



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2021 – 02:05 PM EST

PDB ID : 7RUU  
Title : Structure of Human ATP:Cobalamin Adenosyltransferase R190C bound to adenosylcobalamin  
Authors : Mascarenhas, R.; Gouda, H.; Koutmos, M.; Banerjee, R.  
Deposited on : 2021-08-18  
Resolution : 1.85 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 : 2.23.2  
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) : 2.23.2

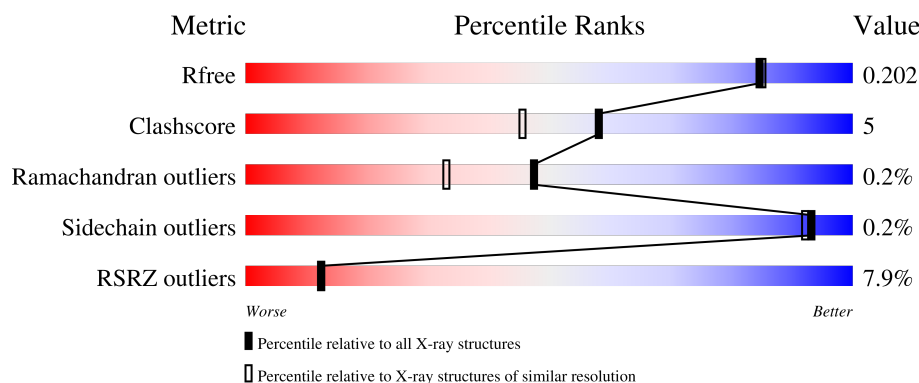
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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 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  $\leq 5\%$ . 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	196	<div> <div>5%</div> <div>73%</div> <div>22%</div> </div>
1	B	196	<div> <div>8%</div> <div>73%</div> <div>24%</div> </div>
1	C	196	<div> <div>6%</div> <div>69%</div> <div>7%</div> <div>24%</div> </div>
1	D	196	<div> <div>5%</div> <div>66%</div> <div>8%</div> <div>26%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5330 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 Corrinoid adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	4	0
			1185	753	196	230	6			
1	B	148	Total	C	N	O	S	0	3	0
			1145	728	190	221	6			
1	C	148	Total	C	N	O	S	0	2	0
			1152	734	190	222	6			
1	D	145	Total	C	N	O	S	0	4	0
			1141	725	188	221	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP Q96EY8
A	190	CYS	ARG	engineered mutation	UNP Q96EY8
B	55	MET	-	initiating methionine	UNP Q96EY8
B	190	CYS	ARG	engineered mutation	UNP Q96EY8
C	55	MET	-	initiating methionine	UNP Q96EY8
C	190	CYS	ARG	engineered mutation	UNP Q96EY8
D	55	MET	-	initiating methionine	UNP Q96EY8
D	190	CYS	ARG	engineered mutation	UNP Q96EY8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

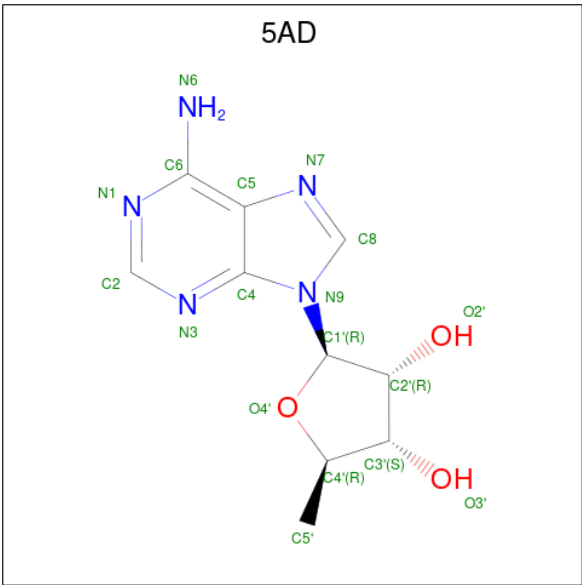


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

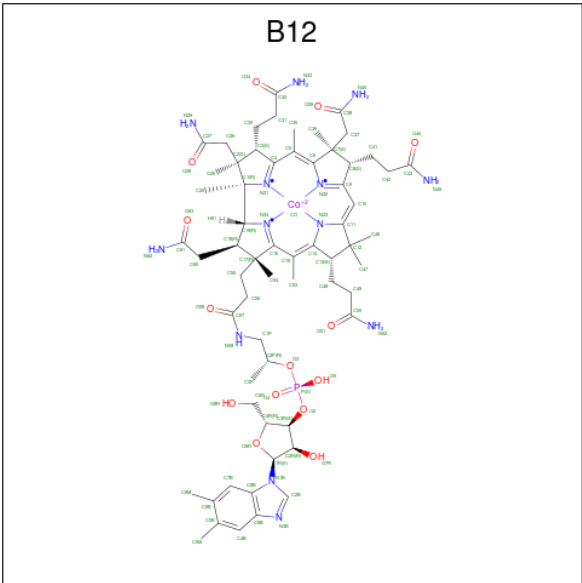
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	C	1	Total K 1 1	0	0

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	10	5	3		
4	B	1	Total	C	N	O	0	0
			18	10	5	3		
4	C	1	Total	C	N	O	0	0
			18	10	5	3		
4	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
5	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
5	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
5	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

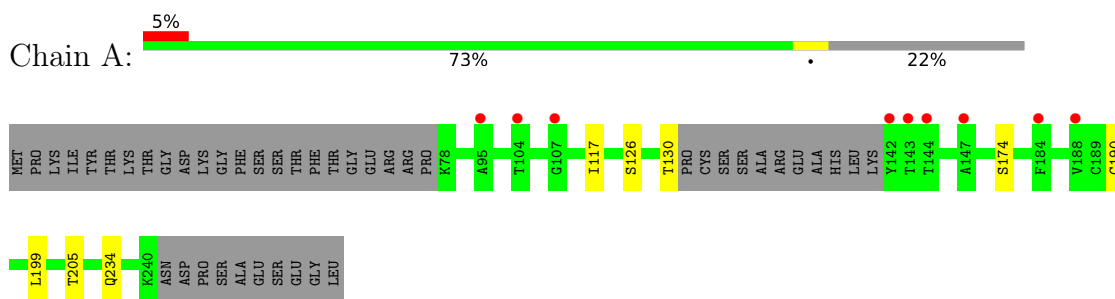
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	63	Total 63	O 63	0	0
6	C	43	Total 43	O 43	0	0
6	D	63	Total 63	O 63	0	0

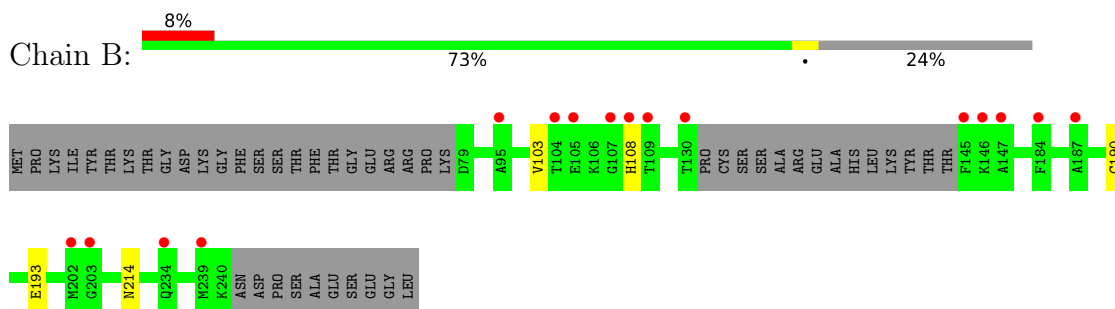
### 3 Residue-property plots [i](#)

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.

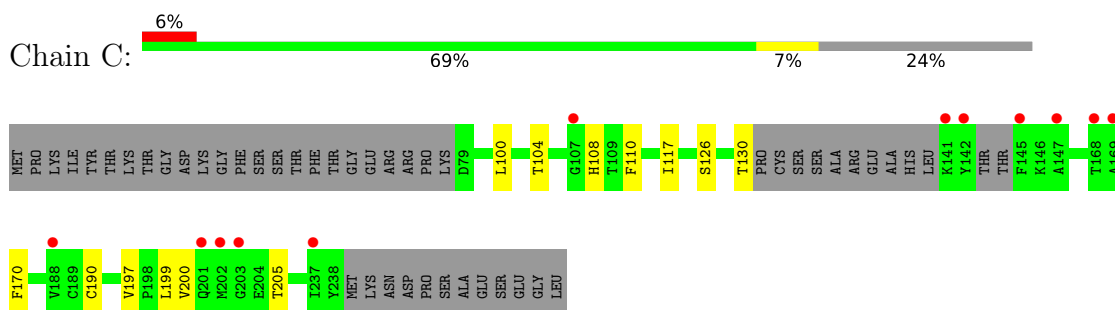
- Molecule 1: Corrinnoid adenosyltransferase



