



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:40 AM UTC

PDB ID : 7RUV / pdb_00007ruv
Title : Structure of Human ATP:Cobalamin Adenosyltransferase E193K bound to adenosylcobalamin
Authors : Mascarenhas, R.; Gouda, H.; Koutmos, M.; Banerjee, R.
Deposited on : 2021-08-18
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

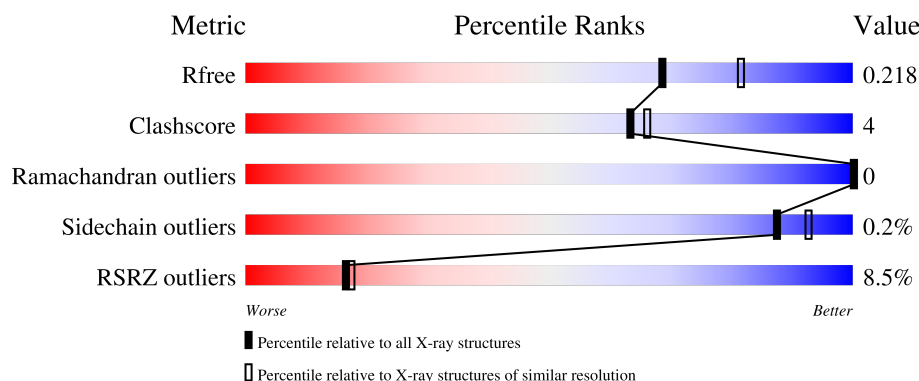
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	7% 73% 23%
1	B	196	7% 72% 25%
1	C	196	6% 76% 23%
1	D	196	7% 73% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5180 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	150	Total	C	N	O	S	0	0	0
			1163	742	195	221	5			
1	B	147	Total	C	N	O	S	0	0	0
			1137	728	191	212	6			
1	C	151	Total	C	N	O	S	0	0	0
			1160	739	194	221	6			
1	D	151	Total	C	N	O	S	0	0	0
			1162	741	196	221	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP Q96EY8
A	193	LYS	GLU	engineered mutation	UNP Q96EY8
B	55	MET	-	initiating methionine	UNP Q96EY8
B	193	LYS	GLU	engineered mutation	UNP Q96EY8
C	55	MET	-	initiating methionine	UNP Q96EY8
C	193	LYS	GLU	engineered mutation	UNP Q96EY8
D	55	MET	-	initiating methionine	UNP Q96EY8
D	193	LYS	GLU	engineered mutation	UNP Q96EY8

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

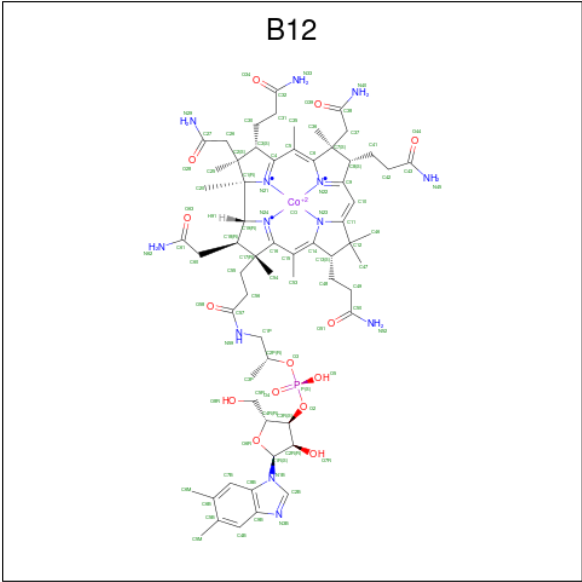
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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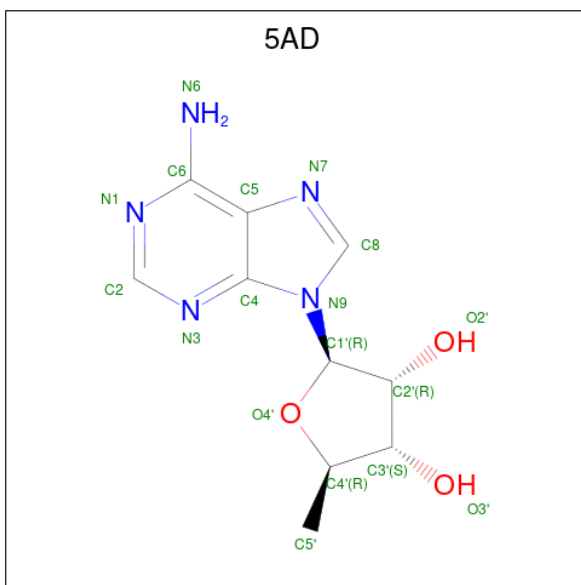
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P) (labeled as "Ligand of Interest" by depositor).



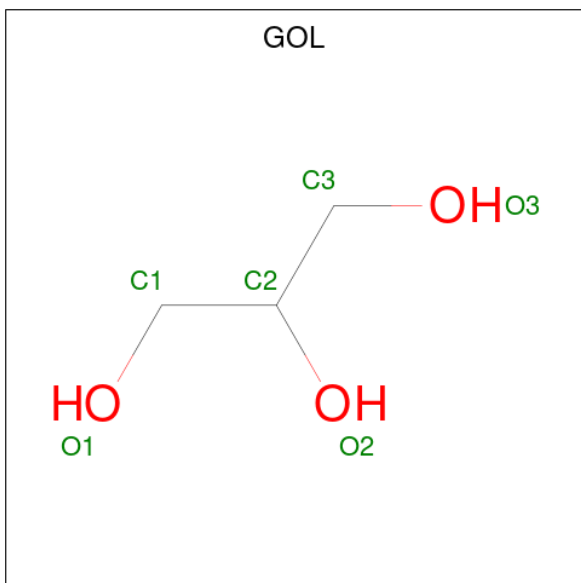
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 5 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: C₁₀H₁₃N₅O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

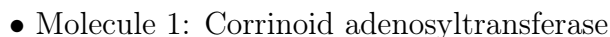
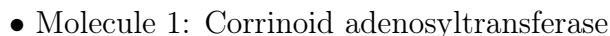
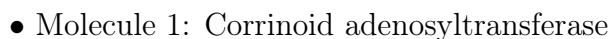


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	24	Total	O	0	0
			24	24		
7	C	32	Total	O	0	0
			32	32		
7	D	21	Total	O	0	0
			21	21		

- Molecule 1: Corrinoid adenosyltransferase



LYS
ASN
ASP
PRO
SER
ALA
GLU
SER
GLU
GLY
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	121.18Å 121.18Å 169.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.00 – 2.10 33.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (33.00-2.10) 96.0 (33.00-2.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.185 , 0.217 0.186 , 0.218	Depositor DCC
R_{free} test set	2626 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5180	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 5AD, K, MG, B12

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	0.35	0/1182	0.46	0/1598
1	B	0.33	0/1155	0.44	0/1559
1	C	0.33	0/1180	0.45	0/1599
1	D	0.30	0/1182	0.43	0/1601
All	All	0.33	0/4699	0.44	0/6357

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	1163	0	1154	4	0
1	B	1137	0	1135	3	0
1	C	1160	0	1141	2	0
1	D	1162	0	1149	5	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	91	0	88	9	0
4	B	91	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	91	0	88	7	0
4	D	91	0	88	10	0
5	A	18	0	10	1	0
5	B	18	0	10	2	0
5	C	18	0	10	1	0
5	D	18	0	10	2	0
6	C	6	0	8	0	0
7	A	36	0	0	0	0
7	B	24	0	0	0	0
7	C	32	0	0	0	0
7	D	21	0	0	0	0
All	All	5180	0	4979	40	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 (40) 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)
4:A:303:B12:O8R	4:A:303:B12:N62	2.23	0.71
4:B:301:B12:H362	4:B:301:B12:H351	1.80	0.63
4:A:303:B12:H59	4:A:303:B12:H5R2	1.63	0.63
4:C:503:B12:H362	4:C:503:B12:H351	1.80	0.61
4:A:303:B12:H362	4:A:303:B12:H351	1.85	0.59
4:D:301:B12:C61	4:D:301:B12:H252	2.36	0.56
1:D:130:THR:HG21	1:D:143:THR:H	1.71	0.56
4:A:303:B12:H601	4:A:303:B12:H252	1.90	0.54
4:D:301:B12:C16	5:D:302:5AD:H4'	2.40	0.52
4:B:301:B12:C16	5:B:302:5AD:H4'	2.39	0.52
1:A:157:ILE:O	1:A:161:THR:HG23	2.10	0.51
4:A:303:B12:C16	5:A:304:5AD:H4'	2.42	0.50
4:C:503:B12:H5R2	4:C:503:B12:H562	1.92	0.50
1:D:103:VAL:HG13	1:D:108:HIS:HB2	1.94	0.49
1:A:128:LEU:HD23	1:A:205:THR:HG21	1.93	0.49
4:C:503:B12:C16	5:C:504:5AD:H4'	2.43	0.49
4:D:301:B12:H621	4:D:301:B12:H18	1.54	0.49
4:C:503:B12:H543	4:C:503:B12:H531	1.96	0.48
4:D:301:B12:H362	4:D:301:B12:H351	1.96	0.48
4:D:301:B12:H562	4:D:301:B12:O8R	2.16	0.46
1:A:170:PHE:CZ	4:A:303:B12:H202	2.50	0.46
4:A:303:B12:H5R2	4:A:303:B12:N59	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:HG22	1:D:143:THR:OG1	2.15	0.46
1:C:170:PHE:CZ	4:C:503:B12:H202	2.52	0.45
1:D:170:PHE:CZ	4:D:301:B12:H202	2.52	0.44
4:B:301:B12:H552	4:B:301:B12:H531	1.99	0.44
1:B:79:ASP:HB3	1:B:82:VAL:HG23	2.00	0.44
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.66	0.44
4:D:301:B12:H253	4:D:301:B12:H301	1.79	0.43
4:D:301:B12:H262	4:D:301:B12:H91	1.80	0.43
4:B:301:B12:N24	5:B:302:5AD:H4'	2.34	0.42
4:A:303:B12:H621	4:A:303:B12:C5R	2.32	0.42
4:C:503:B12:H5R1	4:C:503:B12:H621	1.84	0.42
1:D:157:ILE:O	1:D:161:THR:OG1	2.34	0.41
1:B:86:VAL:HG11	4:D:301:B12:H13	2.02	0.41
4:D:301:B12:N24	5:D:302:5AD:H4'	2.34	0.41
1:A:103:VAL:HG13	1:A:108:HIS:HB2	2.03	0.41
4:A:303:B12:H543	4:A:303:B12:H531	2.02	0.40
1:C:174:SER:OG	1:C:175:GLY:N	2.52	0.40
4:C:503:B12:H3	4:C:503:B12:N29	2.37	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	144/196 (74%)	144 (100%)	0	0	100	100
1	B	139/196 (71%)	136 (98%)	3 (2%)	0	100	100
1	C	147/196 (75%)	143 (97%)	4 (3%)	0	100	100
1	D	147/196 (75%)	143 (97%)	4 (3%)	0	100	100
All	All	577/784 (74%)	566 (98%)	11 (2%)	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	122/164 (74%)	122 (100%)	0	100	100
1	B	119/164 (73%)	118 (99%)	1 (1%)	73	81
1	C	121/164 (74%)	121 (100%)	0	100	100
1	D	121/164 (74%)	121 (100%)	0	100	100
All	All	483/656 (74%)	482 (100%)	1 (0%)	87	93

