



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 09:37 AM EST

PDB ID : 7HIG  
Title : Group deposition for combi-soaks of Chikungunya virus nsP3 macrodomain – Crystal structure of Chikungunya virus nsP3 macrodomain in complex with Z1041785508 and Z1165350851 (CHIKV\_MacB-x1495)  
Authors : Aschenbrenner, J.C.; Fairhead, M.; Godoy, A.S.; Balcomb, B.H.; Capkin, E.; Chandran, A.V.; Golding, M.; Koekemoer, L.; Lithgo, R.M.; Marples, P.G.; Ni, X.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M.-A.E.; Fearon, D.; von Delft, F.  
Deposited on : 2024-10-02  
Resolution : 1.39 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11

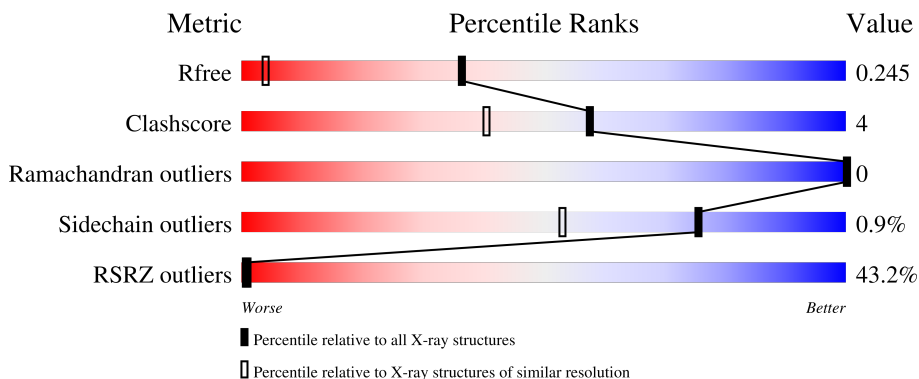
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.39 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))
$R_{free}$	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	C	163	

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.40

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Mol	Chain	Length	Quality of chain
1	D	163	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	B	203	-	-	X	-
2	DMS	B	205	-	-	X	-
2	DMS	C	302	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5970 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	1262	787	220	245	10	0	2	0
1	B	163	1274	793	222	250	9	0	4	0
1	C	163	1274	794	225	246	9	0	3	0
1	D	159	1246	777	217	243	9	0	3	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8JUX6
A	-1	ALA	-	expression tag	UNP Q8JUX6
A	0	MET	-	expression tag	UNP Q8JUX6
A	77	THR	SER	conflict	UNP Q8JUX6
B	-2	GLY	-	expression tag	UNP Q8JUX6
B	-1	ALA	-	expression tag	UNP Q8JUX6
B	0	MET	-	expression tag	UNP Q8JUX6
B	77	THR	SER	conflict	UNP Q8JUX6
C	-2	GLY	-	expression tag	UNP Q8JUX6
C	-1	ALA	-	expression tag	UNP Q8JUX6
C	0	MET	-	expression tag	UNP Q8JUX6
C	77	THR	SER	conflict	UNP Q8JUX6
D	-2	GLY	-	expression tag	UNP Q8JUX6
D	-1	ALA	-	expression tag	UNP Q8JUX6
D	0	MET	-	expression tag	UNP Q8JUX6
D	77	THR	SER	conflict	UNP Q8JUX6

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



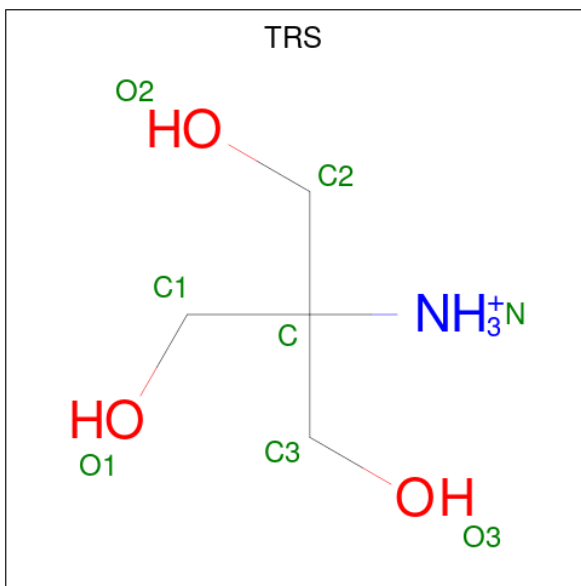
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	D	1	4	2	1	1	0	0
2	D	1	4	2	1	1	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).

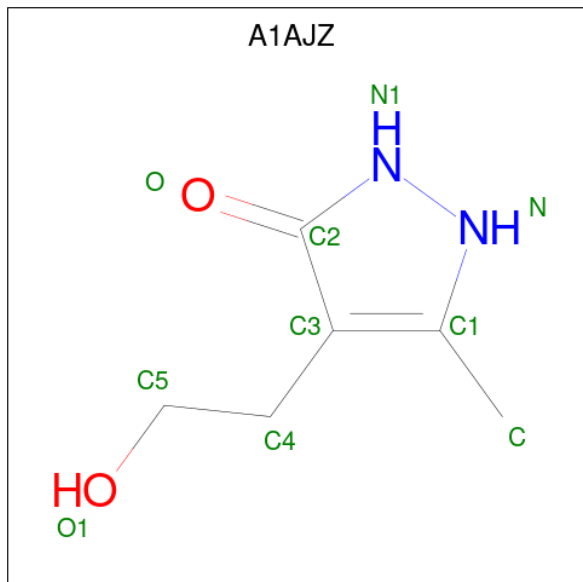


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	1	3	0	0
3	B	1	8	4	1	3	0	0
3	D	1	8	4	1	3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

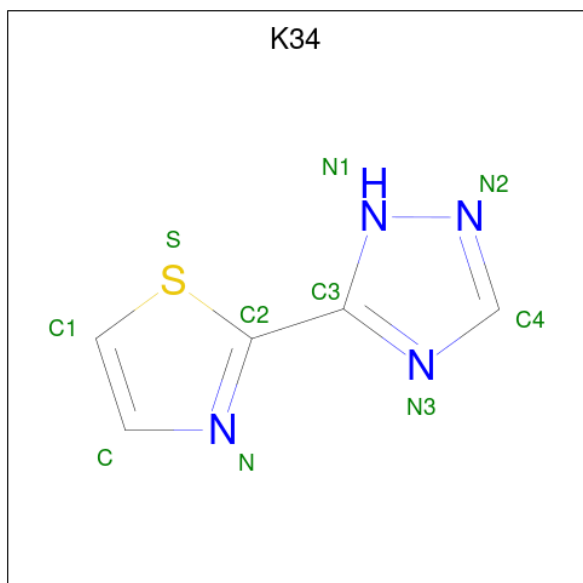
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	2	2	2	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	2	2	2	0	0

- Molecule 5 is 4-(2-hydroxyethyl)-5-methyl-1,2-dihydro-3H-pyrazol-3-one (three-letter code: A1AJZ) (formula:  $C_6H_{10}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	2	2		
5	C	1	Total	C	N	O	0	1
			20	12	4	4		

- Molecule 6 is 5-(1,3-thiazol-2-yl)-1H-1,2,4-triazole (three-letter code: K34) (formula:  $C_5H_4N_4S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	S	0	0
			10	5	4	1		

- Molecule 7 is water.

