



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:06 pm BST

PDB ID : 4TL8  
Title : Crystal structure of N-terminal C1 domain of KaiC  
Authors : Abe, J.; Hiyama, T.B.; Mukaiyama, A.; Son, S.; Akiyama, S.  
Deposited on : 2014-05-29  
Resolution : 1.86 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

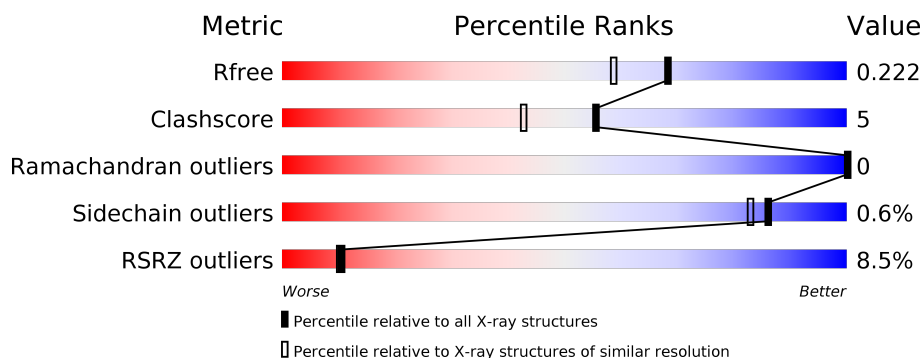
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	253	<div> <div>13%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>15%</div> </div> </div>
1	B	253	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>
1	C	253	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	D	253	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>
1	E	253	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	F	253	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11623 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	6	0
			1735	1101	304	326	4			
1	B	215	Total	C	N	O	S	0	6	0
			1737	1105	301	326	5			
1	C	221	Total	C	N	O	S	0	8	0
			1786	1136	312	334	4			
1	D	217	Total	C	N	O	S	0	5	0
			1760	1115	308	332	5			
1	E	216	Total	C	N	O	S	0	5	0
			1743	1110	303	326	4			
1	F	213	Total	C	N	O	S	0	6	0
			1732	1096	302	330	4			

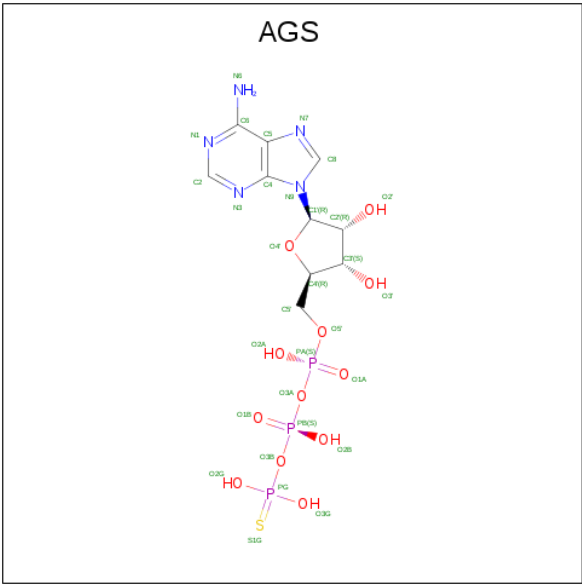
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

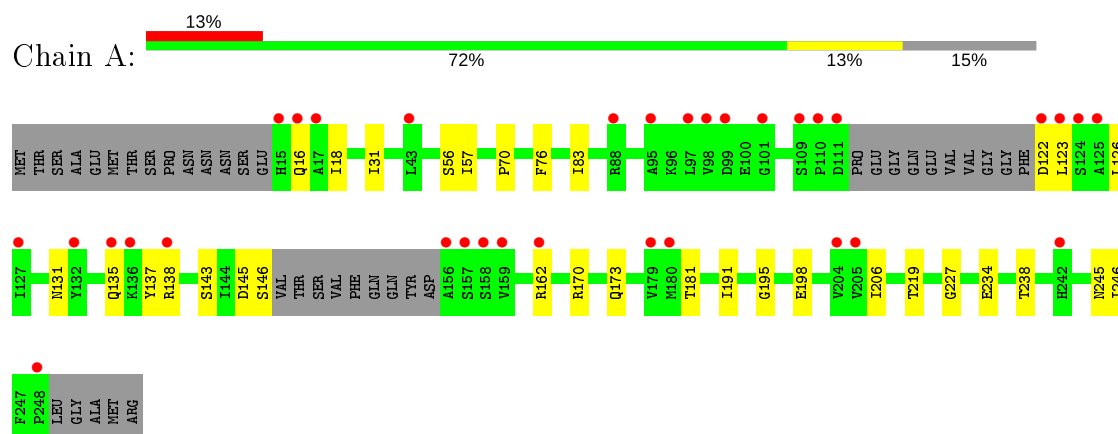
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	181	Total	O	0	0
			181	181		
5	C	178	Total	O	0	0
			178	178		
5	D	178	Total	O	0	0
			178	178		
5	E	139	Total	O	0	0
			139	139		
5	F	137	Total	O	0	0
			137	137		

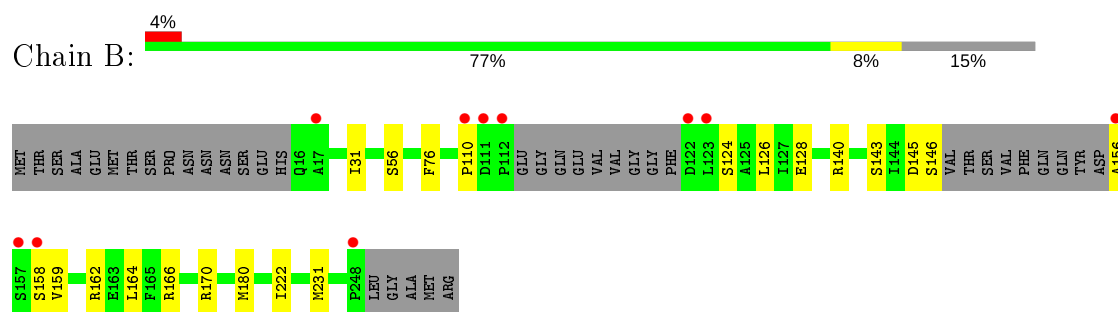
### 3 Residue-property plots [i](#)

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.

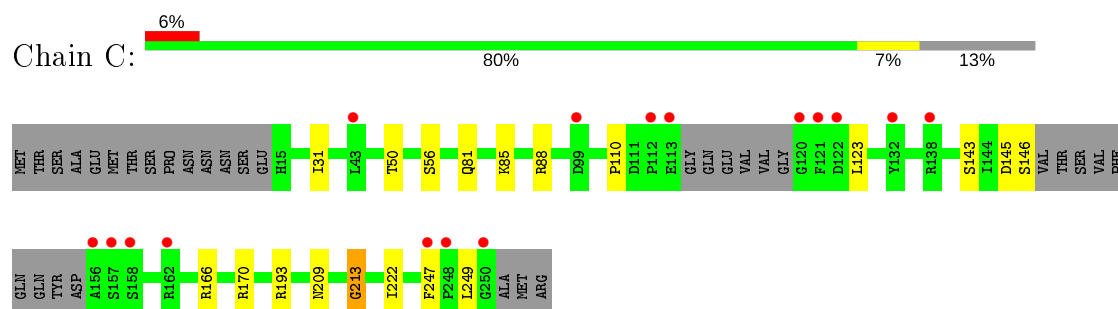
- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC



- Molecule 1: Circadian clock protein kinase KaiC

TTR	ASP	A156	S157	S158	V159	V160	R161	R162	E163	L164	F165	M180	G195	E198	V204	I222	L223	K224	L225	T228	M231	P243	LEU	GLY	ALA	MET	ARG																				
MET	THR	SER	ALA	GLU	MET	THR	PRO	ASN	ASN	ASN	S13	I25	E26	G27	I31	R40	F55	S56	D99	P110	D111	PRO	GLU	GLY	GLN	GLU	VAL	VAL	GLY	GLY	PHE	D122	P125	V132	G135	R138	I143	I144	D145	S146	VAL	THR	SER	VAL	PHE	GLN	GLN