- Molecule 1: Corrinnoid adenosyltransferase

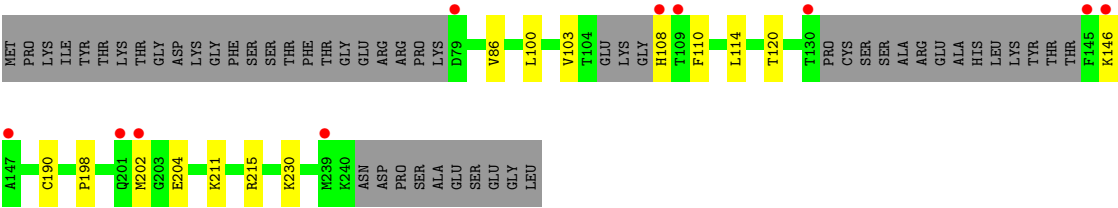


- Molecule 1: Corrinnoid adenosyltransferase



- Molecule 1: Corrinnoid adenosyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.81Å 121.81Å 171.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.16 – 1.85 39.75 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.16-1.85) 99.8 (39.75-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.177 , 0.202 0.178 , 0.202	Depositor DCC
$R_{free}$ test set	4077 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: ACT, K, B12, 5AD

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	0.40	0/1205	0.49	0/1634
1	B	0.38	0/1167	0.48	0/1582
1	C	0.34	0/1171	0.47	0/1584
1	D	0.35	0/1159	0.48	0/1569
All	All	0.37	0/4702	0.48	0/6369

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	1185	0	1153	4	0
1	B	1145	0	1120	3	0
1	C	1152	0	1127	8	0
1	D	1141	0	1120	13	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	8	0	6	1	0
3	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	18	0	10	1	0
4	B	18	0	10	1	0
4	C	18	0	10	2	0
4	D	18	0	10	2	0
5	A	91	0	88	4	0
5	B	91	0	88	5	0
5	C	91	0	88	8	0
5	D	91	0	88	6	0
6	A	79	0	0	1	0
6	B	63	0	0	1	0
6	C	43	0	0	1	0
6	D	63	0	0	2	0
All	All	5330	0	4927	48	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 (48) 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:D:211:LYS:HE2	1:D:215:ARG:NH2	1.92	0.84
1:D:190:CYS:SG	6:D:454:HOH:O	2.46	0.72
1:B:190:CYS:SG	6:B:455:HOH:O	2.49	0.71
5:B:303:B12:H362	5:B:303:B12:H351	1.72	0.71
1:D:103:VAL:HG13	1:D:108:HIS:HB2	1.75	0.69
1:A:190:CYS:SG	6:A:468:HOH:O	2.52	0.68
1:D:211:LYS:HE2	1:D:215:ARG:CZ	2.25	0.67
5:D:303:B12:H351	5:D:303:B12:H362	1.79	0.65
1:A:126:SER:O	1:A:130:THR:HG23	2.02	0.60
1:C:117:ILE:HA	2:C:301:ACT:H3	1.85	0.59
4:D:302:5AD:H4'	5:D:303:B12:C16	2.32	0.58
1:B:103:VAL:HG13	1:B:108:HIS:HB2	1.86	0.58
5:A:305:B12:H362	5:A:305:B12:H351	1.86	0.58
4:C:303:5AD:H4'	5:C:304:B12:N24	2.21	0.55
1:C:126:SER:O	1:C:130:THR:HG23	2.07	0.54
5:D:303:B12:H3	5:D:303:B12:N29	2.22	0.54
5:A:305:B12:H601	5:A:305:B12:H252	1.91	0.53
1:D:198:PRO:O	1:D:202:MET:HG2	2.09	0.51
4:D:302:5AD:H4'	5:D:303:B12:N24	2.26	0.51
5:C:304:B12:H531	5:C:304:B12:H543	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:303:5AD:H4'	5:C:304:B12:C16	2.42	0.50
1:A:199:LEU:HB3	1:A:205:THR:HG23	1.95	0.48
1:C:197:VAL:O	1:C:200:VAL:HG22	2.14	0.48
5:C:304:B12:H362	5:C:304:B12:H351	1.96	0.48
1:B:193:GLU:OE2	1:B:214:ASN:HB2	2.13	0.48
1:C:170:PHE:CZ	5:C:304:B12:H202	2.50	0.47
1:C:190:CYS:SG	6:C:440:HOH:O	2.60	0.47
1:C:100:LEU:O	1:C:104:THR:HG23	2.15	0.47
1:C:199:LEU:HB3	1:C:205:THR:HG23	1.97	0.47
1:D:110:PHE:HA	6:D:443:HOH:O	2.15	0.46
1:A:117:ILE:HA	2:A:301:ACT:H3	1.98	0.45
4:A:304:5AD:H4'	5:A:305:B12:C16	2.48	0.44
1:D:202:MET:SD	1:D:204:GLU:HG3	2.57	0.44
4:B:302:5AD:H4'	5:B:303:B12:C16	2.47	0.44
5:B:303:B12:H601	5:B:303:B12:H252	2.00	0.44
5:C:304:B12:H601	5:C:304:B12:H252	1.99	0.44
5:D:303:B12:H552	5:D:303:B12:H531	1.99	0.43
1:D:230:LYS:HA	1:D:230:LYS:HD2	1.78	0.43
1:D:120:THR:HG1	2:D:301:ACT:H1	1.84	0.42
1:C:108:HIS:HB3	1:C:110:PHE:CE2	2.54	0.42
5:C:304:B12:H13	1:D:86:VAL:CG1	2.50	0.41
5:A:305:B12:H552	5:A:305:B12:H531	2.02	0.41
1:D:146:LYS:N	1:D:146:LYS:HE2	2.36	0.41
5:B:303:B12:H262	5:B:303:B12:H91	1.88	0.41
5:C:304:B12:H13	1:D:86:VAL:HG11	2.01	0.41
5:D:303:B12:H262	5:D:303:B12:H91	1.86	0.40
5:B:303:B12:H552	5:B:303:B12:H531	2.03	0.40
1:D:100:LEU:HD13	1:D:114:LEU:HB2	2.03	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	152/196 (78%)	149 (98%)	2 (1%)	1 (1%)	22	9
1	B	147/196 (75%)	145 (99%)	2 (1%)	0	100	100
1	C	144/196 (74%)	142 (99%)	2 (1%)	0	100	100
1	D	143/196 (73%)	139 (97%)	4 (3%)	0	100	100
All	All	586/784 (75%)	575 (98%)	10 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	SER

### 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	124/164 (76%)	123 (99%)	1 (1%)	81	76
1	B	120/164 (73%)	120 (100%)	0	100	100
1	C	121/164 (74%)	121 (100%)	0	100	100
1	D	122/164 (74%)	122 (100%)	0	100	100
All	All	487/656 (74%)	486 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	GLN

Sometimes 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 [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](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	B12	B	303	-	80,101,101	1.05	3 (3%)	101,166,166	1.64	16 (15%)
5	B12	D	303	-	80,101,101	0.98	2 (2%)	101,166,166	1.68	17 (16%)
2	ACT	A	301	-	1,3,3	1.71	0	0,3,3	-	-
2	ACT	D	304	-	1,3,3	6.93	1 (100%)	0,3,3	-	-
4	5AD	B	302	-	17,20,20	1.62	4 (23%)	15,30,30	1.87	4 (26%)
5	B12	C	304	-	80,101,101	1.01	4 (5%)	101,166,166	1.68	15 (14%)
5	B12	A	305	-	80,101,101	0.99	3 (3%)	101,166,166	1.64	16 (15%)
2	ACT	D	301	-	1,3,3	6.60	1 (100%)	0,3,3	-	-
4	5AD	C	303	-	17,20,20	1.80	5 (29%)	15,30,30	1.80	4 (26%)
4	5AD	D	302	-	17,20,20	1.89	6 (35%)	15,30,30	1.73	3 (20%)
4	5AD	A	304	-	17,20,20	1.87	4 (23%)	15,30,30	1.83	4 (26%)
2	ACT	C	301	-	1,3,3	3.40	1 (100%)	0,3,3	-	-
2	ACT	B	301	-	1,3,3	6.94	1 (100%)	0,3,3	-	-

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
5	B12	B	303	-	-	3/51/223/223	0/3/11/11
5	B12	D	303	-	-	4/51/223/223	0/3/11/11
4	5AD	B	302	-	-	0/0/20/20	0/3/3/3
5	B12	A	305	-	-	3/51/223/223	0/3/11/11
4	5AD	C	303	-	-	0/0/20/20	0/3/3/3
4	5AD	D	302	-	-	0/0/20/20	0/3/3/3
4	5AD	A	304	-	-	0/0/20/20	0/3/3/3
5	B12	C	304	-	-	4/51/223/223	0/3/11/11

