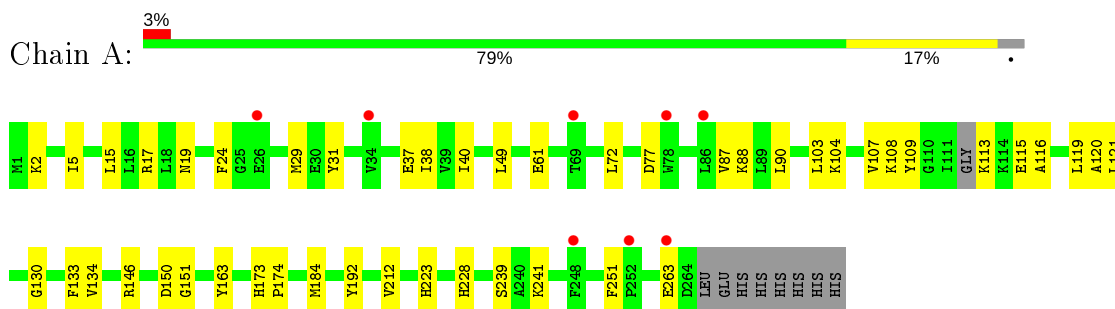
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	32	Total	O	0	0
			32	32		
5	C	37	Total	O	0	0
			37	37		
5	D	50	Total	O	0	0
			50	50		

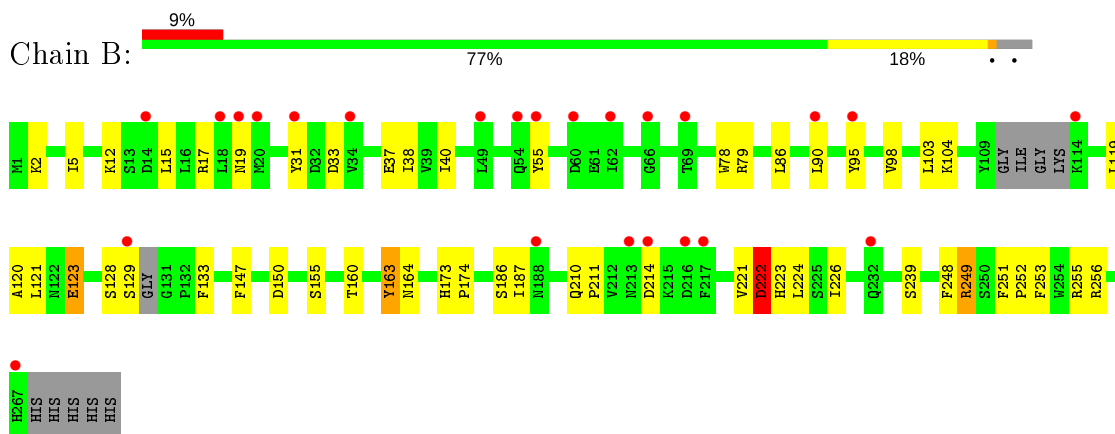
### 3 Residue-property plots [i](#)

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.

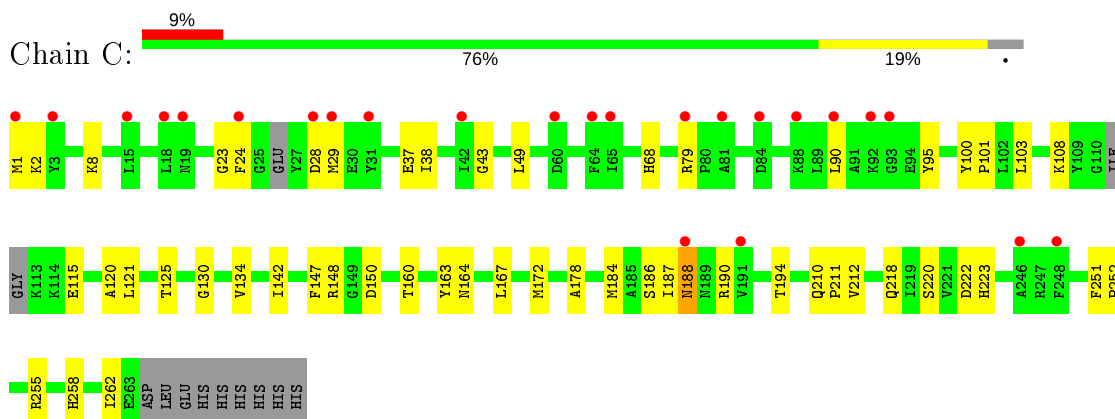
- Molecule 1: NAD kinase 1



- Molecule 1: NAD kinase 1

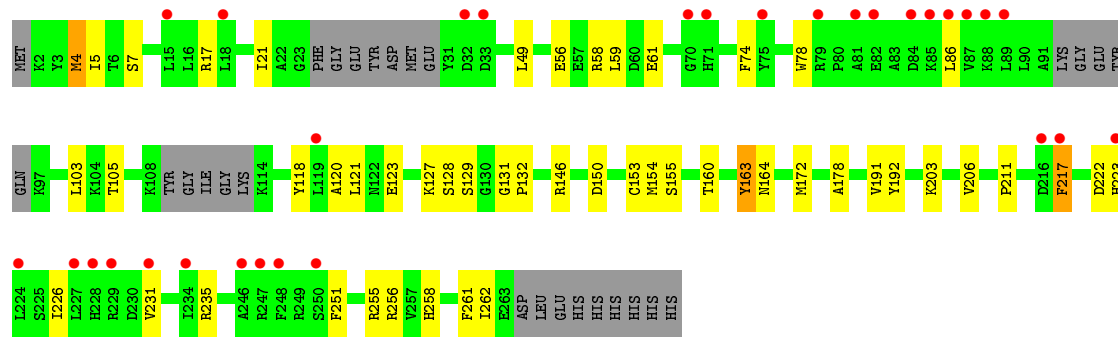


- Molecule 1: NAD kinase 1



- Molecule 1: NAD kinase 1

Chain D:  11% 71% 18% 10%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.77Å 118.95Å 66.90Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	44.14 - 2.62 44.14 - 2.62	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.14-2.62) 99.8 (44.14-2.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.242 , 0.278 0.244 , 0.277	Depositor DCC
$R_{free}$ test set	970 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtrriage
Anisotropy	0.327	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.025 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% 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: GOL, 5AG, 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.22	0/2120	0.38	0/2869
1	B	0.22	0/2129	0.41	0/2879
1	C	0.22	0/2075	0.40	0/2808
1	D	0.22	0/1945	0.40	0/2633
All	All	0.22	0/8269	0.40	0/11189

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)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	1988	28	0
1	B	2080	0	2015	29	0
1	C	2026	0	1933	29	0
1	D	1901	0	1833	34	0
2	A	13	0	5	1	0
2	B	13	0	5	2	0
3	A	6	0	8	1	0
4	A	36	0	0	5	0
4	B	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	36	0	0	4	0
4	D	36	0	0	3	0
5	A	54	0	0	2	0
5	B	32	0	0	1	0
5	C	37	0	0	0	0
5	D	50	0	0	0	0
All	All	8421	0	7787	124	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 8.