- Chain E:**
- 
- | Position | Amino Acid | Conservation (%) |
|----------|------------|------------------|
| 1        | MET        | ~0.05            |
| 2        | THR        | ~0.05            |
| 3        | SER        | ~0.05            |
| 4        | GLN        | ~0.05            |
| 5        | ALA        | ~0.05            |
| 6        | GLU        | ~0.05            |
| 7        | MET        | ~0.05            |
| 8        | THR        | ~0.05            |
| 9        | SER        | ~0.05            |
| 10       | PRO        | ~0.05            |
| 11       | ASN        | ~0.05            |
| 12       | ASN        | ~0.05            |
| 13       | ASN        | ~0.05            |
| 14       | SER        | ~0.05            |
| 15       | GLU        | ~0.05            |
| 16       | HIS        | ~0.05            |
| 17       | G16        | ~0.05            |
| 18       | S48        | ~0.05            |
| 19       | S56        | ~0.05            |
| 20       | R88        | ~0.05            |
| 21       | F110       | ~0.05            |
| 22       | ASP        | ~0.05            |
| 23       | PRO        | ~0.05            |
| 24       | GLU        | ~0.05            |
| 25       | GLY        | ~0.05            |
| 26       | GLN        | ~0.05            |
| 27       | GLU        | ~0.05            |
| 28       | VAL        | ~0.05            |
| 29       | VAL        | ~0.05            |
| 30       | GLY        | ~0.05            |
| 31       | G120       | ~0.05            |
| 32       | F121       | ~0.05            |
| 33       | D122       | ~0.05            |
| 34       | L123       | ~0.05            |
| 35       | S124       | ~0.05            |
| 36       | A125       | ~0.05            |
| 37       | L126       | ~0.05            |
| 38       | I127       | ~0.05            |
| 39       | E128       | ~0.05            |
| 40       | M131       | ~0.05            |
| 41       | Y132       | ~0.05            |
| 42       | Q135       | ~0.05            |
| 43       | K136       | ~0.05            |
| 44       | Y137       | ~0.05            |
| 45       | R138       | ~0.05            |
| 46       | A139       | ~0.05            |
| 47       | R140       | ~0.05            |
| 48       | S143       | ~0.05            |
| 49       | I144       | ~0.05            |
| 50       | D145       | ~0.05            |
| 51       | S146       | ~0.05            |
| 52       | VAL        | ~0.05            |
| 53       | THR        | ~0.05            |
| 54       | CPR        | ~0.05            |

- Chain F:
- 
- 6% 72% 11% 16%
- Y137 R138 S143 I144 D145 S146 VAL THR SER VAL PHE GLN TYR ASP A156 S157 S158 V159 R162 R170 I174 M180 E183 I191 A192 R193 E198 M209 V210 L211 R217 L225 P243 LEU GLY ALA MET ARG
- MET THR SER ALA GLU MET THR SER PRO ASN ASN ASN SER GLU HIS GLN A17 S41 T50 S56 F76 Q81 R88 D99 K102 I103 F104 I105 L106 P110 D111 PRO GLU GLN GLN VAL VAL GLY GLY PHE D122 S123 L124 A125 L126 N131 Q135 Q136

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.93Å 133.22Å 150.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.59 – 1.86 37.59 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.8 (37.59-1.86) 97.8 (37.59-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.28 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.180 , 0.222 0.181 , 0.222	Depositor DCC
$R_{free}$ test set	6644 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, CL