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ACT	CH3-C	6.94	1.57	1.48
2	D	304	ACT	CH3-C	6.93	1.57	1.48
2	D	301	ACT	CH3-C	6.60	1.57	1.48
4	A	304	5AD	C2'-C1'	4.39	1.60	1.53
4	C	303	5AD	O2'-C2'	-3.41	1.35	1.43
2	C	301	ACT	CH3-C	3.40	1.53	1.48
4	D	302	5AD	C2-N3	3.33	1.37	1.32
4	D	302	5AD	O2'-C2'	-3.32	1.35	1.43
4	A	304	5AD	O2'-C2'	-3.26	1.35	1.43
4	B	302	5AD	O2'-C2'	-3.25	1.35	1.43
4	C	303	5AD	O3'-C3'	-3.16	1.35	1.43
4	C	303	5AD	O4'-C1'	3.09	1.45	1.41
4	D	302	5AD	C5'-C4'	2.93	1.58	1.51
4	B	302	5AD	O3'-C3'	-2.72	1.36	1.43
4	B	302	5AD	O4'-C1'	2.69	1.44	1.41
4	D	302	5AD	O3'-C3'	-2.69	1.36	1.43
4	A	304	5AD	O3'-C3'	-2.68	1.36	1.43
4	B	302	5AD	C2'-C1'	2.68	1.57	1.53
4	A	304	5AD	O4'-C1'	2.67	1.44	1.41
5	D	303	B12	C35-C5	2.61	1.57	1.52
5	C	304	B12	C54-C17	2.55	1.59	1.55
4	D	302	5AD	O4'-C1'	2.54	1.44	1.41
4	C	303	5AD	C2-N3	2.40	1.36	1.32
5	A	305	B12	C54-C17	2.37	1.59	1.55
5	B	303	B12	C35-C5	2.34	1.56	1.52
4	C	303	5AD	C2'-C1'	2.31	1.57	1.53
4	D	302	5AD	C2'-C1'	2.28	1.57	1.53
5	A	305	B12	C35-C5	2.25	1.56	1.52
5	B	303	B12	C6B-C5B	2.22	1.46	1.40
5	C	304	B12	C35-C5	2.16	1.56	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	B12	C54-C17	2.15	1.59	1.55
5	B	303	B12	C11-C10	-2.13	1.37	1.40
5	C	304	B12	C6B-C5B	2.10	1.46	1.40
5	C	304	B12	CO-N23	-2.02	1.84	1.94
5	A	305	B12	C55-C17	-2.02	1.50	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	304	B12	C54-C17-C18	-5.57	104.77	112.98
5	C	304	B12	C16-C15-C14	-5.53	115.64	124.27
5	B	303	B12	C16-C15-C14	-5.36	115.91	124.27
5	A	305	B12	C16-C15-C14	-5.33	115.96	124.27
5	D	303	B12	C16-C15-C14	-5.30	116.00	124.27
5	B	303	B12	C7B-C8B-C9B	5.30	125.79	120.54
5	C	304	B12	C7B-C8B-C9B	5.08	125.56	120.54
5	D	303	B12	C7B-C8B-C9B	4.98	125.47	120.54
5	A	305	B12	C7B-C8B-C9B	4.90	125.39	120.54
5	A	305	B12	C2P-C1P-N59	-4.84	105.80	112.93
5	D	303	B12	C56-C55-C17	-4.84	106.14	115.50
5	B	303	B12	C56-C55-C17	-4.75	106.32	115.50
5	D	303	B12	C54-C17-C18	-4.70	106.04	112.98
5	C	304	B12	C2P-C1P-N59	-4.50	106.30	112.93
5	A	305	B12	C56-C55-C17	-4.28	107.22	115.50
5	A	305	B12	C54-C17-C18	-3.68	107.55	112.98
4	C	303	5AD	N3-C2-N1	3.68	134.42	128.68
5	D	303	B12	C2P-C1P-N59	-3.63	107.58	112.93
5	C	304	B12	C55-C17-C16	3.58	121.85	109.92
4	B	302	5AD	N3-C2-N1	3.57	134.26	128.68
5	C	304	B12	C1P-N59-C57	-3.56	114.94	122.69
5	B	303	B12	C54-C17-C18	-3.52	107.79	112.98
4	A	304	5AD	N3-C2-N1	3.52	134.17	128.68
5	D	303	B12	C55-C17-C16	3.51	121.61	109.92
5	C	304	B12	C13-C14-C15	-3.51	118.95	131.68
5	A	305	B12	C55-C17-C16	3.49	121.56	109.92
4	B	302	5AD	C5'-C4'-C3'	-3.46	112.06	115.70
4	D	302	5AD	N3-C2-N1	3.44	134.06	128.68
5	B	303	B12	C2P-C1P-N59	-3.33	108.03	112.93
4	B	302	5AD	C4-C5-N7	3.28	112.82	109.40
5	D	303	B12	C13-C14-C15	-3.26	119.86	131.68
4	A	304	5AD	C5'-C4'-C3'	-3.22	112.32	115.70
5	B	303	B12	C5B-C4B-C9B	-3.20	116.69	121.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	5AD	C4-C5-N7	3.18	112.72	109.40
5	A	305	B12	C1P-N59-C57	-3.17	115.78	122.69
5	A	305	B12	C5B-C4B-C9B	-3.17	116.73	121.22
4	A	304	5AD	C4-C5-N7	3.14	112.67	109.40
4	C	303	5AD	C4-C5-N7	3.10	112.63	109.40
5	B	303	B12	C1P-N59-C57	-3.10	115.94	122.69
5	A	305	B12	C13-C14-C15	-3.08	120.49	131.68
5	B	303	B12	C55-C17-C16	3.05	120.10	109.92
5	D	303	B12	C5B-C4B-C9B	-3.05	116.90	121.22
5	B	303	B12	C13-C14-C15	-3.03	120.69	131.68
5	B	303	B12	C6-C5-C4	-2.99	119.61	124.27
5	C	304	B12	C5B-C4B-C9B	-2.97	117.01	121.22
4	C	303	5AD	C5'-C4'-C3'	-2.96	112.59	115.70
5	C	304	B12	C1-C19-C18	-2.91	117.12	121.93
4	D	302	5AD	C2-N1-C6	-2.83	113.91	118.75
5	B	303	B12	C55-C17-C18	2.80	116.55	111.14
5	A	305	B12	C1-C19-C18	-2.68	117.50	121.93
4	C	303	5AD	C2-N1-C6	-2.66	114.20	118.75
5	D	303	B12	C1P-N59-C57	-2.66	116.90	122.69
5	C	304	B12	C55-C17-C18	2.66	116.27	111.14
5	D	303	B12	C55-C17-C18	2.66	116.27	111.14
5	A	305	B12	C6-C5-C4	-2.60	120.21	124.27
5	C	304	B12	C5M-C5B-C6B	-2.58	115.45	120.74
4	B	302	5AD	C2-N1-C6	-2.58	114.34	118.75
5	B	303	B12	C5M-C5B-C6B	-2.57	115.48	120.74
5	D	303	B12	C36-C7-C37	2.56	115.19	110.83
4	A	304	5AD	C2-N1-C6	-2.53	114.42	118.75
5	D	303	B12	C6-C5-C4	-2.51	120.35	124.27
5	C	304	B12	C56-C55-C17	-2.43	110.79	115.50
5	B	303	B12	C36-C7-C37	2.39	114.91	110.83
5	D	303	B12	C4B-C5B-C6B	2.33	123.84	119.91
5	D	303	B12	C3-C4-C5	-2.32	123.25	131.68
5	A	305	B12	C3-C4-C5	-2.31	123.31	131.68
5	B	303	B12	C3-C4-C5	-2.30	123.33	131.68
5	B	303	B12	C4B-C5B-C6B	2.27	123.73	119.91
5	A	305	B12	C2R-C3R-C4R	-2.23	99.26	103.22
5	B	303	B12	O28-C27-N29	-2.20	116.50	122.50
5	C	304	B12	O28-C27-N29	-2.19	116.52	122.50
5	C	304	B12	C3-C4-C5	-2.15	123.88	131.68
5	A	305	B12	O28-C27-N29	-2.15	116.64	122.50
5	D	303	B12	O7R-C2R-C3R	2.13	117.22	111.17
5	A	305	B12	O6R-C1R-C2R	-2.13	103.81	106.93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	B12	O28-C27-C26	2.07	128.53	121.99
5	D	303	B12	O44-C43-N45	-2.07	116.86	122.50
5	D	303	B12	O2-C3R-C2R	2.07	119.17	111.68
5	C	304	B12	C36-C7-C37	2.06	114.35	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	B12	C1P-C2P-O3-P
5	A	305	B12	C3P-C2P-O3-P
5	B	303	B12	C14-C13-C48-C49
5	B	303	B12	C1P-C2P-O3-P
5	B	303	B12	C3P-C2P-O3-P
5	C	304	B12	C1P-C2P-O3-P
5	C	304	B12	C3P-C2P-O3-P
5	D	303	B12	C1P-C2P-O3-P
5	D	303	B12	C3P-C2P-O3-P
5	D	303	B12	C3-C30-C31-C32
5	A	305	B12	C14-C13-C48-C49
5	C	304	B12	C14-C13-C48-C49
5	D	303	B12	C14-C13-C48-C49
5	C	304	B12	C3-C30-C31-C32