All (124) 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:150:ASP:OD1	4:C:301:5AG:N6	2.18	0.77
1:C:125:THR:HG1	1:C:220:SER:HG	1.34	0.75
1:B:17:ARG:NH2	1:B:31:TYR:OH	2.21	0.73
1:B:15:LEU:O	1:B:19:ASN:ND2	2.24	0.70
4:B:302:5AG:N7	4:B:302:5AG:NAH	2.42	0.68
4:C:301:5AG:NAH	4:C:301:5AG:N7	2.43	0.67
4:B:302:5AG:N6	1:D:150:ASP:OD1	2.28	0.66
1:C:1:MET:N	1:C:29:MET:SD	2.67	0.66
4:A:303:5AG:NAH	4:A:303:5AG:N7	2.44	0.66
1:D:160:THR:HG21	1:D:172:MET:HG2	1.78	0.66
1:B:121:LEU:N	1:B:222:ASP:OD2	2.26	0.65
1:A:223:HIS:HB2	4:A:303:5AG:CBB	2.27	0.65
4:A:303:5AG:SAK	4:A:303:5AG:OBF	2.53	0.65
4:A:303:5AG:N6	1:C:150:ASP:OD1	2.29	0.65
1:B:79:ARG:NH2	5:B:402:HOH:O	2.29	0.64
1:A:108:LYS:NZ	1:A:115:GLU:OE1	2.30	0.64
1:D:211:PRO:HB3	1:D:217:PHE:HZ	1.62	0.64
1:B:33:ASP:O	1:B:55:TYR:OH	2.17	0.63
1:B:222:ASP:N	1:B:222:ASP:OD1	2.29	0.63
1:C:38:ILE:HG21	1:C:90:LEU:HD11	1.81	0.62
1:B:103:LEU:HB3	1:B:120:ALA:HB3	1.82	0.62
1:C:172:MET:HE1	1:C:178:ALA:HB3	1.82	0.61
1:D:74:PHE:O	1:D:256:ARG:NH2	2.34	0.61
1:B:38:ILE:HG21	1:B:90:LEU:HD11	1.85	0.59
2:B:301:CIT:O1	2:B:301:CIT:O7	2.21	0.58
1:A:2:LYS:O	1:A:37:GLU:N	2.34	0.57
1:A:263:GLU:HA	1:C:190:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:301:5AG:CBH	4:D:301:5AG:CAI	2.83	0.56
4:B:302:5AG:CAW	4:B:302:5AG:SAK	2.94	0.55
1:B:78:TRP:CD2	1:B:86:LEU:HD21	2.42	0.54
1:C:103:LEU:HB3	1:C:120:ALA:HB3	1.90	0.53
1:D:123:GLU:HB2	1:D:155:SER:HA	1.90	0.53
1:C:142:ILE:HD13	1:D:255:ARG:HD2	1.90	0.53
1:B:5:ILE:HG12	1:B:40:ILE:HB	1.92	0.52
1:A:5:ILE:HG12	1:A:40:ILE:HB	1.92	0.52
1:B:98:VAL:HG11	2:B:301:CIT:H41	1.91	0.51
1:B:95:TYR:HB3	1:B:248:PHE:CE1	2.45	0.51
1:C:2:LYS:O	1:C:37:GLU:N	2.34	0.51
1:D:217:PHE:HE2	1:D:231:VAL:HB	1.76	0.51
1:B:123:GLU:HB3	1:B:155:SER:HA	1.92	0.51
1:B:253:PHE:HD1	1:B:256:ARG:HH21	1.58	0.50
1:A:49:LEU:HD23	1:A:121:LEU:HD23	1.92	0.50
1:B:128:SER:HB2	1:B:133:PHE:HB2	1.93	0.50
4:A:303:5AG:CAA	1:C:148:ARG:HH22	2.25	0.50
1:D:123:GLU:HB2	1:D:154:MET:O	2.12	0.50
1:B:187:ILE:HD11	1:D:261:PHE:HE1	1.77	0.49
1:A:88:LYS:NZ	5:A:403:HOH:O	2.38	0.49
1:C:223:HIS:O	1:C:223:HIS:ND1	2.42	0.49
1:D:103:LEU:HB3	1:D:120:ALA:HB3	1.95	0.48
1:D:78:TRP:CE2	1:D:86:LEU:HD21	2.48	0.48
1:D:49:LEU:HD23	1:D:121:LEU:HD23	1.95	0.48
1:A:15:LEU:O	1:A:19:ASN:ND2	2.43	0.48
1:D:4:MET:HG2	1:D:5:ILE:H	1.79	0.48
1:A:109:TYR:OH	1:A:228:HIS:ND1	2.39	0.48
1:C:68:HIS:CE1	1:C:79:ARG:HG2	2.49	0.48
1:B:2:LYS:O	1:B:37:GLU:N	2.31	0.47
1:C:49:LEU:HD23	1:C:121:LEU:HD23	1.96	0.47
1:A:107:VAL:HG13	1:A:116:ALA:HB3	1.97	0.47
1:C:134:VAL:HG12	1:C:212:VAL:HG21	1.96	0.47
1:A:184:MET:HB3	3:A:302:GOL:H12	1.96	0.47
1:C:108:LYS:NZ	1:C:115:GLU:OE1	2.39	0.47
1:A:38:ILE:HD13	1:A:90:LEU:HD22	1.97	0.47
1:A:173:HIS:CE1	2:A:301:CIT:H42	2.50	0.47
1:B:249:ARG:HA	1:B:249:ARG:HD3	1.66	0.47
4:C:301:5AG:SAK	4:C:301:5AG:CAW	3.02	0.46
1:B:163:TYR:OH	1:D:150:ASP:OD2	2.31	0.46
1:D:258:HIS:ND1	1:D:262:ILE:HB	2.31	0.46
1:A:104:LYS:HB2	1:A:239:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:HB2	1:B:239:SER:HB2	1.98	0.46
1:D:206:VAL:HG11	1:D:235:ARG:NH2	2.32	0.45
1:B:252:PRO:HD2	1:B:255:ARG:HD3	1.97	0.45
1:C:188:ASN:OD1	1:C:194:THR:OG1	2.34	0.45