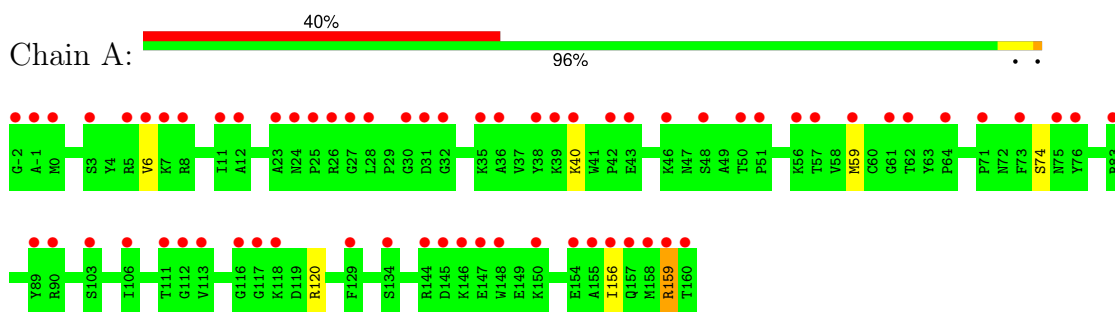
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	227	Total	O	0	0
			227	227		
7	B	204	Total	O	0	0
			204	204		
7	C	196	Total	O	0	0
			196	196		
7	D	153	Total	O	0	0
			153	153		



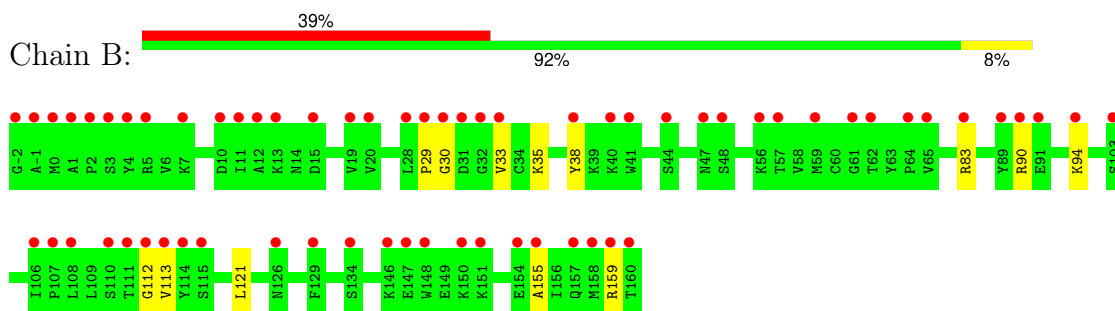
### 3 Residue-property plots [i](#)

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. 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. 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.

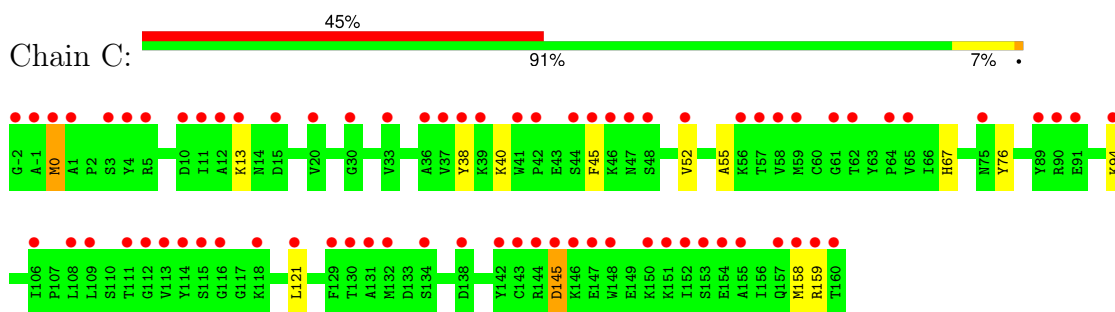
- Molecule 1: Non-structural protein 3



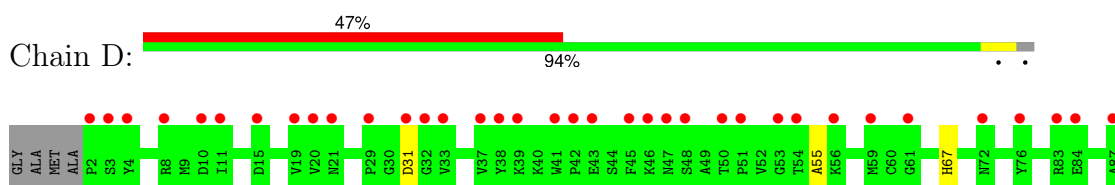
- Molecule 1: Non-structural protein 3

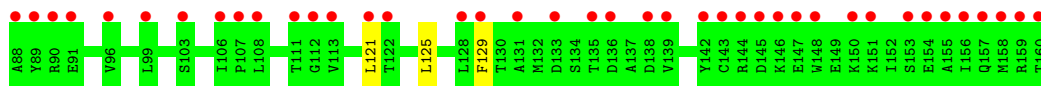


- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.61Å 87.61Å 85.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.71 – 1.39 34.71 – 1.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.71-1.39) 98.9 (34.71-1.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.181 , 0.208 0.229 , 0.245	Depositor DCC
$R_{free}$ test set	7345 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.029 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4388e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CL, K34, DMS, TRS, A1AJZ

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	0.81	1/1285 (0.1%)	0.90	2/1739 (0.1%)
1	B	0.86	0/1297	0.86	0/1756
1	C	0.84	0/1297	0.86	0/1754
1	D	0.80	0/1269	0.86	0/1717
All	All	0.83	1/5148 (0.0%)	0.87	2/6966 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	SER	CA-CB	-5.06	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	120	ARG	NE-CZ-NH1	6.16	123.38	120.30

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	1262	0	1256	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1274	0	1262	18	0
1	C	1274	0	1272	17	0
1	D	1246	0	1236	5	0
2	A	28	0	42	3	0
2	B	12	0	18	8	0
2	C	4	0	6	6	0
2	D	20	0	30	2	0
3	A	8	0	12	0	0
3	B	8	0	12	4	0
3	D	8	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	0	0	0
5	C	20	0	0	1	0
6	C	10	0	0	0	0
7	A	227	0	0	0	0
7	B	204	0	0	2	0
7	C	196	0	0	8	0
7	D	153	0	0	1	0
All	All	5970	0	5158	46	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 4.