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	0.58	0/1774	0.63	0/2388
1	B	0.68	0/1776	0.72	0/2391
1	C	0.67	0/1827	0.74	1/2459 (0.0%)
1	D	0.70	0/1787	0.75	1/2405 (0.0%)
1	E	0.70	0/1776	0.74	0/2390
1	F	0.70	0/1758	0.77	3/2366 (0.1%)
All	All	0.67	0/10698	0.72	5/14399 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	F	217	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	C	213	GLY	N-CA-C	-5.84	98.50	113.10
1	D	225	LEU	CA-CB-CG	5.27	127.41	115.30
1	F	211	LEU	CA-CB-CG	5.17	127.20	115.30
1	F	225	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	16	GLN	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1754	23	0
1	B	1737	0	1765	18	0
1	C	1786	0	1808	16	0
1	D	1760	0	1765	17	0
1	E	1743	0	1767	21	0
1	F	1732	0	1737	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	2	0
4	F	31	0	12	0	0
5	A	119	0	0	1	0
5	B	181	0	0	2	0
5	C	178	0	0	4	0
5	D	178	0	0	2	0
5	E	139	0	0	1	0
5	F	137	0	0	2	0
All	All	11623	0	10668	108	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 (108) 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:C:193:ARG:NH1	1:D:195:GLY:O	1.91	1.04
1:A:195:GLY:O	1:F:193:ARG:NH2	2.03	0.91
1:E:16:GLN:O	1:E:16:GLN:HG2	1.70	0.90
1:B:124:SER:OG	1:B:166:ARG:NH2	2.05	0.90
1:F:81:GLN:NE2	5:F:504:HOH:O	2.12	0.83
1:E:127:ILE:HG21	1:E:170:ARG:HD3	1.69	0.75
1:A:238:THR:OG1	1:A:245[A]:ASN:OD1	2.14	0.66
1:D:158:SER:HA	1:D:161:ARG:HB3	1.78	0.65
1:D:198:GLU:OE1	5:D:545:HOH:O	2.15	0.65
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.26	0.64
1:F:41:SER:OG	5:F:536:HOH:O	1.96	0.63
1:E:123:LEU:HD13	1:E:127:ILE:HD11	1.82	0.62
1:B:158:SER:O	1:B:162:ARG:HG3	1.99	0.61
1:F:191:ILE:HG21	1:F:198:GLU:HB3	1.83	0.61
1:F:156:ALA:HB3	1:F:159:VAL:HG12	1.81	0.60
1:E:156:ALA:HB3	1:E:159:VAL:HG12	1.86	0.58
1:B:164:LEU:HD11	1:B:180:MET:HE1	1.88	0.56
1:B:156:ALA:HB3	1:B:159:VAL:HG12	1.88	0.55
1:A:76:PHE:HZ	1:A:126:LEU:HD21	1.71	0.55
1:F:56[A]:SER:HB2	1:F:143:SER:HB3	1.90	0.54
1:A:122:ASP:OD1	1:A:123:LEU:N	2.40	0.54
1:D:31[A]:ILE:HG22	1:D:222:ILE:HD12	1.91	0.53
1:B:140:ARG:HD2	5:B:469:HOH:O	2.09	0.52
1:E:162:ARG:HG3	1:E:162:ARG:HH11	1.74	0.52
1:E:191:ILE:HG21	1:E:198:GLU:HB3	1.91	0.52
1:E:56[A]:SER:HB2	1:E:143:SER:HB3	1.92	0.52
1:F:104:PHE:HE2	1:F:106:LEU:HD12	1.74	0.50
1:A:162:ARG:NH1	1:F:110:PRO:HG3	2.26	0.50
1:A:16:GLN:OE1	5:A:401:HOH:O	2.20	0.50
1:C:110:PRO:HG2	1:D:165:PHE:CE1	2.48	0.49
1:D:31[B]:ILE:HG22	1:D:222:ILE:HD12	1.95	0.49
1:C:146[B]:SER:OG	5:C:488:HOH:O	2.06	0.48
1:A:170:ARG:HD3	1:A:173:GLN:OE1	2.12	0.48
1:C:213:GLY:O	5:C:561:HOH:O	2.17	0.48
1:A:162:ARG:HA	1:A:162:ARG:NE	2.28	0.48
1:E:123:LEU:HD11	1:E:166:ARG:CZ	2.44	0.48
1:E:145[A]:ASP:HA	1:E:146[A]:SER:HA	1.59	0.48
1:C:166:ARG:O	1:C:170:ARG:HG2	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LYS:HE3	1:D:40:ARG:NH2	2.29	0.48
1:A:145[A]:ASP:HA	1:A:146[A]:SER:HA	1.67	0.47
1:F:170:ARG:O	1:F:174:ILE:HG13	2.14	0.47
1:B:164:LEU:CD1	1:B:180:MET:HE1	2.44	0.47
1:D:156:ALA:O	1:D:159:VAL:HG12	2.15	0.47
1:D:145[A]:ASP:HA	1:D:146[A]:SER:HA	1.67	0.47
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.97	0.47
1:B:56[A]:SER:HB2	1:B:143:SER:HB3	1.97	0.46
1:C:170:ARG:NH1	5:C:512:HOH:O	2.30	0.46
1:D:56[A]:SER:HB2	1:D:143:SER:HB3	1.97	0.46
1:F:183:GLU:OE2	1:F:193:ARG:NH1	2.49	0.46
1:C:88[A]:ARG:HD3	5:C:418:HOH:O	2.14	0.46
1:F:122:ASP:HB2	1:F:125:ALA:CB	2.46	0.46
1:E:131:ASN:O	1:E:135:GLN:HG2	2.16	0.46
1:A:131:ASN:O	1:A:135:GLN:HG2	2.16	0.45
1:D:25:ILE:O	5:D:551:HOH:O	2.21	0.45
1:F:145[A]:ASP:HA	1:F:146[A]:SER:HA	1.71	0.45
1:B:166:ARG:O	1:B:170:ARG:HG2	2.17	0.45
1:F:122:ASP:HB2	1:F:125:ALA:HB3	1.97	0.45
1:C:31:ILE:HG22	1:C:222:ILE:HD12	1.97	0.45
1:E:162:ARG:HH11	1:E:162:ARG:CG	2.29	0.45
1:A:16:GLN:HB2	1:F:88:ARG:HB3	2.00	0.44
1:F:76:PHE:O	1:F:110:PRO:HD3	2.18	0.44
1:A:18:ILE:HD13	1:A:227:GLY:O	2.17	0.44
1:B:180:MET:HB3	1:B:180:MET:HE3	1.69	0.44
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.99	0.44
1:E:161:ARG:HG3	1:E:200:VAL:HG11	1.99	0.44
1:B:31[A]:ILE:HG22	1:B:222:ILE:HD12	2.00	0.43
1:C:247:PHE:O	1:C:249:LEU:HD23	2.18	0.43
1:C:145[A]:ASP:HA	1:C:146[A]:SER:HA	1.57	0.43
1:E:88:ARG:NE	5:E:401:HOH:O	2.44	0.43
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.83	0.43
1:D:31[B]:ILE:HD13	1:D:231:MET:SD	2.59	0.43
1:D:159:VAL:O	1:D:163:GLU:HG2	2.18	0.43
1:B:140:ARG:NH1	5:B:525:HOH:O	2.50	0.43
1:D:204:VAL:HG23	1:D:224:LYS:HE2	2.01	0.43
1:B:124:SER:O	1:B:128:GLU:HG2	2.18	0.43
1:A:70:PRO:HG2	1:A:138:ARG:O	2.17	0.43
1:B:145[A]:ASP:HA	1:B:146[A]:SER:HA	1.67	0.43
1:E:158:SER:O	1:E:162:ARG:HG3	2.19	0.43
1:D:180[B]:MET:HB3	1:D:180[B]:MET:HE3	1.75	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:CZ	1:A:162:ARG:HA	2.49	0.42
1:A:146[A]:SER:HA	1:A:181:THR:OG1	2.19	0.42
1:E:56[B]:SER:HB3	1:E:143:SER:HB3	2.01	0.42
1:F:191:ILE:CG2	1:F:198:GLU:HB3	2.48	0.42
1:A:56[A]:SER:HB2	1:A:143:SER:HB3	2.00	0.42
1:E:48[B]:SER:HA	4:E:303:AGS:S1G	2.60	0.42
1:F:180:MET:HB3	1:F:180:MET:HE3	1.93	0.42
1:B:56[B]:SER:HB3	1:B:143:SER:HB3	2.00	0.42
1:C:50:THR:HG22	1:C:209:ASN:HB2	2.00	0.42
1:E:123:LEU:HD11	1:E:166:ARG:NH2	2.35	0.42
1:C:56[B]:SER:HB3	1:C:143:SER:HB3	2.01	0.42
1:A:16:GLN:OE1	1:F:88:ARG:HD3	2.20	0.41
1:D:27:GLY:O	1:D:31[B]:ILE:HG12	2.19	0.41
1:E:123:LEU:HD12	1:E:124:SER:HA	2.02	0.41
1:F:131:ASN:O	1:F:135:GLN:HG2	2.20	0.41
1:E:48[A]:SER:HA	4:E:303:AGS:S1G	2.60	0.41
1:B:76:PHE:O	1:B:110:PRO:HD3	2.20	0.41
1:B:31[B]:ILE:HG23	1:B:231[B]:MET:HB2	2.02	0.41
1:A:191:ILE:HB	1:A:198:GLU:HB3	2.03	0.41
1:E:127:ILE:HD12	1:E:170:ARG:HD2	2.03	0.41
1:C:85:LYS:HE3	1:D:40:ARG:HH21	1.84	0.41
1:C:123:LEU:HD12	1:C:123:LEU:HA	1.77	0.41
1:A:191:ILE:HD12	1:A:206:ILE:HD11	2.02	0.40
1:A:57:ILE:HD11	1:A:83:ILE:HG23	2.02	0.40
1:C:56[A]:SER:HB2	1:C:143:SER:HB3	2.02	0.40
1:A:137:TYR:O	1:A:138:ARG:HB2	2.21	0.40
1:A:219:THR:HB	1:A:234:GLU:HB3	2.03	0.40
1:B:31[A]:ILE:HD13	1:B:31[A]:ILE:HG21	1.87	0.40
1:F:102:LYS:HA	1:F:102:LYS:HD3	1.96	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	214/253 (85%)	210 (98%)	4 (2%)	0	100	100
1	B	214/253 (85%)	208 (97%)	6 (3%)	0	100	100
1	C	220/253 (87%)	214 (97%)	6 (3%)	0	100	100
1	D	215/253 (85%)	211 (98%)	4 (2%)	0	100	100
1	E	214/253 (85%)	211 (99%)	3 (1%)	0	100	100
1	F	212/253 (84%)	208 (98%)	4 (2%)	0	100	100
All	All	1289/1518 (85%)	1262 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/217 (88%)	190 (100%)	0	100	100
1	B	191/217 (88%)	191 (100%)	0	100	100
1	C	195/217 (90%)	194 (100%)	1 (0%)	88	86
1	D	191/217 (88%)	190 (100%)	1 (0%)	88	86
1	E	190/217 (88%)	187 (98%)	3 (2%)	62	49
1	F	189/217 (87%)	187 (99%)	2 (1%)	73	65
All	All	1146/1302 (88%)	1139 (99%)	7 (1%)	86	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	81	GLN
1	D	228	THR
1	E	16	GLN
1	E	170	ARG
1	E	212	GLU
1	F	122	ASP
1	F	191	ILE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
4	AGS	E	303	2	26,33,33	0.85	1 (3%)	26,52,52	1.34	3 (11%)
4	AGS	C	303	2	26,33,33	0.95	1 (3%)	26,52,52	1.11	1 (3%)
4	AGS	B	303	2	26,33,33	1.00	1 (3%)	26,52,52	0.97	2 (7%)
4	AGS	A	303	2	26,33,33	0.81	1 (3%)	26,52,52	1.03	2 (7%)
4	AGS	F	301	2	26,33,33	0.79	0	26,52,52	1.25	2 (7%)
4	AGS	D	303	2	26,33,33	0.91	1 (3%)	26,52,52	1.02	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	E	303	2	-	6/17/38/38	0/3/3/3
4	AGS	C	303	2	-	4/17/38/38	0/3/3/3
4	AGS	B	303	2	-	4/17/38/38	0/3/3/3
4	AGS	A	303	2	-	7/17/38/38	0/3/3/3
4	AGS	F	301	2	-	4/17/38/38	0/3/3/3
4	AGS	D	303	2	-	7/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	AGS	PG-S1G	3.38	1.98	1.90
4	D	303	AGS	PG-S1G	3.12	1.97	1.90
4	A	303	AGS	PG-S1G	2.85	1.96	1.90
4	E	303	AGS	O5'-C5'	-2.51	1.35	1.44
4	B	303	AGS	PG-S1G	2.27	1.95	1.90

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	303	AGS	O2G-PG-O3B	4.08	118.26	104.64
4	F	301	AGS	O2G-PG-O3B	3.88	117.61	104.64
4	C	303	AGS	O2G-PG-O3B	3.10	114.98	104.64
4	D	303	AGS	O2G-PG-O3B	3.00	114.65	104.64
4	B	303	AGS	O2G-PG-O3B	2.72	113.71	104.64
4	A	303	AGS	C5-C6-N6	2.51	124.16	120.35
4	E	303	AGS	PA-O3A-PB	-2.30	124.92	132.83
4	A	303	AGS	O2G-PG-O3B	2.22	112.04	104.64
4	F	301	AGS	C5-C6-N6	2.18	123.67	120.35
4	B	303	AGS	C5-C6-N6	2.17	123.65	120.35
4	E	303	AGS	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	303	AGS	PB-O3B-PG-O2G
4	E	303	AGS	PB-O3B-PG-O3G
4	C	303	AGS	PB-O3B-PG-O2G
4	C	303	AGS	PB-O3B-PG-O3G
4	B	303	AGS	PB-O3B-PG-O2G
4	B	303	AGS	PB-O3B-PG-O3G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	F	301	AGS	PB-O3B-PG-O2G
4	F	301	AGS	PB-O3B-PG-O3G
4	D	303	AGS	PB-O3B-PG-O2G
4	D	303	AGS	PB-O3B-PG-O3G
4	D	303	AGS	C5'-O5'-PA-O2A
4	A	303	AGS	C5'-O5'-PA-O2A
4	A	303	AGS	C5'-O5'-PA-O3A
4	C	303	AGS	PA-O3A-PB-O1B
4	B	303	AGS	PA-O3A-PB-O1B
4	F	301	AGS	PA-O3A-PB-O2B
4	D	303	AGS	PA-O3A-PB-O1B
4	E	303	AGS	PA-O3A-PB-O2B
4	B	303	AGS	PA-O3A-PB-O2B
4	F	301	AGS	PG-O3B-PB-O2B
4	D	303	AGS	PG-O3B-PB-O2B
4	A	303	AGS	PB-O3B-PG-O2G
4	A	303	AGS	PB-O3B-PG-O3G
4	E	303	AGS	PA-O3A-PB-O1B
4	A	303	AGS	PA-O3A-PB-O1B
4	E	303	AGS	PG-O3B-PB-O1B
4	E	303	AGS	C5'-O5'-PA-O3A
4	D	303	AGS	C5'-O5'-PA-O3A
4	C	303	AGS	PA-O3A-PB-O2B
4	A	303	AGS	PA-O3A-PB-O2B
4	D	303	AGS	C5'-O5'-PA-O1A
4	A	303	AGS	C5'-O5'-PA-O1A