1:D:4:MET:HE3	1:D:4:MET:HB3	1.60	0.45
1:D:4:MET:HG2	1:D:5:ILE:N	2.32	0.45
1:B:147:PHE:CE1	1:B:186:SER:HB3	2.52	0.44
1:C:134:VAL:HG22	1:C:148:ARG:HG3	1.99	0.44
4:C:301:5AG:SAK	4:C:301:5AG:CAY	3.06	0.44
1:C:252:PRO:HB2	1:C:255:ARG:HB2	2.00	0.44
1:D:146:ARG:HG2	1:D:192:TYR:HD1	1.81	0.44
1:A:173:HIS:HA	1:A:174:PRO:HD3	1.86	0.44
1:B:160:THR:HA	1:B:164:ASN:HB3	2.00	0.44
1:D:160:THR:HA	1:D:164:ASN:HB3	1.99	0.44
1:C:167:LEU:HD11	1:C:184:MET:HE2	2.00	0.44
1:C:2:LYS:HB2	1:C:37:GLU:HG3	2.00	0.44
1:B:210:GLN:HA	1:B:211:PRO:HD3	1.80	0.43
1:D:49:LEU:HD13	1:D:222:ASP:HB3	2.00	0.43
1:A:146:ARG:HG2	1:A:192:TYR:CD2	2.53	0.43
1:D:105:THR:HB	1:D:118:TYR:HB2	2.01	0.43
1:D:128:SER:OG	1:D:129:SER:N	2.50	0.43
1:B:128:SER:OG	1:B:129:SER:N	2.49	0.43
1:D:17:ARG:O	1:D:21:ILE:HG12	2.19	0.43
1:D:123:GLU:OE1	4:D:301:5AG:OAX	2.37	0.43
1:B:150:ASP:OD2	1:D:163:TYR:OH	2.32	0.43
1:D:217:PHE:CE2	1:D:231:VAL:HB	2.54	0.43
1:A:146:ARG:HG2	1:A:192:TYR:HD2	1.84	0.42
1:D:123:GLU:HG3	1:D:153:CYS:SG	2.59	0.42
1:A:113:LYS:N	5:A:407:HOH:O	2.52	0.42
1:A:133:PHE:CD2	1:A:151:GLY:HA2	2.54	0.42
1:A:119:LEU:HD11	1:A:241:LYS:HD2	2.01	0.42
1:C:147:PHE:CE1	1:C:186:SER:HB2	2.55	0.42
1:D:56:GLU:HA	1:D:59:LEU:HG	2.01	0.42
1:C:24:PHE:CZ	1:C:90:LEU:HD22	2.54	0.42
1:A:24:PHE:CD1	1:A:29:MET:HG3	2.54	0.42
1:C:210:GLN:HA	1:C:211:PRO:HD3	1.84	0.42
1:B:173:HIS:HA	1:B:174:PRO:HD3	1.87	0.41
1:C:258:HIS:ND1	1:C:262:ILE:HB	2.36	0.41
1:A:103:LEU:HB3	1:A:120:ALA:HB3	2.02	0.41
1:D:131:GLY:HA3	1:D:132:PRO:HD3	1.87	0.41
1:A:24:PHE:CD1	1:A:87:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ARG:NH2	1:D:61:GLU:OE1	2.46	0.41
1:A:77:ASP:OD1	1:A:77:ASP:N	2.48	0.41
1:C:100:TYR:HA	1:C:101:PRO:HD3	1.90	0.41
1:D:123:GLU:OE2	4:D:301:5AG:OAX	2.39	0.41
1:A:17:ARG:NH2	1:A:31:TYR:OH	2.48	0.41
1:B:223:HIS:O	1:B:223:HIS:ND1	2.49	0.41
1:C:1:MET:N	1:C:28:ASP:O	2.43	0.41
1:C:8:LYS:HB2	1:C:43:GLY:HA3	2.02	0.41
1:A:61:GLU:N	1:A:61:GLU:OE2	2.54	0.41
1:A:134:VAL:HG12	1:A:212:VAL:HG21	2.02	0.40
1:B:221:VAL:O	1:B:224:LEU:HB3	2.22	0.40
1:C:160:THR:HA	1:C:164:ASN:HB3	2.04	0.40
1:D:172:MET:HE1	1:D:178:ALA:HB3	2.03	0.40
1:C:148:ARG:O	1:C:187:ILE:HG22	2.21	0.40
1:D:127:LYS:O	1:D:217:PHE:HB3	2.21	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	260/272 (96%)	242 (93%)	17 (6%)	1 (0%)	34	55
1	B	256/272 (94%)	240 (94%)	15 (6%)	1 (0%)	34	55
1	C	254/272 (93%)	236 (93%)	15 (6%)	3 (1%)	13	25
1	D	237/272 (87%)	224 (94%)	13 (6%)	0	100	100
All	All	1007/1088 (93%)	942 (94%)	60 (6%)	5 (0%)	29	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	ASP
1	C	23	GLY
1	C	222	ASP
1	A	130	GLY
1	C	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	220/237 (93%)	217 (99%)	3 (1%)	67	84
1	B	224/237 (94%)	215 (96%)	9 (4%)	31	55
1	C	212/237 (90%)	207 (98%)	5 (2%)	49	72
1	D	200/237 (84%)	191 (96%)	9 (4%)	27	50
All	All	856/948 (90%)	830 (97%)	26 (3%)	41	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	163	TYR
1	A	251	PHE
1	B	12	LYS
1	B	119	LEU
1	B	123	GLU
1	B	163	TYR
1	B	214	ASP
1	B	222	ASP
1	B	226	ILE
1	B	249	ARG
1	B	251	PHE
1	C	95	TYR
1	C	163	TYR
1	C	188	ASN
1	C	218	GLN
1	C	251	PHE