All (46) 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:B:33:VAL:H	2:B:203:DMS:H11	1.47	0.80
1:B:83:ARG:HD3	3:B:202:TRS:H12	1.64	0.78
1:C:52:VAL:CG2	7:C:518:HOH:O	2.35	0.74
1:C:52:VAL:HG21	7:C:518:HOH:O	1.88	0.73
1:D:31:ASP:O	2:D:204:DMS:H12	1.95	0.67
1:C:40:LYS:NZ	2:C:302:DMS:H11	2.09	0.67
2:C:302:DMS:H12	7:C:559:HOH:O	1.93	0.67
1:C:52:VAL:HG23	7:C:551:HOH:O	1.94	0.67
1:B:113:VAL:HG22	2:B:205:DMS:C2	2.30	0.62
1:B:94:LYS:NZ	7:B:301:HOH:O	2.24	0.61
5:C:304[A]:A1AJZ:O1	7:C:401:HOH:O	2.16	0.60
1:A:156:ILE:O	1:A:159:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13[B]:LYS:NZ	7:C:403:HOH:O	2.33	0.59
1:B:113:VAL:HG22	2:B:205:DMS:H21	1.85	0.58
1:B:159:ARG:HD3	7:B:436:HOH:O	2.06	0.54
1:C:40:LYS:HD3	2:C:302:DMS:H11	1.90	0.53
1:C:0:MET:HE1	7:D:351:HOH:O	2.09	0.52
1:B:113:VAL:CG2	2:B:205:DMS:H21	2.39	0.52
1:A:6:VAL:HG12	2:A:204:DMS:S	2.49	0.51
1:C:52:VAL:HG21	1:C:76:TYR:OH	2.10	0.51
1:B:33:VAL:H	2:B:203:DMS:C1	2.19	0.51
1:C:145:ASP:HB3	7:C:415:HOH:O	2.10	0.51
1:C:40:LYS:CE	2:C:302:DMS:H11	2.41	0.50
1:B:113:VAL:CG2	2:B:205:DMS:C2	2.90	0.49
1:C:121:LEU:C	1:C:121:LEU:HD23	2.33	0.48
1:B:90:ARG:HH12	3:B:202:TRS:H22	1.77	0.48
1:A:59[A]:MET:HG2	2:A:203:DMS:H11	1.96	0.47
1:C:40:LYS:NZ	2:C:302:DMS:C1	2.75	0.46
1:B:121:LEU:C	1:B:121:LEU:HD23	2.36	0.46
1:D:121:LEU:C	1:D:121:LEU:HD23	2.36	0.46
1:B:90:ARG:HH12	3:B:202:TRS:C2	2.29	0.45
1:A:40:LYS:HD3	2:A:201:DMS:H11	1.99	0.45
1:C:40:LYS:HZ2	2:C:302:DMS:H11	1.80	0.45
1:B:30:GLY:O	1:B:35:LYS:HB2	2.17	0.44
1:D:55:ALA:HA	1:D:67:HIS:O	2.18	0.44
1:C:52:VAL:HG22	7:C:518:HOH:O	2.12	0.44
1:B:155:ALA:O	1:B:159:ARG:HG3	2.18	0.44
1:B:33:VAL:HB	2:B:203:DMS:H11	2.00	0.43
1:B:90:ARG:NH1	3:B:202:TRS:C2	2.82	0.43
1:B:112[A]:GLY:N	2:B:203:DMS:H22	2.34	0.43
1:C:94:LYS:HB3	1:C:94:LYS:HE2	1.88	0.42
1:D:125:LEU:HG	1:D:129:PHE:CE2	2.55	0.42
1:D:31:ASP:O	2:D:204:DMS:C1	2.67	0.42
1:B:29:PRO:HG3	1:B:38:TYR:CE1	2.56	0.41
1:C:38:TYR:HA	1:C:45:PHE:CE1	2.57	0.40
1:C:55:ALA:HA	1:C:67:HIS:O	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	163/163 (100%)	162 (99%)	1 (1%)	0	100	100
1	B	165/163 (101%)	165 (100%)	0	0	100	100
1	C	164/163 (101%)	161 (98%)	3 (2%)	0	100	100
1	D	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
All	All	652/652 (100%)	647 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	136/134 (102%)	135 (99%)	1 (1%)	81	61
1	B	137/134 (102%)	137 (100%)	0	100	100
1	C	137/134 (102%)	133 (97%)	4 (3%)	37	9
1	D	136/134 (102%)	136 (100%)	0	100	100
All	All	546/536 (102%)	541 (99%)	5 (1%)	75	53

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

Mol	Chain	Res	Type
1	A	159	ARG
1	C	0	MET

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Mol	Chain	Res	Type
1	C	145	ASP
1	C	158	MET
1	C	159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	GLN
1	C	157	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	A1AJZ	A	207	-	10,10,10	0.38	0	11,13,13	1.37	1 (9%)
5	A1AJZ	C	304[B]	-	10,10,10	0.35	0	11,13,13	1.32	1 (9%)
3	TRS	D	202	-	7,7,7	0.20	0	9,9,9	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	C	302	-	3,3,3	0.49	0	3,3,3	0.27	0
2	DMS	D	208	-	3,3,3	0.25	0	3,3,3	0.06	0
2	DMS	A	211	-	3,3,3	0.32	0	3,3,3	0.22	0
2	DMS	A	208	-	3,3,3	0.26	0	3,3,3	0.10	0
2	DMS	A	209	-	3,3,3	0.30	0	3,3,3	0.17	0
2	DMS	A	203	-	3,3,3	0.19	0	3,3,3	0.24	0
6	K34	C	303	-	9,11,11	0.95	1 (11%)	5,14,14	6.33	4 (80%)
5	A1AJZ	C	304[A]	-	10,10,10	0.38	0	11,13,13	1.28	1 (9%)
2	DMS	B	205	-	3,3,3	0.32	0	3,3,3	0.27	0
2	DMS	A	201	-	3,3,3	0.85	0	3,3,3	0.46	0
2	DMS	D	201	-	3,3,3	0.29	0	3,3,3	0.06	0
2	DMS	D	205	-	3,3,3	0.19	0	3,3,3	0.06	0
3	TRS	B	202	-	7,7,7	0.21	0	9,9,9	0.61	0
3	TRS	A	202	-	7,7,7	0.19	0	9,9,9	0.33	0
2	DMS	B	203	-	3,3,3	0.31	0	3,3,3	0.54	0
2	DMS	B	204	-	3,3,3	0.27	0	3,3,3	0.09	0
2	DMS	A	210	-	3,3,3	0.28	0	3,3,3	0.26	0
2	DMS	D	204	-	3,3,3	0.16	0	3,3,3	0.19	0
2	DMS	A	204	-	3,3,3	0.63	0	3,3,3	0.67	0
2	DMS	D	203	-	3,3,3	0.32	0	3,3,3	0.14	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
5	A1AJZ	C	304[A]	-	-	0/3/3/3	0/1/1/1
5	A1AJZ	A	207	-	-	0/3/3/3	0/1/1/1
5	A1AJZ	C	304[B]	-	-	0/3/3/3	0/1/1/1
6	K34	C	303	-	-	0/1/4/4	0/2/2/2
3	TRS	D	202	-	-	0/9/9/9	-
3	TRS	B	202	-	-	6/9/9/9	-
3	TRS	A	202	-	-	0/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	303	K34	C4-N2	2.21	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	303	K34	C4-N3-C3	12.91	106.37	101.63
6	C	303	K34	N3-C3-N1	-4.72	110.80	114.72
5	A	207	A1AJZ	C4-C3-C1	3.66	132.12	126.19
5	C	304[B]	A1AJZ	C4-C3-C1	3.45	131.78	126.19
5	C	304[A]	A1AJZ	C4-C3-C1	3.34	131.59	126.19
6	C	303	K34	C2-C3-N1	2.37	126.34	124.11
6	C	303	K34	C-N-C2	2.18	110.01	104.39

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	TRS	C2-C-C1-O1
3	B	202	TRS	C3-C-C1-O1
3	B	202	TRS	N-C-C1-O1
3	B	202	TRS	N-C-C3-O3
3	B	202	TRS	C2-C-C3-O3
3	B	202	TRS	C1-C-C3-O3