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

Mol	Chain	Res	Type
1	B	177	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	C	108	HIS
1	D	81	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

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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
6	GOL	C	501	-	5,5,5	0.68	0	5,5,5	1.18	1 (20%)
4	B12	B	301	-	94,101,101	1.09	4 (4%)	149,166,166	1.69	31 (20%)
5	5AD	B	302	-	20,20,20	1.67	6 (30%)	28,30,30	1.57	6 (21%)
4	B12	D	301	-	94,101,101	1.08	5 (5%)	149,166,166	1.66	24 (16%)
4	B12	C	503	-	94,101,101	1.10	9 (9%)	149,166,166	1.68	29 (19%)
4	B12	A	303	-	94,101,101	1.09	5 (5%)	149,166,166	1.63	28 (18%)
5	5AD	D	302	-	20,20,20	1.81	7 (35%)	28,30,30	1.56	6 (21%)
5	5AD	C	504	-	20,20,20	1.54	5 (25%)	28,30,30	1.66	8 (28%)
5	5AD	A	304	-	20,20,20	1.70	6 (30%)	28,30,30	1.61	6 (21%)

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
6	GOL	C	501	-	-	2/4/4/4	-
4	B12	B	301	-	-	5/56/223/223	0/3/11/11
5	5AD	B	302	-	-	3/4/20/20	0/3/3/3
4	B12	D	301	-	-	9/56/223/223	0/3/11/11
4	B12	C	503	-	-	8/56/223/223	0/3/11/11
4	B12	A	303	-	-	9/56/223/223	0/3/11/11
5	5AD	D	302	-	-	2/4/20/20	0/3/3/3
5	5AD	C	504	-	-	2/4/20/20	0/3/3/3
5	5AD	A	304	-	-	3/4/20/20	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	B12	C14-N23	3.93	1.40	1.35
4	A	303	B12	C14-N23	3.47	1.39	1.35
5	C	504	5AD	O2'-C2'	-3.37	1.34	1.43
4	B	301	B12	C54-C17	3.34	1.60	1.54
5	D	302	5AD	O2'-C2'	-3.33	1.34	1.43
5	B	302	5AD	O2'-C2'	-3.26	1.34	1.43
4	B	301	B12	C14-N23	3.15	1.39	1.35
5	A	304	5AD	O2'-C2'	-3.09	1.35	1.43
4	C	503	B12	C54-C17	3.07	1.59	1.54
4	B	301	B12	C35-C5	3.05	1.57	1.50
4	A	303	B12	C35-C5	3.03	1.57	1.50
5	B	302	5AD	O3'-C3'	-3.00	1.35	1.43
5	D	302	5AD	C3'-C4'	2.98	1.56	1.52
5	D	302	5AD	O3'-C3'	-2.97	1.35	1.43
5	A	304	5AD	O3'-C3'	-2.95	1.35	1.43
4	C	503	B12	C14-N23	2.91	1.39	1.35
4	D	301	B12	C54-C17	2.88	1.59	1.54
5	B	302	5AD	C5-N7	2.75	1.44	1.39
5	C	504	5AD	O3'-C3'	-2.64	1.36	1.43
4	C	503	B12	C35-C5	2.61	1.56	1.50
4	A	303	B12	C54-C17	2.60	1.58	1.54
5	B	302	5AD	C4-N9	2.57	1.43	1.37
5	A	304	5AD	C4-N9	2.57	1.43	1.37
4	D	301	B12	C2B-N1B	-2.49	1.33	1.37
5	D	302	5AD	C4-N9	2.48	1.42	1.37
5	D	302	5AD	O4'-C1'	2.48	1.47	1.42
4	D	301	B12	C35-C5	2.37	1.55	1.50
4	B	301	B12	C2B-N1B	-2.34	1.33	1.37
5	A	304	5AD	C5-N7	2.34	1.43	1.39
5	B	302	5AD	C4-N3	2.32	1.38	1.34
4	D	301	B12	C55-C17	-2.31	1.49	1.54
4	C	503	B12	C3R-C4R	2.20	1.58	1.52
5	D	302	5AD	C8-N9	2.20	1.41	1.37
5	D	302	5AD	C5-N7	2.19	1.43	1.39
4	C	503	B12	C30-C3	2.18	1.59	1.54
5	C	504	5AD	O4'-C1'	2.16	1.47	1.42
5	C	504	5AD	C4-N9	2.14	1.42	1.37
4	C	503	B12	C2B-N1B	-2.14	1.33	1.37
4	C	503	B12	C6B-C5B	2.10	1.46	1.40
5	B	302	5AD	C8-N9	2.09	1.41	1.37
5	A	304	5AD	C4-N3	2.08	1.38	1.34
5	A	304	5AD	C8-N9	2.08	1.41	1.37
4	A	303	B12	C6B-C5B	2.06	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	B12	P-O2	2.05	1.65	1.59
4	A	303	B12	C30-C3	2.04	1.59	1.54
4	C	503	B12	C48-C13	2.04	1.59	1.54
5	C	504	5AD	C8-N9	2.00	1.41	1.37