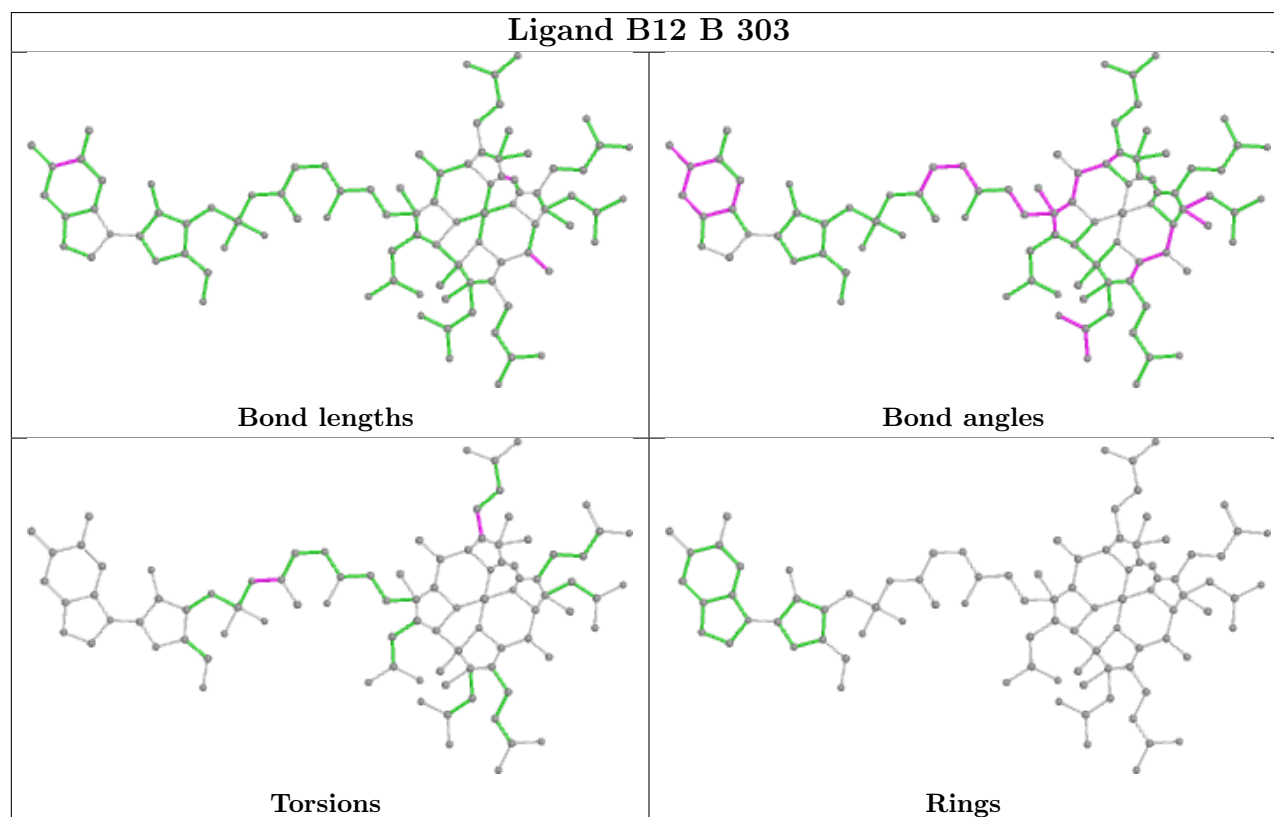
There are no ring outliers.

11 monomers are involved in 26 short contacts:

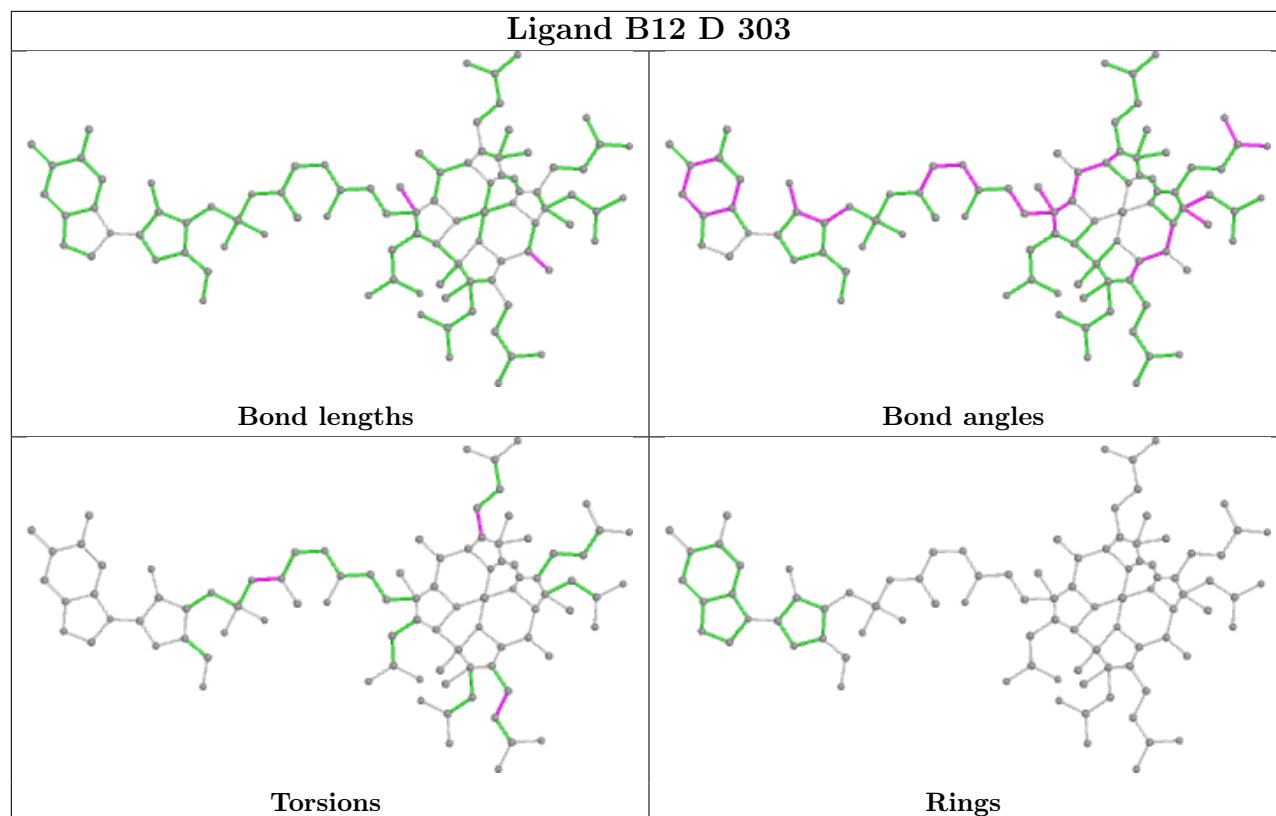
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	303	B12	5	0
5	D	303	B12	6	0
2	A	301	ACT	1	0
4	B	302	5AD	1	0
5	C	304	B12	8	0
5	A	305	B12	4	0
2	D	301	ACT	1	0
4	C	303	5AD	2	0
4	D	302	5AD	2	0
4	A	304	5AD	1	0
2	C	301	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

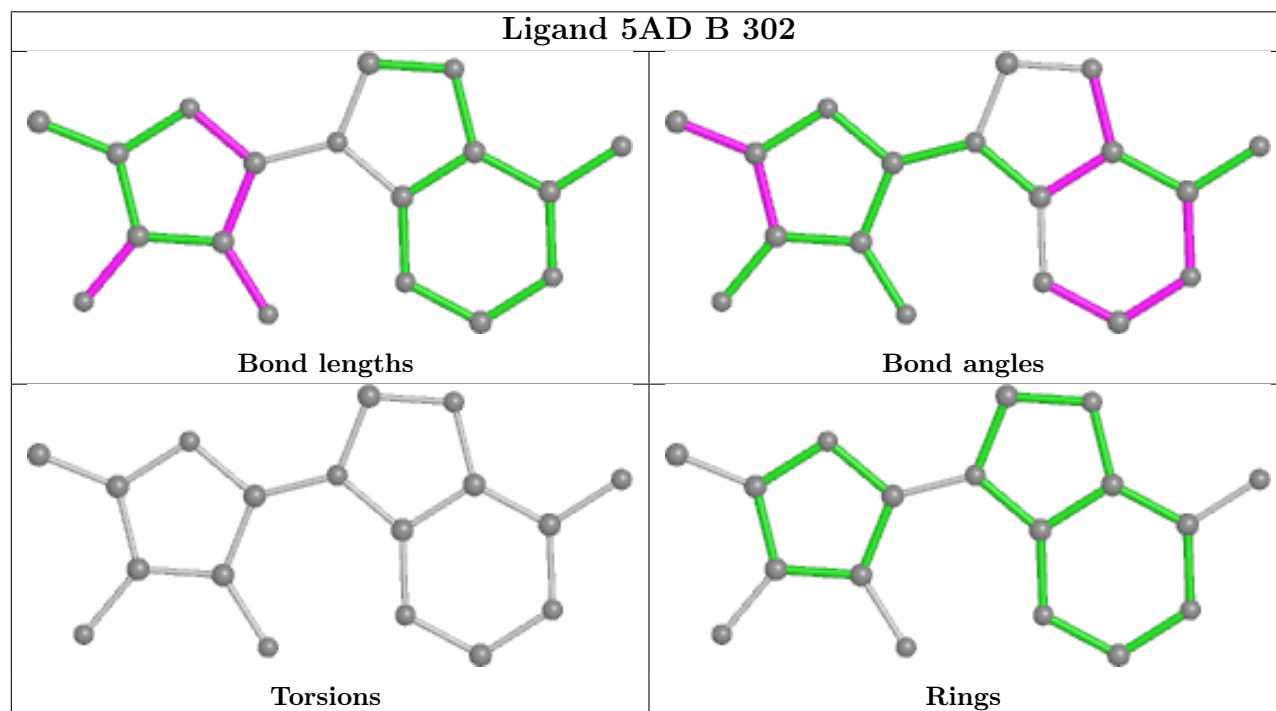
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