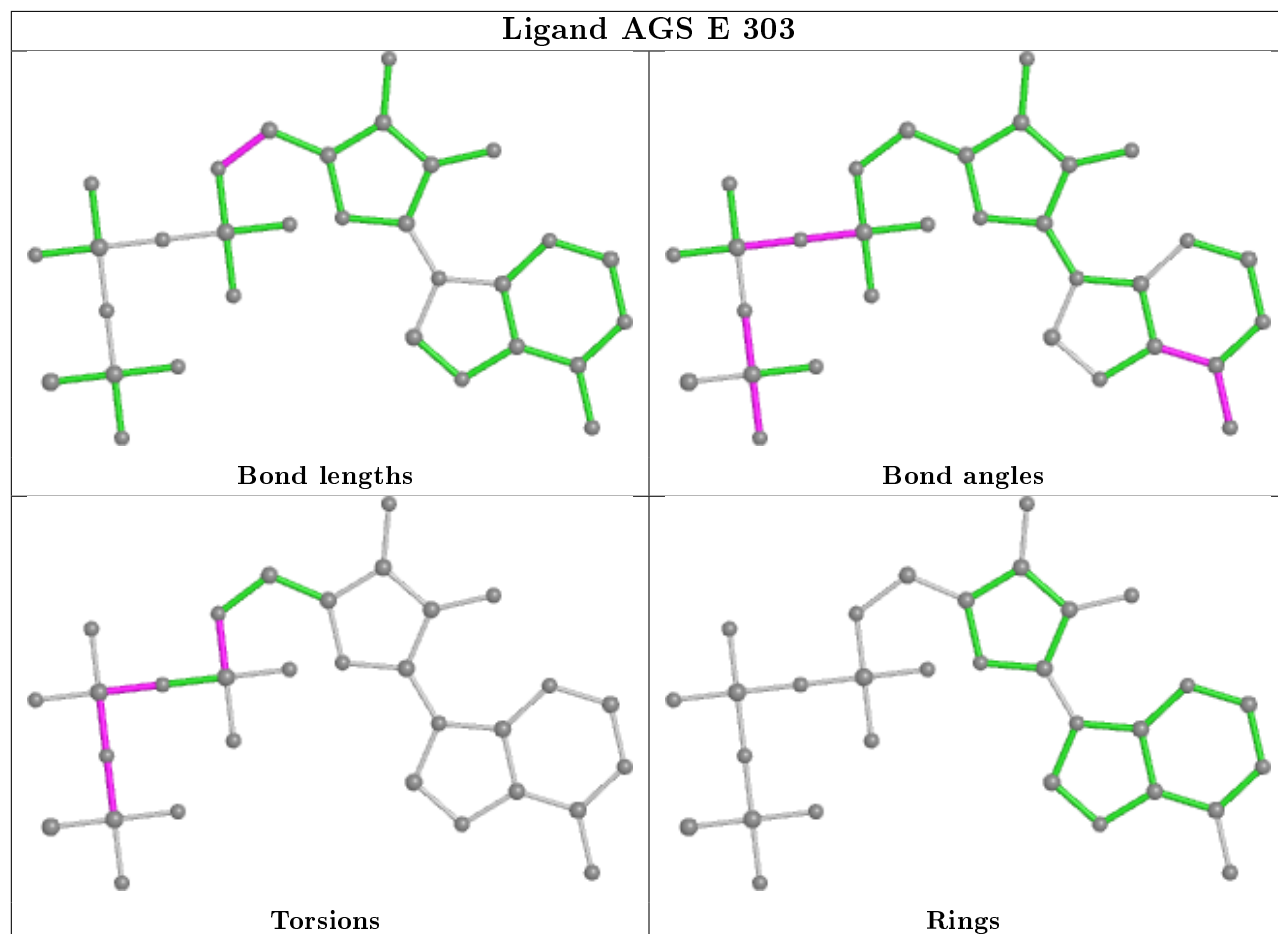
There are no ring outliers.

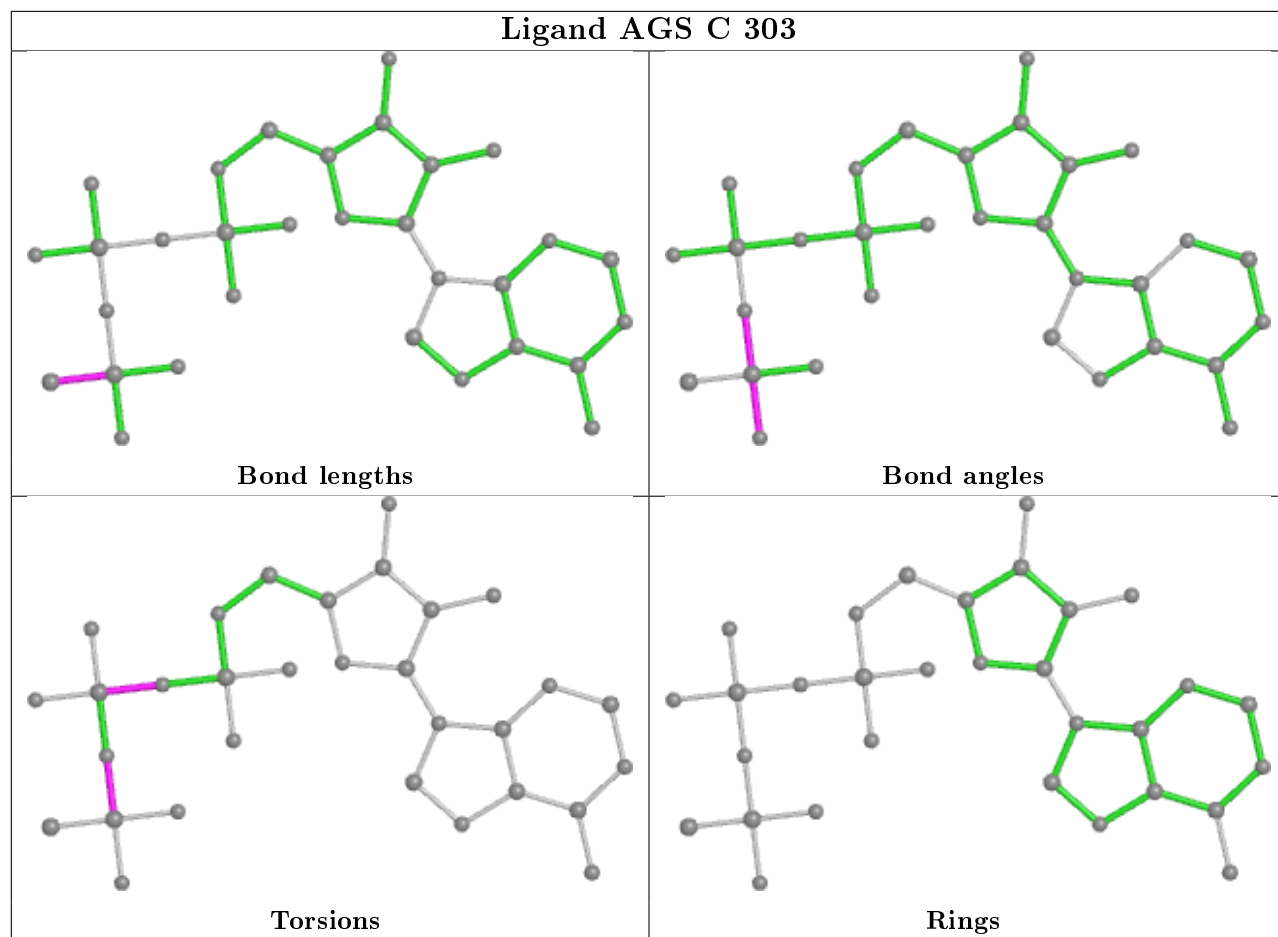
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	303	AGS	2	0