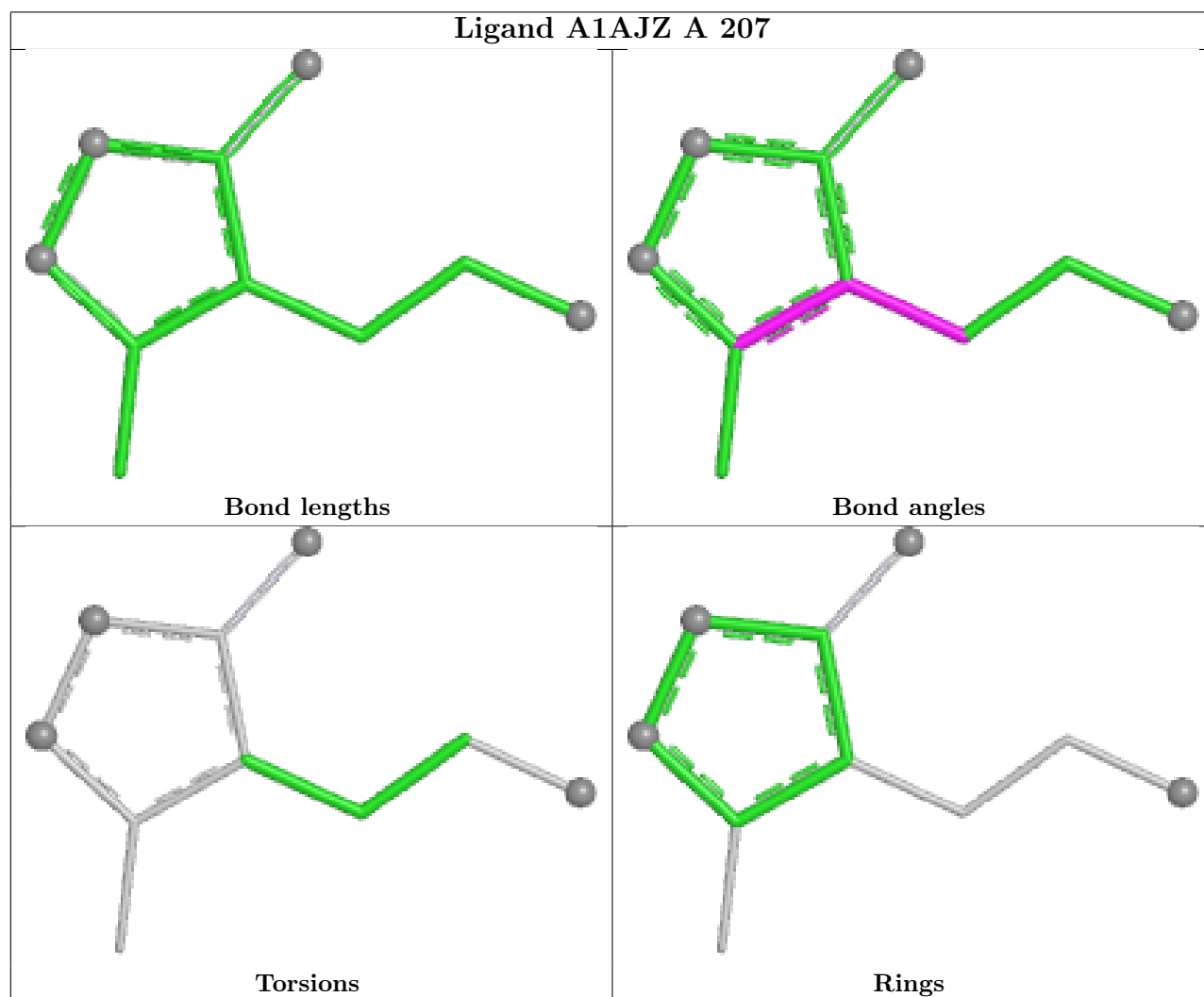
There are no ring outliers.

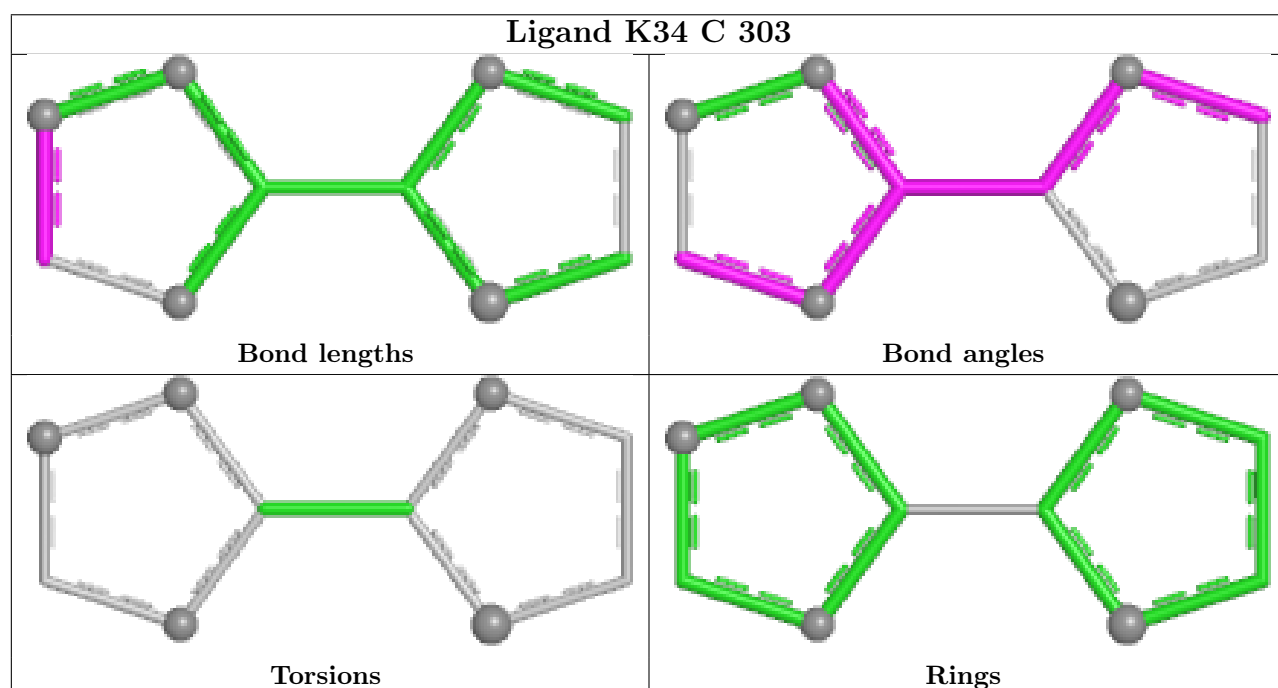
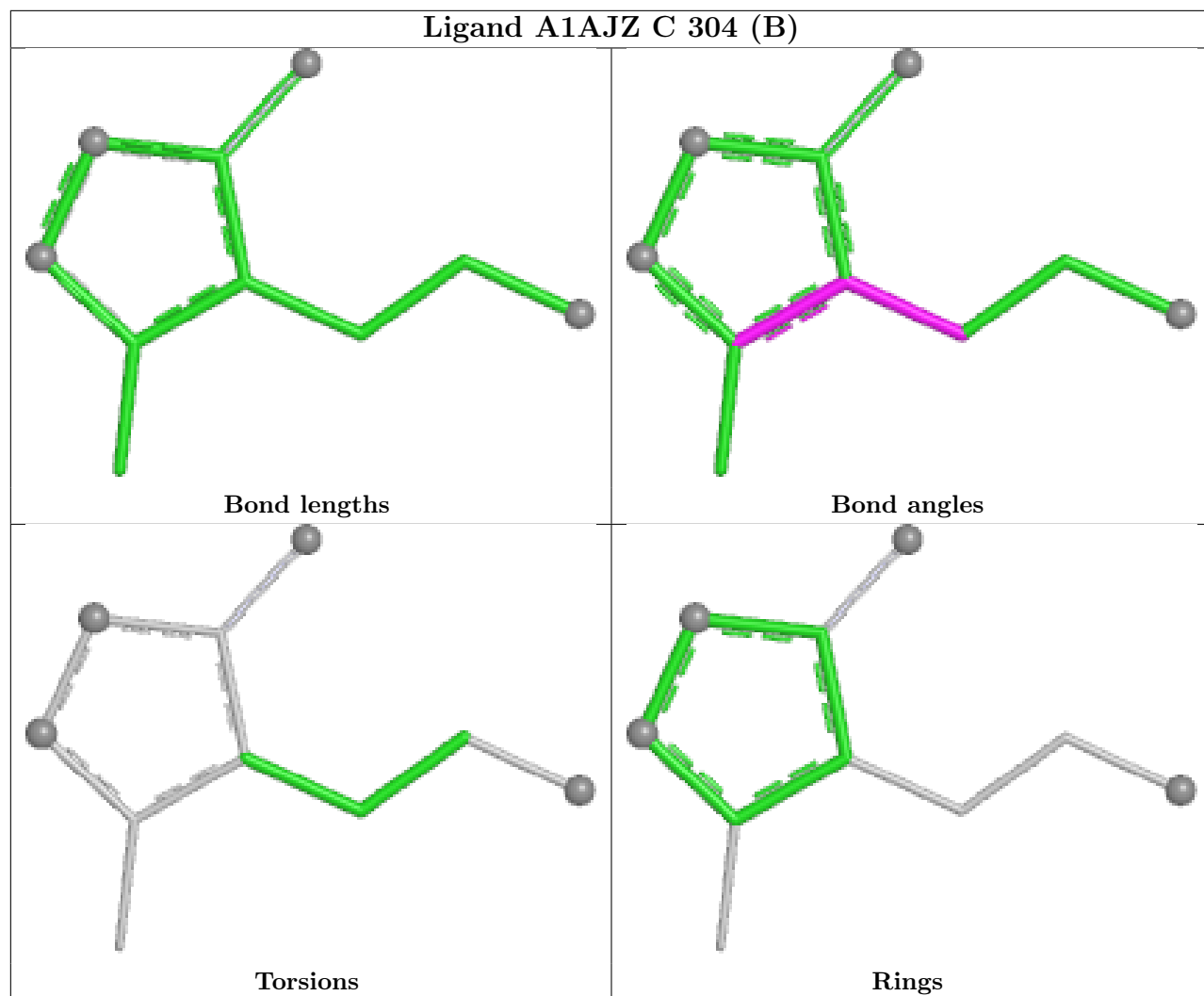
9 monomers are involved in 24 short contacts:

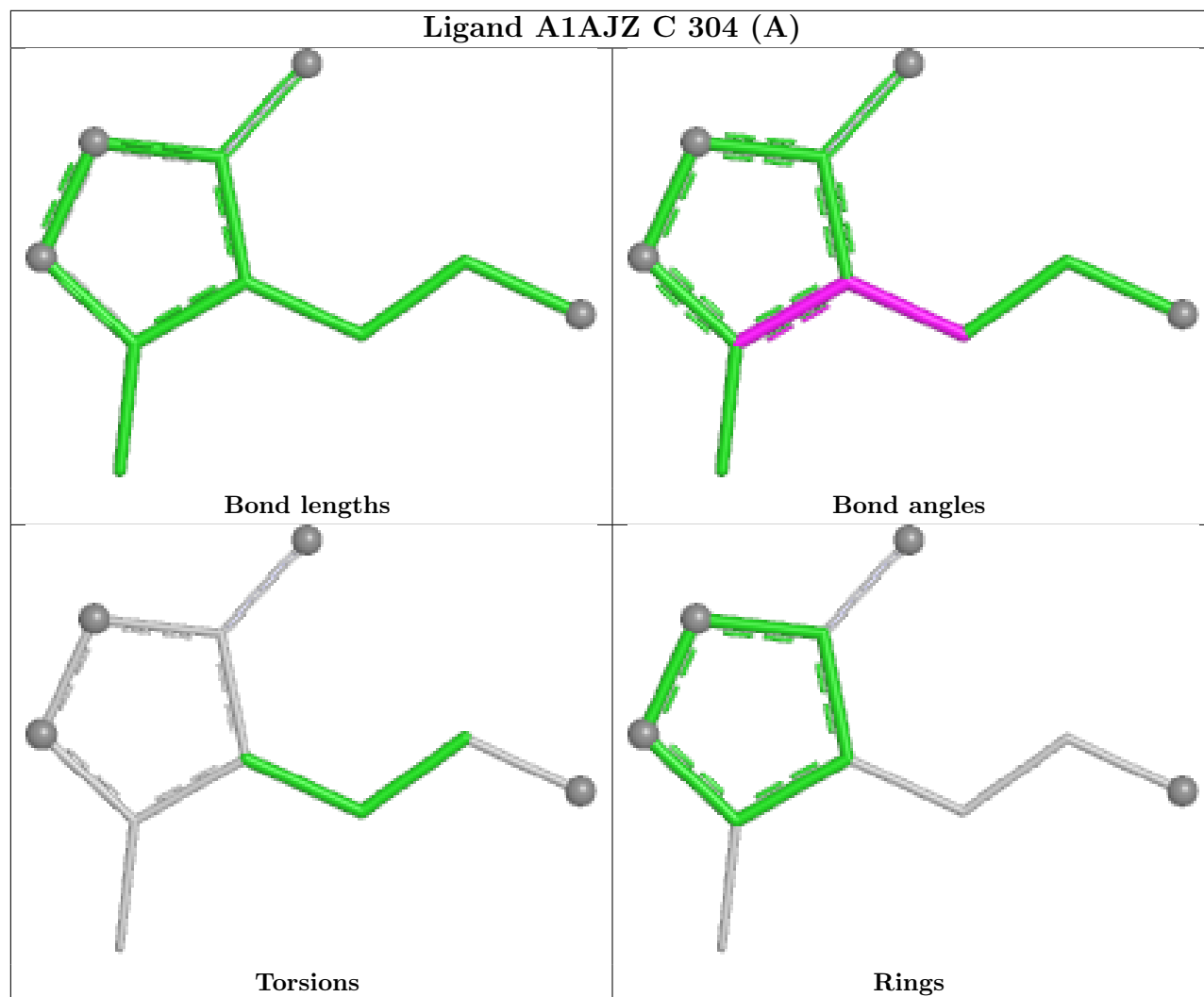
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	DMS	6	0
2	A	203	DMS	1	0
5	C	304[A]	A1AJZ	1	0
2	B	205	DMS	4	0
2	A	201	DMS	1	0
3	B	202	TRS	4	0
2	B	203	DMS	4	0
2	D	204	DMS	2	0
2	A	204	DMS	1	0

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 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](#)

**Warning:** The R factor obtained from EDS is 0.2413, which does not match the depositor's R factor of 0.18078. Please interpret the results in this section carefully.