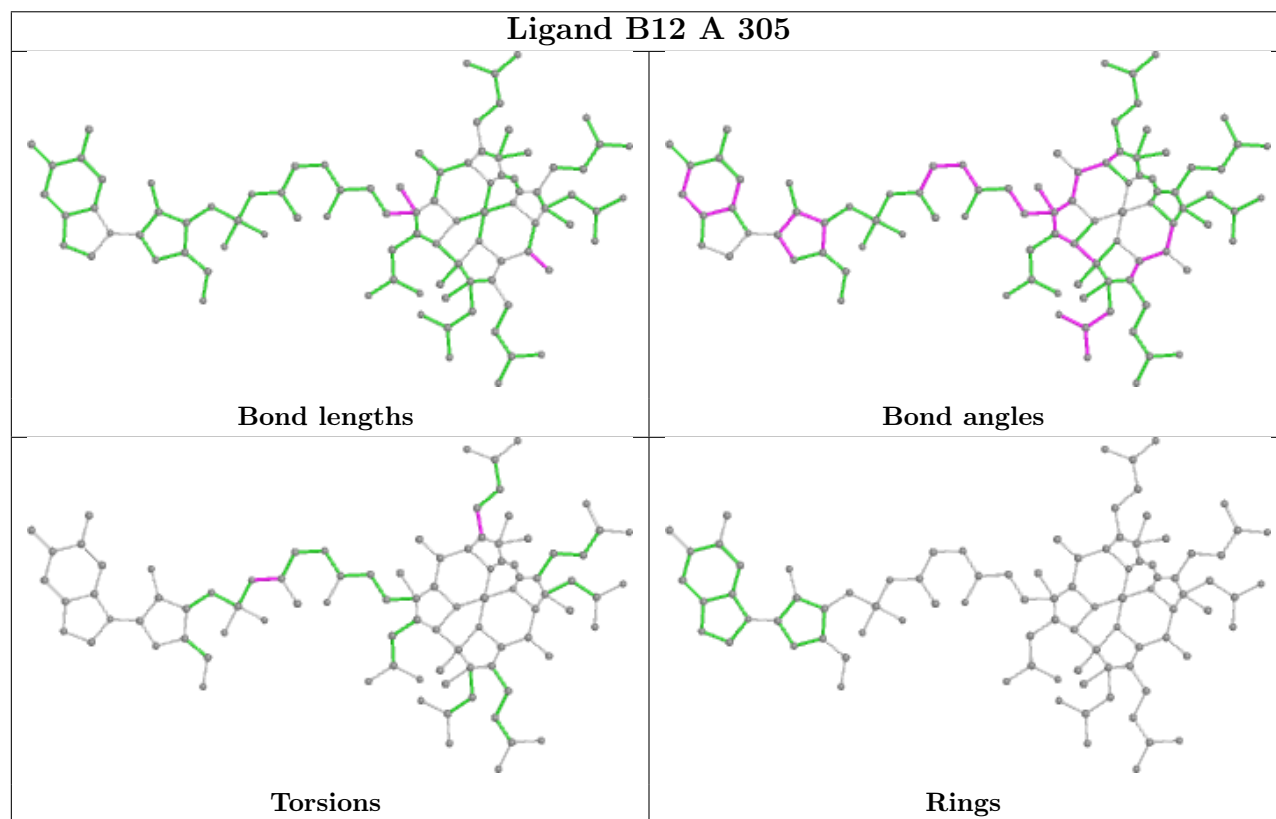
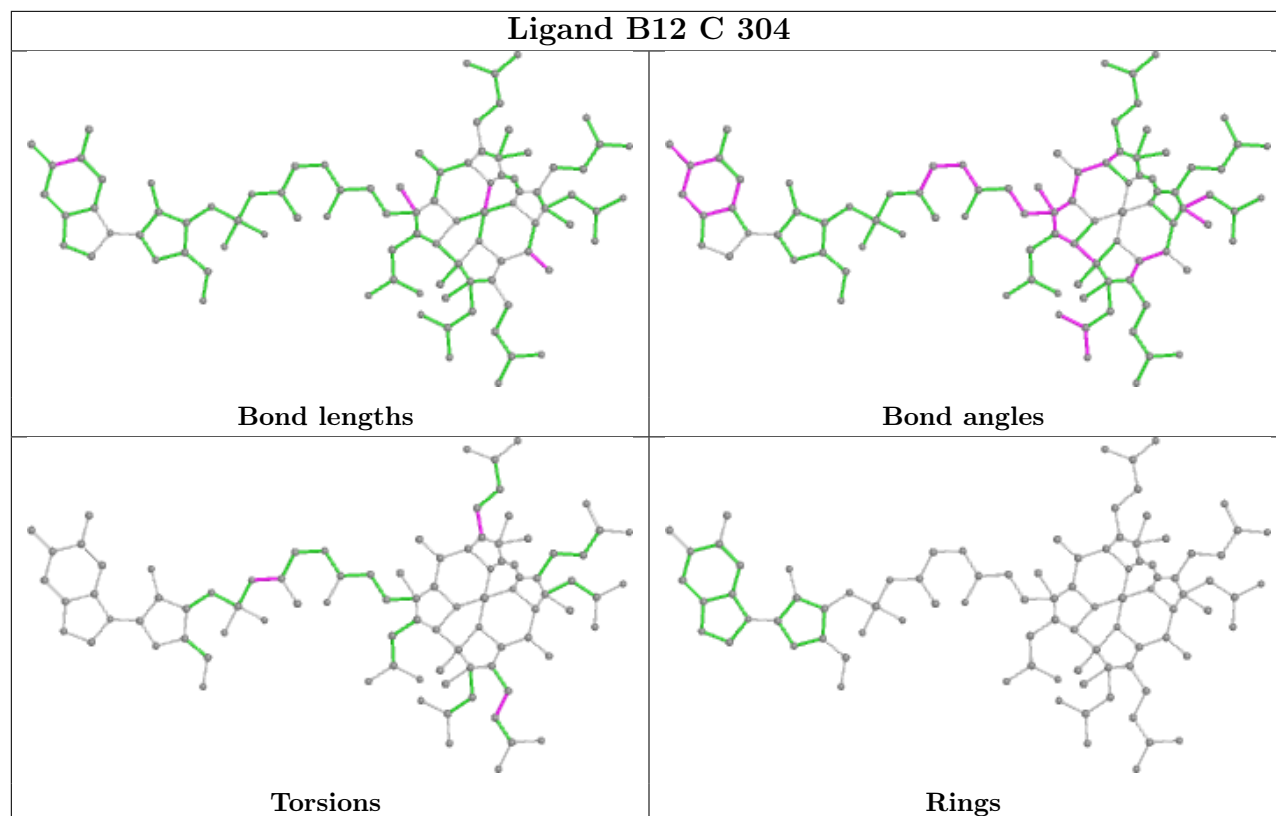