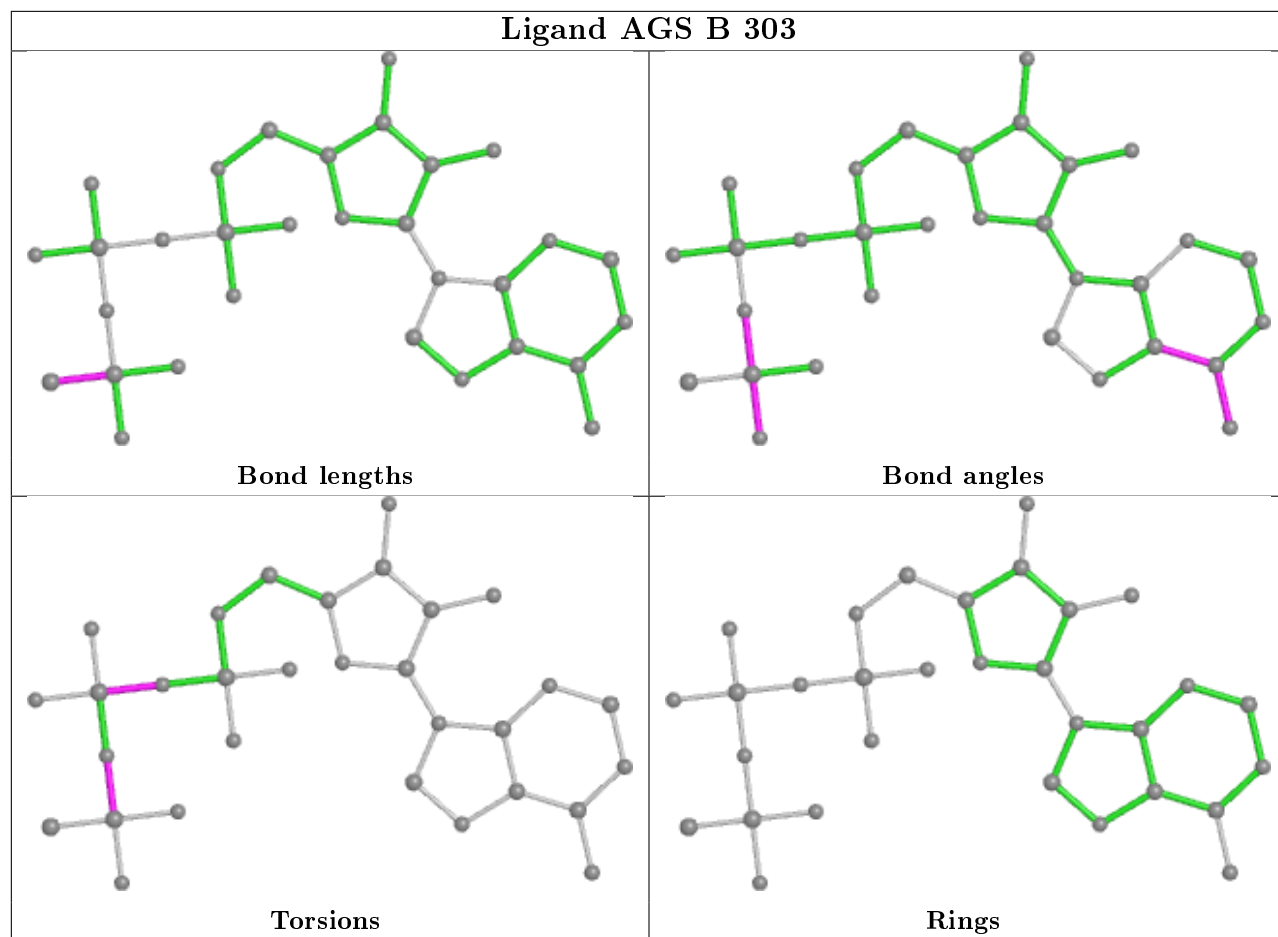
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

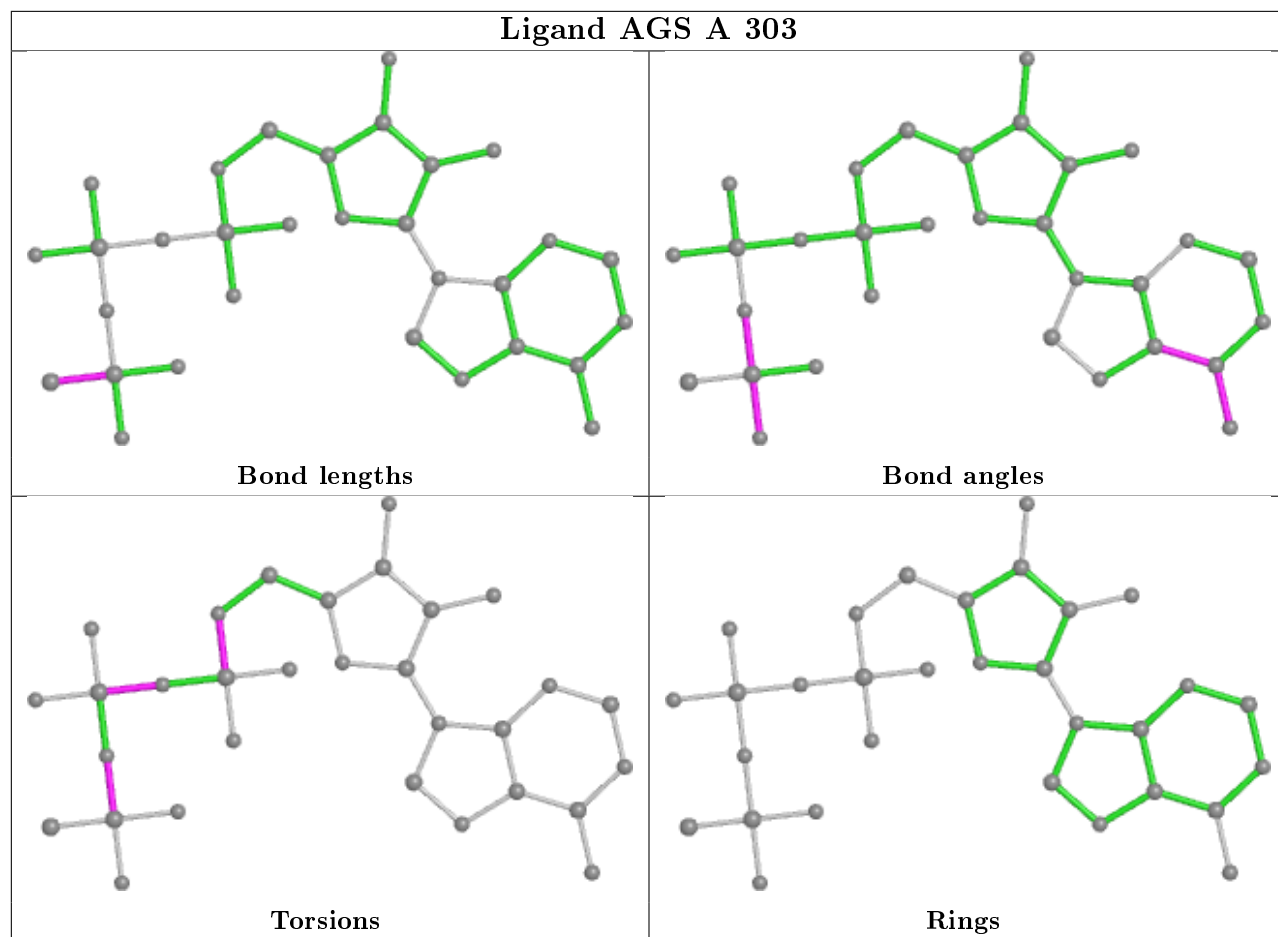
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