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Mol	Chain	Res	Type
1	D	4	MET
1	D	7	SER
1	D	163	TYR
1	D	191	VAL
1	D	203	LYS
1	D	217	PHE
1	D	223	HIS
1	D	226	ILE
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 monosaccharides 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CIT	B	301	-	3,12,12	1.36	0	3,17,17	2.14	1 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	5AG	A	303	-	36,39,39	1.35	4 (11%)	36,54,54	1.76	7 (19%)
3	GOL	A	302	-	5,5,5	0.37	0	5,5,5	0.24	0
4	5AG	B	302	-	36,39,39	1.65	5 (13%)	36,54,54	2.26	9 (25%)
4	5AG	C	301	-	36,39,39	2.10	8 (22%)	36,54,54	1.57	7 (19%)
2	CIT	A	301	-	3,12,12	1.28	0	3,17,17	1.57	1 (33%)
4	5AG	D	301	-	36,39,39	1.53	6 (16%)	36,54,54	1.74	8 (22%)

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	CIT	B	301	-	-	4/6/16/16	-
4	5AG	A	303	-	-	6/15/37/37	0/4/4/4
3	GOL	A	302	-	-	2/4/4/4	-
4	5AG	B	302	-	-	3/15/37/37	0/4/4/4
4	5AG	C	301	-	-	6/15/37/37	0/4/4/4
2	CIT	A	301	-	-	1/6/16/16	-
4	5AG	D	301	-	-	4/15/37/37	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	5AG	C8-N9	-6.63	1.29	1.36
4	C	301	5AG	C8-SAK	-5.12	1.61	1.75
4	B	302	5AG	C8-N9	-4.78	1.31	1.36
4	A	303	5AG	C8-N9	-4.75	1.31	1.36
4	B	302	5AG	OBF-CBA	-4.06	1.35	1.45
4	B	302	5AG	C8-SAK	-3.50	1.66	1.75
4	D	301	5AG	C8-N9	-3.49	1.33	1.36
4	D	301	5AG	OBF-CAV	-3.46	1.36	1.41
4	C	301	5AG	C4-N3	-3.41	1.30	1.35
4	A	303	5AG	C2-N1	3.03	1.39	1.33
4	D	301	5AG	C4-N3	-2.95	1.31	1.35
4	B	302	5AG	C4-N3	-2.93	1.31	1.35
4	D	301	5AG	C8-SAK	-2.88	1.67	1.75
4	C	301	5AG	OBF-CAV	-2.66	1.37	1.41
4	A	303	5AG	NBD-NBC	2.65	1.30	1.23
4	A	303	5AG	C8-SAK	-2.64	1.68	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	5AG	OBF-CBA	-2.60	1.39	1.45
4	D	301	5AG	CBB-CBA	-2.41	1.48	1.51
4	C	301	5AG	C6-C5	-2.34	1.34	1.43
4	C	301	5AG	C5-C4	-2.20	1.35	1.40
4	D	301	5AG	NBD-NBC	2.12	1.28	1.23
4	C	301	5AG	C8-N7	-2.12	1.27	1.33
4	B	302	5AG	C6-C5	-2.04	1.35	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	5AG	OBF-CBA-CBB	-7.87	100.88	109.09
4	A	303	5AG	OBF-CBA-CBB	5.41	114.74	109.09
4	D	301	5AG	N3-C2-N1	-5.39	120.25	128.68
4	B	302	5AG	N3-C2-N1	-5.01	120.84	128.68
4	A	303	5AG	N3-C2-N1	-4.79	121.19	128.68
4	C	301	5AG	CAJ-SAK-C8	-4.54	96.04	101.86
4	C	301	5AG	N3-C2-N1	-4.27	122.01	128.68
4	B	302	5AG	CAF-CAG-NAH	-4.14	99.48	111.99
4	B	302	5AG	OBF-CBA-CAY	-3.94	97.31	105.11
4	D	301	5AG	CAV-N9-C4	-3.85	119.97	126.71
4	B	302	5AG	CBJ-CAC-CAB	-3.40	115.56	120.65
4	D	301	5AG	CBB-NBC-NBD	3.39	122.97	115.60
2	B	301	CIT	C3-C2-C1	-3.37	109.59	114.98
4	D	301	5AG	OBF-CBA-CBB	-3.26	105.69	109.09
4	A	303	5AG	OBF-CAV-CAW	-2.98	102.57	106.93
4	D	301	5AG	OAX-CAW-CAY	-2.56	103.54	111.82
2	A	301	CIT	C3-C4-C5	-2.56	110.89	114.98
4	B	302	5AG	OBF-CAV-CAW	-2.49	103.29	106.93
4	B	302	5AG	CAW-CAY-CBA	-2.49	97.81	102.64
4	B	302	5AG	CAF-CAE-CAD	2.38	124.44	120.54
4	C	301	5AG	N6-C6-N1	2.36	123.47	118.57
4	C	301	5AG	OAZ-CAY-CAW	-2.35	104.22	111.82
4	C	301	5AG	OBF-CAV-CAW	-2.28	103.59	106.93
4	D	301	5AG	CAY-CAW-CAV	2.24	104.35	100.98
4	A	303	5AG	CBJ-CAC-CAB	-2.22	117.33	120.65
4	B	302	5AG	CAD-CAC-CAB	2.21	122.92	120.09
4	C	301	5AG	CBB-NBC-NBD	2.19	120.36	115.60
4	D	301	5AG	CAG-CAF-CAE	2.14	117.82	112.87
4	A	303	5AG	OBF-CBA-CAY	-2.11	100.94	105.11
4	D	301	5AG	OBF-CBA-CAY	2.08	109.22	105.11
4	C	301	5AG	CAY-CAW-CAV	2.05	104.07	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	5AG	CBA-CBB-NBC	-2.05	106.60	111.15
4	A	303	5AG	CAY-CAW-CAV	2.02	104.01	100.98

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	CIT	C1-C2-C3-C6
4	A	303	5AG	OBF-CBA-CBB-NBC
4	A	303	5AG	CAY-CBA-CBB-NBC
4	B	302	5AG	CAY-CBA-CBB-NBC
4	C	301	5AG	CAE-CAF-CAG-NAH
4	D	301	5AG	CAE-CAF-CAG-NAH
4	D	301	5AG	OBF-CBA-CBB-NBC
4	D	301	5AG	CAY-CBA-CBB-NBC
2	B	301	CIT	C1-C2-C3-O7
3	A	302	GOL	O1-C1-C2-C3
4	C	301	5AG	OBG-CAI-CAJ-SAK
2	B	301	CIT	C1-C2-C3-C4
4	B	302	5AG	CBB-NBC-NBD-NBE
4	B	302	5AG	CBA-CBB-NBC-NBD
4	C	301	5AG	CBA-CBB-NBC-NBD
4	A	303	5AG	NAH-CAI-CAJ-SAK
4	C	301	5AG	NAH-CAI-CAJ-SAK
3	A	302	GOL	O1-C1-C2-O2
2	B	301	CIT	O7-C3-C4-C5
4	A	303	5AG	OBG-CAI-CAJ-SAK
4	C	301	5AG	CAY-CBA-CBB-NBC
4	A	303	5AG	CBH-CAE-CAF-CAG
2	A	301	CIT	C1-C2-C3-O7
4	A	303	5AG	CAD-CAE-CAF-CAG
4	C	301	5AG	CAA-CAB-CAC-CBJ
4	D	301	5AG	CAA-CAB-CAC-CAD

There are no ring outliers.

7 monomers are involved in 19 short contacts:

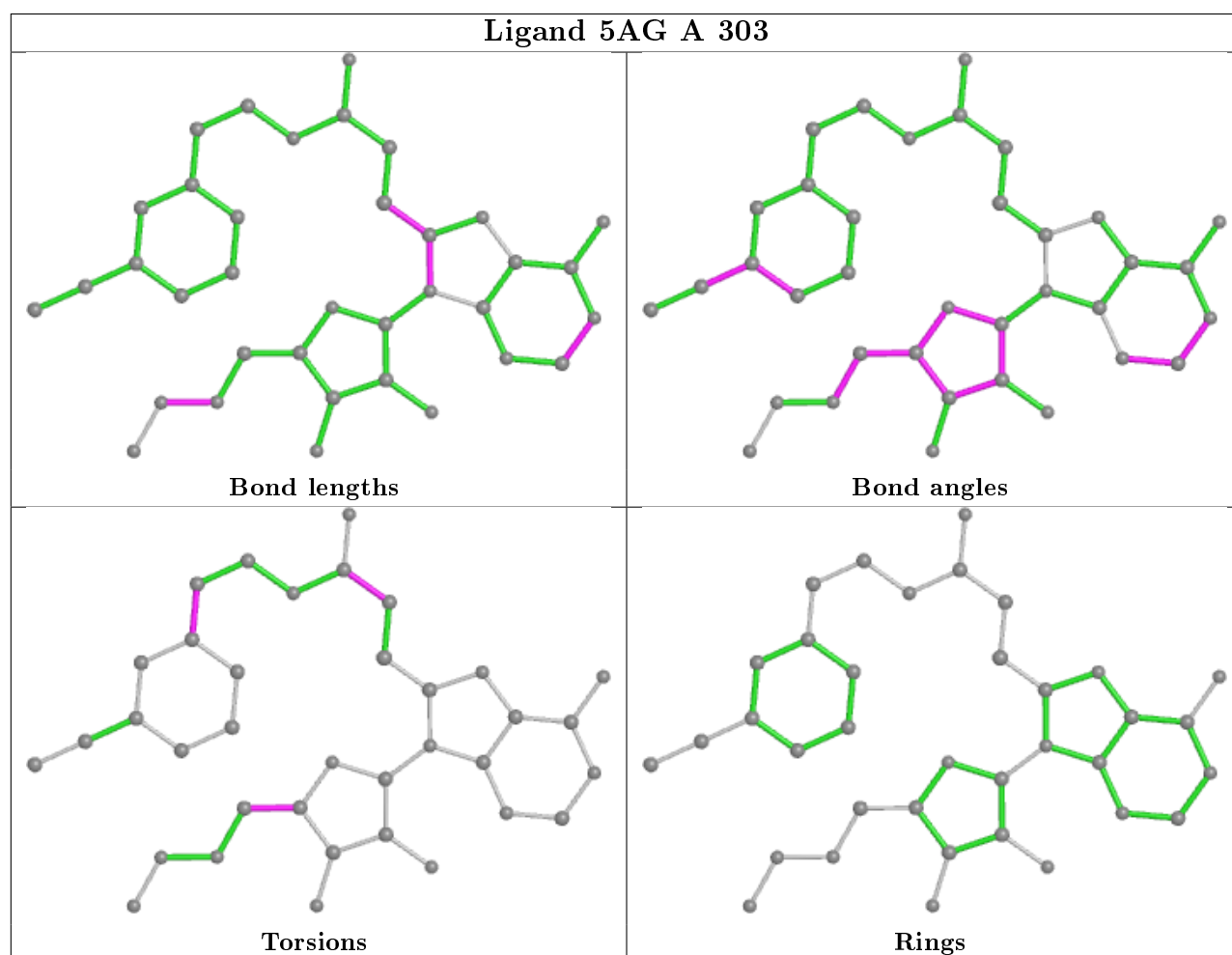
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CIT	2	0
4	A	303	5AG	5	0
3	A	302	GOL	1	0