## Ligand B12 D 303

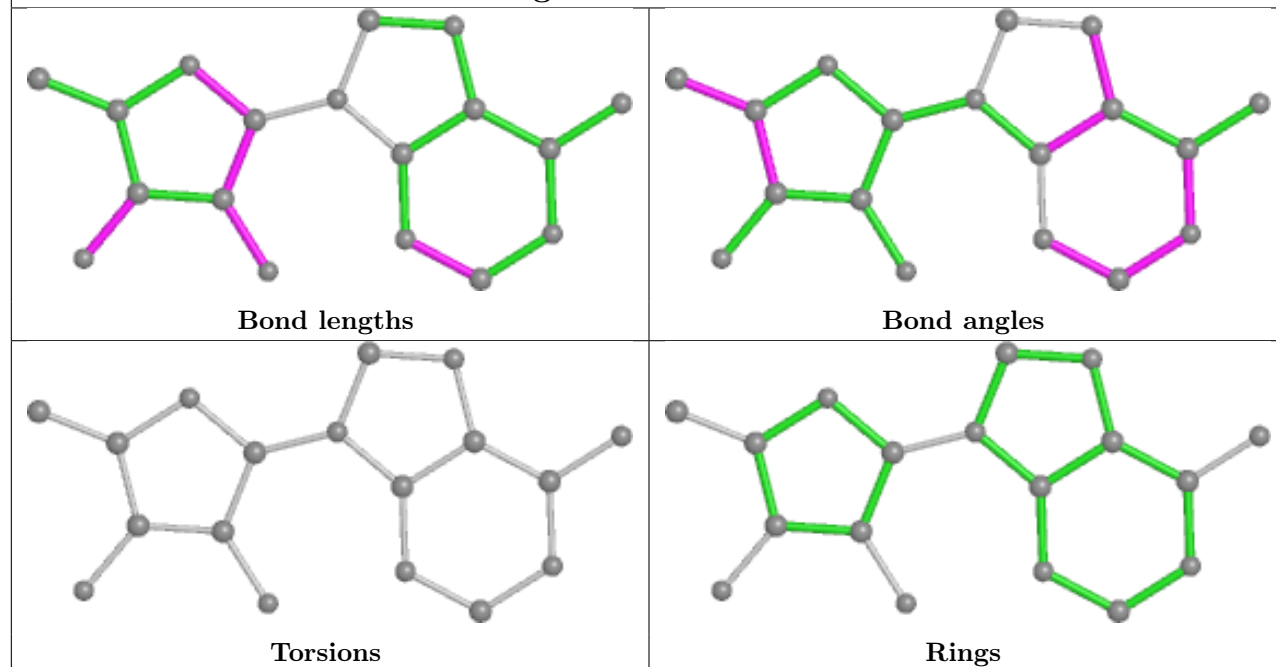


## Ligand 5AD B 302

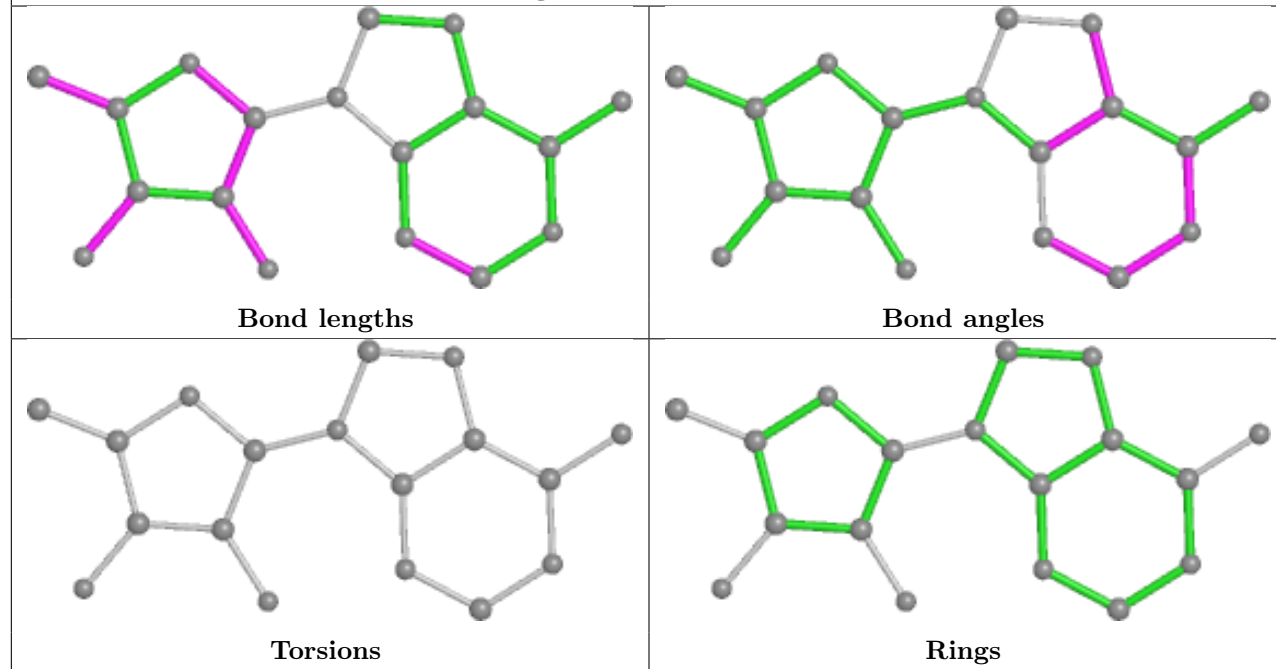


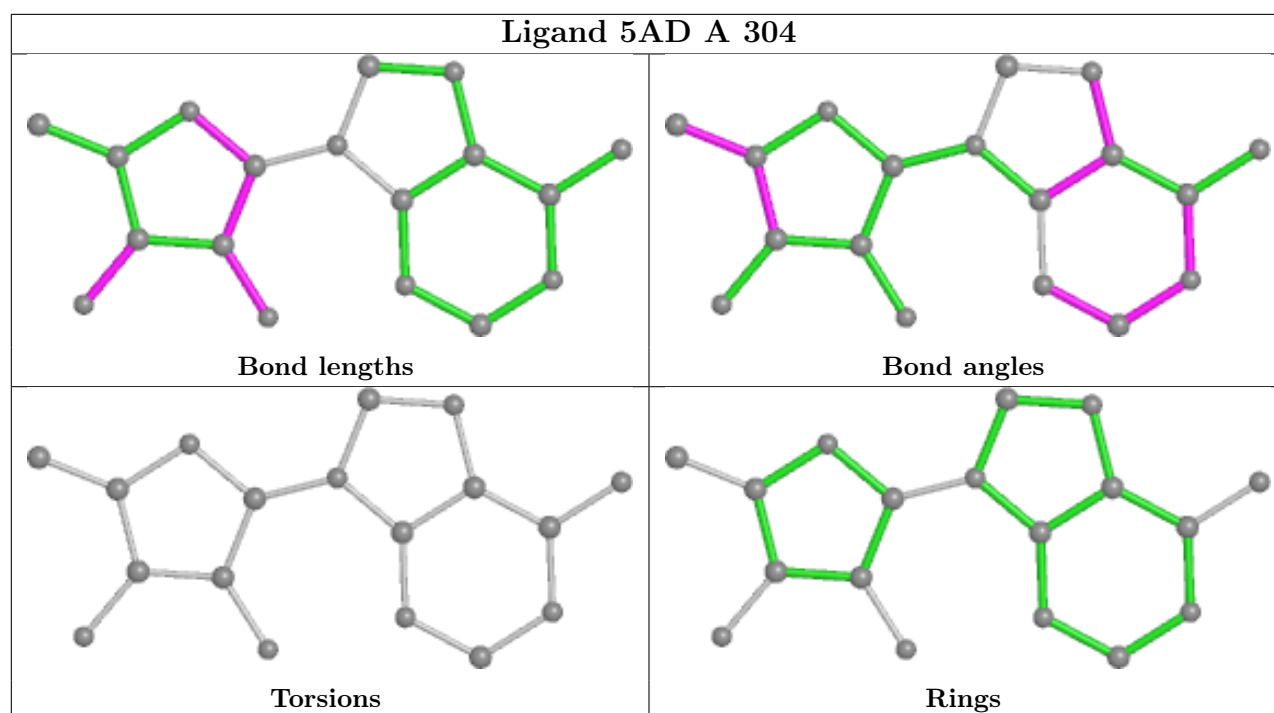


## Ligand 5AD C 303



## Ligand 5AD D 302





## 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	152/196 (77%)	0.31	9 (5%) 22 22	23, 33, 63, 88	0
1	B	148/196 (75%)	0.32	16 (10%) 5 5	27, 41, 65, 83	0
1	C	148/196 (75%)	0.43	12 (8%) 12 12	27, 40, 68, 82	0
1	D	145/196 (73%)	0.16	10 (6%) 16 16	27, 39, 68, 76	0
All	All	593/784 (75%)	0.31	47 (7%) 12 12	23, 39, 67, 88	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	THR	9.2
1	A	144	THR	7.3
1	A	107	GLY	6.1
1	C	142	TYR	5.6
1	A	142	TYR	5.6
1	B	145	PHE	5.5
1	C	237	ILE	5.0
1	D	109	THR	4.7
1	C	168	THR	4.2
1	B	146	LYS	4.2
1	C	107	GLY	4.1
1	B	147	ALA	4.0
1	D	79	ASP	3.7
1	D	202	MET	3.6
1	D	147	ALA	3.4
1	D	239	MET	3.3
1	D	146	LYS	3.2
1	C	145	PHE	3.2
1	B	104	THR	3.2
1	D	130	THR	3.2
1	C	147	ALA	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	108	HIS	3.1
1	B	108	HIS	3.0
1	A	188	VAL	2.8
1	B	234	GLN	2.8
1	C	202	MET	2.8
1	C	141	LYS	2.8
1	D	145	PHE	2.7
1	B	105	GLU	2.7
1	B	184	PHE	2.6
1	B	107	GLY	2.6
1	B	109	THR	2.5
1	A	147	ALA	2.5
1	A	104	THR	2.5
1	B	239	MET	2.4
1	C	203	GLY	2.4
1	A	95	ALA	2.4
1	C	201	GLN	2.4
1	B	203	GLY	2.3
1	C	188	VAL	2.3
1	B	187	ALA	2.3
1	B	130	THR	2.2
1	B	202	MET	2.1
1	D	201	GLN	2.1
1	A	184	PHE	2.1
1	B	95	ALA	2.1
1	C	169	ALA	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](#)