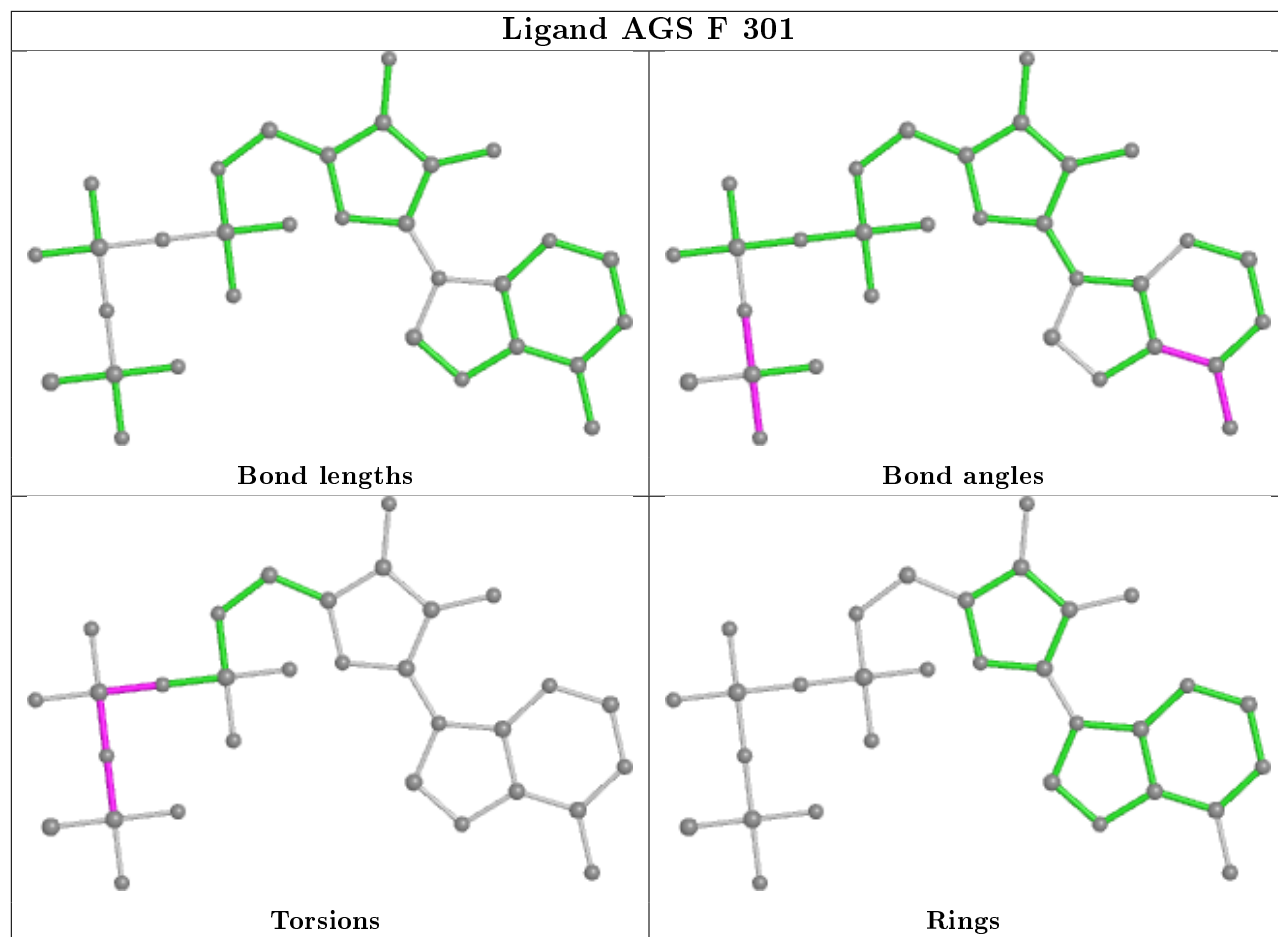


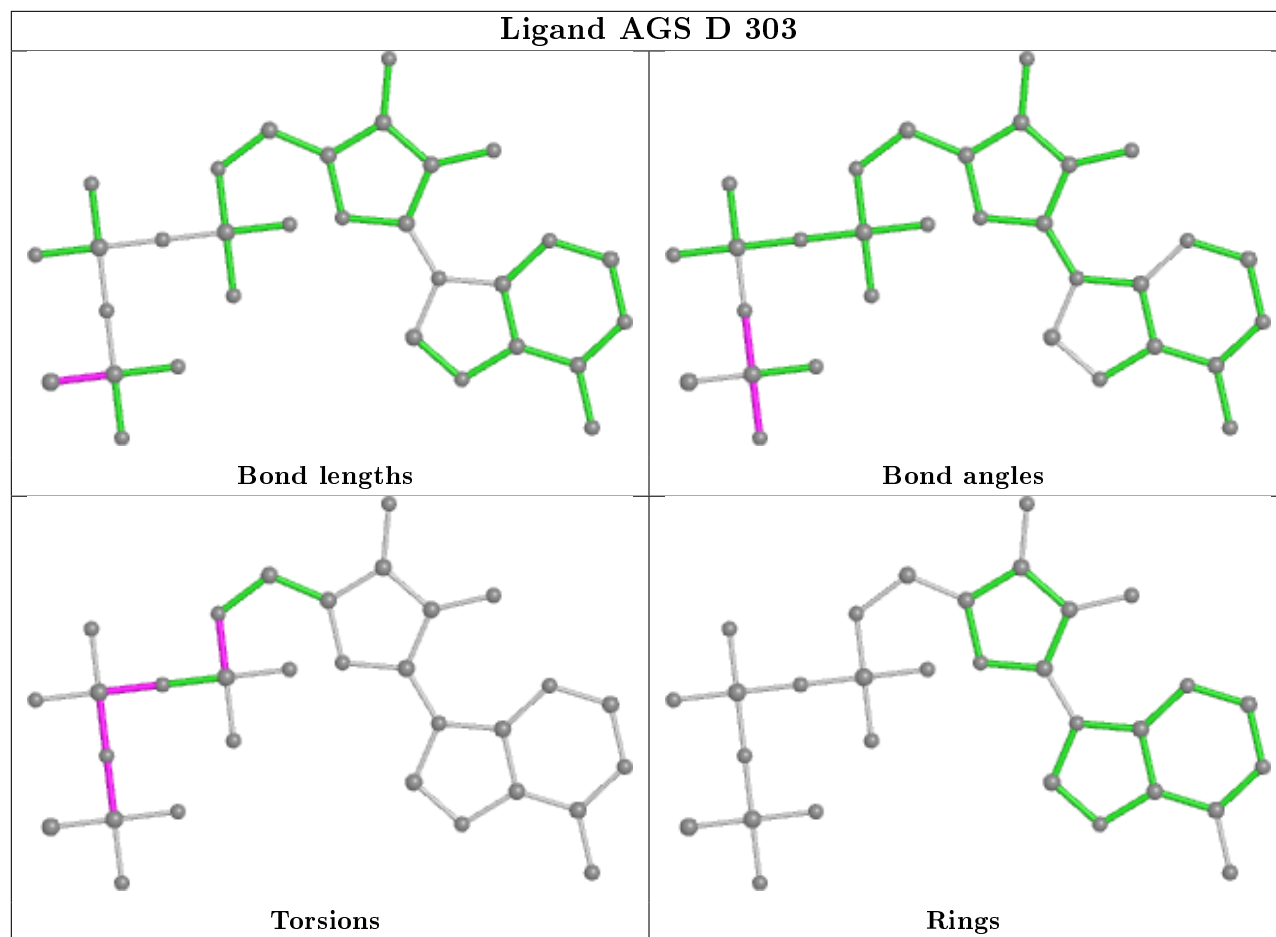
## Ligand AGS B 303





## Ligand AGS F 301





## 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	215/253 (84%)	0.59	33 (15%) <b>2</b> <b>2</b>	17, 35, 68, 94	0
1	B	215/253 (84%)	0.13	10 (4%) 31 30	16, 27, 52, 88	0
1	C	221/253 (87%)	0.11	16 (7%) 15 15	14, 26, 50, 104	0
1	D	217/253 (85%)	0.14	13 (5%) 21 21	13, 25, 52, 90	0
1	E	216/253 (85%)	0.37	22 (10%) 6 6	12, 28, 65, 103	0
1	F	213/253 (84%)	0.42	16 (7%) 14 14	13, 28, 59, 95	0
All	All	1297/1518 (85%)	0.29	110 (8%) 10 10	12, 28, 60, 104	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	120	GLY	9.9
1	F	158	SER	7.0
1	C	120	GLY	6.9
1	E	121	PHE	6.8
1	E	132	TYR	6.7
1	F	123	LEU	6.5
1	F	156	ALA	6.4
1	C	250	GLY	6.1
1	B	248	PRO	5.8
1	A	132	TYR	5.8
1	F	122	ASP	5.0
1	B	112	PRO	5.0
1	E	123	LEU	5.0
1	A	156	ALA	4.5
1	D	122	ASP	4.5
1	A	16	GLN	4.4
1	C	247	PHE	4.4
1	A	159	VAL	4.4
1	F	99	ASP	4.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	138	ARG	4.2
1	C	156	ALA	4.1
1	A	138	ARG	4.1
1	A	162	ARG	4.0
1	D	132	TYR	3.9
1	A	248	PRO	3.9
1	C	113	GLU	3.9
1	E	156	ALA	3.9
1	A	122	ASP	3.8
1	E	158	SER	3.8
1	A	123	LEU	3.6
1	F	111	ASP	3.6
1	B	111	ASP	3.5
1	E	135	GLN	3.5
1	E	159	VAL	3.5
1	E	16	GLN	3.5
1	B	156	ALA	3.4
1	E	249	LEU	3.4
1	A	110	PRO	3.3
1	A	136	LYS	3.2
1	A	95	ALA	3.2
1	F	138	ARG	3.2
1	E	247	PHE	3.2
1	A	99	ASP	3.1
1	C	162	ARG	3.1
1	A	158	SER	3.1
1	A	125	ALA	3.0
1	E	125	ALA	3.0
1	E	157	SER	3.0
1	C	121	PHE	3.0
1	E	248	PRO	3.0
1	A	109	SER	3.0
1	D	156	ALA	3.0
1	F	157	SER	3.0
1	F	110	PRO	3.0
1	E	122	ASP	3.0
1	D	125	ALA	2.9
1	E	128	GLU	2.7
1	D	146[A]	SER	2.7
1	C	157	SER	2.7
1	A	124	SER	2.7
1	B	122	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	15	HIS	2.6
1	A	101	GLY	2.6
1	C	99	ASP	2.6
1	A	204	VAL	2.6
1	C	132	TYR	2.5
1	C	248	PRO	2.5
1	F	159	VAL	2.5
1	D	135	GLN	2.5
1	B	158	SER	2.5
1	A	98	VAL	2.5
1	A	135	GLN	2.5
1	F	126	LEU	2.5
1	C	122	ASP	2.4
1	F	124	SER	2.4
1	F	88	ARG	2.4
1	E	137	TYR	2.4
1	F	137	TYR	2.4