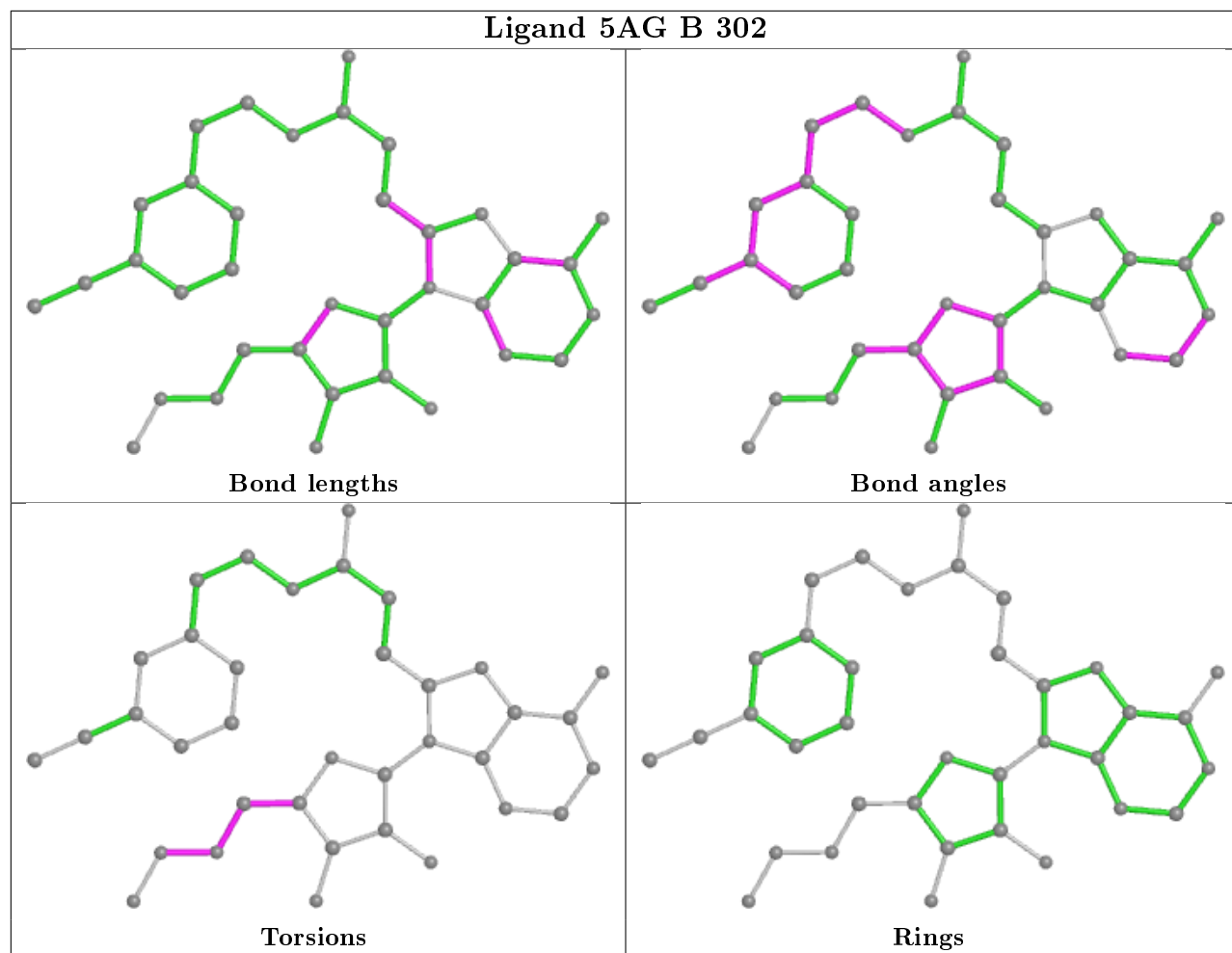
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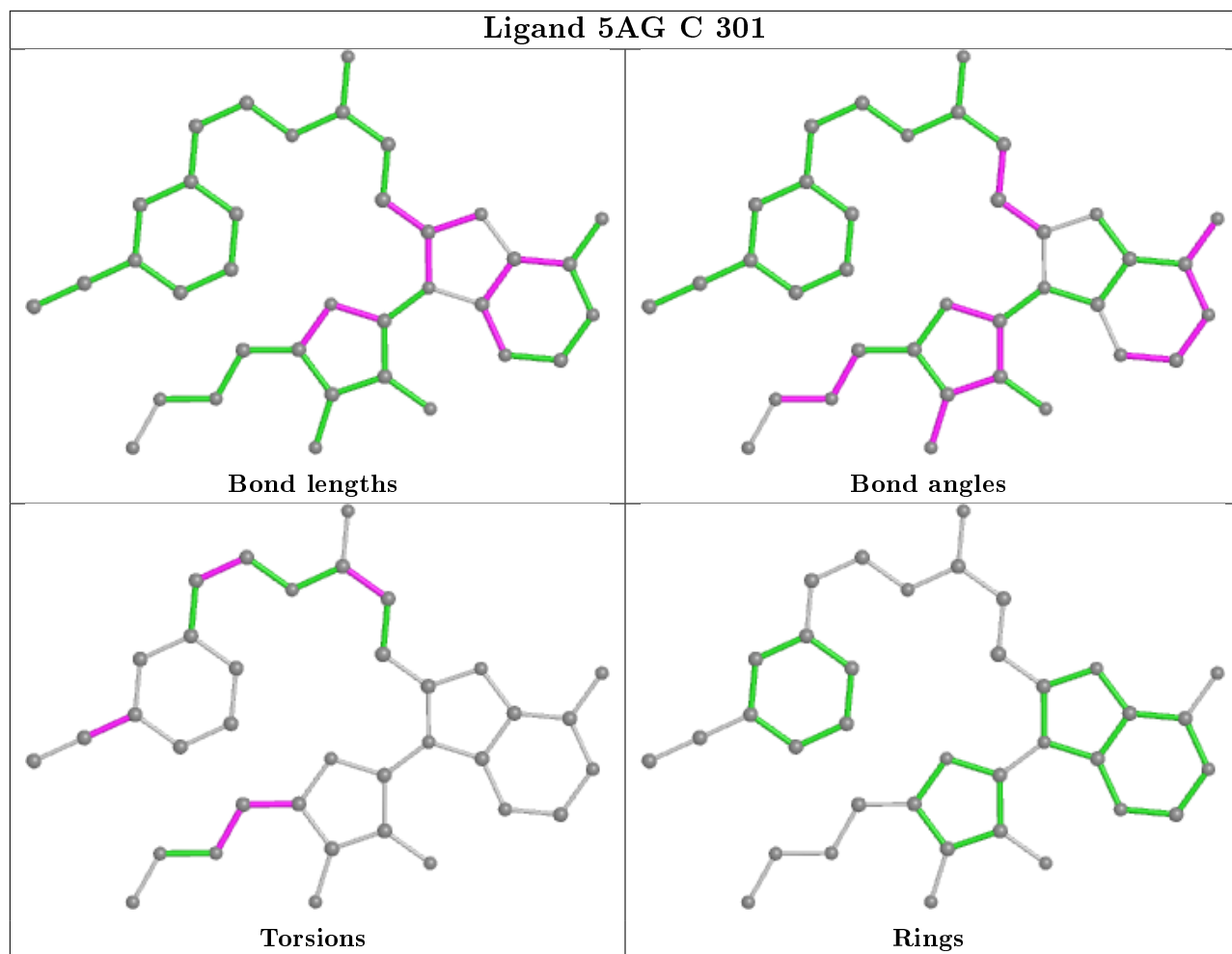
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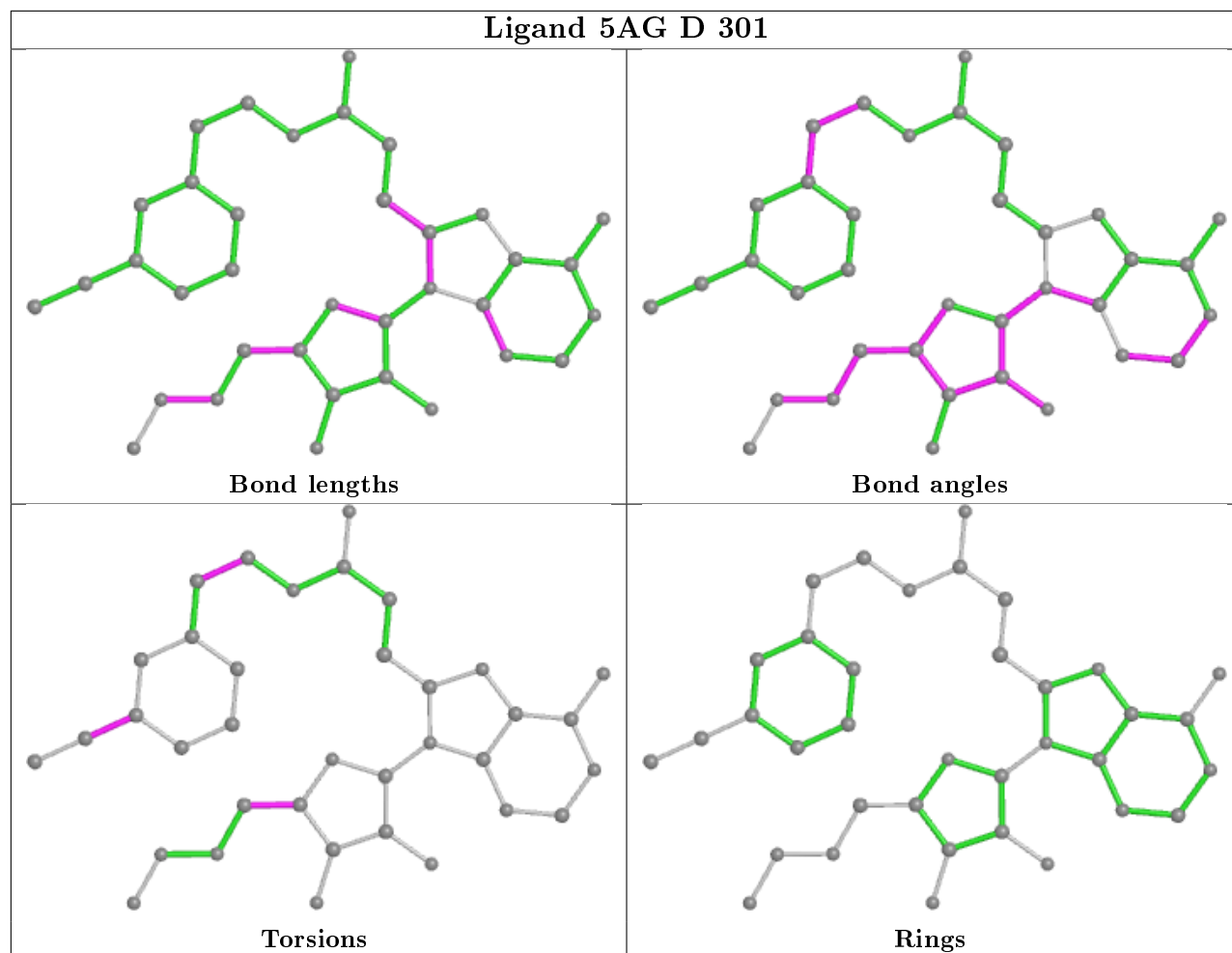
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	5AG	3	0
4	C	301	5AG	4	0
2	A	301	CIT	1	0
4	D	301	5AG	3	0