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	163/163 (100%)	2.09	66 (40%) 1 1	4, 15, 26, 37	56 (34%)
1	B	163/163 (100%)	2.17	64 (39%) 1 1	4, 16, 25, 36	58 (35%)
1	C	163/163 (100%)	2.41	74 (45%) 1 1	5, 18, 29, 39	57 (34%)
1	D	159/163 (97%)	2.63	76 (47%) 0 1	5, 20, 33, 47	56 (35%)
All	All	648/652 (99%)	2.33	280 (43%) 1 1	4, 17, 29, 47	227 (35%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106[A]	ILE	9.2
1	A	106[A]	ILE	9.1
1	D	106[A]	ILE	8.7
1	D	113	VAL	8.2
1	B	106[A]	ILE	8.2
1	A	-1	ALA	8.1
1	D	11	ILE	8.1
1	C	89	TYR	8.0
1	A	112	GLY	7.9
1	D	142	TYR	7.8
1	A	113	VAL	7.8
1	D	20	VAL	7.8
1	B	113	VAL	7.6
1	D	155	ALA	7.5
1	D	19	VAL	7.4
1	C	61	GLY	7.3
1	D	131	ALA	7.3
1	B	65	VAL	7.3
1	C	62	THR	7.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	128	LEU	7.2
1	A	160	THR	7.2
1	A	111	THR	7.2
1	D	143	CYS	7.1
1	D	139	VAL	7.1
1	B	114	TYR	7.0
1	B	129	PHE	6.9
1	C	-1	ALA	6.8
1	C	142	TYR	6.8
1	C	64	PRO	6.7
1	D	156	ILE	6.7
1	C	129	PHE	6.7
1	D	87	ALA	6.7
1	C	4	TYR	6.6
1	A	134	SER	6.5
1	B	30	GLY	6.4
1	A	156	ILE	6.4
1	B	89	TYR	6.4
1	C	20	VAL	6.4
1	D	88	ALA	6.4
1	B	33	VAL	6.3
1	D	3[A]	SER	6.3
1	C	160	THR	6.3
1	D	32	GLY	6.3
1	B	64	PRO	6.2
1	A	64	PRO	6.2
1	B	111[A]	THR	6.2
1	A	28	LEU	6.2
1	D	89	TYR	6.2
1	D	148	TRP	6.1
1	B	-1	ALA	6.1
1	C	11	ILE	6.0
1	B	4	TYR	6.0
1	D	129	PHE	6.0
1	C	130	THR	6.0
1	B	28	LEU	5.9
1	D	108	LEU	5.9
1	B	61	GLY	5.9
1	A	51	PRO	5.9
1	C	131	ALA	5.9
1	A	0	MET	5.9
1	A	27	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	3	SER	5.9
1	B	20	VAL	5.7
1	B	108	LEU	5.7
1	A	11	ILE	5.7
1	B	155	ALA	5.7
1	A	50	THR	5.7
1	D	160	THR	5.7
1	B	2	PRO	5.6
1	A	89	TYR	5.6
1	A	32	GLY	5.6
1	D	107	PRO	5.6
1	B	0	MET	5.6
1	C	52	VAL	5.5
1	D	146	LYS	5.5
1	B	29	PRO	5.5
1	B	11	ILE	5.5
1	A	-2	GLY	5.4
1	C	157	GLN	5.4
1	B	62	THR	5.4
1	A	23	ALA	5.4
1	C	12	ALA	5.4
1	A	62	THR	5.4
1	A	148	TRP	5.4
1	D	103	SER	5.3
1	C	57	THR	5.3
1	C	108	LEU	5.3
1	D	2	PRO	5.3
1	A	3	SER	5.3
1	B	32	GLY	5.3
1	B	112[A]	GLY	5.3
1	D	112	GLY	5.3
1	C	143	CYS	5.2
1	C	13[A]	LYS	5.2
1	C	148	TRP	5.2
1	D	153	SER	5.2
1	C	155	ALA	5.2
1	C	10	ASP	5.1
1	A	129	PHE	5.1
1	A	155	ALA	5.0
1	D	21	ASN	5.0
1	C	33	VAL	5.0
1	A	57	THR	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	47	ASN	4.9
1	A	48	SER	4.9
1	D	29	PRO	4.9
1	B	56	LYS	4.9
1	C	46	LYS	4.8
1	C	145	ASP	4.8
1	C	42	PRO	4.8
1	B	160	THR	4.7
1	C	90[A]	ARG	4.7
1	B	44	SER	4.7
1	B	57	THR	4.7
1	B	107	PRO	4.7
1	C	158	MET	4.6
1	C	116	GLY	4.6
1	D	158	MET	4.6
1	B	115	SER	4.6
1	B	126	ASN	4.6
1	C	-2	GLY	4.6
1	C	138	ASP	4.6
1	C	118	LYS	4.5
1	B	47	ASN	4.5
1	A	59[A]	MET	4.5
1	A	158	MET	4.5
1	A	30	GLY	4.5
1	A	61	GLY	4.5
1	A	159	ARG	4.5
1	A	83	ARG	4.5
1	B	19	VAL	4.4
1	A	35	LYS	4.4
1	C	146	LYS	4.4
1	D	8	ARG	4.4
1	B	158	MET	4.4
1	C	3	SER	4.4
1	D	157	GLN	4.3
1	B	103	SER	4.3
1	A	76	TYR	4.3
1	B	59	MET	4.3
1	D	51	PRO	4.3
1	D	144	ARG	4.2
1	A	103	SER	4.2
1	D	31	ASP	4.2
1	B	1	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	39	LYS	4.2
1	D	53	GLY	4.2
1	D	59[A]	MET	4.2
1	D	46	LYS	4.2
1	C	112	GLY	4.2
1	D	111	THR	4.2
1	D	90	ARG	4.2
1	A	6	VAL	4.2
1	C	0	MET	4.1
1	D	154	GLU	4.1
1	D	145	ASP	4.0
1	B	83	ARG	4.0
1	B	148	TRP	4.0
1	A	157	GLN	4.0
1	B	-2	GLY	4.0
1	D	54	THR	4.0
1	B	91[A]	GLU	4.0
1	C	153	SER	3.9
1	B	15	ASP	3.9
1	B	31	ASP	3.9
1	C	111	THR	3.9
1	C	48	SER	3.9
1	B	147	GLU	3.8
1	A	24	ASN	3.8
1	D	48	SER	3.8
1	D	43	GLU	3.8
1	A	40	LYS	3.8
1	D	151	LYS	3.8
1	C	56	LYS	3.7
1	B	110	SER	3.7
1	D	76	TYR	3.7
1	A	46	LYS	3.7
1	A	56	LYS	3.7
1	A	144	ARG	3.7
1	B	48	SER	3.7
1	A	25	PRO	3.7
1	C	134	SER	3.6
1	D	56	LYS	3.6
1	D	10	ASP	3.6
1	B	12	ALA	3.6
1	B	157	GLN	3.6
1	C	150	LYS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	38	TYR	3.6
1	C	154	GLU	3.6
1	A	5	ARG	3.6
1	C	159	ARG	3.5
1	D	159	ARG	3.5
1	B	94	LYS	3.5
1	C	132	MET	3.5
1	B	10	ASP	3.4
1	B	150	LYS	3.4
1	C	59	MET	3.4
1	B	134	SER	3.4
1	B	159	ARG	3.3
1	A	145	ASP	3.3
1	C	147	GLU	3.3
1	C	94	LYS	3.3
1	A	42	PRO	3.3
1	A	150	LYS	3.3
1	B	90	ARG	3.3
1	C	91	GLU	3.3
1	C	114	TYR	3.2
1	D	138	ASP	3.2
1	A	118	LYS	3.2
1	B	38	TYR	3.2
1	A	31	ASP	3.1
1	D	91	GLU	3.1
1	D	61	GLY	3.1
1	A	146	LYS	3.1
1	C	58	VAL	3.1
1	D	147	GLU	3.1
1	B	7	LYS	3.1
1	C	47	ASN	3.1
1	C	151	LYS	3.0
1	C	144	ARG	3.0
1	A	7	LYS	3.0
1	B	13	LYS	3.0
1	B	146	LYS	3.0
1	C	37	VAL	2.9
1	C	113	VAL	2.9
1	A	90	ARG	2.9
1	D	41	TRP	2.9
1	C	39	LYS	2.9
1	D	96	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	50	THR	2.9
1	A	117	GLY	2.8
1	A	43	GLU	2.8
1	A	39	LYS	2.8
1	C	1	ALA	2.8
1	A	147	GLU	2.7
1	C	44	SER	2.7
1	A	116	GLY	2.7
1	A	26	ARG	2.7
1	A	8	ARG	2.7
1	D	37	VAL	2.7
1	C	121	LEU	2.6
1	D	45	PHE	2.6
1	C	5	ARG	2.6
1	D	83	ARG	2.6
1	A	38	TYR	2.6
1	D	133	ASP	2.6
1	A	75	ASN	2.6
1	C	115	SER	2.5
1	C	41	TRP	2.5
1	D	122	THR	2.5
1	D	99	LEU	2.5
1	D	84	GLU	2.5
1	B	154	GLU	2.5
1	C	45	PHE	2.4
1	D	121	LEU	2.4
1	D	135	THR	2.4
1	A	73	PHE	2.4
1	C	152	ILE	2.4
1	B	5	ARG	2.3
1	A	12	ALA	2.3
1	D	150	LYS	2.3
1	D	4	TYR	2.3
1	D	72	ASN	2.3
1	A	36	ALA	2.3
1	C	30	GLY	2.2
1	D	38	TYR	2.2
1	A	71	PRO	2.2
1	D	136	ASP	2.2
1	C	109	LEU	2.2
1	C	15	ASP	2.2
1	C	36	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	15	ASP	2.1
1	C	75	ASN	2.1
1	D	33	VAL	2.1
1	D	42	PRO	2.1
1	A	154	GLU	2.1
1	B	40	LYS	2.1
1	B	41	TRP	2.1
1	C	65	VAL	2.1
1	B	151	LYS	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DMS	A	209	4/4	0.60	0.32	35,37,37,39	4
2	DMS	D	201	4/4	0.61	0.27	30,36,37,37	4
5	A1AJZ	A	207	10/10	0.66	0.31	35,37,39,40	10
2	DMS	B	203	4/4	0.67	0.41	34,36,39,41	4
2	DMS	A	204	4/4	0.71	0.22	25,42,50,56	0
3	TRS	D	202	8/8	0.73	0.19	29,31,32,34	8
2	DMS	A	208	4/4	0.75	0.51	73,74,74,76	4
3	TRS	B	202	8/8	0.76	0.20	24,29,31,33	8
5	A1AJZ	C	304[A]	10/10	0.76	0.18	18,19,20,20	10
5	A1AJZ	C	304[B]	10/10	0.76	0.18	20,21,21,22	10
2	DMS	B	204	4/4	0.77	0.24	30,35,37,38	4
2	DMS	D	208	4/4	0.80	0.20	45,49,50,53	4
2	DMS	D	205	4/4	0.80	0.23	37,44,47,48	4
2	DMS	D	204	4/4	0.83	0.27	37,48,49,49	4