1	D	13	SER	2.3
1	B	123	LEU	2.3
1	E	140	ARG	2.3
1	E	162	ARG	2.3
1	D	99	ASP	2.3
1	A	97	LEU	2.3
1	D	110	PRO	2.2
1	A	111	ASP	2.2
1	C	138	ARG	2.2
1	A	205	VAL	2.2
1	A	157	SER	2.2
1	E	110	PRO	2.2
1	D	138	ARG	2.2
1	A	88	ARG	2.1
1	C	43	LEU	2.1
1	A	17	ALA	2.1
1	A	180	MET	2.1
1	A	242	HIS	2.1
1	D	55	PHE	2.1
1	B	110	PRO	2.1
1	B	157	SER	2.1
1	D	111	ASP	2.0
1	D	157	SER	2.0
1	A	179	VAL	2.0
1	C	112	PRO	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	162	ARG	2.0
1	A	43	LEU	2.0
1	A	127	ILE	2.0
1	C	158	SER	2.0
1	B	17	ALA	2.0
1	E	136	LYS	2.0
1	F	146[A]	SER	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<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
4	AGS	E	303	31/31	0.97	0.09	13,18,26,32	0
4	AGS	F	301	31/31	0.97	0.09	15,20,29,30	0
4	AGS	B	303	31/31	0.98	0.10	15,18,25,26	0
2	MG	C	301	1/1	0.98	0.07	19,19,19,19	0
2	MG	A	301	1/1	0.98	0.06	25,25,25,25	0
4	AGS	C	303	31/31	0.98	0.08	14,18,23,25	0
2	MG	E	301	1/1	0.98	0.04	19,19,19,19	0
4	AGS	A	303	31/31	0.98	0.09	19,24,29,32	0
3	CL	F	303	1/1	0.99	0.04	19,19,19,19	0
2	MG	F	302	1/1	0.99	0.09	20,20,20,20	0
3	CL	A	302	1/1	0.99	0.04	25,25,25,25	0
2	MG	D	301	1/1	0.99	0.09	18,18,18,18	0
2	MG	B	301	1/1	0.99	0.09	17,17,17,17	0
4	AGS	D	303	31/31	0.99	0.09	14,17,24,26	0
3	CL	E	302	1/1	0.99	0.04	22,22,22,22	0
3	CL	B	302	1/1	1.00	0.07	24,24,24,24	0

*Continued on next page...*

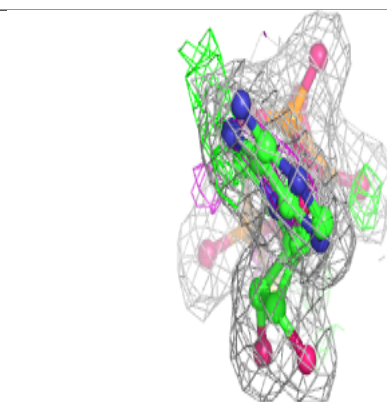
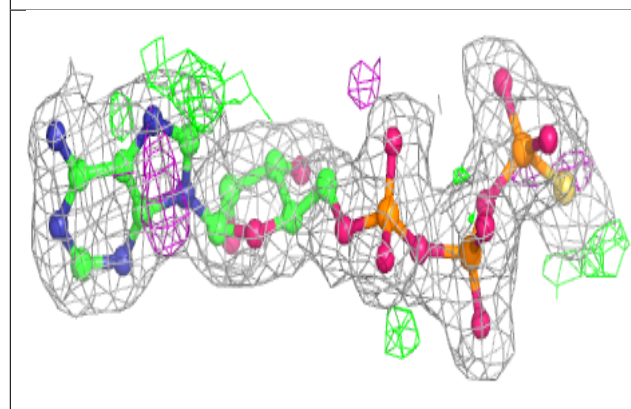
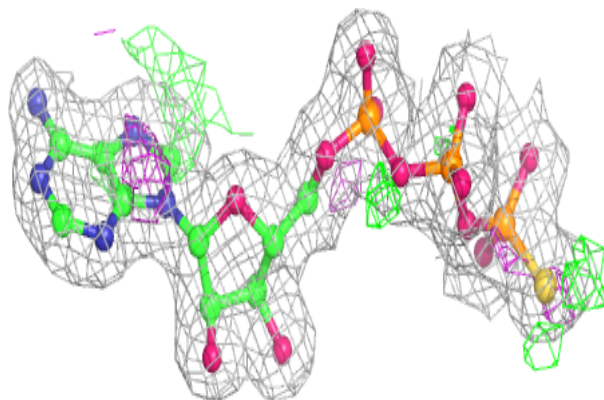
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	D	302	1/1	1.00	0.05	17,17,17,17	0
3	CL	C	302	1/1	1.00	0.03	20,20,20,20	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.

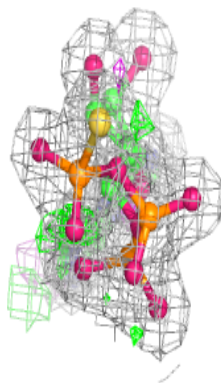
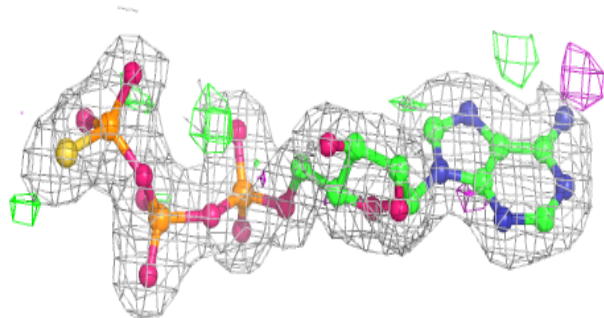
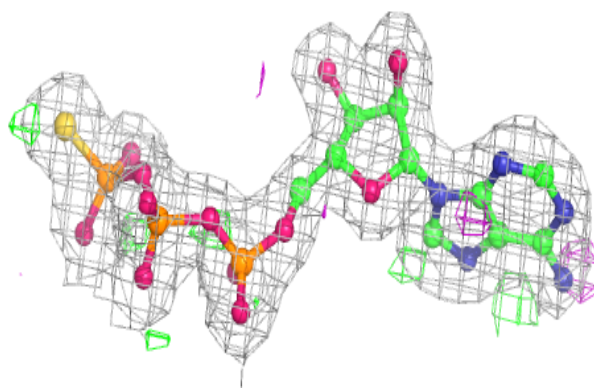
**Electron density around AGS E 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

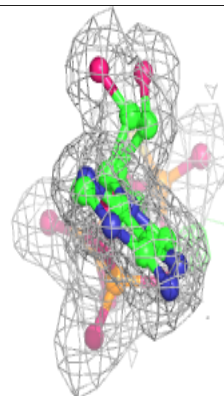
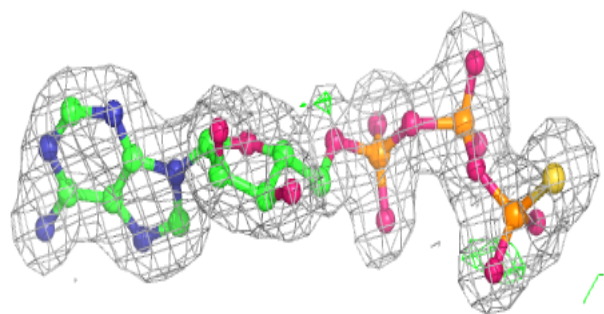
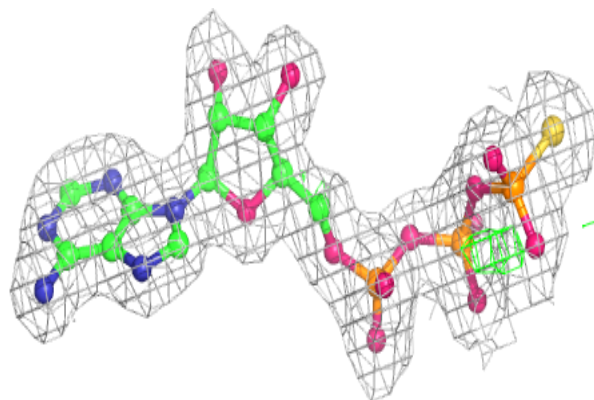