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	263/272 (96%)	0.17	8 (3%) 50 44	25, 54, 94, 136	43 (16%)
1	B	262/272 (96%)	0.75	24 (9%) 9 6	35, 80, 131, 176	43 (16%)
1	C	260/272 (95%)	0.60	24 (9%) 9 6	34, 71, 137, 183	37 (14%)
1	D	245/272 (90%)	0.77	30 (12%) 4 2	35, 78, 136, 169	34 (13%)
All	All	1030/1088 (94%)	0.57	86 (8%) 11 8	25, 70, 131, 183	157 (15%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	MET	6.1
1	D	89	LEU	5.0
1	C	81	ALA	4.6
1	D	227	LEU	4.6
1	B	214	ASP	4.6
1	D	248	PHE	4.6
1	B	216	ASP	4.4
1	D	86	LEU	4.4
1	B	217	PHE	4.3
1	C	15	LEU	3.8
1	C	3	TYR	3.8
1	D	71	HIS	3.8
1	B	213	ASN	3.7
1	C	31	TYR	3.6
1	C	93	GLY	3.6
1	D	231	VAL	3.5
1	C	29	MET	3.4
1	D	81	ALA	3.4
1	B	60	ASP	3.4
1	D	119	LEU	3.4
1	D	70	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	79	ARG	3.3
1	D	88	LYS	3.2
1	C	28	ASP	3.2
1	A	263	GLU	3.1
1	C	65	ILE	3.1
1	A	248	PHE	3.0
1	B	55	TYR	3.0
1	B	31	TYR	3.0
1	C	19	ASN	2.9
1	D	223	HIS	2.9
1	B	14	ASP	2.9
1	B	188	ASN	2.8
1	D	229	ARG	2.8
1	B	90	LEU	2.8
1	D	84	ASP	2.8
1	D	87	VAL	2.7
1	D	15	LEU	2.7
1	C	92	LYS	2.7
1	D	33	ASP	2.7
1	D	85	LYS	2.7
1	A	69	THR	2.6
1	C	64	PHE	2.6
1	C	84	ASP	2.6
1	D	234	ILE	2.6
1	C	90	LEU	2.6
1	C	248	PHE	2.5
1	D	82	GLU	2.5
1	A	26	GLU	2.5
1	D	250	SER	2.5
1	C	1	MET	2.5
1	B	69	THR	2.5
1	B	114	LYS	2.5
1	D	75	TYR	2.4
1	A	78	TRP	2.4
1	B	34	VAL	2.4
1	D	32	ASP	2.4
1	A	252	PRO	2.3
1	B	129	SER	2.3
1	B	19	ASN	2.3
1	D	247	ARG	2.3
1	A	34	VAL	2.3
1	D	228	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	217	PHE	2.3
1	D	224	LEU	2.3
1	C	88	LYS	2.3
1	B	95	TYR	2.3
1	C	79	ARG	2.3
1	C	60	ASP	2.3
1	D	216	ASP	2.3
1	A	86	LEU	2.2
1	C	24	PHE	2.2
1	C	191	VAL	2.2
1	C	188	ASN	2.1
1	B	232	GLN	2.1
1	B	18	LEU	2.1
1	B	267	HIS	2.1
1	C	42	ILE	2.1
1	B	62	ILE	2.1
1	B	66	GLY	2.1
1	B	49	LEU	2.1
1	D	246	ALA	2.0
1	C	246	ALA	2.0
1	B	54	GLN	2.0
1	C	18	LEU	2.0
1	D	18	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