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	B12	C19-N24-C16	7.15	115.10	107.29
4	A	303	B12	C19-N24-C16	6.54	114.44	107.29
4	C	503	B12	C19-N24-C16	5.76	113.59	107.29
4	D	301	B12	C19-N24-C16	5.41	113.20	107.29
4	A	303	B12	C18-C17-C16	5.10	106.84	100.69
4	D	301	B12	C18-C17-C16	5.09	106.83	100.69
4	C	503	B12	C54-C17-C18	-4.94	105.89	112.99
4	D	301	B12	C54-C17-C18	-4.84	106.04	112.99
4	B	301	B12	C18-C17-C16	4.75	106.42	100.69
4	C	503	B12	C18-C17-C16	4.73	106.39	100.69
4	D	301	B12	C2P-C1P-N59	-4.50	106.30	112.92
4	B	301	B12	C56-C55-C17	-4.44	107.02	115.58
4	B	301	B12	C54-C17-C18	-4.40	106.67	112.99
4	C	503	B12	C2P-C1P-N59	-4.29	106.61	112.92
4	D	301	B12	C1P-N59-C57	-4.28	113.50	122.69
4	A	303	B12	C56-C55-C17	-4.12	107.63	115.58
4	D	301	B12	C56-C55-C17	-4.01	107.85	115.58
4	B	301	B12	C2P-C1P-N59	-3.98	107.06	112.92
4	C	503	B12	C9-N22-C6	3.89	109.96	105.28
5	C	504	5AD	N3-C2-N1	3.88	134.46	128.58
5	A	304	5AD	N3-C2-N1	3.83	134.38	128.58
5	D	302	5AD	N3-C2-N1	3.83	134.37	128.58
4	D	301	B12	C13-C14-C15	-3.81	118.52	124.32
4	B	301	B12	C9-N22-C6	3.80	109.86	105.28
4	D	301	B12	C9-N22-C6	3.80	109.86	105.28
5	B	302	5AD	N3-C2-N1	3.79	134.33	128.58
4	B	301	B12	C17-C16-N24	-3.73	105.47	111.17
4	A	303	B12	C54-C17-C16	-3.69	93.29	112.41
4	A	303	B12	C17-C16-N24	-3.68	105.55	111.17
4	D	301	B12	C17-C16-N24	-3.67	105.56	111.17
4	D	301	B12	C16-C15-C14	-3.67	115.66	121.26
4	B	301	B12	C15-C16-N24	3.65	127.62	122.42
4	C	503	B12	C16-C15-C14	-3.63	115.72	121.26
4	A	303	B12	C54-C17-C18	-3.39	108.13	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	B12	C54-C17-C16	-3.36	95.01	112.41
4	C	503	B12	C13-C14-C15	-3.33	119.25	124.32
4	C	503	B12	C7B-C8B-C9B	3.30	126.43	122.47
4	D	301	B12	C55-C17-C16	3.21	122.86	116.59
4	D	301	B12	C54-C17-C16	-3.17	95.97	112.41
4	C	503	B12	C5M-C5B-C6B	-3.17	114.29	120.76
4	A	303	B12	C7B-C8B-C9B	3.15	126.25	122.47
4	B	301	B12	C54-C17-C16	-3.15	96.09	112.41
4	C	503	B12	C15-C16-N24	3.13	126.88	122.42
4	C	503	B12	C1P-N59-C57	-3.09	116.06	122.69
4	A	303	B12	C9-N22-C6	3.06	108.96	105.28
4	A	303	B12	C1P-N59-C57	-3.05	116.14	122.69
4	B	301	B12	C5M-C5B-C6B	-3.05	114.53	120.76
4	D	301	B12	C7B-C8B-C9B	2.99	126.06	122.47
4	C	503	B12	C56-C55-C17	-2.99	109.82	115.58
4	A	303	B12	C2P-C1P-N59	-2.98	108.54	112.92
4	B	301	B12	C16-C15-C14	-2.97	116.73	121.26
4	B	301	B12	C13-C14-C15	-2.97	119.80	124.32
4	A	303	B12	C15-C16-N24	2.96	126.64	122.42
4	D	301	B12	C15-C16-N24	2.95	126.62	122.42
5	A	304	5AD	C5'-C4'-C3'	-2.93	112.62	115.70
4	A	303	B12	C16-C15-C14	-2.91	116.82	121.26
4	C	503	B12	C55-C17-C16	2.91	122.28	116.59
4	C	503	B12	C17-C16-N24	-2.90	106.74	111.17
4	A	303	B12	C4B-C5B-C6B	2.88	123.91	119.69
5	B	302	5AD	C5'-C4'-C3'	-2.88	112.68	115.70
4	B	301	B12	C4B-C5B-C6B	2.87	123.90	119.69
5	C	504	5AD	C5'-C4'-C3'	-2.86	112.70	115.70
5	A	304	5AD	C1'-N9-C8	2.82	133.35	127.09
5	C	504	5AD	C4-N9-C8	-2.80	102.80	105.74
5	A	304	5AD	C2-N1-C6	-2.79	114.14	118.73
4	A	303	B12	C55-C17-C16	2.77	122.01	116.59
4	A	303	B12	C1-C19-C18	-2.77	117.42	121.90
5	B	302	5AD	C2-N1-C6	-2.76	114.19	118.73
4	C	503	B12	C4B-C5B-C6B	2.76	123.73	119.69
5	A	304	5AD	C4-N9-C8	-2.76	102.84	105.74
4	D	301	B12	C4B-C5B-C6B	2.72	123.69	119.69
5	D	302	5AD	C2-N1-C6	-2.72	114.26	118.73
5	D	302	5AD	C4-N9-C8	-2.72	102.88	105.74
5	C	504	5AD	C1'-N9-C8	2.72	133.13	127.09
4	B	301	B12	C53-C15-C16	2.67	124.89	120.36
4	B	301	B12	C8B-C9B-N3B	-2.66	107.12	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	504	5AD	C2-N1-C6	-2.66	114.36	118.73
5	C	504	5AD	O4'-C1'-N9	-2.65	103.01	108.09
4	B	301	B12	C13-C14-N23	2.64	112.67	109.09
4	B	301	B12	C9B-N3B-C2B	2.63	107.63	104.40
4	B	301	B12	C55-C17-C18	2.61	116.11	111.12
4	D	301	B12	C5M-C5B-C6B	-2.59	115.47	120.76
5	D	302	5AD	N9-C8-N7	2.58	117.60	113.94
4	A	303	B12	C13-C14-C15	-2.57	120.41	124.32
4	A	303	B12	C5M-C5B-C6B	-2.56	115.53	120.76
4	B	301	B12	O58-C57-N59	2.56	128.05	123.03
5	B	302	5AD	N9-C8-N7	2.52	117.52	113.94
4	A	303	B12	C53-C15-C16	2.49	124.60	120.36
5	D	302	5AD	C5'-C4'-C3'	-2.48	113.09	115.70
5	B	302	5AD	C4-N9-C8	-2.47	103.15	105.74
5	A	304	5AD	N9-C8-N7	2.46	117.43	113.94
4	A	303	B12	C31-C32-N33	2.46	124.36	116.49
4	C	503	B12	C2-C1-C19	-2.46	114.80	118.61
4	C	503	B12	C18-C19-N24	2.44	106.00	102.33
4	C	503	B12	O6R-C1R-N1B	-2.44	103.40	108.09
4	A	303	B12	C26-C2-C1	-2.41	106.28	110.00
4	A	303	B12	C18-C19-N24	2.39	105.93	102.33
4	A	303	B12	C55-C17-C18	2.36	115.62	111.12
4	C	503	B12	C1-C19-C18	-2.33	118.13	121.90
4	A	303	B12	O2-C3R-C2R	2.32	119.99	111.68
4	B	301	B12	C7B-C8B-C9B	2.31	125.24	122.47
4	B	301	B12	C55-C17-C16	2.25	120.99	116.59
4	D	301	B12	C53-C15-C16	2.23	124.15	120.36
4	C	503	B12	O6R-C4R-C5R	-2.22	104.53	109.22
4	C	503	B12	O28-C27-N29	-2.21	116.62	122.53
4	A	303	B12	C8B-C9B-N3B	-2.21	107.61	110.00
4	B	301	B12	C31-C32-N33	2.19	123.51	116.49
4	C	503	B12	O3-C2P-C1P	-2.19	102.60	106.94
4	C	503	B12	C55-C17-C18	2.19	115.30	111.12
5	B	302	5AD	C1'-N9-C8	2.18	131.94	127.09
4	B	301	B12	C25-C2-C26	2.18	114.07	109.74
4	B	301	B12	C20-C1-C19	2.18	111.44	109.35
4	C	503	B12	O44-C43-N45	-2.17	116.73	122.53
5	D	302	5AD	C1'-N9-C8	2.17	131.92	127.09
4	D	301	B12	O2-C3R-C2R	2.17	119.47	111.68
4	A	303	B12	C9B-N3B-C2B	2.17	107.06	104.40
4	C	503	B12	C8B-C9B-N3B	-2.16	107.66	110.00
4	B	301	B12	C9B-C4B-C5B	-2.15	116.85	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	B12	O28-C27-N29	-2.14	116.82	122.53
4	B	301	B12	O28-C27-N29	-2.13	116.83	122.53
6	C	501	GOL	C3-C2-C1	-2.12	104.02	111.80
4	D	301	B12	C2-C26-C27	-2.12	109.31	115.19
5	C	504	5AD	N9-C8-N7	2.11	116.93	113.94
4	D	301	B12	C31-C30-C3	-2.11	108.67	114.65
4	B	301	B12	C56-C57-N59	-2.11	112.50	116.34
4	B	301	B12	O44-C43-N45	-2.10	116.94	122.53
4	D	301	B12	C30-C3-C4	2.10	114.58	109.66
4	B	301	B12	C2-C1-C19	-2.09	115.36	118.61
4	C	503	B12	O2-C3R-C2R	2.09	119.18	111.68
4	C	503	B12	C53-C15-C16	2.09	123.91	120.36
4	C	503	B12	C9B-C4B-C5B	-2.08	116.97	120.83
4	A	303	B12	O44-C43-N45	-2.07	117.00	122.53
4	B	301	B12	C1-C19-C18	-2.07	118.55	121.90
4	D	301	B12	O51-C50-C49	-2.06	114.81	121.04
4	A	303	B12	C9B-C4B-C5B	-2.06	117.01	120.83
4	D	301	B12	O39-C38-C37	-2.05	115.62	121.98
5	C	504	5AD	C2-N3-C4	-2.05	106.83	111.83
4	D	301	B12	C25-C2-C26	2.04	113.78	109.74
4	B	301	B12	C36-C7-C37	2.02	114.17	110.74

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	B12	C1P-C2P-O3-P
4	A	303	B12	C3P-C2P-O3-P
4	A	303	B12	O6R-C4R-C5R-O8R
4	B	301	B12	C14-C13-C48-C49
4	B	301	B12	C1P-C2P-O3-P
4	B	301	B12	C3P-C2P-O3-P
4	C	503	B12	C1P-C2P-O3-P
4	C	503	B12	C3P-C2P-O3-P
4	D	301	B12	C14-C13-C48-C49
4	D	301	B12	C18-C60-C61-O63
4	D	301	B12	C18-C60-C61-N62
4	D	301	B12	C1P-C2P-O3-P
4	D	301	B12	C3P-C2P-O3-P
6	C	501	GOL	C1-C2-C3-O3
4	C	503	B12	O6R-C4R-C5R-O8R
4	A	303	B12	C3R-C4R-C5R-O8R

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Mol	Chain	Res	Type	Atoms
4	A	303	B12	C14-C13-C48-C49
4	C	503	B12	C3R-C4R-C5R-O8R
4	D	301	B12	C16-C17-C55-C56
6	C	501	GOL	O2-C2-C3-O3
4	C	503	B12	C14-C13-C48-C49
4	D	301	B12	C3-C30-C31-C32
4	D	301	B12	C4-C3-C30-C31
5	B	302	5AD	C2'-C1'-N9-C8
5	C	504	5AD	C2'-C1'-N9-C8
5	D	302	5AD	C2'-C1'-N9-C8
4	A	303	B12	C2P-O3-P-O4
4	C	503	B12	C2P-O3-P-O4
4	C	503	B12	C18-C60-C61-O63
4	C	503	B12	C18-C60-C61-N62
5	A	304	5AD	C2'-C1'-N9-C8
4	D	301	B12	C2-C3-C30-C31
4	A	303	B12	C42-C41-C8-C9
4	B	301	B12	O6R-C4R-C5R-O8R
4	B	301	B12	C3-C30-C31-C32
4	A	303	B12	C18-C60-C61-O63
4	A	303	B12	C18-C60-C61-N62
5	B	302	5AD	O4'-C1'-N9-C8
5	A	304	5AD	C2'-C1'-N9-C4
5	B	302	5AD	C2'-C1'-N9-C4
5	C	504	5AD	C2'-C1'-N9-C4
5	A	304	5AD	O4'-C1'-N9-C8
5	D	302	5AD	O4'-C1'-N9-C8