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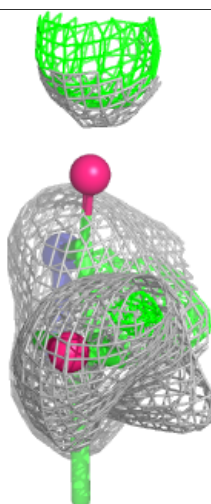
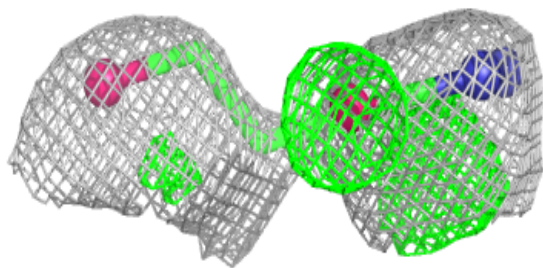
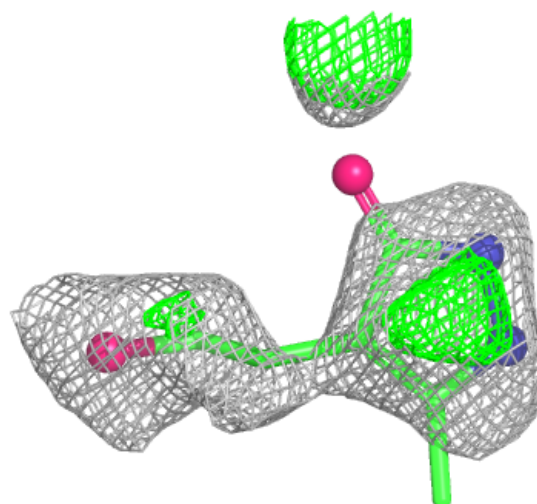
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DMS	D	203	4/4	0.83	0.23	40,42,43,43	4
3	TRS	A	202	8/8	0.84	0.22	31,35,39,40	8
2	DMS	B	205	4/4	0.86	0.23	27,33,35,35	4
2	DMS	A	201	4/4	0.87	0.16	37,42,45,46	0
2	DMS	A	203	4/4	0.88	0.22	33,36,38,42	4
2	DMS	A	211	4/4	0.88	0.17	57,63,68,71	0
2	DMS	C	302	4/4	0.89	0.14	36,40,41,43	0
6	K34	C	303	10/10	0.94	0.10	12,12,13,13	10
2	DMS	A	210	4/4	0.95	0.14	27,30,32,32	4
4	CL	C	301	1/1	0.96	0.15	29,29,29,29	0
4	CL	D	206	1/1	0.96	0.12	35,35,35,35	0
4	CL	D	207	1/1	0.98	0.14	27,27,27,27	0
4	CL	A	206	1/1	0.99	0.08	19,19,19,19	0
4	CL	B	201	1/1	0.99	0.03	21,21,21,21	0
4	CL	A	205	1/1	0.99	0.04	19,19,19,19	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.