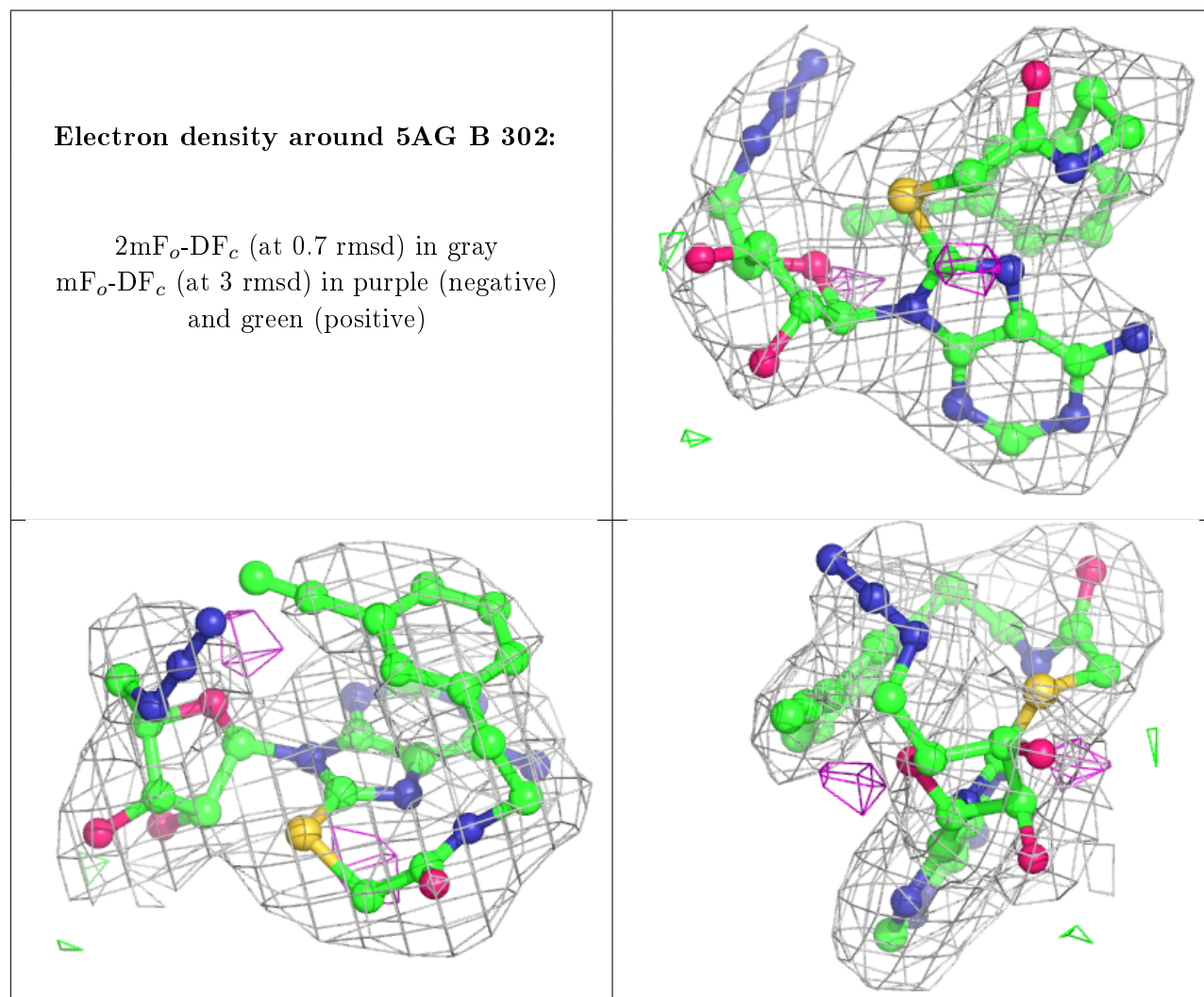
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

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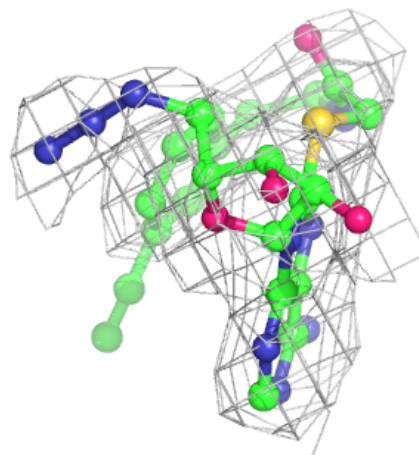
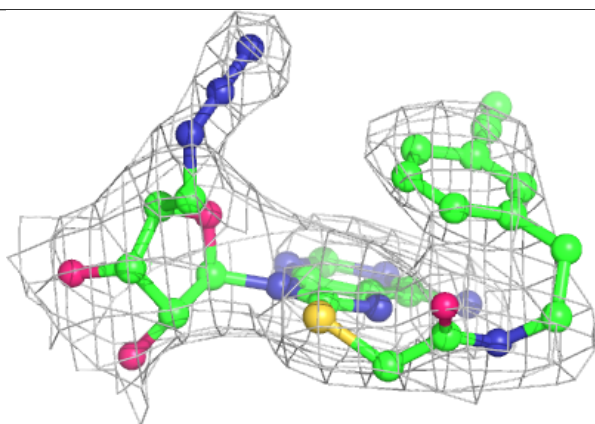
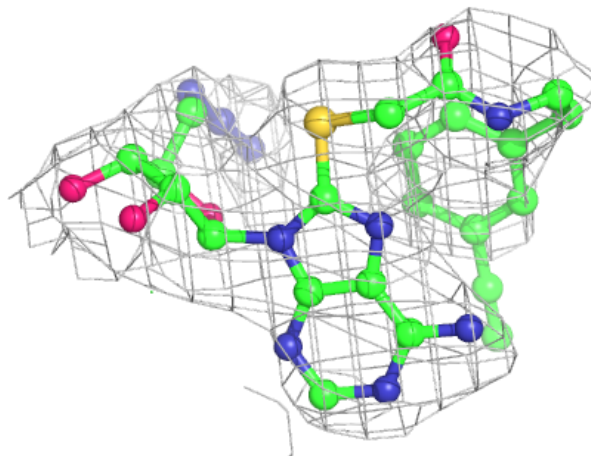
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	B	301	13/13	0.85	0.24	55,65,66,68	13
2	CIT	A	301	13/13	0.86	0.27	29,31,45,49	13
4	5AG	B	302	36/36	0.89	0.17	49,68,82,84	0
3	GOL	A	302	6/6	0.89	0.31	74,76,80,84	0
4	5AG	D	301	36/36	0.91	0.18	59,77,85,97	0
4	5AG	A	303	36/36	0.92	0.18	28,48,69,70	0
4	5AG	C	301	36/36	0.93	0.15	36,44,67,70	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.