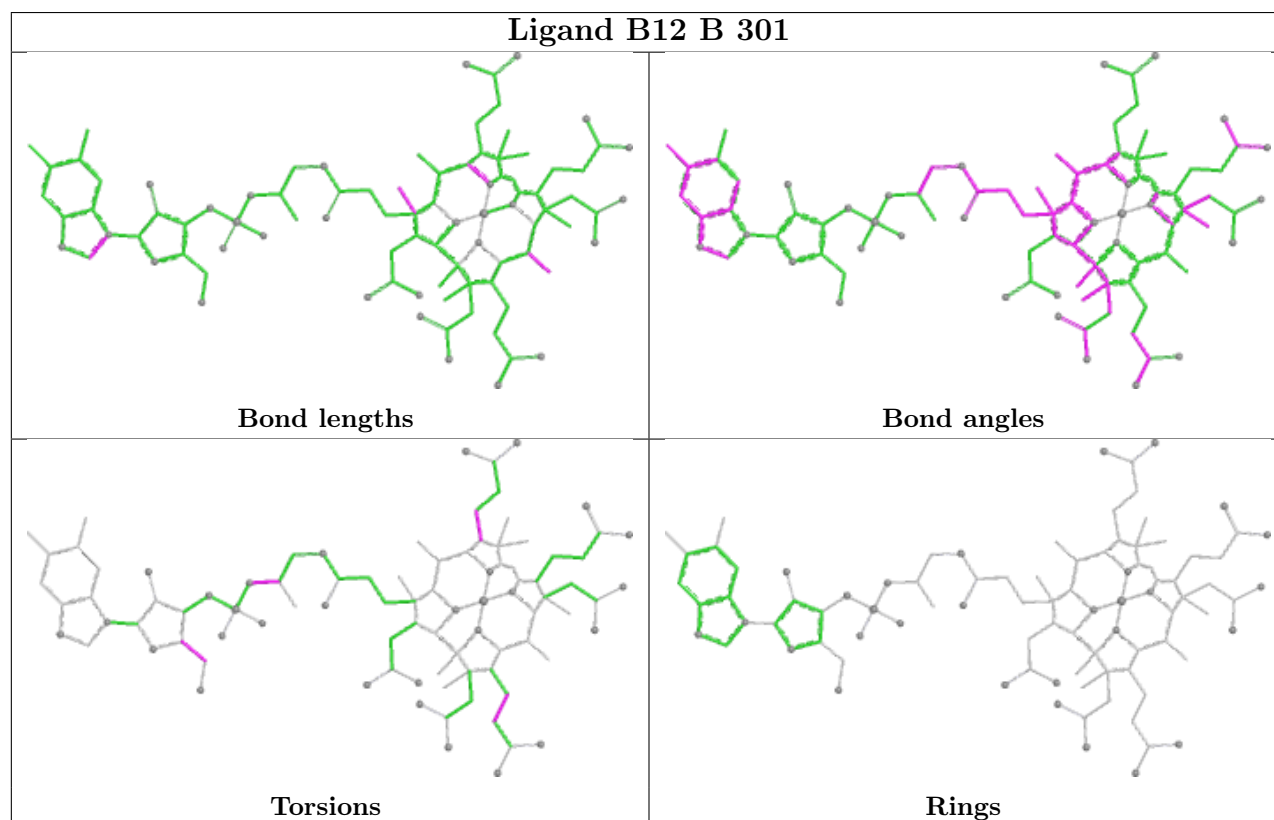
There are no ring outliers.

8 monomers are involved in 30 short contacts:

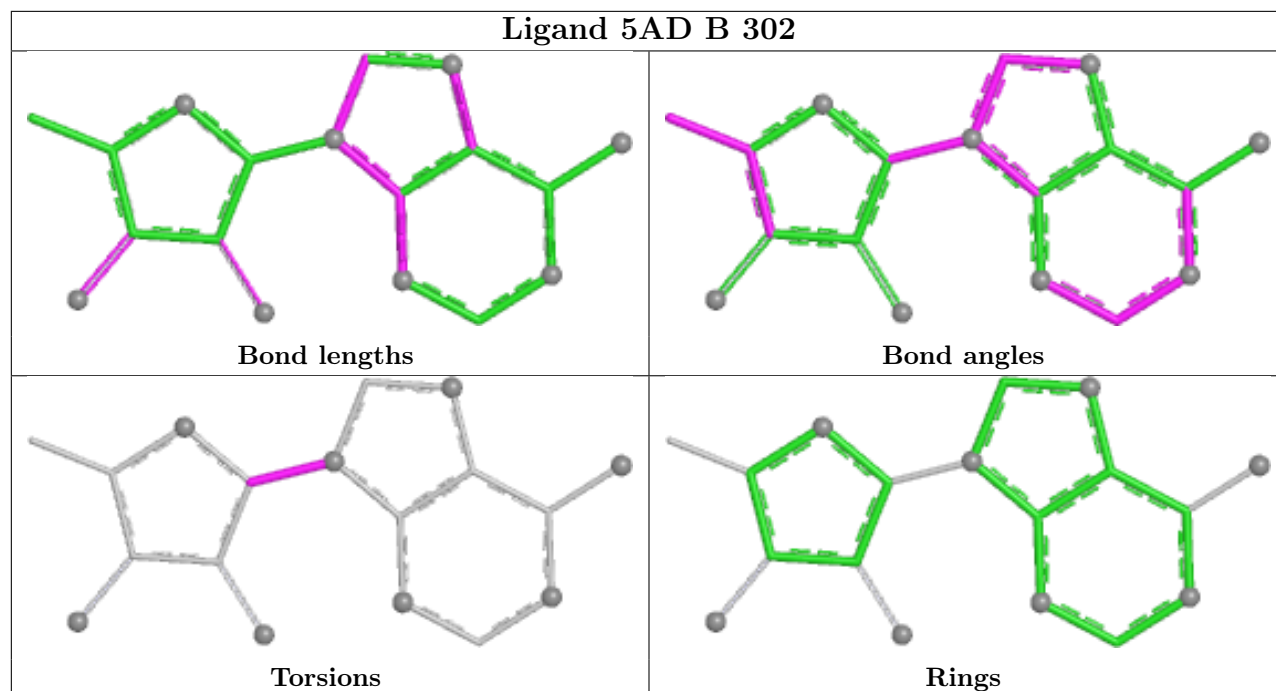
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	B12	4	0
5	B	302	5AD	2	0
4	D	301	B12	10	0
4	C	503	B12	7	0
4	A	303	B12	9	0
5	D	302	5AD	2	0
5	C	504	5AD	1	0
5	A	304	5AD	1	0

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

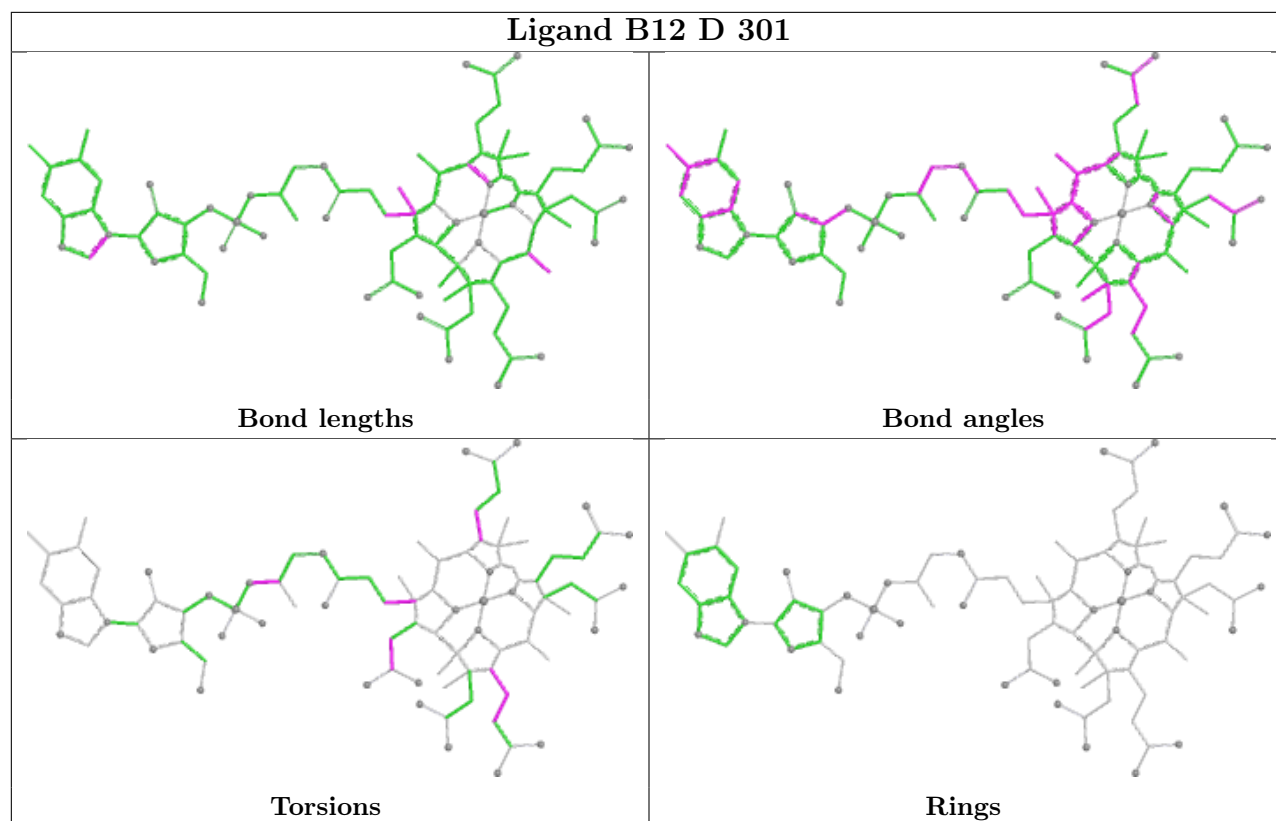
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