**Electron density around AGS F 301:**

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

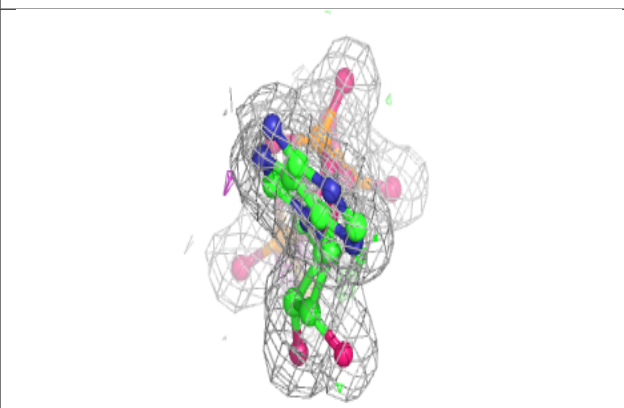
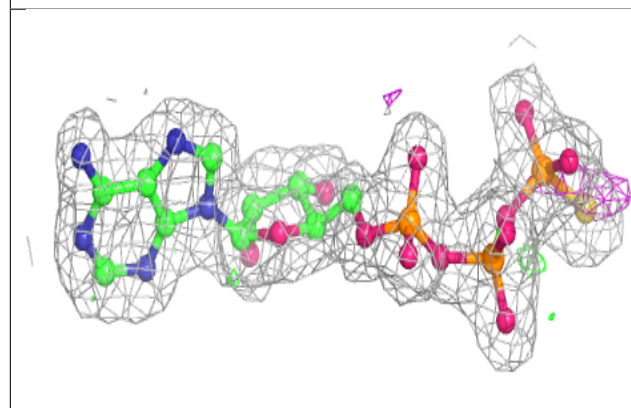
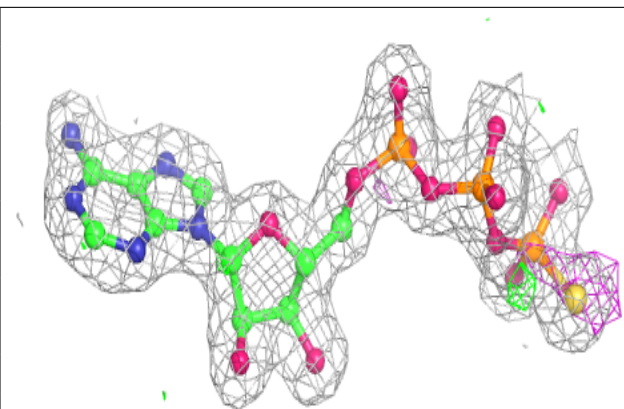
**Electron density around AGS B 303:**

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

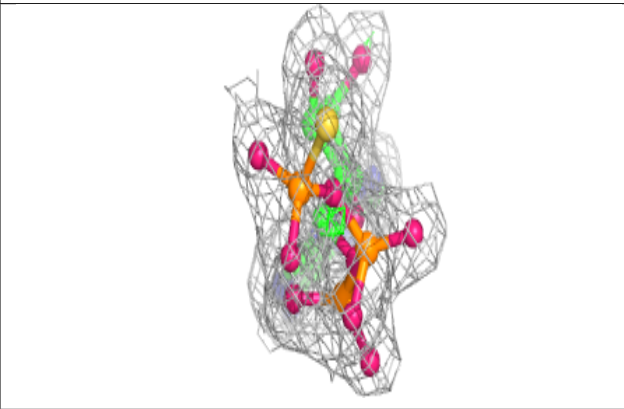
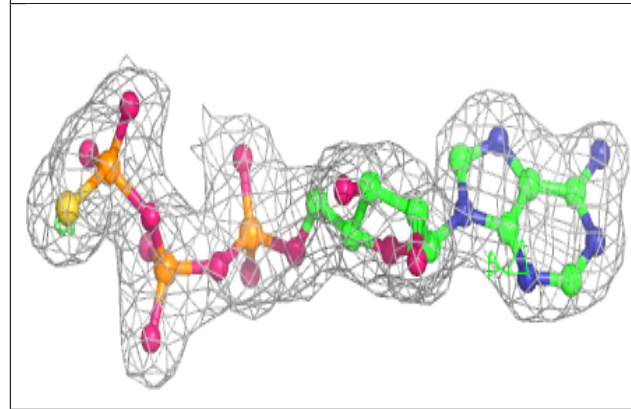
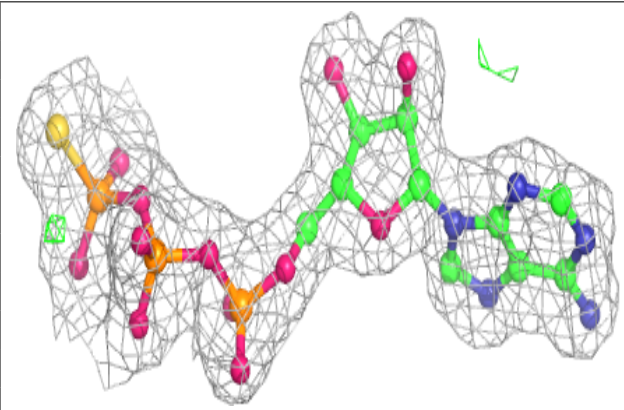


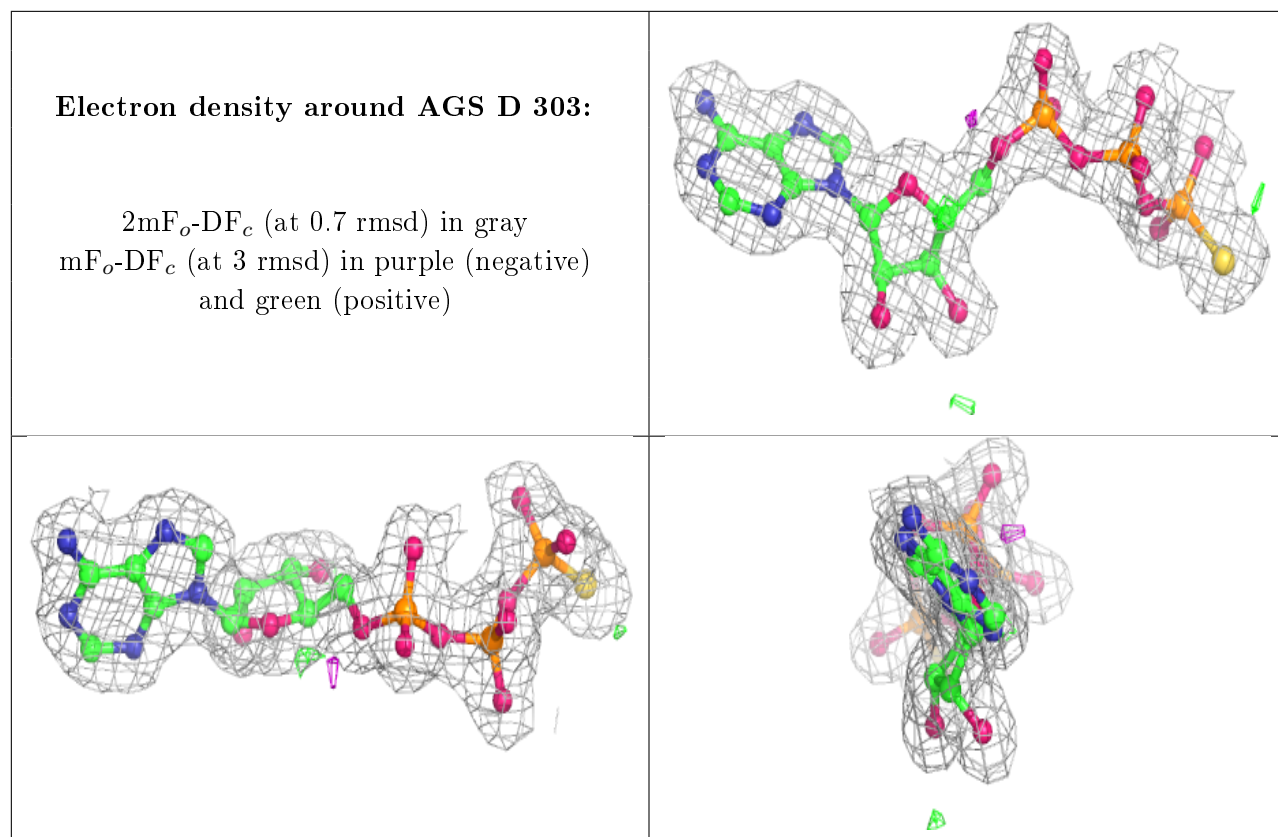
**Electron density around AGS C 303:**

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

**Electron density around AGS 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.