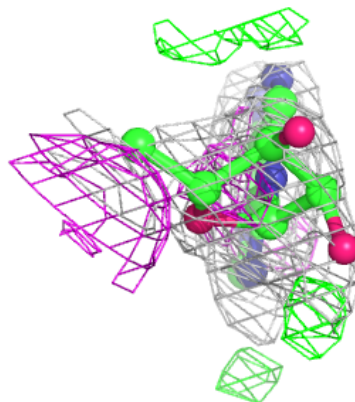
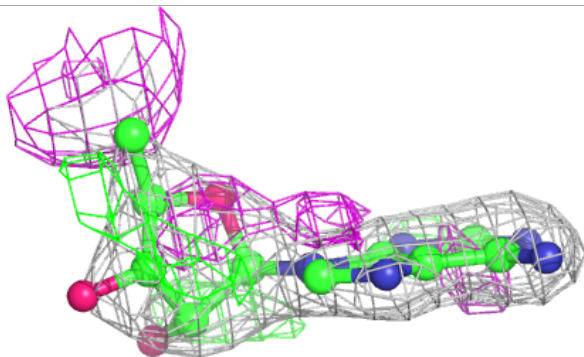
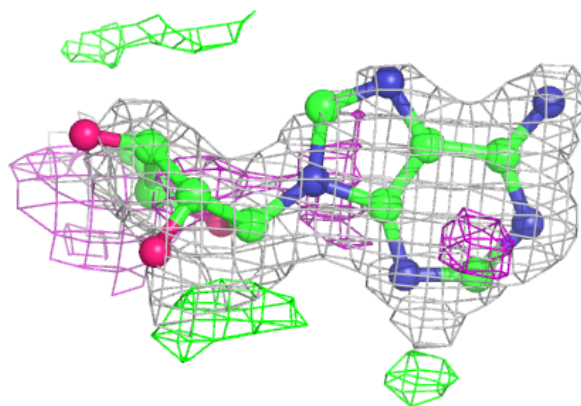
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	D	304	4/4	0.86	0.15	56,65,69,70	0
4	5AD	C	303	18/18	0.88	0.28	38,68,77,79	0
5	B12	C	304	91/91	0.88	0.19	41,61,70,77	0
4	5AD	D	302	18/18	0.91	0.12	26,40,44,44	0
2	ACT	A	301	4/4	0.91	0.15	26,40,45,46	0
2	ACT	C	301	4/4	0.92	0.11	36,52,55,55	0
2	ACT	D	301	4/4	0.96	0.13	45,48,49,56	0
4	5AD	A	304	18/18	0.96	0.07	28,32,34,36	0
4	5AD	B	302	18/18	0.96	0.10	29,34,37,37	0
5	B12	D	303	91/91	0.96	0.08	27,33,50,64	0
5	B12	B	303	91/91	0.97	0.09	24,31,43,53	0
2	ACT	B	301	4/4	0.97	0.09	41,42,49,52	0
5	B12	A	305	91/91	0.97	0.09	24,30,39,55	0
3	K	C	302	1/1	0.99	0.09	41,41,41,41	0
3	K	A	302	1/1	0.99	0.14	37,37,37,37	1
3	K	A	303	1/1	0.99	0.13	42,42,42,42	1

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.

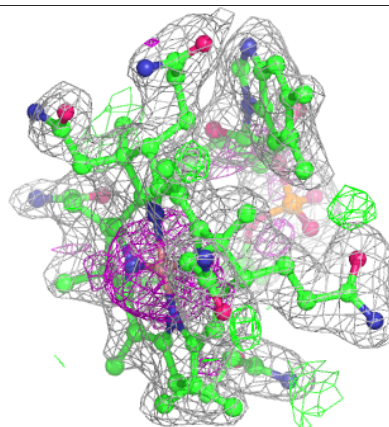
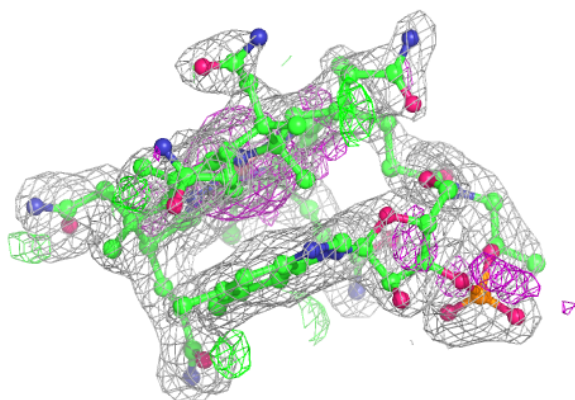
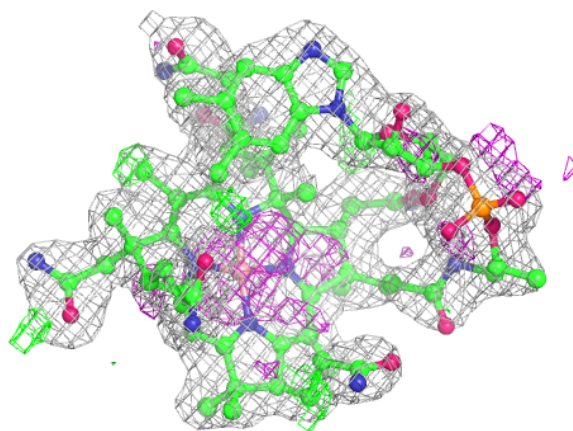
**Electron density around 5AD C 303:**

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



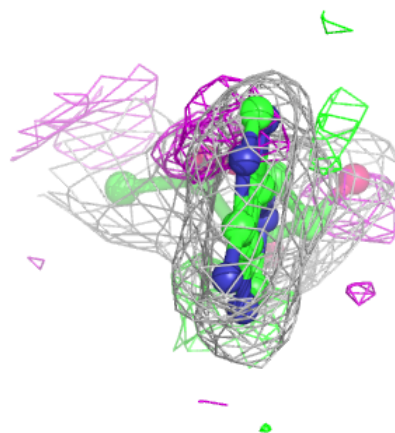
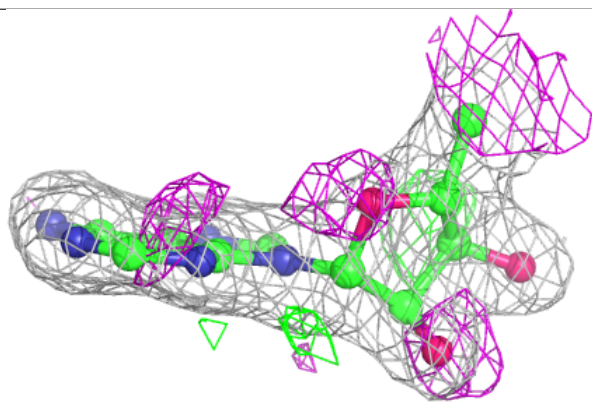
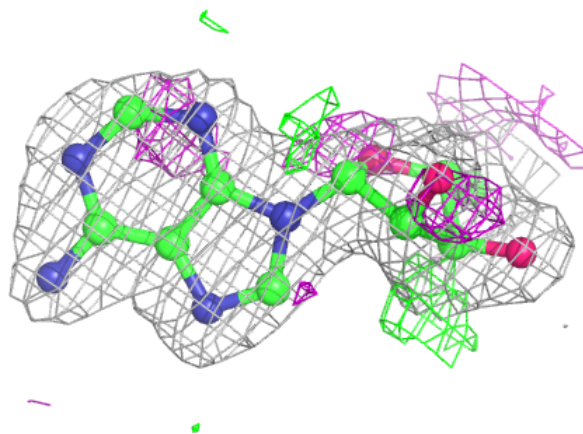
**Electron density around B12 C 304:**

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



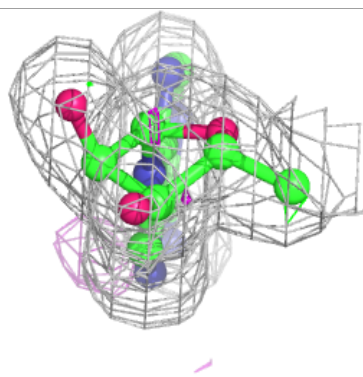
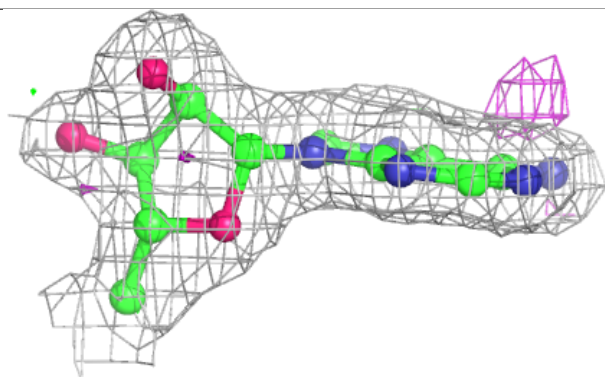
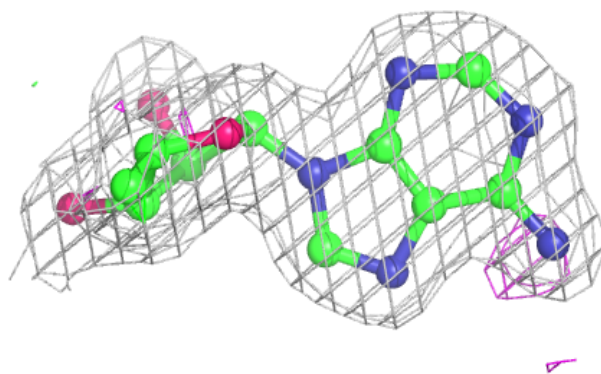
**Electron density around 5AD D 302:**

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

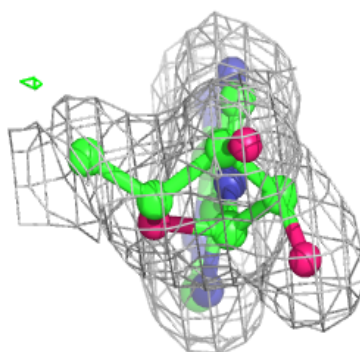
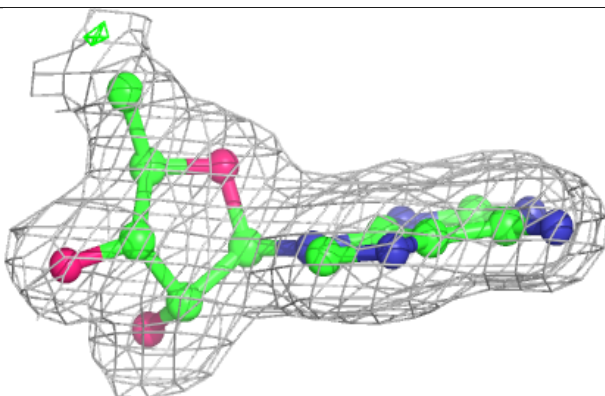
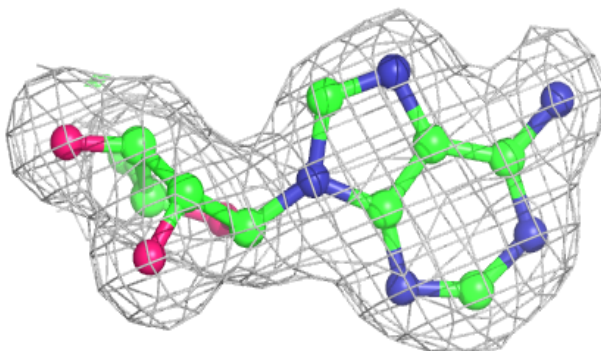