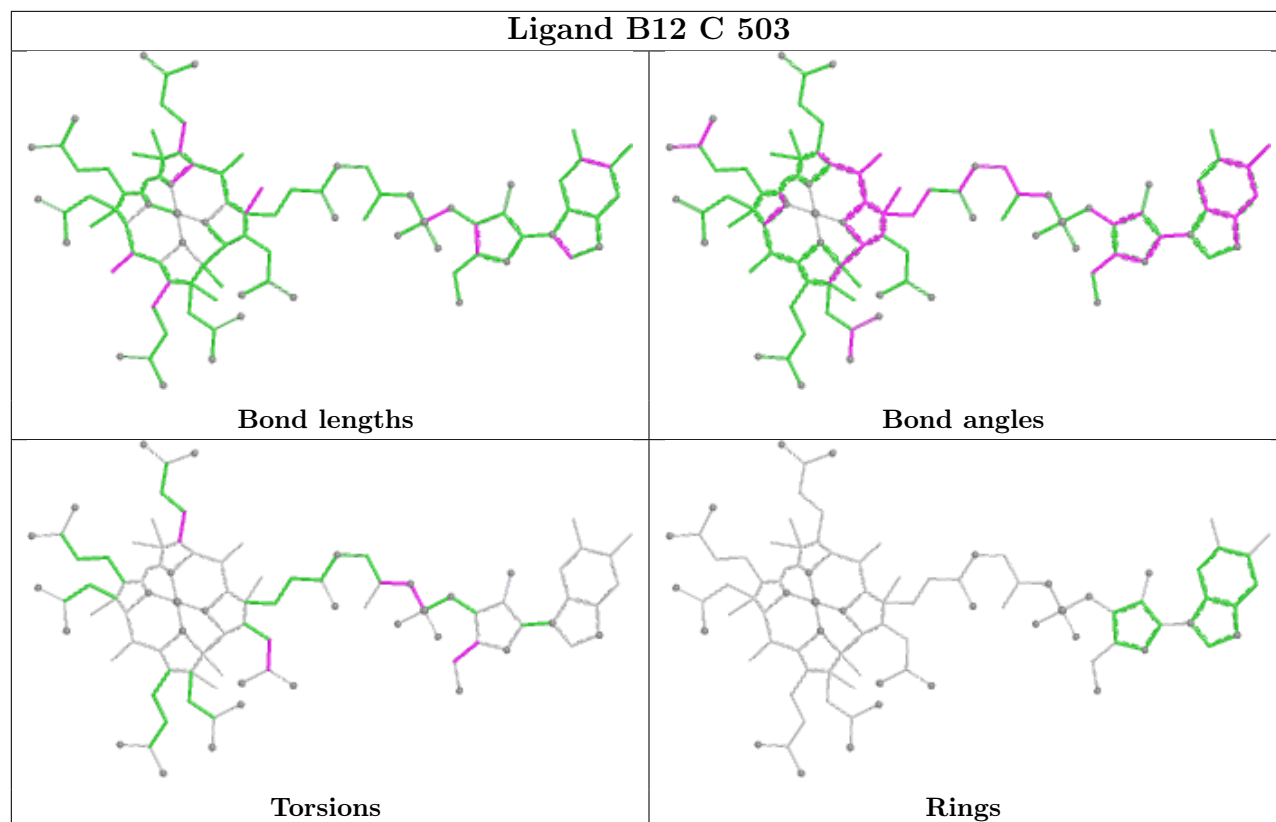
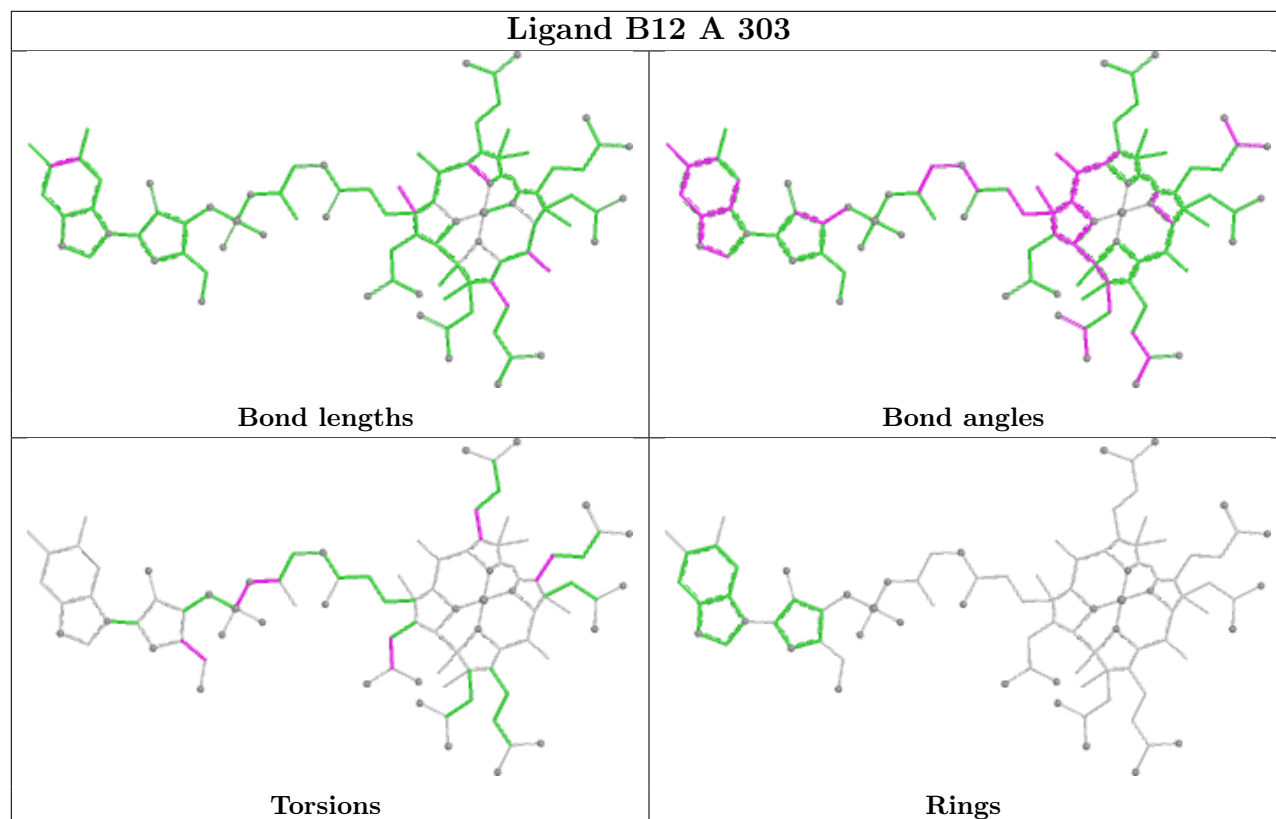