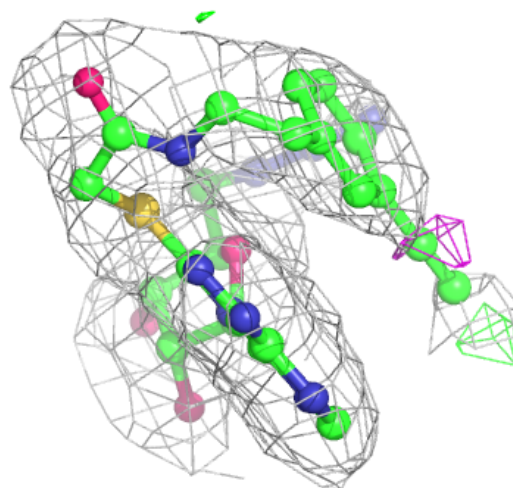
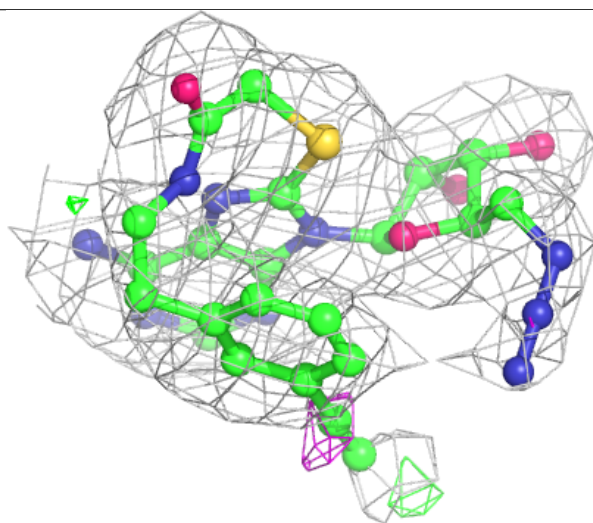
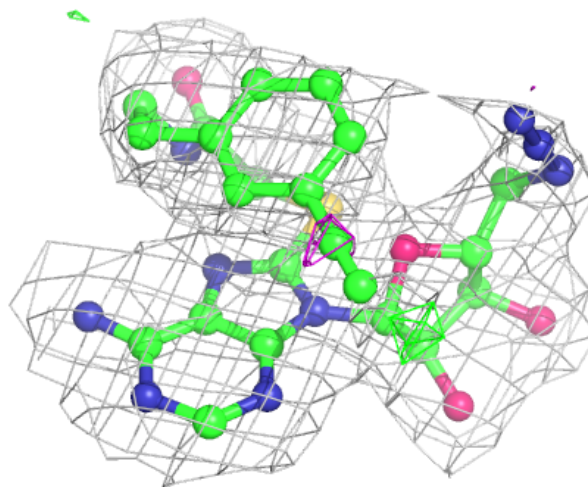
**Electron density around 5AG D 301:**

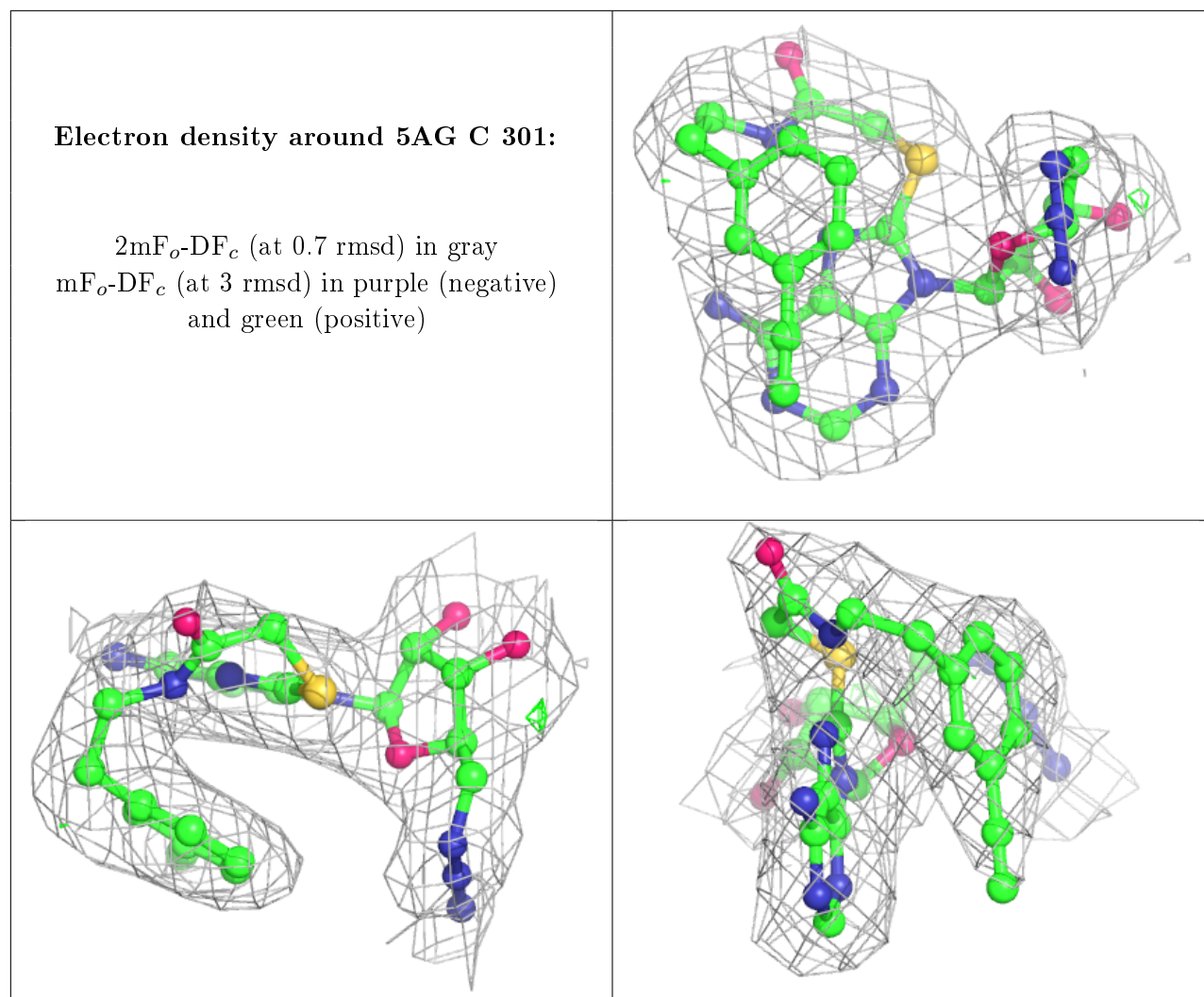
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 5AG A 303:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.