**Electron density around 5AD A 304:**

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

**Electron density around 5AD B 302:**

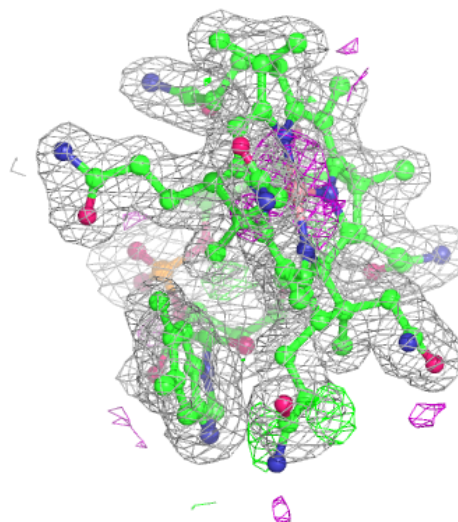
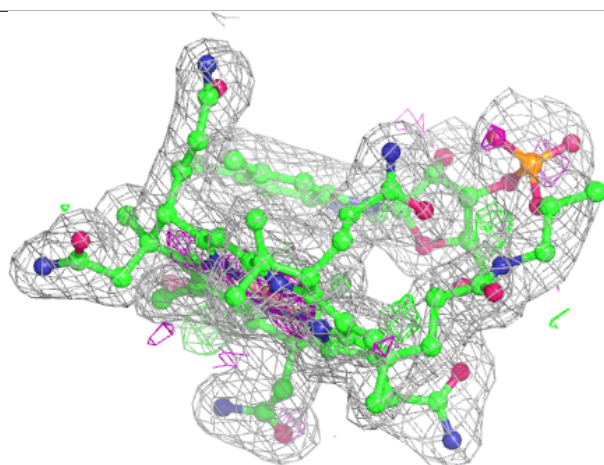
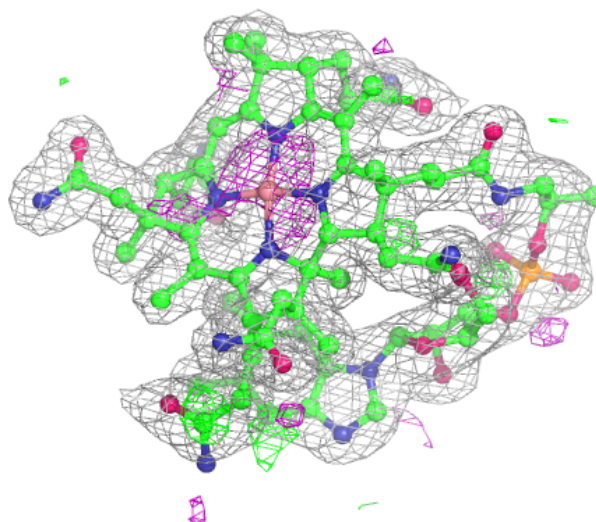
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





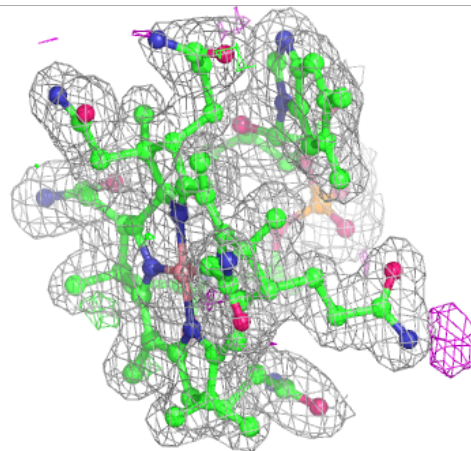
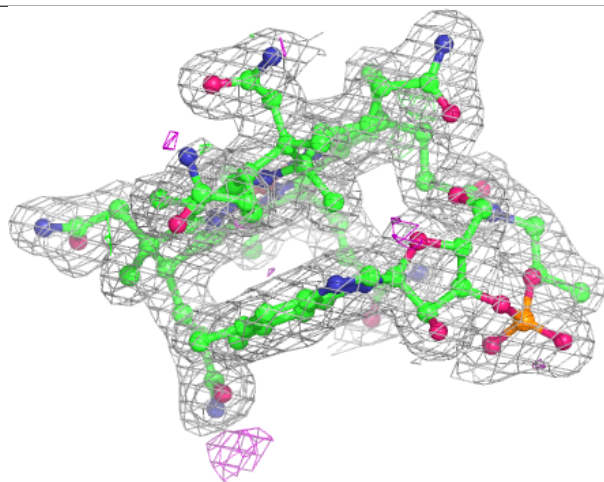
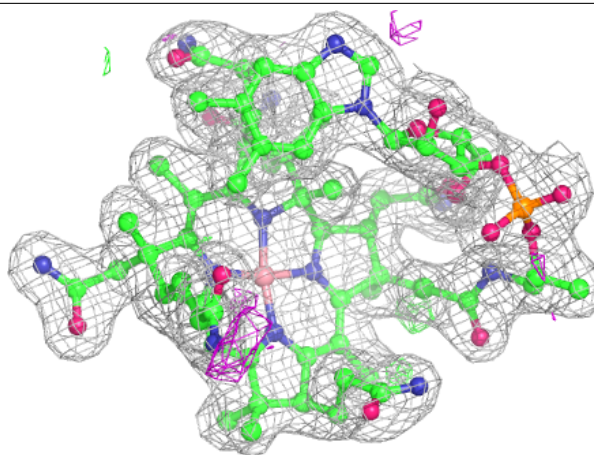
**Electron density around B12 D 303:**

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



**Electron density around B12 B 303:**

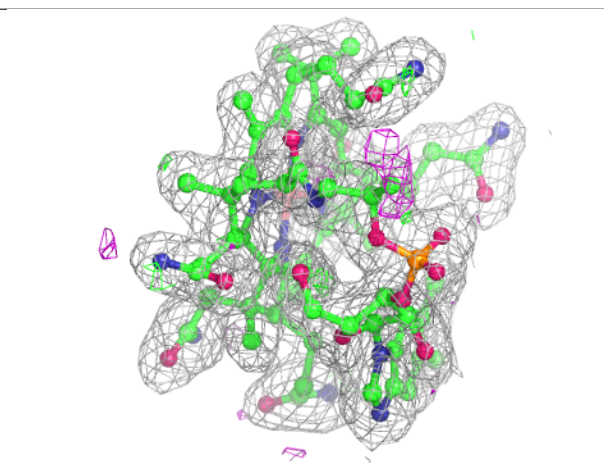
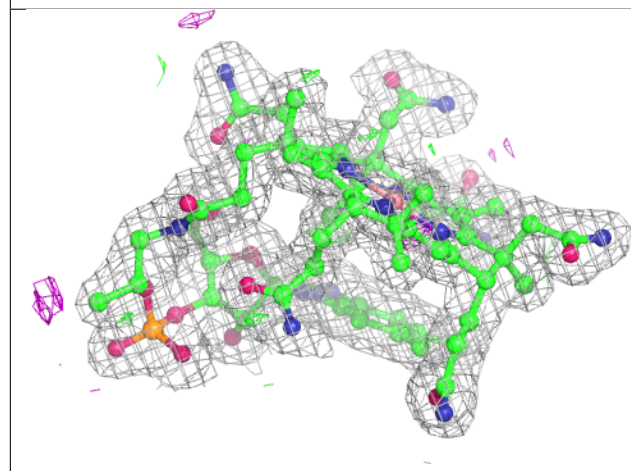
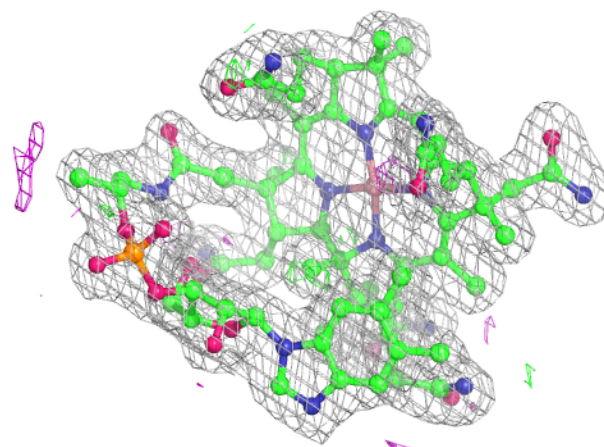
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around B12 A 305:**

$2mF_o-DF_c$  (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.