Ligand 5AD B 302

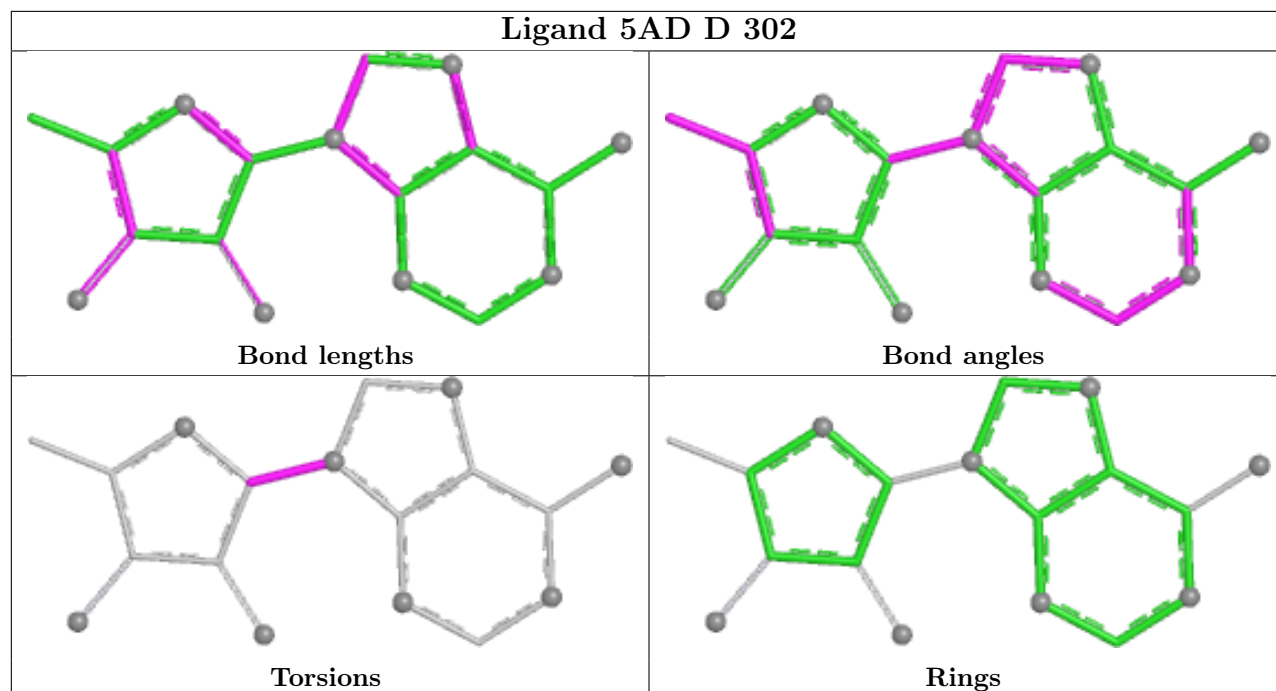


Ligand B12 D 301

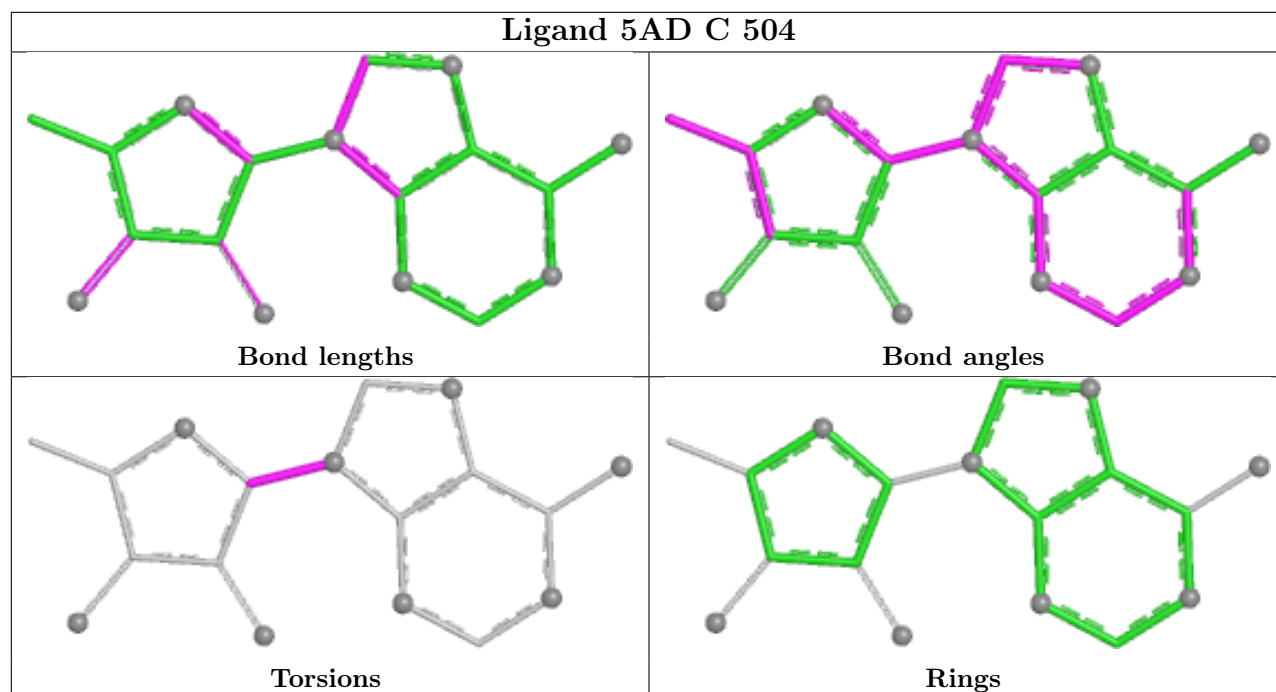


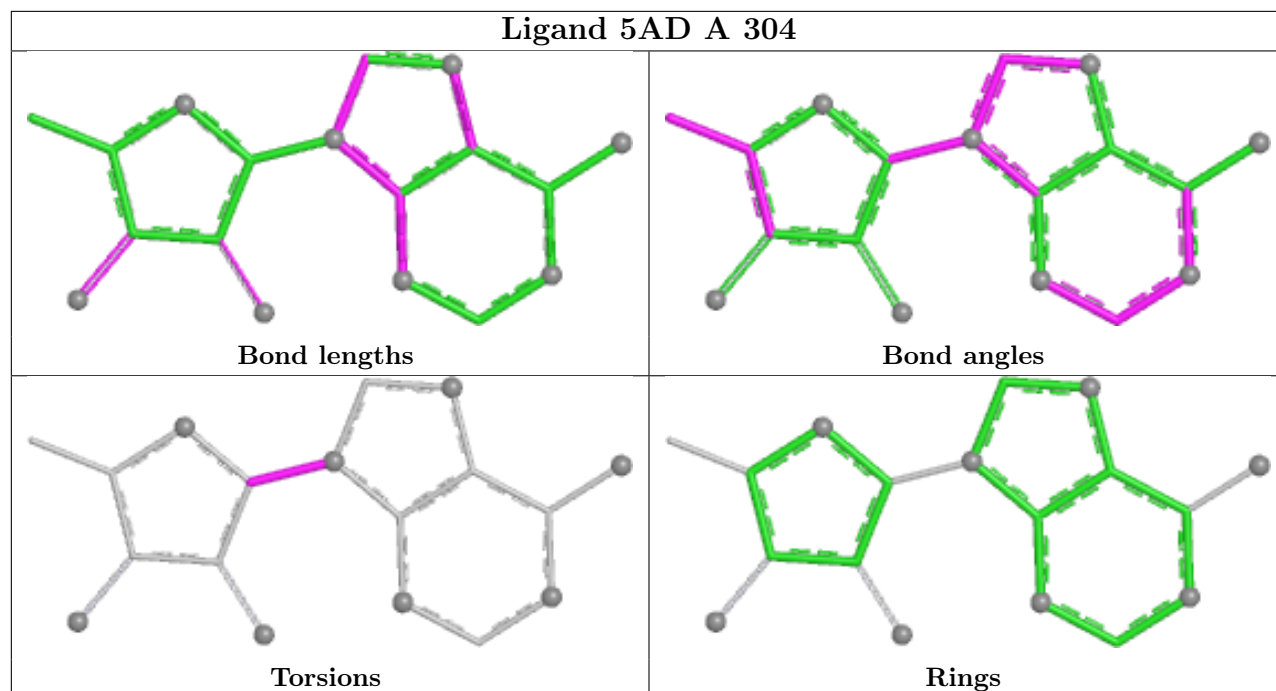
Ligand B12 C 503**Ligand B12 A 303**

Ligand 5AD D 302



Ligand 5AD C 504





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, 95th 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 ²)	Q<0.9
1	A	150/196 (76%)	0.37	14 (9%) 14 15	32, 43, 69, 91	0
1	B	147/196 (75%)	0.37	13 (8%) 15 16	34, 46, 74, 86	0
1	C	151/196 (77%)	0.30	11 (7%) 21 22	33, 48, 68, 79	0
1	D	151/196 (77%)	0.36	13 (8%) 16 17	34, 48, 73, 87	0
All	All	599/784 (76%)	0.35	51 (8%) 16 17	32, 47, 72, 91	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	THR	4.8
1	D	107	GLY	4.3
1	B	107	GLY	4.3
1	B	142	TYR	3.9
1	D	130	THR	3.9
1	A	143	THR	3.9
1	C	239	MET	3.8
1	D	143	THR	3.5
1	B	175	GLY	3.4
1	A	130	THR	3.4
1	B	108	HIS	3.3
1	B	109	THR	3.3
1	A	144	THR	3.2
1	A	142	TYR	3.2
1	B	130	THR	3.1
1	C	107	GLY	3.1
1	B	129	ALA	3.1
1	A	108	HIS	3.1
1	C	130	THR	3.0
1	B	143	THR	3.0
1	A	107	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	239	MET	2.8
1	C	141	LYS	2.8
1	D	239	MET	2.8
1	A	175	GLY	2.8
1	A	129	ALA	2.8
1	A	104	THR	2.8
1	B	144	THR	2.8
1	A	202	MET	2.7
1	C	143	THR	2.7
1	D	108	HIS	2.7
1	D	141	LYS	2.7
1	C	104	THR	2.6
1	D	142	TYR	2.5
1	C	109	THR	2.4
1	D	202	MET	2.4
1	C	108	HIS	2.4
1	D	204	GLU	2.4
1	A	147	ALA	2.4
1	D	109	THR	2.3
1	D	151	LEU	2.3
1	D	129	ALA	2.3
1	C	142	TYR	2.3
1	D	144	THR	2.2
1	B	239	MET	2.2
1	A	109	THR	2.2
1	B	103	VAL	2.2
1	C	158	ASP	2.2
1	C	106	LYS	2.1
1	B	201	GLN	2.0
1	A	215	ARG	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 oligosaccharides in this entry.