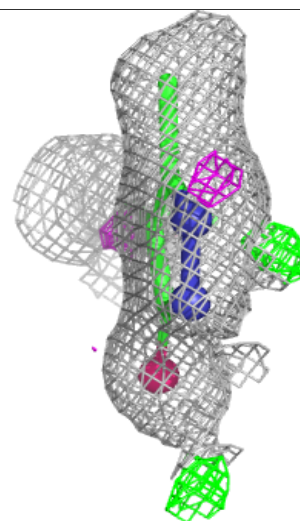
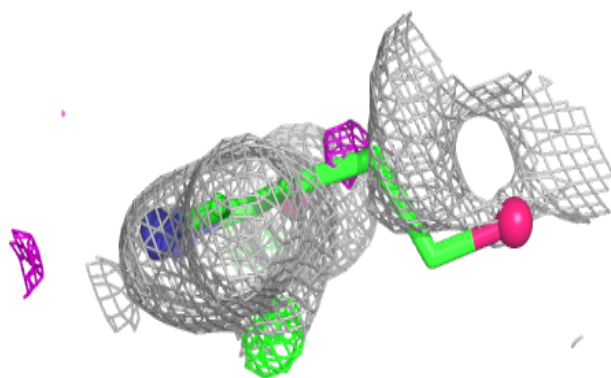
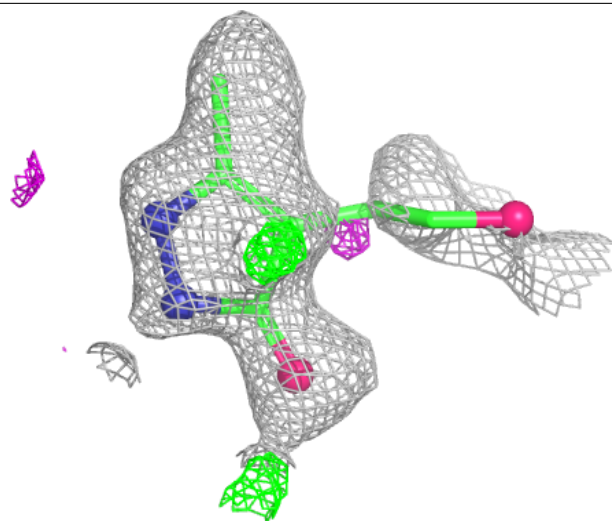
**Electron density around A1AJZ A 207:**

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



**Electron density around A1AJZ C 304 (A):**

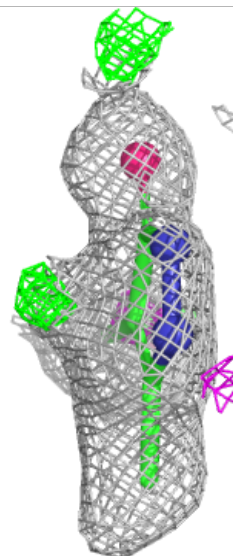
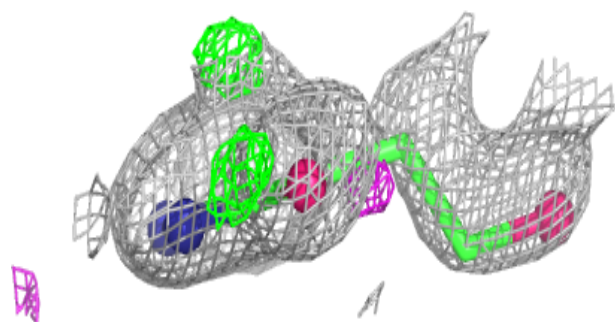
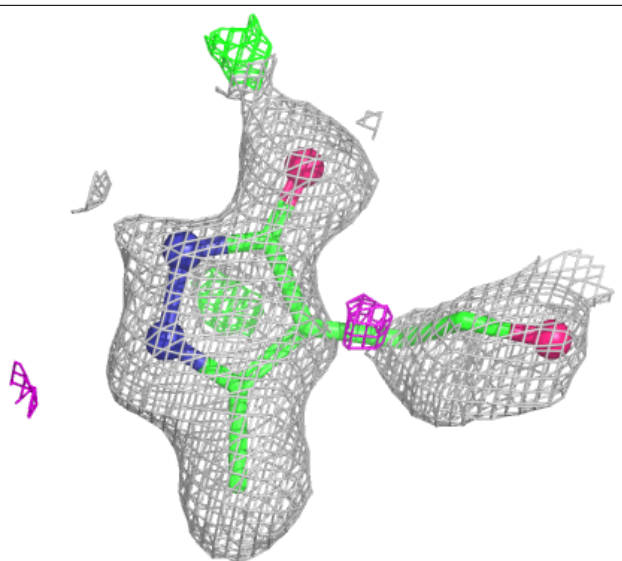
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

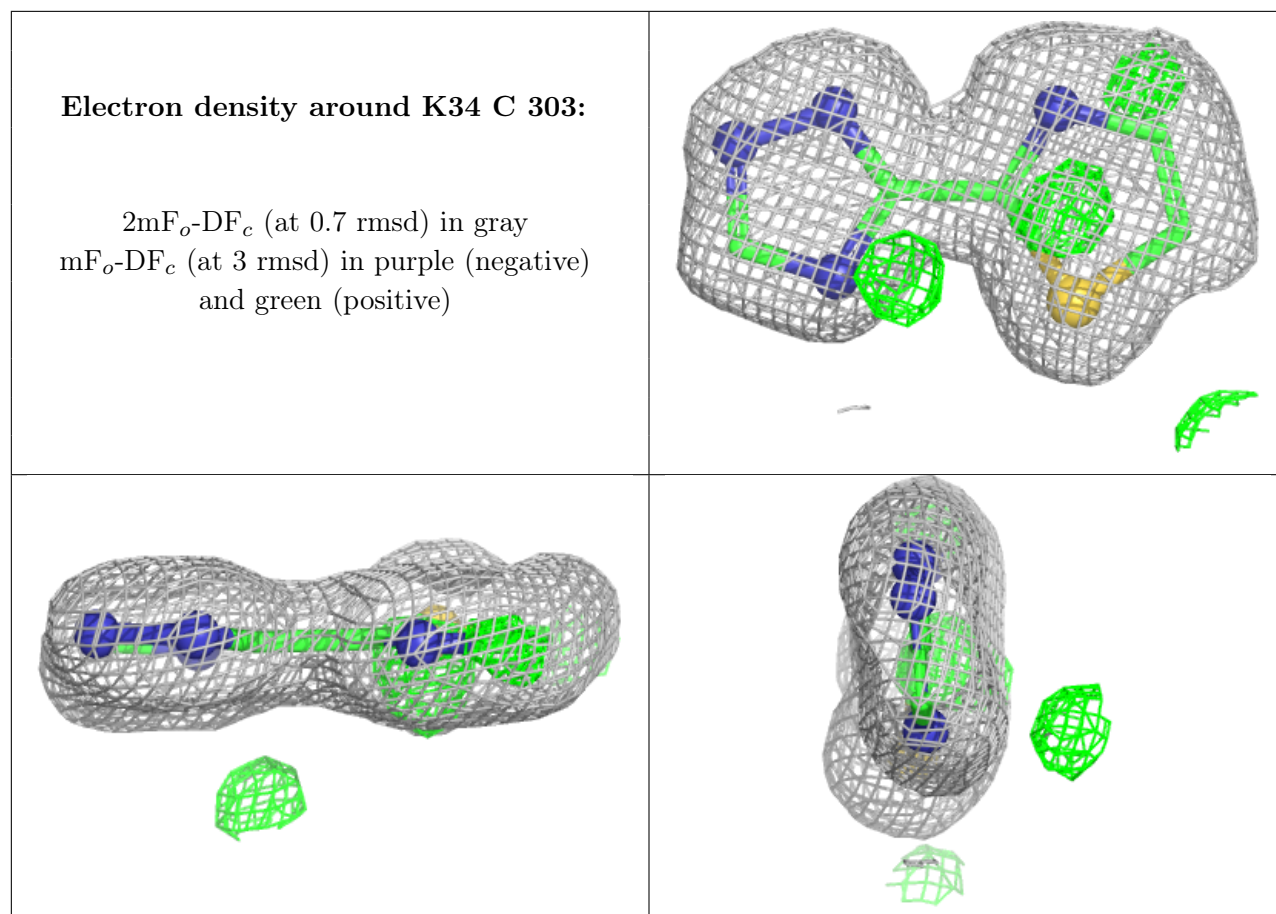




**Electron density around A1AJZ C 304 (B):**

$2mF_o-DF_c$  (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.