6.4 Ligands

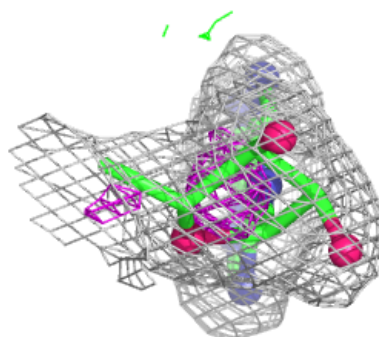
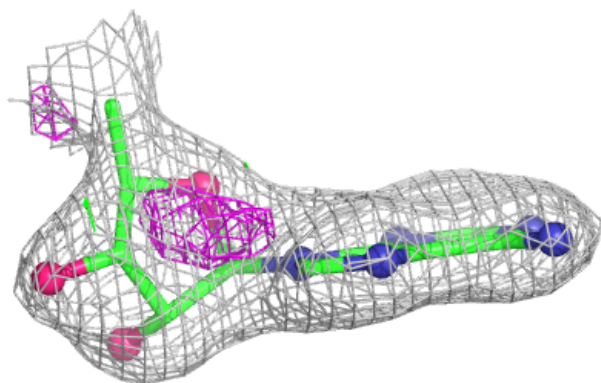
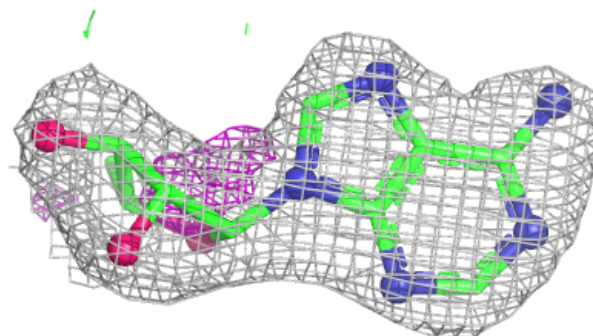
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	C	501	6/6	0.77	0.18	43,57,61,69	0
5	5AD	D	302	18/18	0.91	0.10	47,57,62,63	0
3	MG	C	502	1/1	0.92	0.11	36,36,36,36	0
5	5AD	B	302	18/18	0.96	0.06	32,40,44,45	0
5	5AD	C	504	18/18	0.96	0.06	34,40,43,43	0
4	B12	D	301	91/91	0.96	0.09	41,56,64,77	0
5	5AD	A	304	18/18	0.96	0.07	34,41,45,49	0
4	B12	B	301	91/91	0.97	0.08	33,40,50,58	0
4	B12	C	503	91/91	0.97	0.07	32,38,48,54	0
2	K	A	301	1/1	0.97	0.07	46,46,46,46	1
4	B12	A	303	91/91	0.97	0.08	34,41,47,53	0
3	MG	A	302	1/1	0.98	0.22	45,45,45,45	1

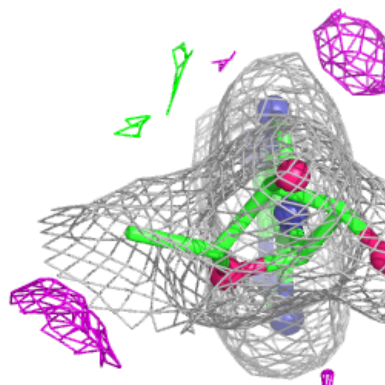
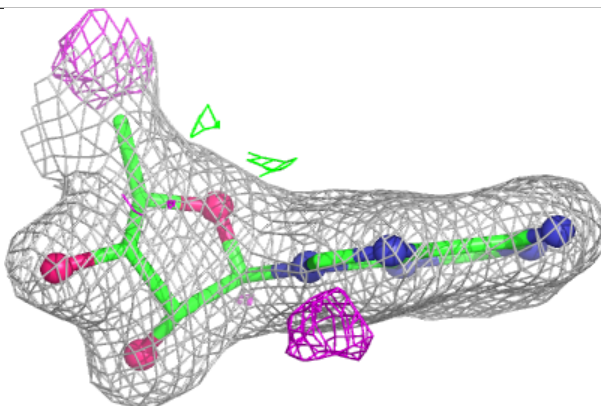
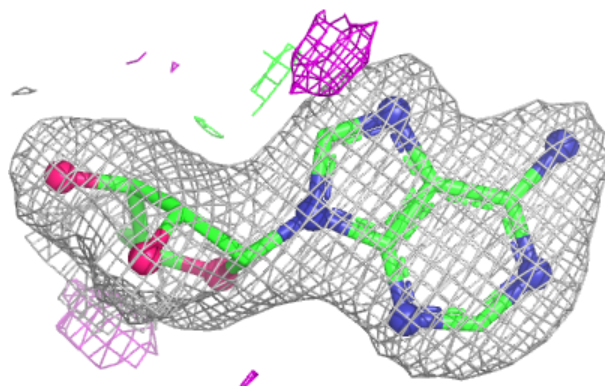
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD 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)

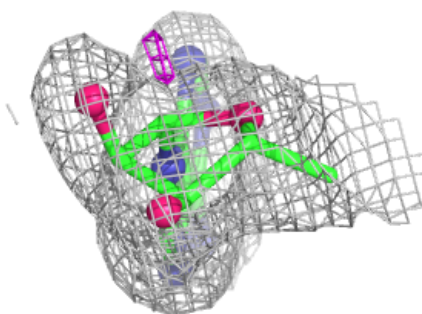
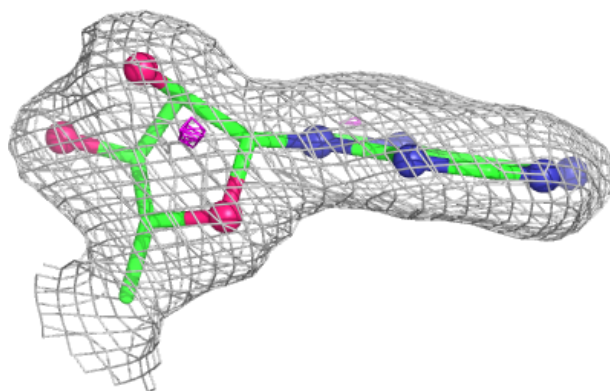
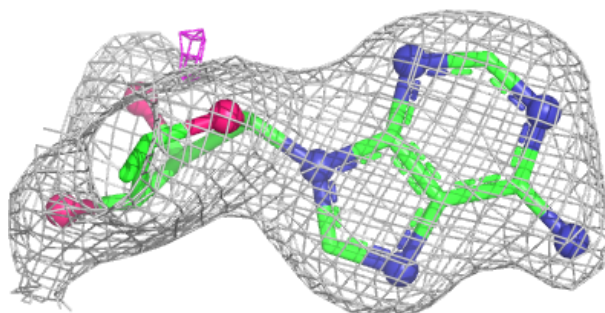
**Electron density around 5AD B 302:**

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



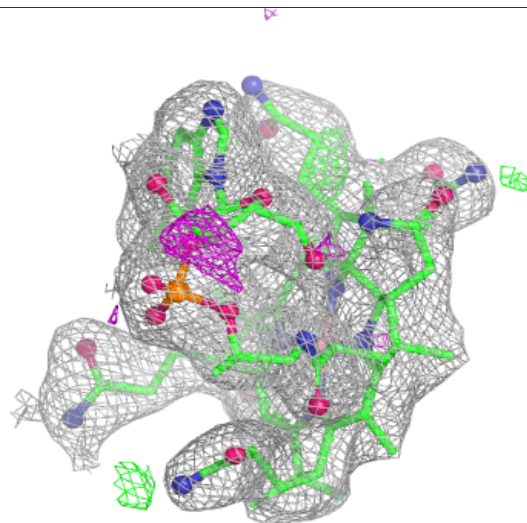
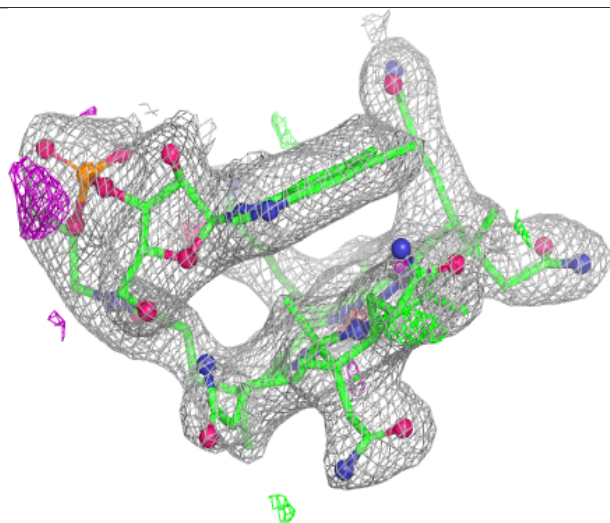
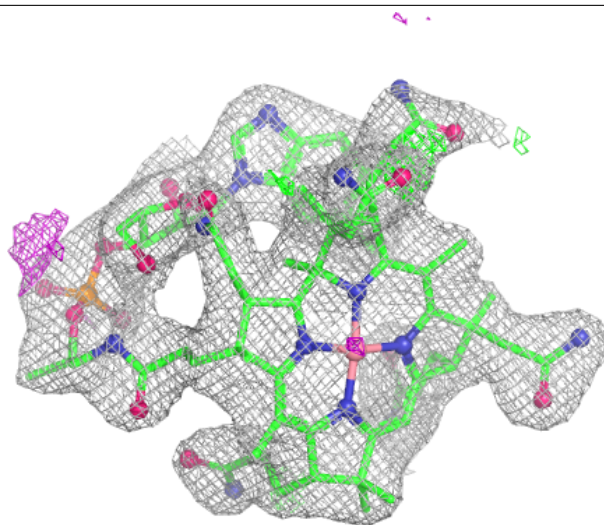
Electron density around 5AD C 504:

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



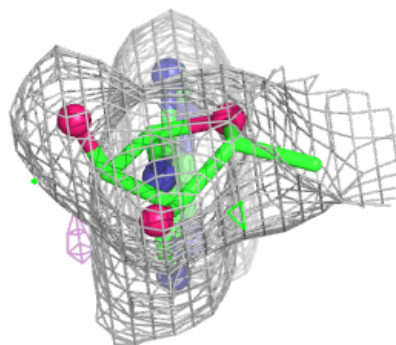
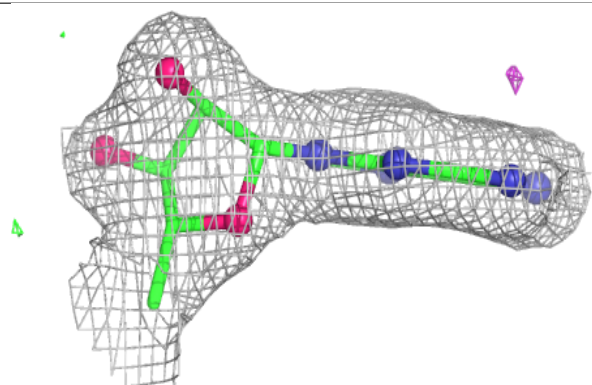
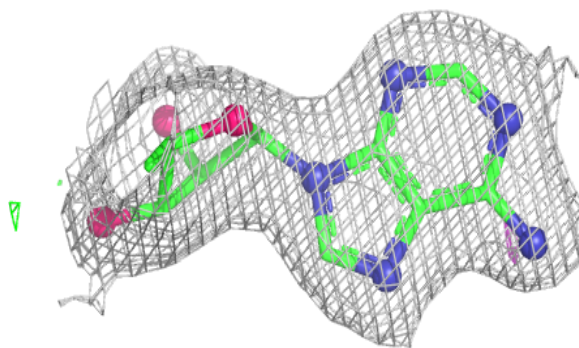
Electron density around B12 D 301:

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



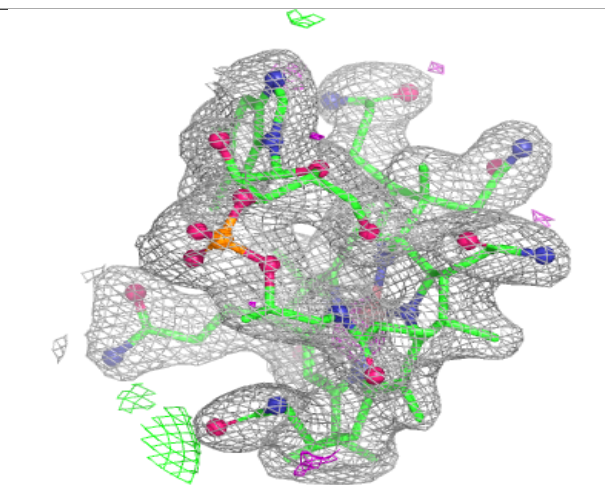
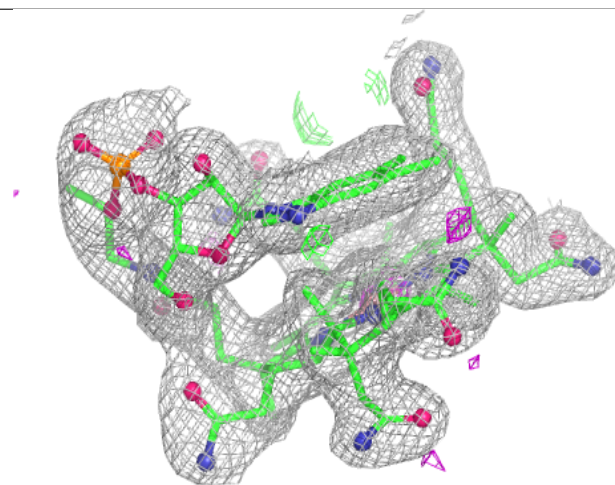
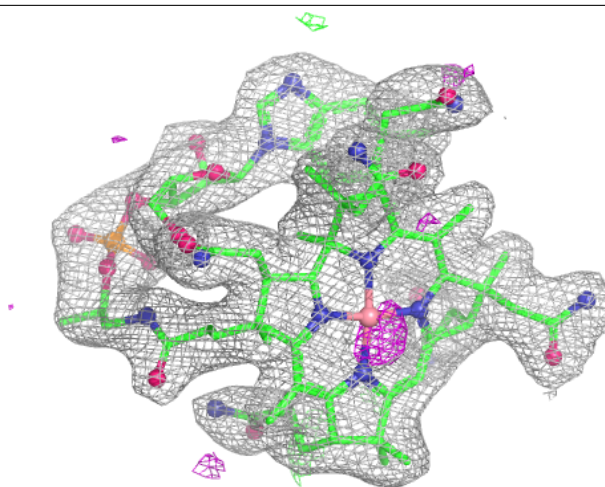
Electron density around 5AD A 304:

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



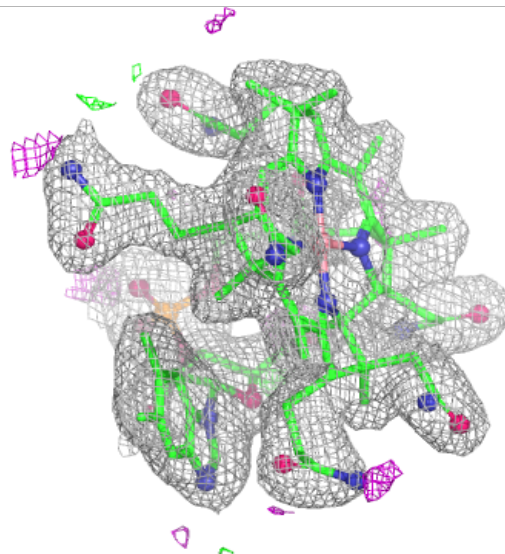
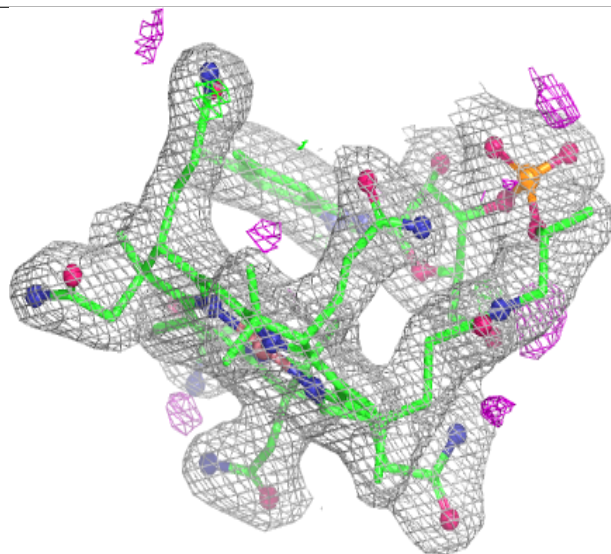
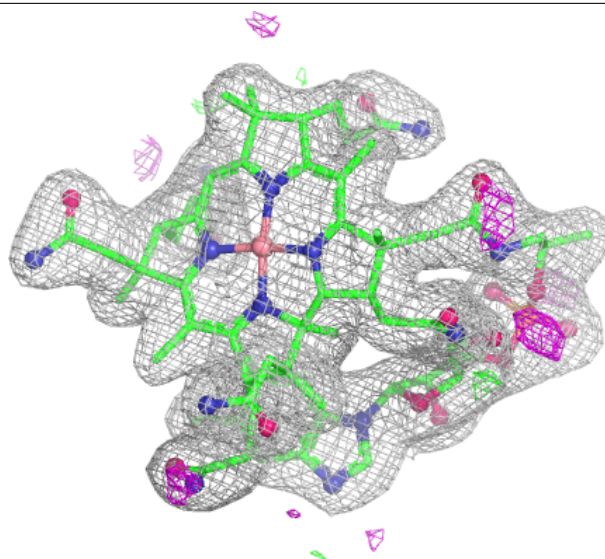
Electron density around B12 B 301:

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



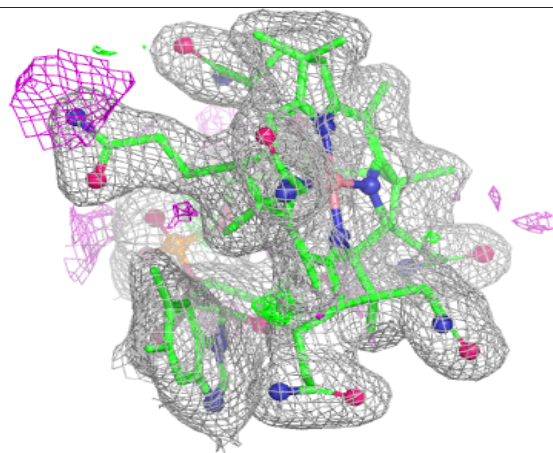
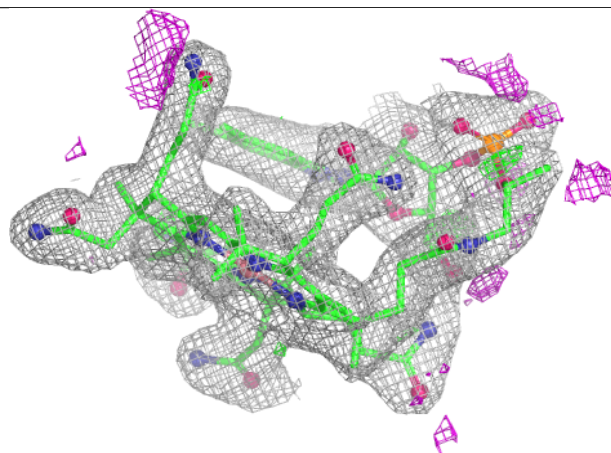
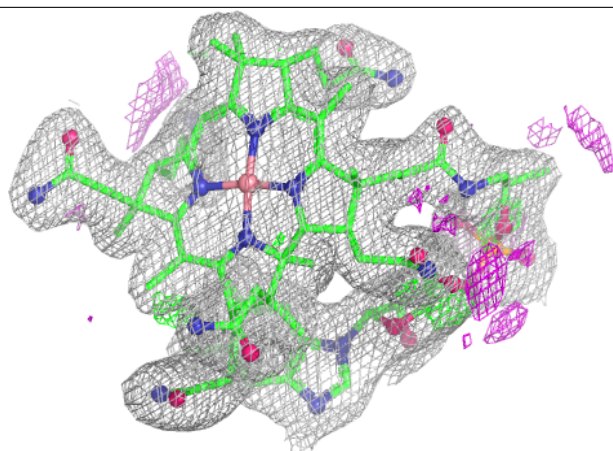
Electron density around B12 C 503:

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



Electron density around B12 A 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.